Title: Topological States in Strongly-Correlated Materials

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Abstract: In the study of strongly-correlated insulators, a long-standing puzzle remained open for over 40 years. Some Kondo insulators (or mixed-valent insulators) display strange electrical transport that cannot be understood if one assumes that it is governed by the three-dimensional bulk. In this talk, I show that some 3D Kondo insulators have the right ingredients to be topological insulators, which we called â€œtopological Kondo insulatorsâ€•. For a topological Kondo insulator, the low-temperature transport is dominated by the 2D surface rather than the 3D bulk, because the bulk of this material is an insulator while its surface is a topologically-protected 2D metal. This theoretical picture offers a natural explanation for the long-standing puzzle mentioned above. In addition, we also find that Kondo insulators can support another type of nontrivial topological structure protected by lattice symmetries, which we called â€œtopological crystalline Kondo insulatorsâ€•. In particular, we predict that SmB$_6$ is both a topological Kondo insulator and a topological crystalline Kondo insulator and I will also discuss recent experiments, which reveal the surface states in SmB$_6$.

Topological States in Strongly-Correlated Materials

Kai Sun

University of Michigan, Ann Arbor

Collaborators

Theory:

Mengxing Ye (U of Michigan) Maxim Dzero (Kent State) Victor Galitski (U of Maryland) and Piers Coleman (Rutgers)

Experiment:

J. W. Allen, Lu Li , Cagliyan Kurdak (U of Michigan), Zachary Fisk (UC-Irvine)

References: Ye, Allen and **KS**, arXiv:1307.7191 (2013)

Theoritical:

Dzero, **KS**, Galitski and Coleman, PRL, 104, 106408 (2010).

Experimental:

Wolgast, Kurdak, **KS**, Allen, Kim and Fisk, arXiv1211.5104 (2012).

Li, Xiang, Yu, Asaba, Lawson, Cai, Tinsman, Berkley, Wolgast, Eo, Kim, Kurdak, Allen, **KS**, Chen, Wang, Fisk, Li arXiv:1306.5221 (2013).

Outline

- Introduction
  - Brief review on SmB_6 and heavy fermion compounds
- Topological Kondo insulator
  - Prediction: SmB_6 is a topological Kondo insulator
- Topological Crystalline Kondo insulator
  - Prediction: SmB_6 is a topological crystalline Kondo insulator
- Experimental evidence

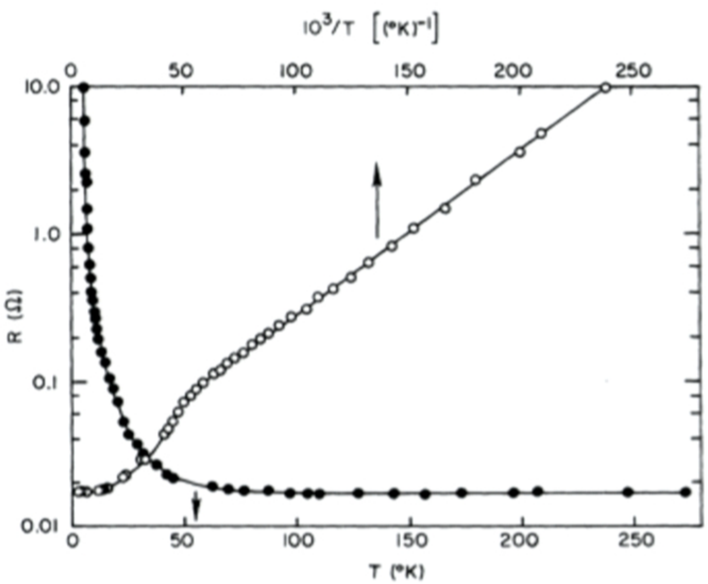
SmB_6: a insulator or a metal?

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)



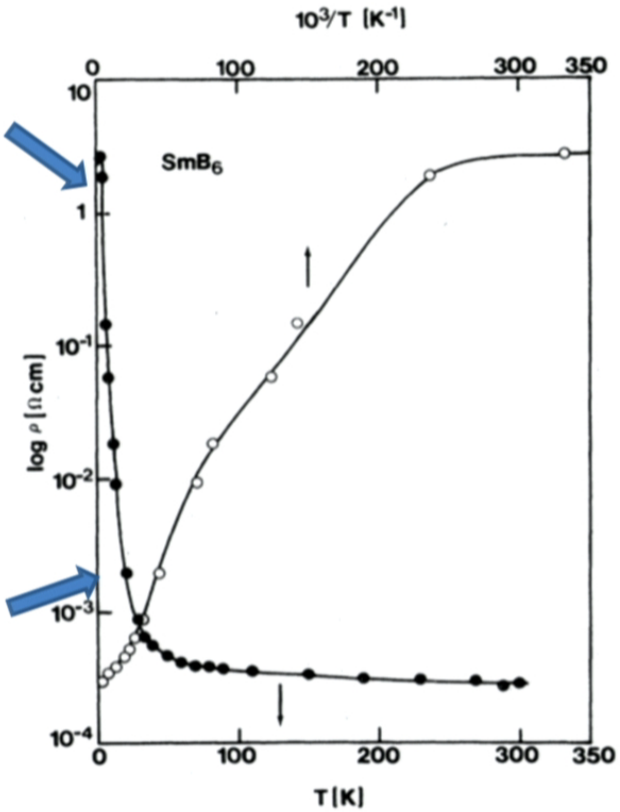
At 3°K the resistivity shows a sharp break and increases only by a factor of 1.3 with decreasing temperature down to 1.6°K. This may be due to the onset of another type of conduction mechanism which bears some relation to the impurity-band phenomena which have been studied so extensively in extrinsic semiconductors. At this time, however, we cannot rule out the possibility that it may be due to trace impurities of other rare-earth ions in the lot of Sm metal from which the samples were prepared (see below).

Low-temperature residual conductivity

Resistivity saturates at low T~4K
metal?

Resistivity increases exponentially at T>4K
Insulator?

Metal or insulator?



J. W. Allen, B. Batlogg and P. Wachter, Phys. Rev. **B 20**, 4807(1979).

Metal or Insulator?

- NOT a metal: residual conductivity is too low for the carrier density (mean-free path to small).

  J. W. Allen, B. Batlogg and P. Wachter, Phys. Rev. B 20, 4807(1979).

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- **Impurities band?** Very unlikely.

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  J. W. Allen, B. Batlogg and P. Wachter, Phys. Rev. B 20, 4807(1979).

- Impurities band? Very unlikely.
  - Mott limit is not satisfied
  - residual conductivity never goes away, even if the sample is very clean.

SmB_6: Kondo Insulator or Exotic Metal?

J. C. Cooley,[1] M. C. Aronson,[1] Z. Fisk,[2] and P. C. Canfield[3]

Physical Review letters 74, 1629, (1995)

Compelling evidence that the metallic states which dominate the low temperature, low pressure transport are intrinsic is found in the evolution of this band as pressure suppresses the gap. As depicted in Fig. 2(b),

A very incomplete list of literature on Kondo insulators

A. Menth, E. Buehler, and T. H. Geballe, "Magnetic and Semiconducting Properties of SmB6" Phys. Rev. Lett. 22, 295 (1969)

R. M. Martin and J. W. Allen, "Theory of mixed valence: Metals or small gap insulators," J. Appl. Phys. 50, 7561 (1979)

J. W. Allen, B. Batlogg, and P. Wachter, "Large low-temperature Hall effect and resistivity in mixed-valent SmB6," Phys. Rev. B 20, 4807–4813 (1979)

G. Aeppli and Z. Fisk, "Kondo Insulators," Comm. Condens. Matter Phys. 16, 155 (1992)

J. C. Cooley, M. C. Aronson, Z. Fisk, and P. C. Canfield, "SmB6: Kondo Insulator or Exotic Metal?" Phys. Rev. Lett. 74, 1629-1632 (1995)

H. Tsunetsugu, M. Sigrist and K. Ueda, "The ground-state phase diagram of the onedimensional Kondo lattice model," Rev. Mod. Phys. 69, 809 (1997)

P. Riseborough, "Heavy fermion semiconductors," Adv. Phys. 49, 257 (2000)

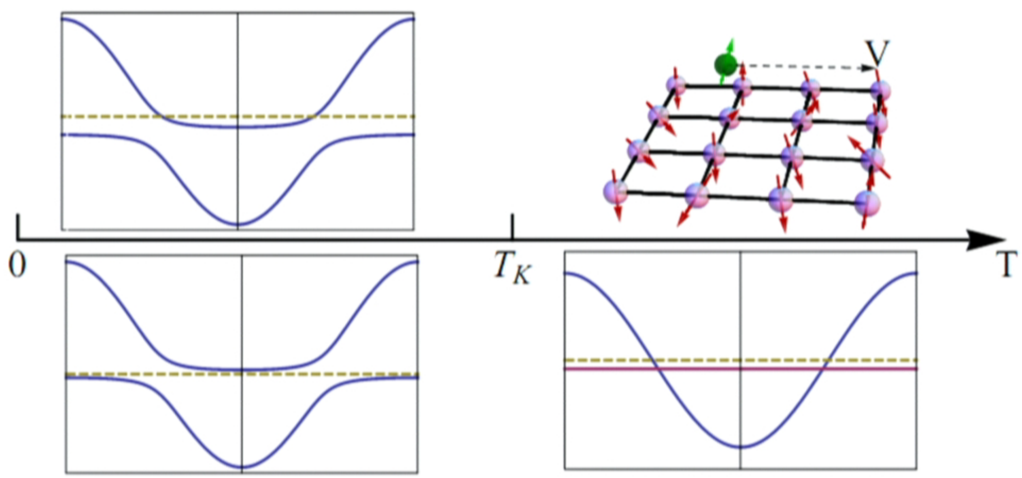
P. Coleman, "Heavy Fermions: Electrons at the Edge of Magnetism", Handbook of Magnetism and Advanced Magnetic Materials, Vol 1, 95-148 (Wiley, 2007)

…

Heavy Fermion in a Nut Shell

- Experimental signature:
  - Fermi liquid with very large effect electron mass ~ 100 me
- Theoretical description (Anderson model or Kondo model):
  - Electrons moving on a lattice of local spins

$$\mathcal{H}_{\mathbf{k}} = \begin{pmatrix} \xi_{\mathbf{k}} I & \Phi_{\mathbf{k}}^{\dagger} \\ \Phi_{\mathbf{k}} & \epsilon\, I \end{pmatrix}$$



Microscopic model: Anderson model

- model: $\hat{H} = \sum_{\mathbf{k},\alpha} \xi_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\alpha} c_{\mathbf{k}\alpha} + \sum_{j\alpha} \left[V \psi^{\dagger}_{j\alpha} f_{j\alpha} + \text{h.c.} \right] + \sum_{j\alpha} \left[\varepsilon_f^{(0)} n_{f,j\alpha} + \frac{U_f}{2} n_{f,j\alpha} n_{f,j\bar{\alpha}} \right]$

- correlation functions

$$\mathcal{G}_{cc}(\mathbf{k}, i\omega) = \left[i\omega - \xi_{\mathbf{k}} - \frac{|V(\mathbf{k})|^2}{i\omega - \varepsilon_f^{(0)} - \Sigma_f(\mathbf{k}, i\omega)} \right]^{-1}$$

$$\mathcal{G}_{ff}(\mathbf{k}, i\omega) = \left[i\omega - \varepsilon_f^{(0)} - \Sigma_f(\mathbf{k}, i\omega) - \frac{|V(\mathbf{k})|^2}{i\omega - \xi_{\mathbf{k}}} \right]^{-1}$$

f-level renormalization due to Hubbard interaction

- approximations:
  - neglect self-energy dispersion: Kondo limit (large U_f)
  - ignore the physics at high Matsubara frequencies

