Topological insulators driven by electron spin

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$$\mathcal{H} = \sum_{a=1,2} \sum_{\mathbf{k}\sigma} \varepsilon_a(\mathbf{k}) \hat{c}^{\dagger}_{\mathbf{k}\sigma a} \hat{c}_{\mathbf{k}\sigma a} + \lambda \sum_{\mathbf{k}} [\Phi_{\alpha\beta}(\mathbf{k}) \hat{c}^{\dagger}_{\mathbf{k}a\alpha} \hat{c}_{\mathbf{k}\bar{a}\beta} + \text{h.c.}]$$

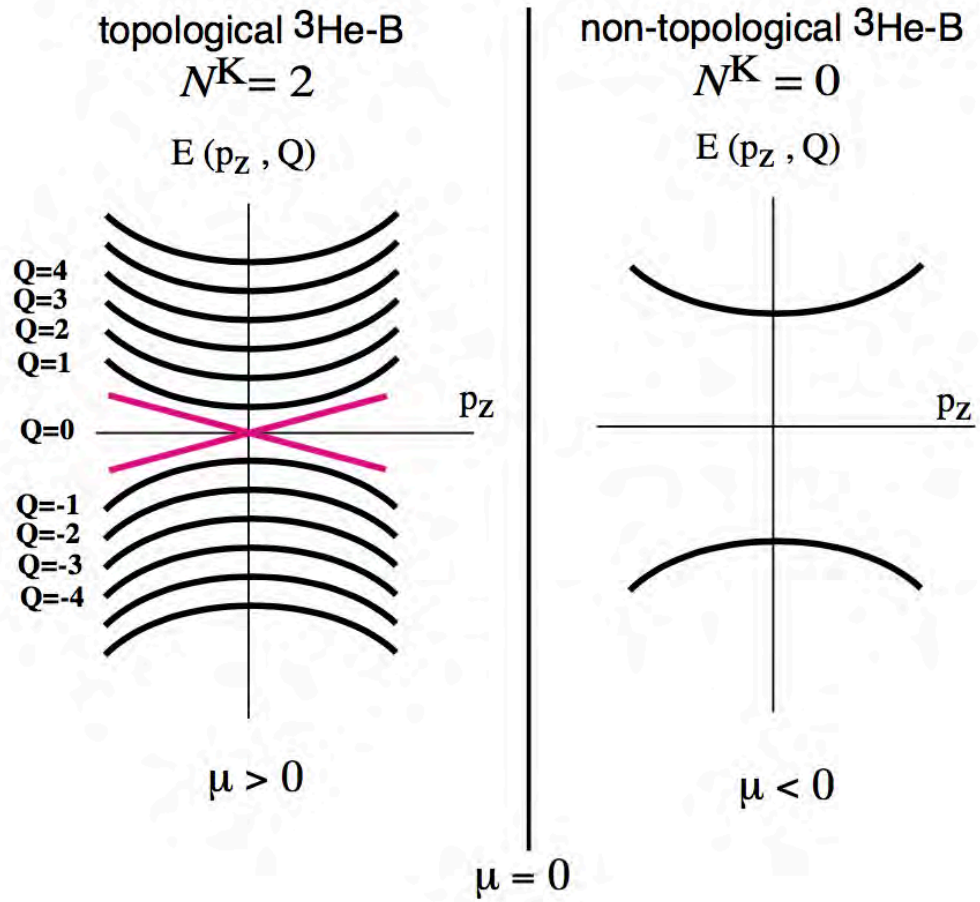
$$+ \sum_{ia\sigma} U_{aa} \hat{n}_{ia\sigma} \hat{n}_{ia\bar{\sigma}}$$

Idea

- superfluid ^{3}He: B-phase

  G. E. Volovik (2010)