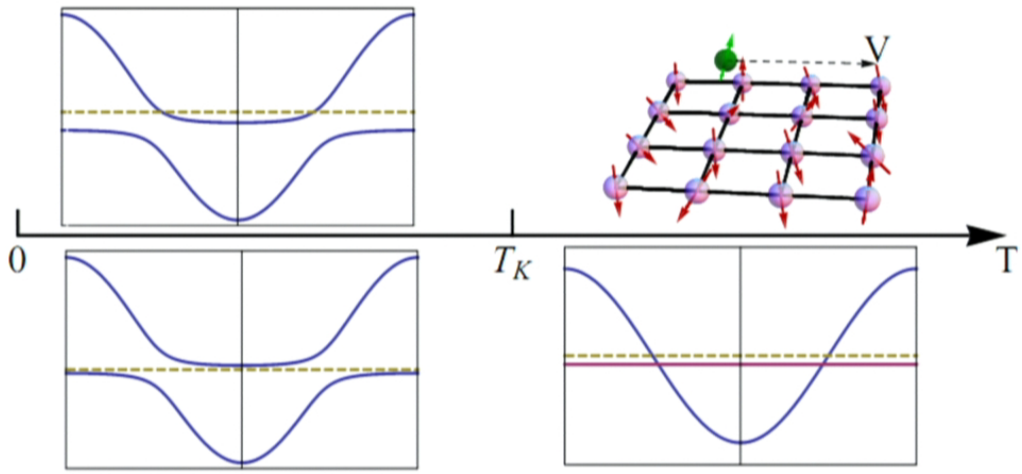
$$\varepsilon_f = Z_{\cancel{\mathbf{k}}} [\varepsilon_f^{(0)} + \Sigma_f(\cancel{\mathbf{k}}, 0)]$$

$$Z_{\cancel{\mathbf{k}}} = \left[1 - \frac{\partial \Sigma_f(\cancel{\mathbf{k}}, \omega)}{\partial \omega} \right]^{-1}_{\omega=0}$$

- hybridization amplitude $\tilde{V}(\mathbf{k}) = \sqrt{Z} V(\mathbf{k})$

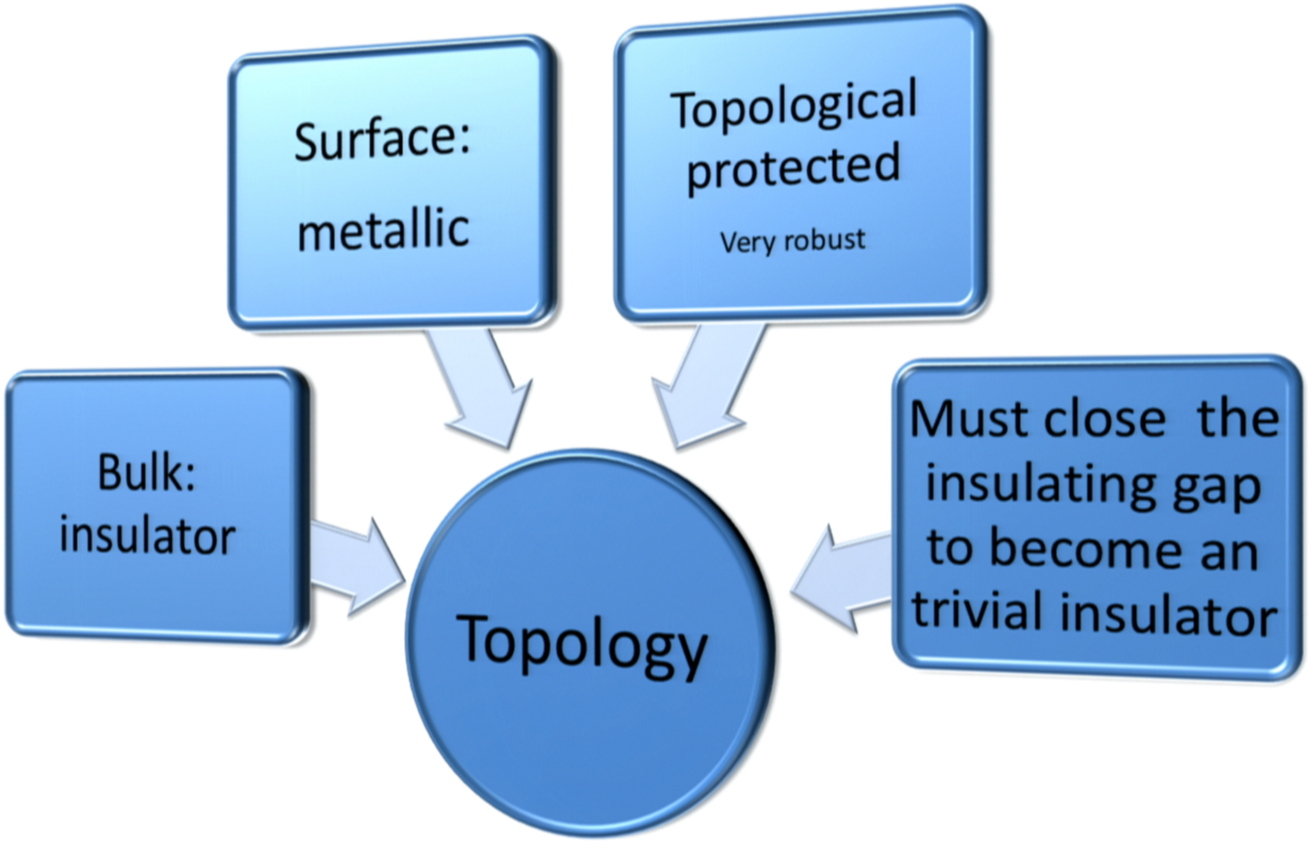
Effective model: Fermi liquid

$$\mathcal{H}_{\mathbf{k}} = \begin{pmatrix} \xi_{\mathbf{k}} I & \Phi^{\dagger}_{\mathbf{k}} \\ \Phi_{\mathbf{k}} & \epsilon\, I \end{pmatrix}$$



Dzero, **KS**, Galitski and Coleman, PRL, (2010).

What is a topological insulator?



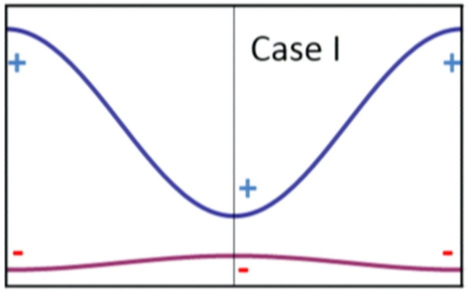
Why topological?

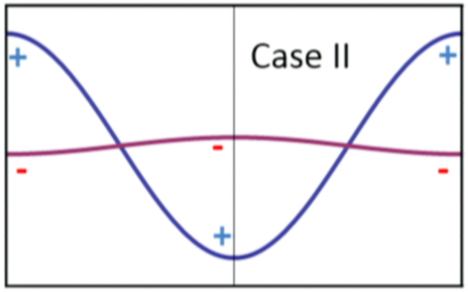
Consider a example where local moments (flat band) and conducting electrons (dispersive bands) have opposite parity. In SmB_6

- dispersive band: $5d$ state of Sm with ($l = 2$ and thus even parity)
- flat bands: $4f$ state of Sm ($l = 3$ and thus odd parity)

First, consider the simple situation: no hybridization between d and f states.

- Two situations: the d and f bands cross or not





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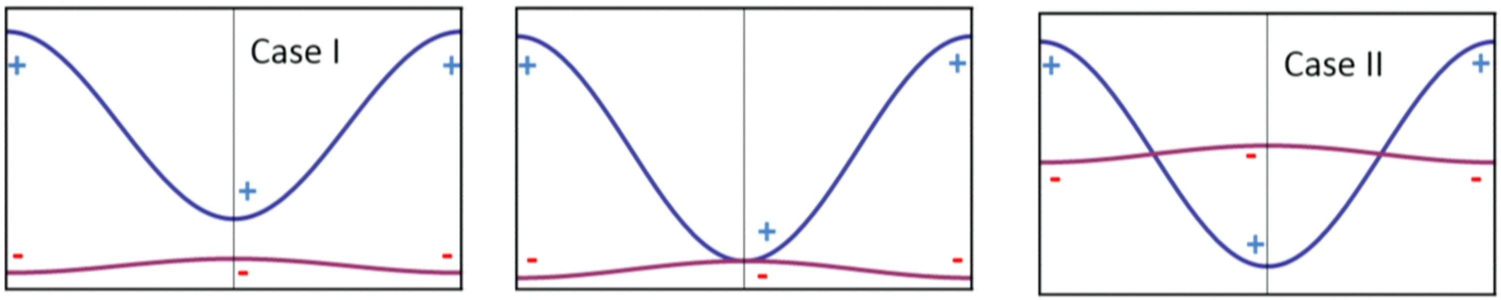
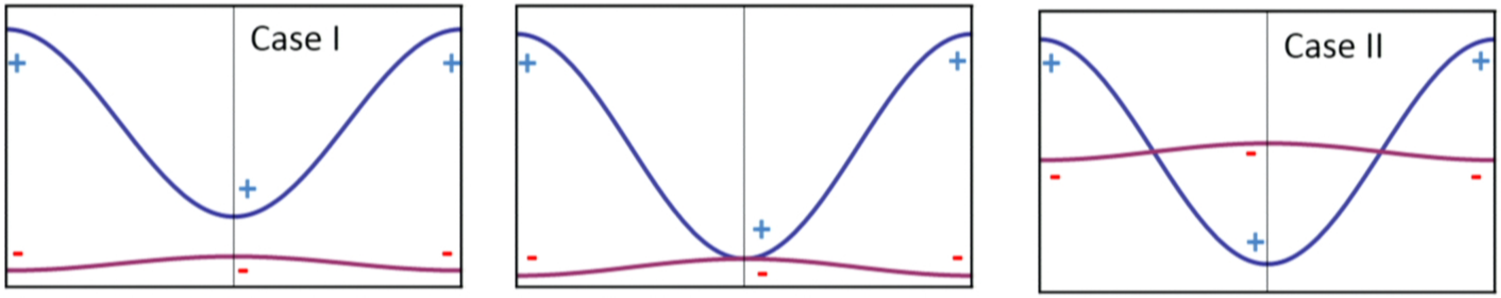
First, consider the simple situation: no hybridization between d and f states.

- Two situations: the d and f bands cross or not
- The marginal case: two bands barely touch

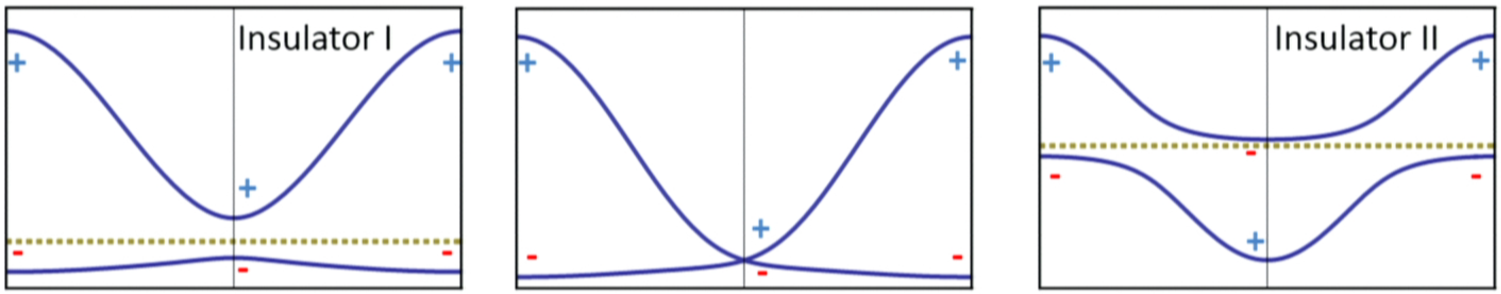


Dzero, **KS**, Galitski and Coleman, PRL, (2010).

Why topological? (with f-d hybridization)

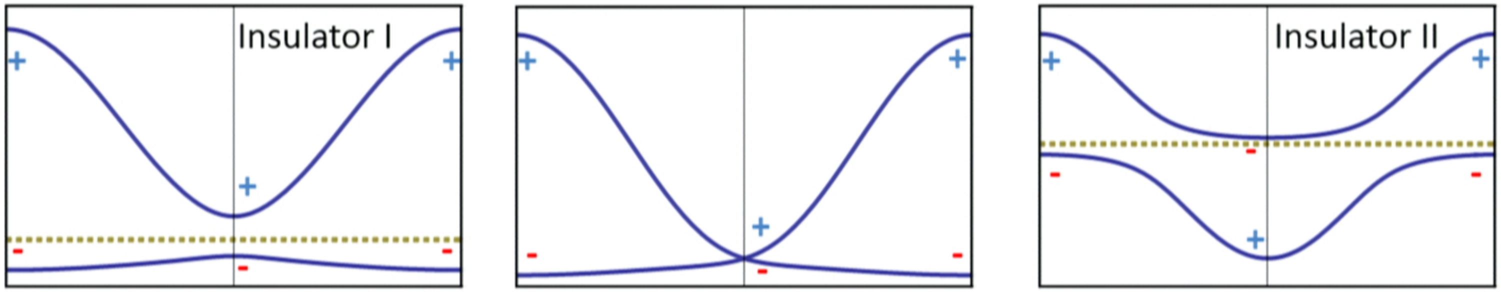


Turn on hybridization between f and d orbitals



Dzero, **KS**, Galitski and Coleman, PRL, (2010).

Key ingredients



(1) Two bands with opposite parities + (2)They cross with each other: band inversion

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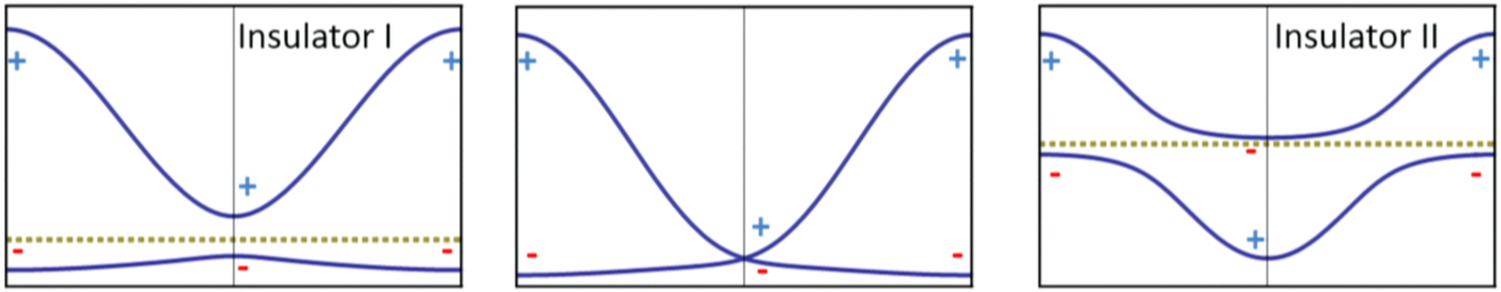

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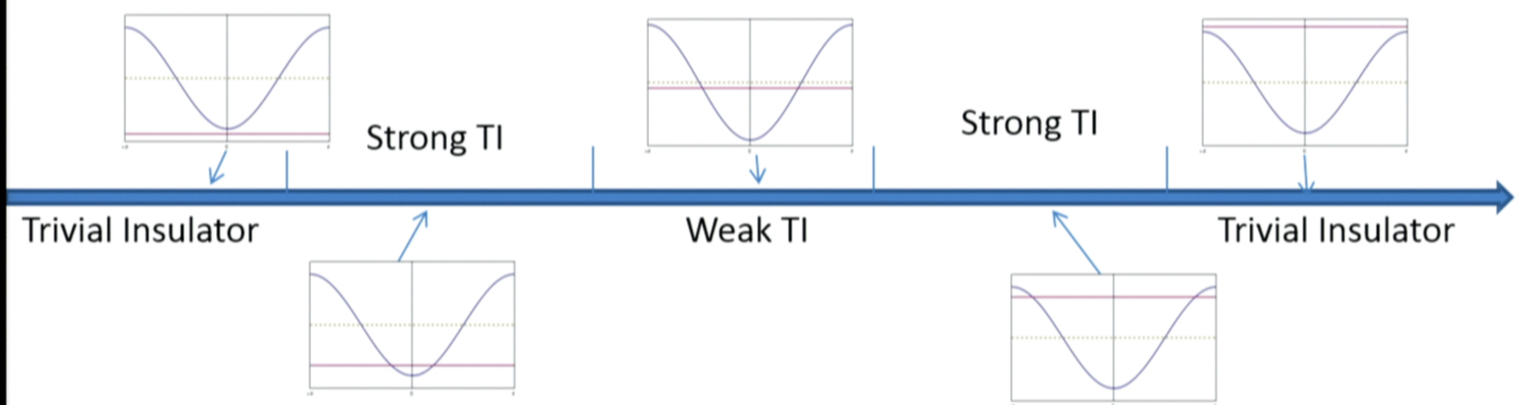

SmB_6 Strong TI
CeNiSn: Weak TI

Dzero, **KS**, Galitski and Coleman, PRL, (2010).

What is the topological structure of SmB_6?

Q: What is the band structure of SmB_6?
A: We don't know the band structure, except for certain momentum points.

Q: Can we determine the topology by only looking at a few points?
A: In general no, because topology is a global property, which cannot be determined by local features, e.g., we cannot distinguish a cylinder from a Möbius strip by looking at a coupling of points.

But, with the help of certain symmetry, it can be done.

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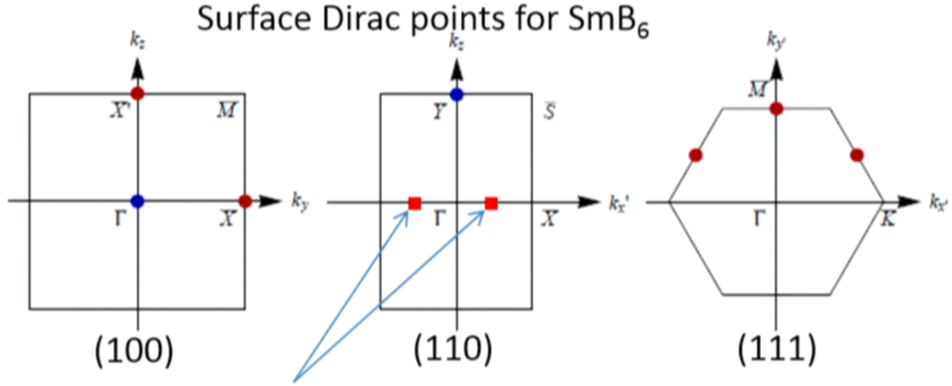
Luckily, our very limited knowledge on SmB_6 band structure to determine the topological nature and the surface states

Surface Dirac points for SmB_6



Surface Dirac points protected by lattice (mirror) symmetries

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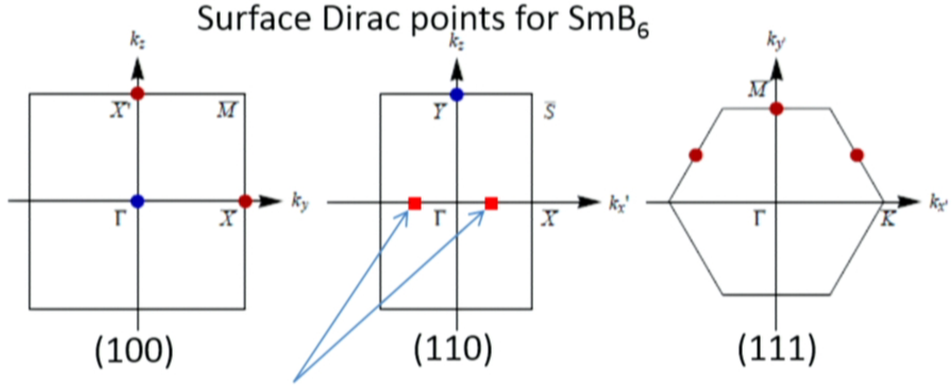

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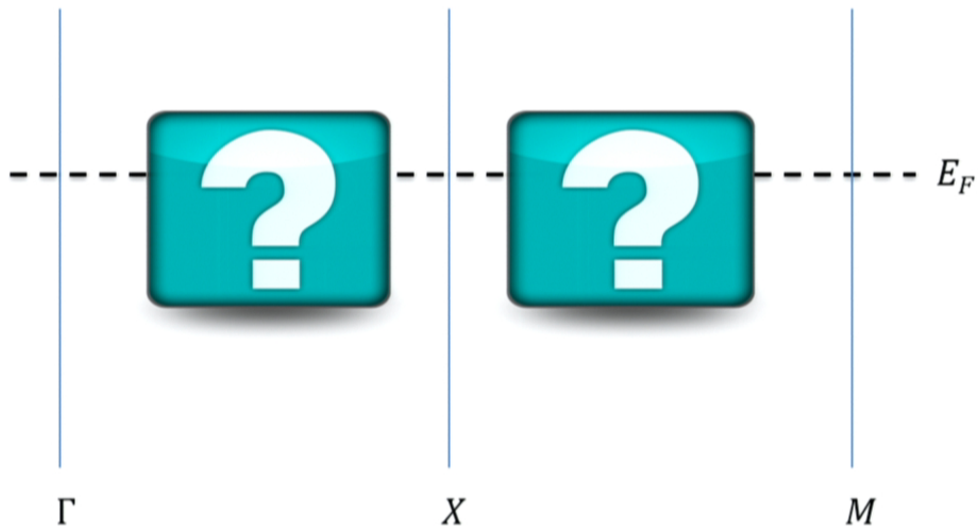

Ye, Allen and **KS**, arXiv:1307.7191

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- Each band is doubly degenerate due time-reversal and space-inversion symmetries.

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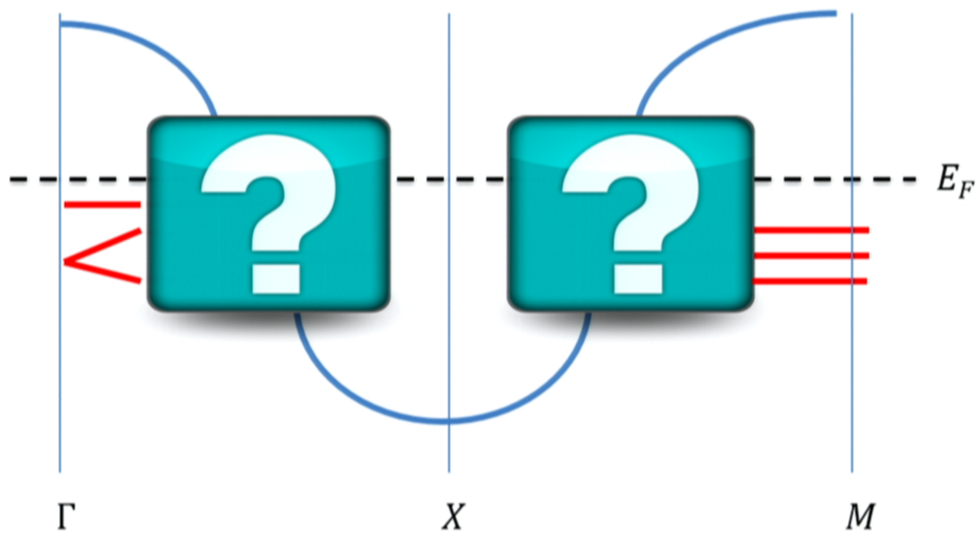

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- Each band is doubly degenerate due time-reversal and space-inversion symmetries.
- The d band is above E_F for most part of the BZ, but is below E_F around X.
- The three f-bands are nearly degenerate and hard to resolve.
- They are below E_F for most part of BZ.

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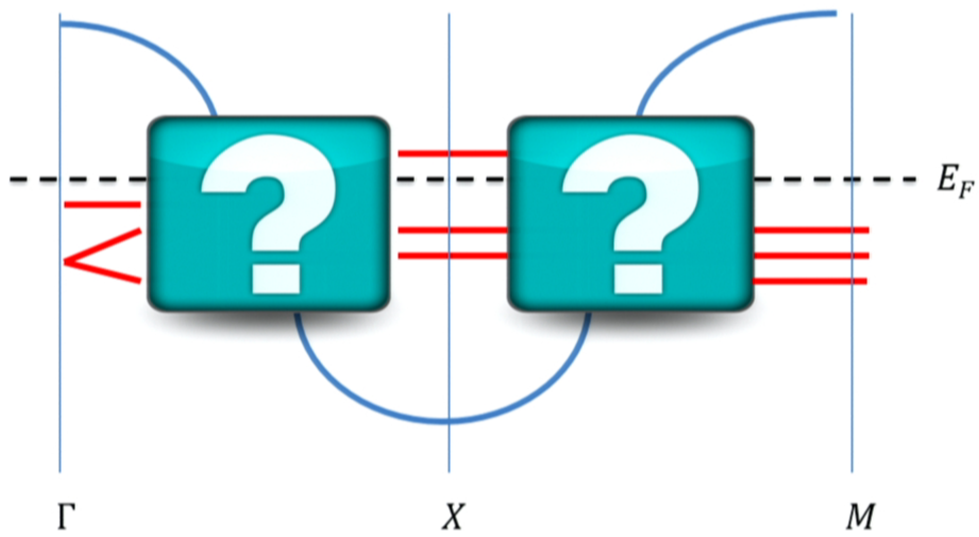

Two bands with opposite parities inverted at X: enough for topology

Ye, Allen and **KS**, arXiv:1307.7191

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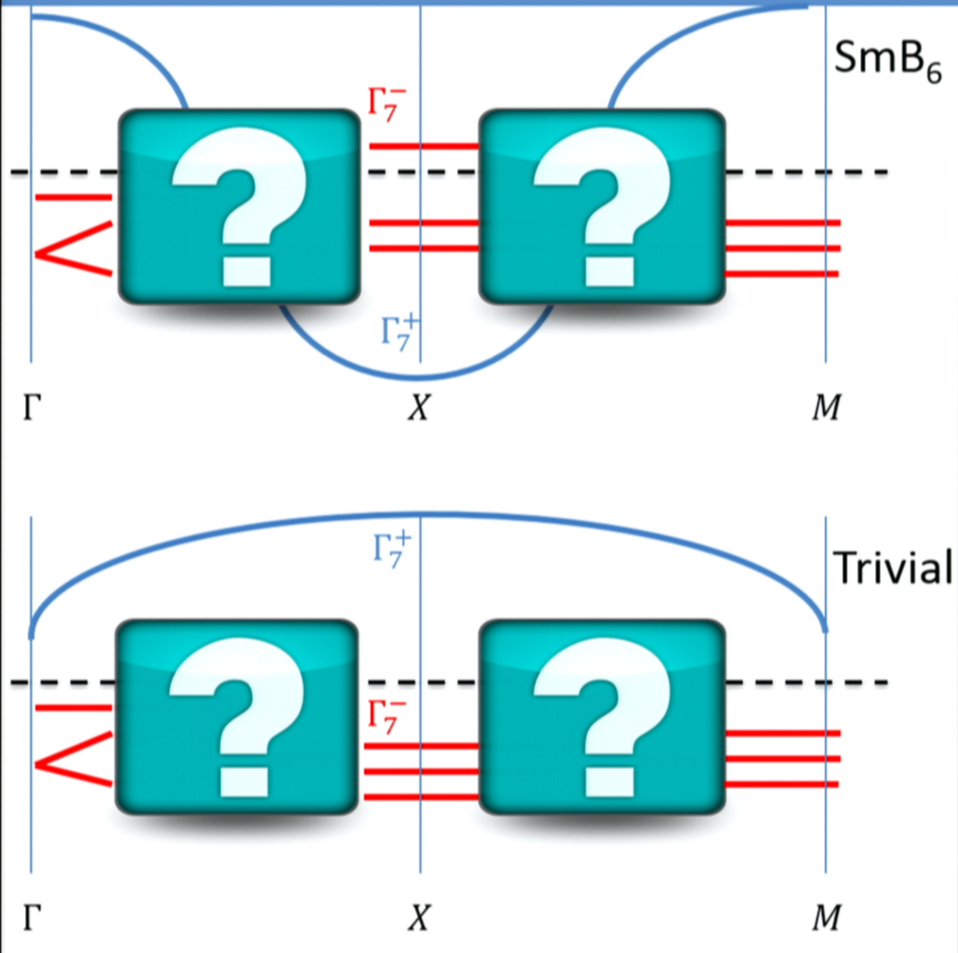
- The d band is above E_F for most part of the BZ, but is below E_F around X.
- The three f-bands are nearly degenerate and hard to resolve.
- They are below E_F for most part of BZ.
- Near X, one f-band must be above E_F to maintain the number of valence bands.

SmB_6 vs a trivial insulator



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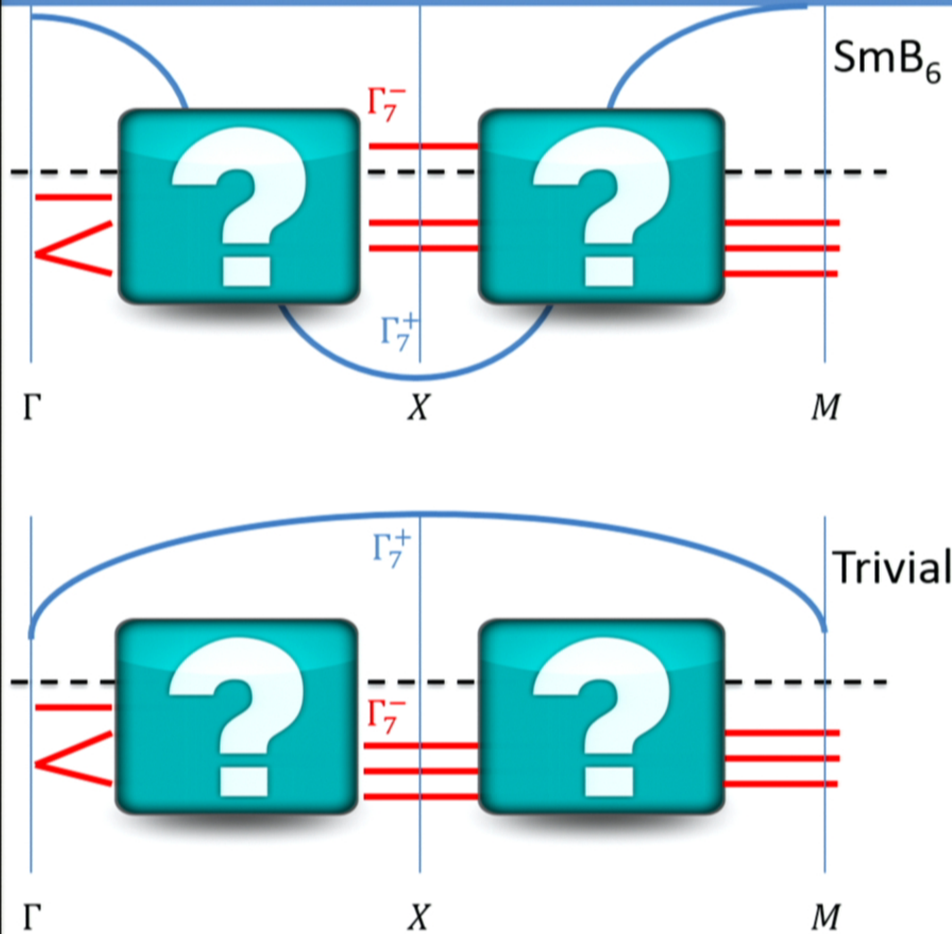

Insulators with inversion symmetry

$$(-1)^{\nu} = \prod_{m=1}^{N}\prod_{i=1}^{8}\xi_m(\Gamma_i),$$

ξ: parity eigenvalues

Γ_i: 8 high symmetry points

m: valence bands

Fu and Kane, PRB, (2007)

Compare these two insulators:

$$\frac{(-1)^{\nu_{\mathrm{SmB_6}}}}{(-1)^{\nu_{\mathrm{trivial}}}} = \prod_{i=1}^{8}\prod_{m=1}^{N}\frac{\xi_m^{\mathrm{SmB_6}}(\Gamma_i)}{\xi_m^{\mathrm{trivial}}(\Gamma_i)}$$

Ye, Allen and **KS**, arXiv:1307.7191

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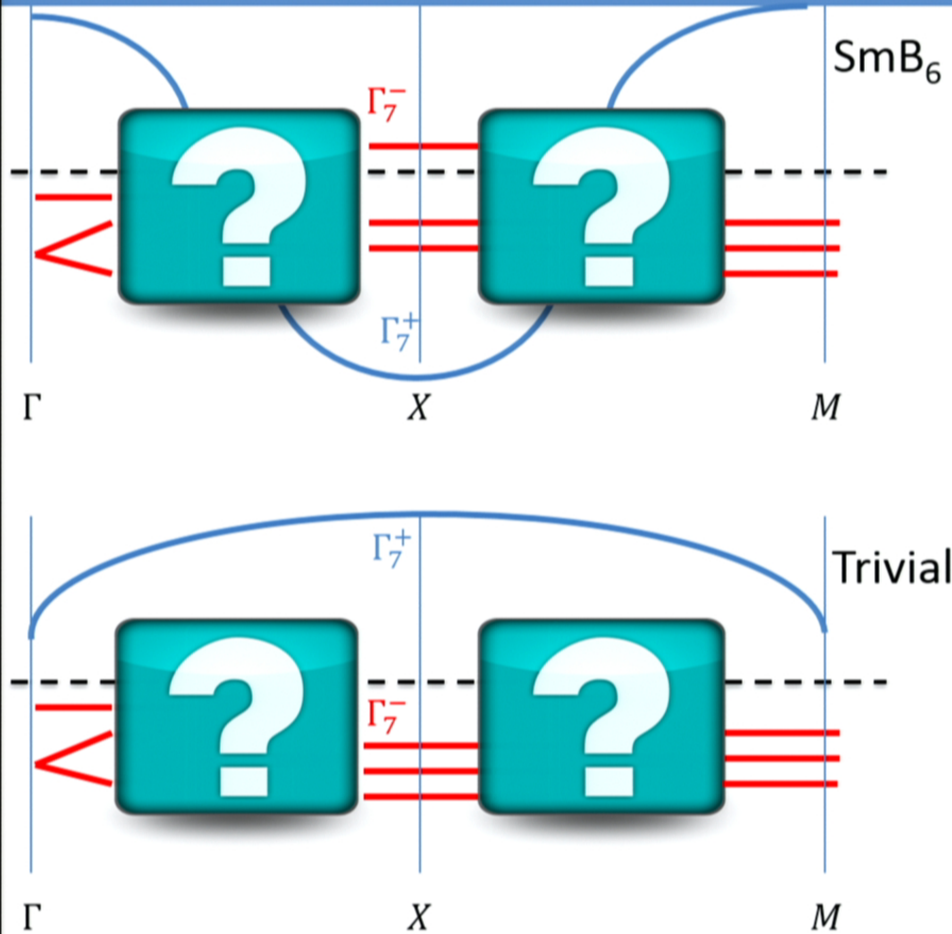

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Most of the eigenvalues cancel out
Only the inverted bands matter

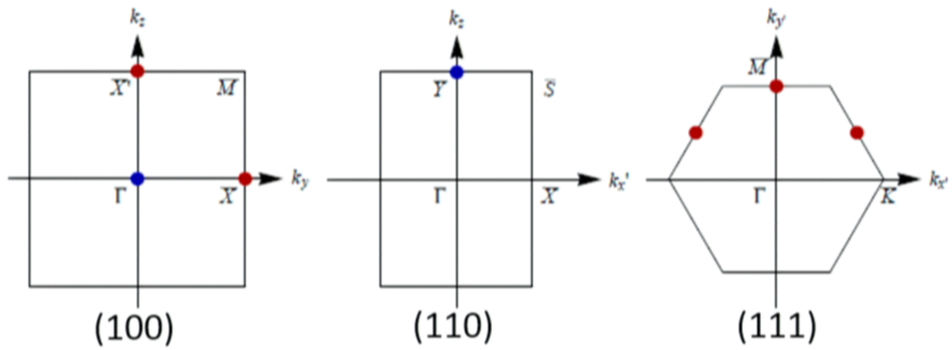
$$(-1)^{\nu_{\mathrm{SmB_6}}} = \left[\frac{\xi_{\mathrm{IV}}^{\mathrm{SmB_6}}(X)}{\xi_{\mathrm{IV}}^{\mathrm{trivial}}(X)}\right]^3 = \left[\frac{\xi_{\mathrm{IV}}^{\mathrm{SmB_6}}(X)}{\xi_{\mathrm{IC}}^{\mathrm{SmB_6}}(X)}\right]^3 = -1$$

Ye, Allen and **KS**, arXiv:1307.7191

Band inversion and surface states

Surface states (Dirac points): if odd number of bulk band inversion points are projected to a surface k-point, there is a Dirac point. (Fu and Kane)

Surface Dirac points for SmB_6



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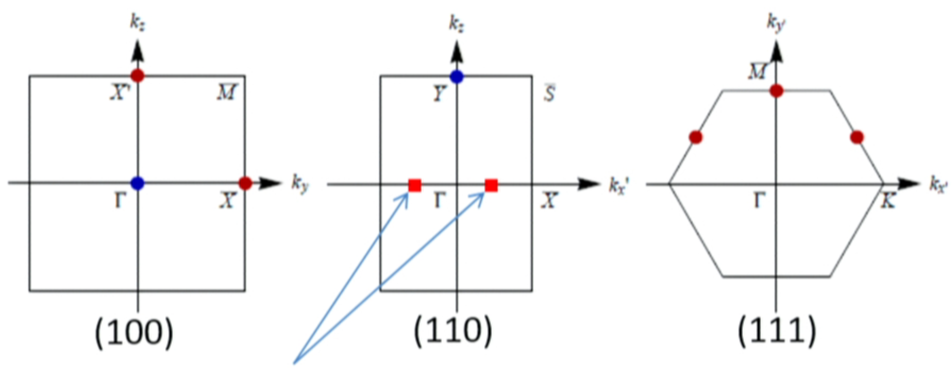
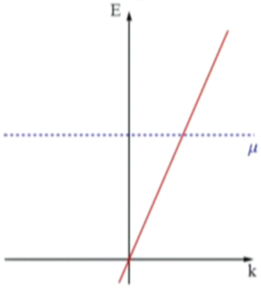


Topological surface states protected by lattice (mirror) symmetries

Ye, Allen and **KS**, arXiv:1307.7191

Mirror Chern number

QHE (Chern insulator): The Chern number ~ number of chiral edge modes



Teo, Fu and Kane, PRB, 2008

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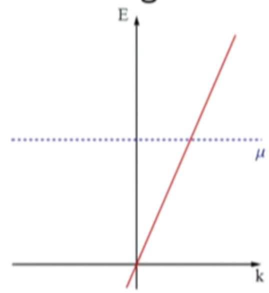
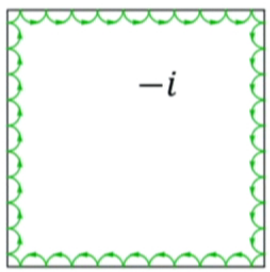
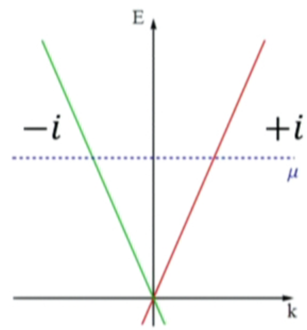


A 2D system with horizontal mirror symmetry:

- States with mirror eigenvalues $+i/-i$ never mix
- Define mirror Chern numbers for states with mirror eigenvalues $+i/-i$: C^+ and C^-.
- $C^+ = -C^-$.
- $|C^+|$ left-moving modes with mirror eigenvalues $+i$, $|C^-|$ right-moving mods with $-i$.
- There are (at least) $|C^+|$ Dirac points on the edge





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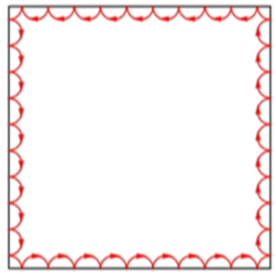

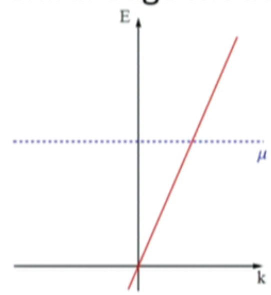

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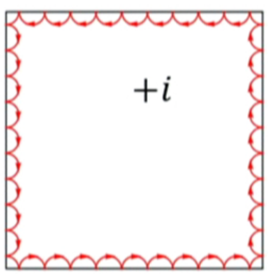
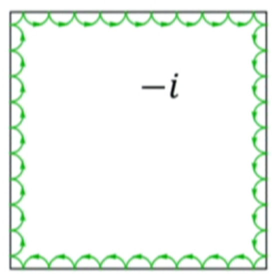
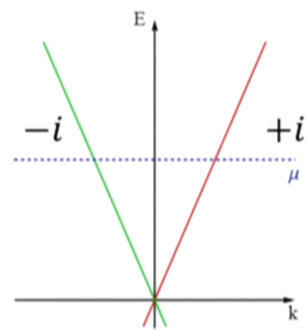
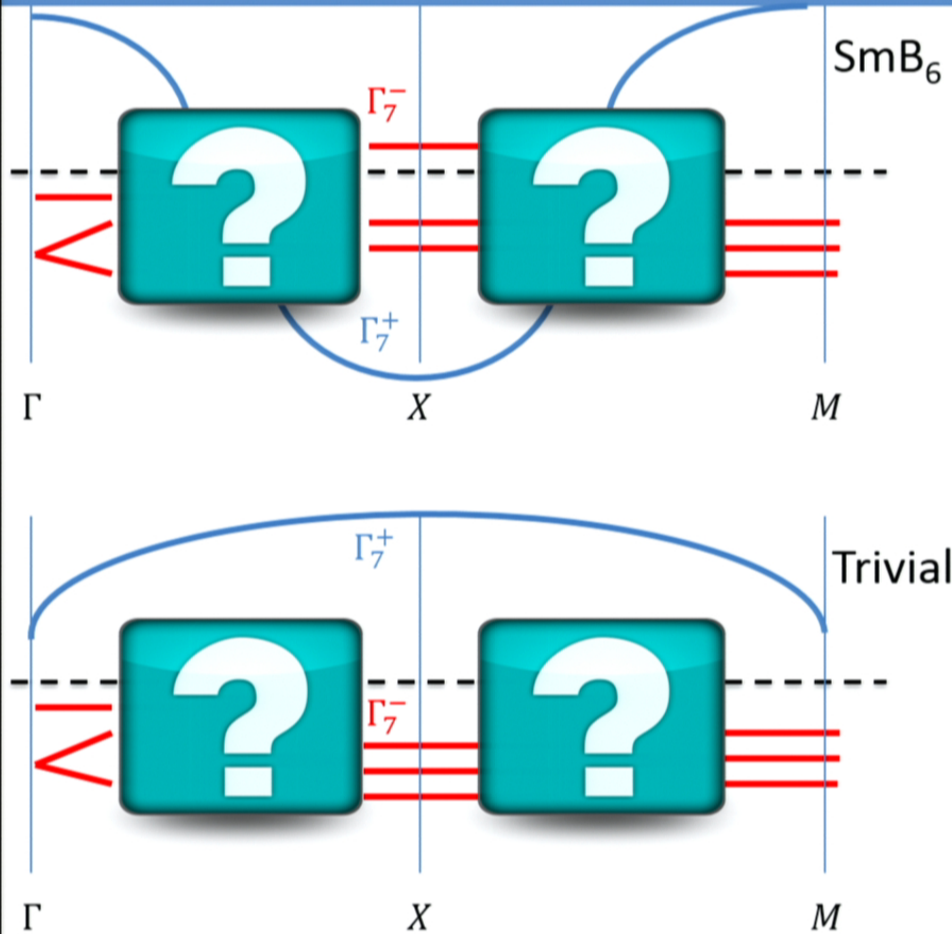






Teo, Fu and Kane, PRB, 2008

$k_z = 0$ plane of SmB_6:
a 2D system with mirror symmetry



With C_n-symmetry, high symmetry points are enough to obtain $C \ mod \ n$.
Fang, Gilbert, Bernevig, PRB 2012

Insulators with C_4-symmetry

$$(i)^{C^+} = \prod_{m=1}^{N} (-1)\eta_m(\Gamma)\eta_m(M)\zeta_m(X)$$

η: eigenvalues of C_4
ζ: eigenvalues of C_2
m: valence bands

Same is true for mirror C number
Compare these two insulators:

$$\frac{(i)^{C^+_{\mathrm{SmB_6}}}}{(i)^{C^+_{\mathrm{trivial}}}} = \prod_{m=1}^{N} \frac{\eta_m^{\mathrm{SmB_6}}(\Gamma)\eta_m^{\mathrm{SmB_6}}(M)\zeta_m^{\mathrm{SmB_6}}(X)}{\eta_m^{\mathrm{trivial}}(\Gamma)\eta_m^{\mathrm{trivial}}(M)\zeta_m^{\mathrm{trivial}}(X)}$$

Most of the eigenvalues cancel out
Only the inverted bands matter

$$(i)^{C^+_{\mathrm{SmB_6}}} = \frac{\zeta_{\mathrm{IV}}^{\mathrm{SmB_6}}(X)}{\zeta_{\mathrm{IV}}^{\mathrm{trivial}}(X)} = \frac{\zeta_{\mathrm{IV}}^{\mathrm{SmB_6}}(X)}{\zeta_{\mathrm{IC}}^{\mathrm{SmB_6}}(X)} = -1$$

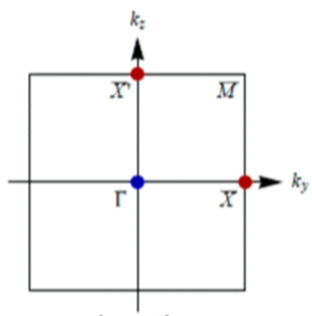
Mirror Chern number is 2

Ye, Allen and **KS**, arXiv:1307.7191

Surface states

- The $k_z = 0$ plane: the mirror Chern number is 2 (up to mod 4).
- The $k_z = \pi$ plane: the mirror Chern number is 1 (up to mod 4).
- For the $(mn0)$ surface, the $k_z = 0$ line shall have 2 Dirac points and the $k_z = \pi$ line shall have 1 Dirac point.

Surface Dirac points for SmB_6



(100)

Ye, Allen and **KS**, arXiv:1307.7191

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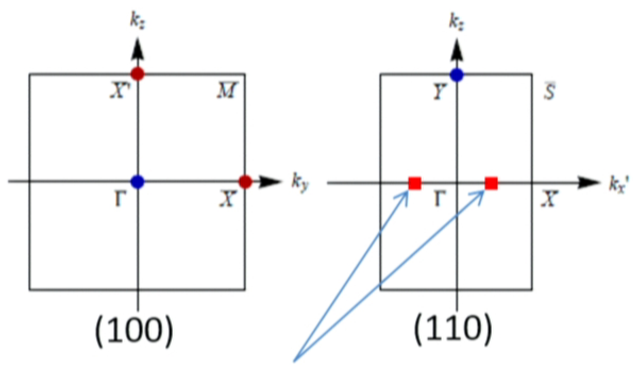

Topological surface states protected by lattice (mirror) symmetries

Ye, Allen and **KS**, arXiv:1307.7191

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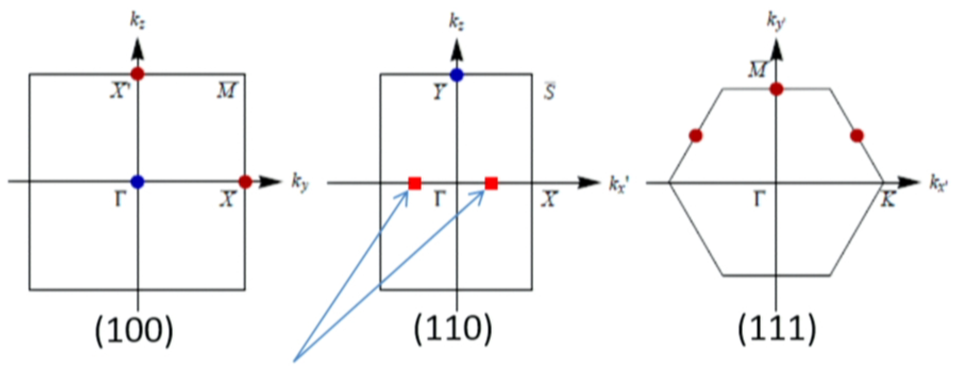
- For the $(mn0)$ surface, the $k_z = 0$ line shall have 2 Dirac points and the $k_z = \pi$ line shall have 1 Dirac point.
- For surfaces like (111), they are not perpendicular to the $k_z = 0$ or π planes, so these two mirror Chern numbers don't tell us anything.

Surface Dirac points for SmB_6



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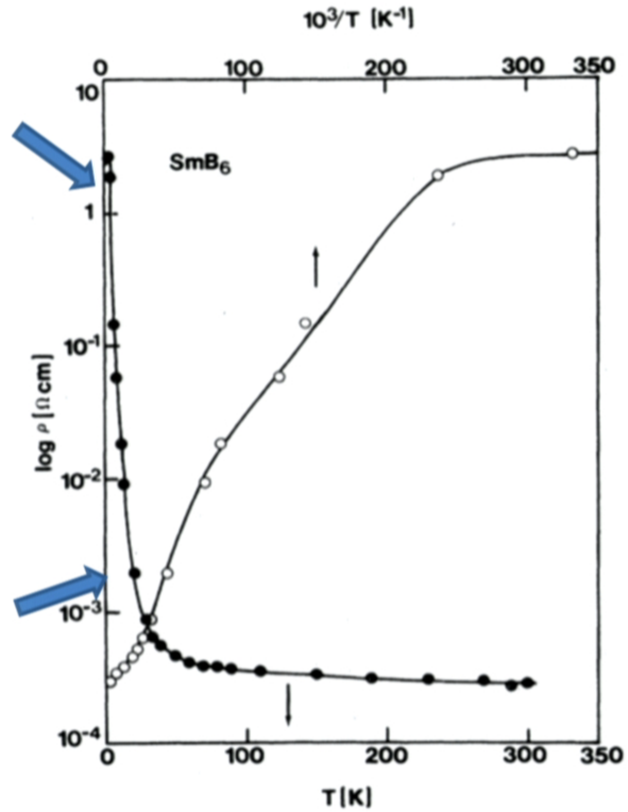
SmB_6: topological Kondo insulator?

Residual resistivity: surface states

Resistivity increases: insulating bulk

Is SmB_6 really a topological insulator?



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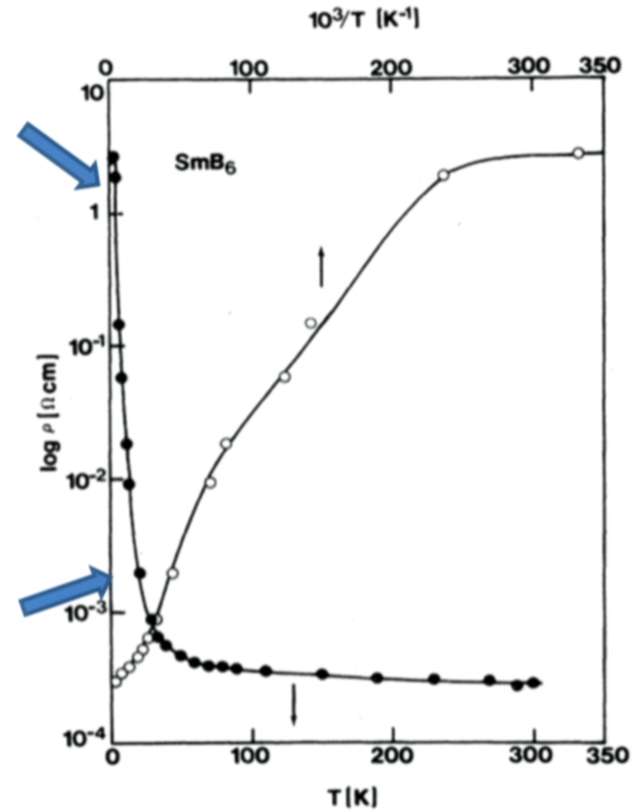
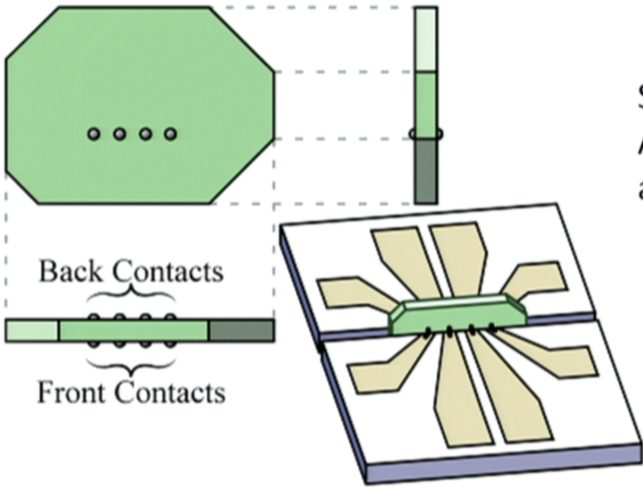


Is SmB_6 really a topological insulator?

Or a more precise question:

Can we really trust those theorists?

Experimental setup



Steven Wolgast, Cagliyan Kurdak, **KS,** J. W. Allen, Dae-Jeong Kim and Zachary Fisk, arXiv1211.5104.

- How to distinguish bulk and surface contributions?
  - Most other 3D TIs have bulk conductivity due to impurity effects.
  - Quantum Hall effect for strained HgTe thin film (Brune et.al. PRL 2011).
- Experimental setup
  - Sample: 3.47 mmX1.32mmX170µm
  - 4 contacts on the top side and 4 contacts on the bottom side

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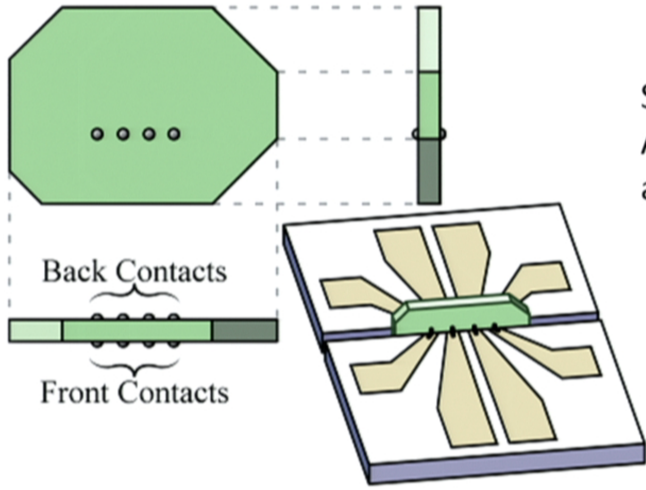

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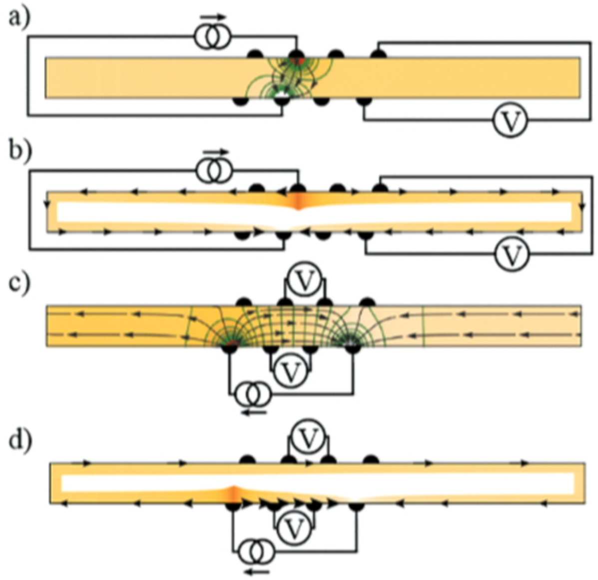
Experimental technique

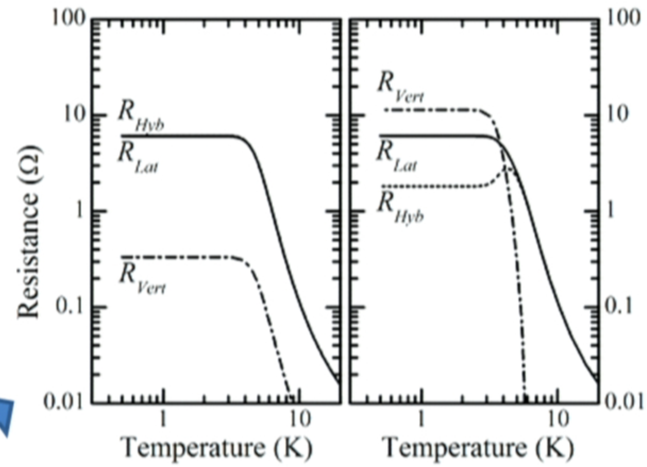


R_{Vert}=V_{Vert}/I
bulk conductor: R_{Vert} very small
surface conductor: R_{Vert} large

R_{Lat}=V_{Lat}/I: I and V on same side
R_{Hyb}=V_{Hyb}/I: I and V on different sides
Bulk conductor: $R_{Lat} \approx R_{Hyb}$
Surface conductor: $R_{Lat} > R_{Hyb}$

Bottom line:
Bulk dominates: $R_{Hyb} \approx R_{Lat} \gg R_{Vert}$
Surface dominates: $R_{Vert} > R_{Lat} > R_{Hyb}$

Numerical results



Bulk conductor:

1. $R_{Hyb} \approx R_{Lat} \gg R_{Vert}$
2. The ratios between Rs are T-independent

$$R = \frac{V}{I} = C\,\rho$$

The resistance R is determined by

1. the resistivity ρ (T-dependent)
2. A coefficient C (determined by geometry)

Topological insulator:

Bulk + surface

High T transport: Bulk dominate

Low T transport: Surface dominate

High T (Bulk): $R_{Hyb} \approx R_{Hyb} \gg R_{Vert}$

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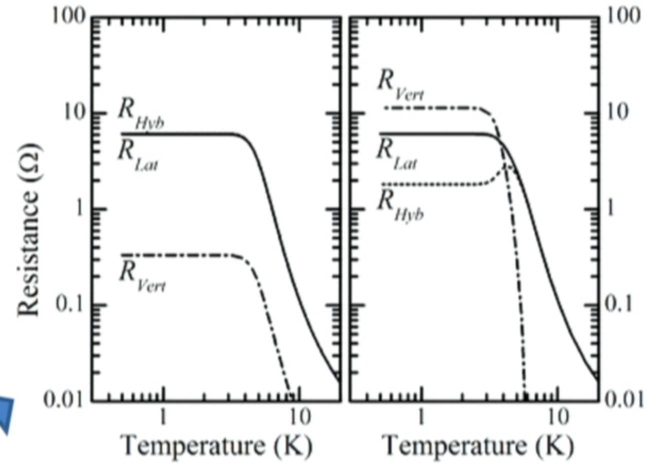

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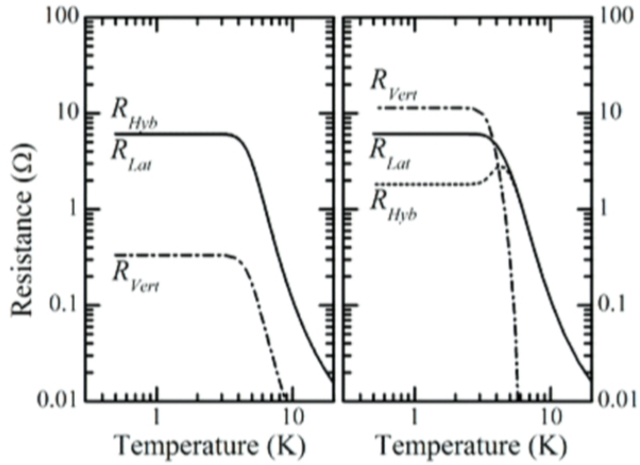

Wolgast, Kurdak, **KS**, Allen, Kim and Fisk, arXiv1211.5104 (2012).

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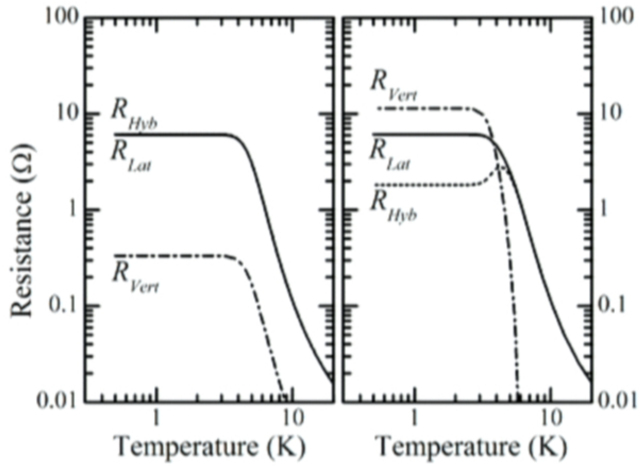
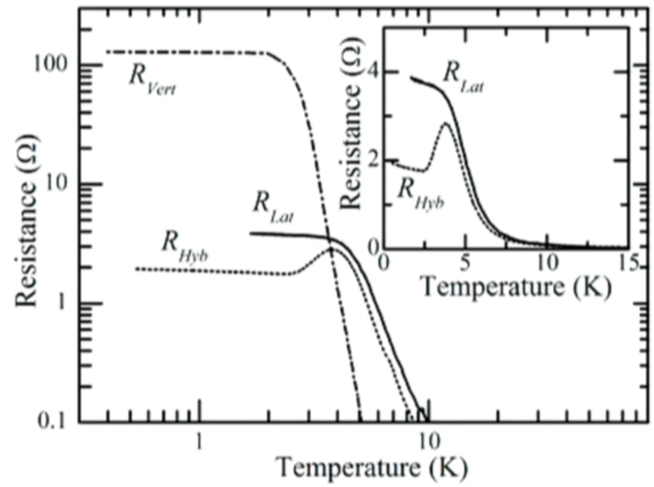


Theory



Experiment

Wolgast, Kurdak, **KS**, Allen, Kim and Fisk, arXiv1211.5104 (2012).

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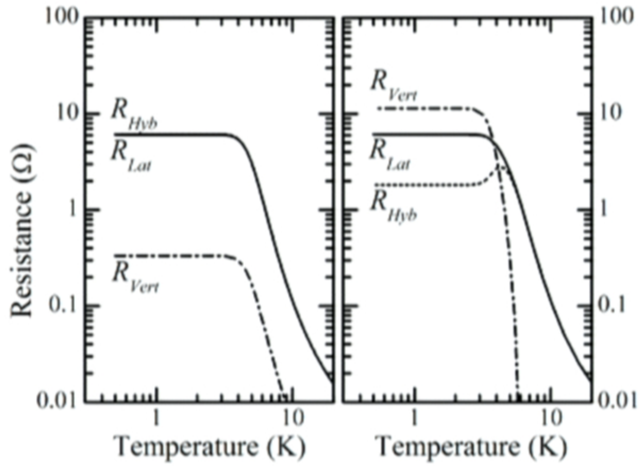

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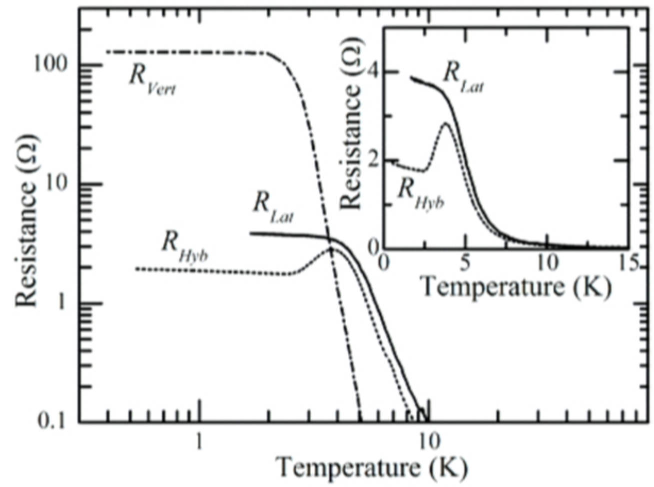
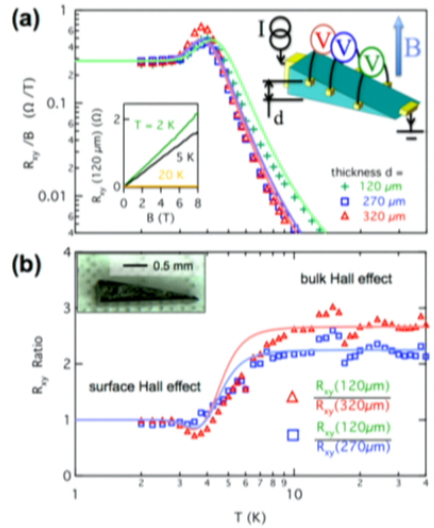


Experiment

- ➢ Bulk conductor at high T
- ➢ Surface conductor at low T: this is the nature of the residual conductivity
- ➢ Robustness: topological protection?
- ➢ Bulk conductivity is zero at low T: an idea topological insulator?

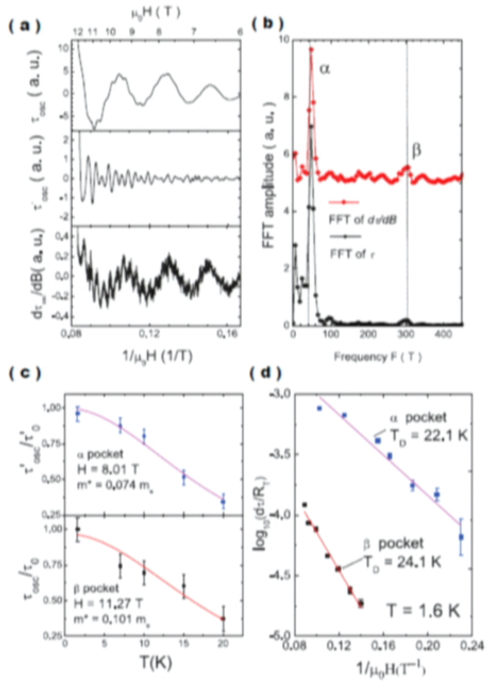
Wolgast, Kurdak, **KS**, Allen, Kim and Fisk, arXiv1211.5104 (2012).

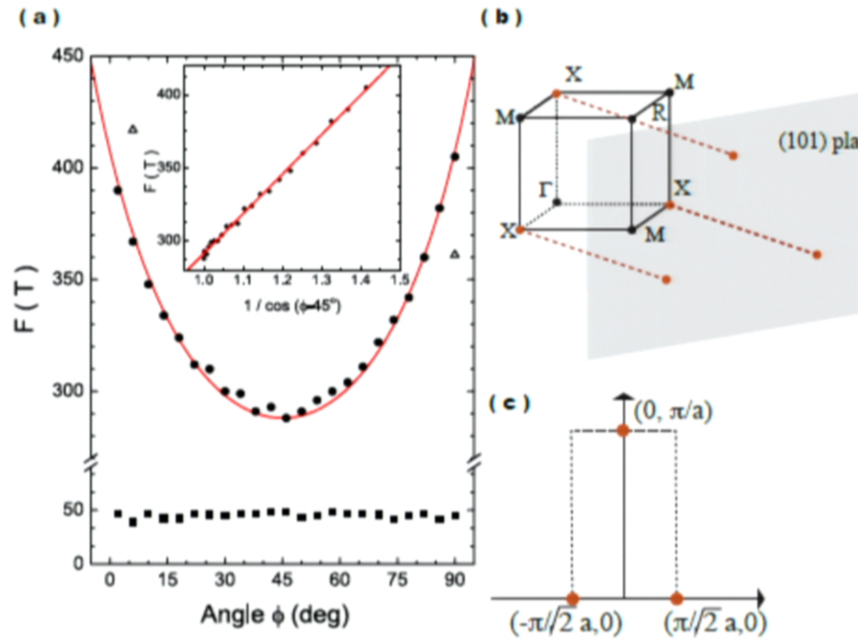
Carrier density



Botimer et. al. arXiv:1211.6769

dHvA oscillations

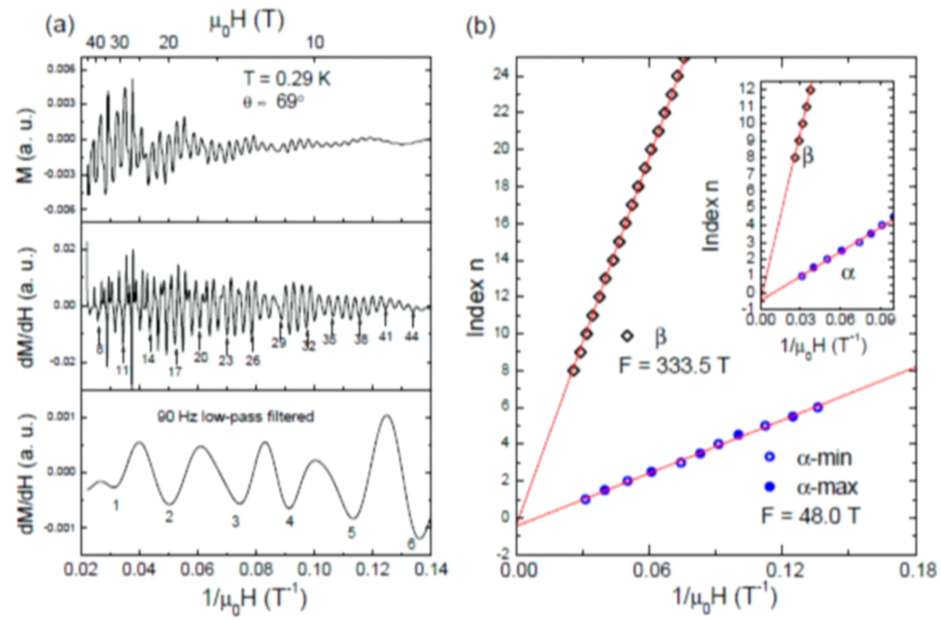




- Two pockets
- One pocket on the (110) surface (from angle dependence)
- The other has a lower resolution, but most likely on the (100) surface

Li, Xiang, Yu, Asaba, Lawson, Cai, Tinsman, Berkley, Wolgast, Eo, Kim, Kurdak, Allen, **KS**, Chen, Wang, Fisk, Li arXiv:1306.5221 (2013).

Surface Dirac points (dHvA oscillations)



Landau index extrapolated to infinite B is an half-integer (for both pockets)

- The surface states contain Dirac points
- Surface states are NOT due to band bending

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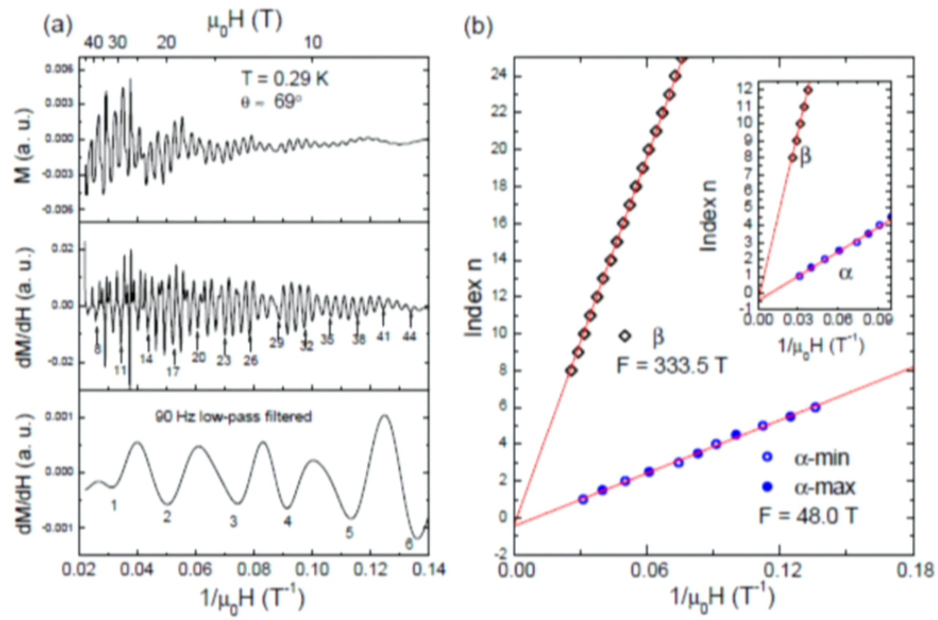

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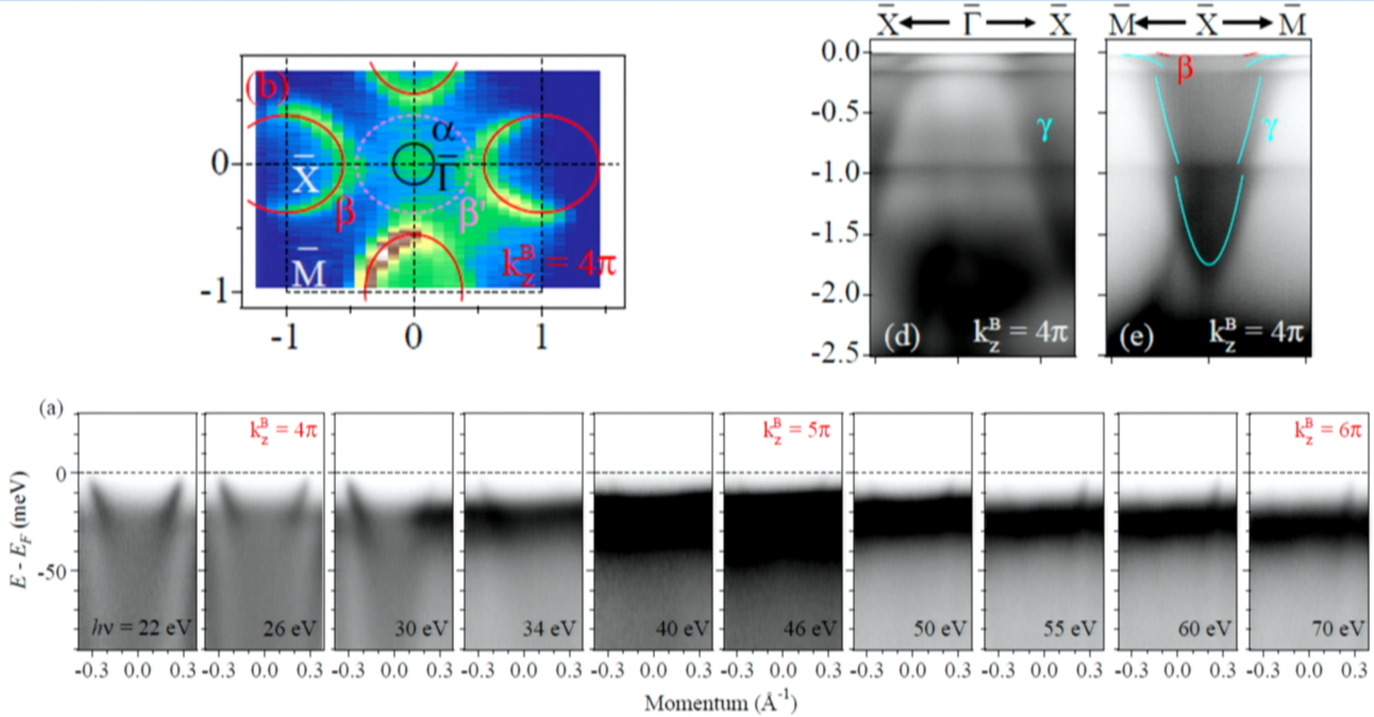
ARPES: three pockets on the (100) surface



Xu, et al., arXiv:1306.3678
Neupane, et al., arXiv:1306.4634
Jiang, et al., arXiv:1306.5664
Frantzeskakis, et al. arXiv:1308.0151
Zhu, et al. arXiv:1309.2945v1

Additional numerical and experimental evidence

- LDA+Gutzwiller (PRL 110, 096401, 2013)
- Magnetic impurities suppresses surface transport (arXiv:1307.0448)
- Weak anti-localization (arXiv:1307.4133)
- STM: (arXiv:1308.1085)

Experiments

- Transport: insulating bulk + a very robust metallic surface
  - Low-T transport (<5K) dominated by the surface
  - people have tried hard to get rid of the “residual resistivity” but failed in the last 40+ years. Now we know the reason (topological protection).
  - Surface transport suppressed by magnetic impurities
  - Surface transport show weak-anti-localization
- Quantum oscillation: surface Dirac points
  - Surface pockets show dHvA oscillations
  - Surface bands contains Dirac points
- ARPES:
  - number and locations of surface pockets agree with the topological theory.

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SmB_6 is an ideal topological insulator

- How about topological crystalline Kondo insulator?
  - Theory: if SmB_6 is a TKI, the same band structure must give us a TCKI.
  - Exp.: need to study the 110 surface with k-sensitive techniques (e.g. ARPES)

Summary

- SmB_6: a topological Kondo insulator and a topological crystalline Kondo insulator.
- SmB_6 : an ideal topological insulator with zero bulk conductivity.
- Other candidates:
  - Topological Kondo insulators:

    SmB_6 and CeNiSn (Dzero, **KS**, Galitski and Coleman, PRL, 2010)

    $CeOs_4As_{12}$ and $CeOs_4Sb_{12}$ (Yan, Muchler, Qi, Zhang and Felser, PRB 2012)

    SmS under pressure (Wolgast, Kurdak, **KS**, Allen, Kim and Fisk, arXiv:1211.5104)

    PuB_6 (Deng, Haule and Kotliar, arXiv:1308.2245)

    YbB_6 (Weng, Zhao, Wang, Fang and Dai, arXiv:1308.5607)

    ...
  - Topological Crystalline Kondo insulators:

    SmB_6 (Ye, Allen and **KS**, arXiv:1307.7191)

    YbB_{12}: a TCKI but not a TKI (Weng, Zhao, Wang, Fang and Dai, arXiv:1308.5607)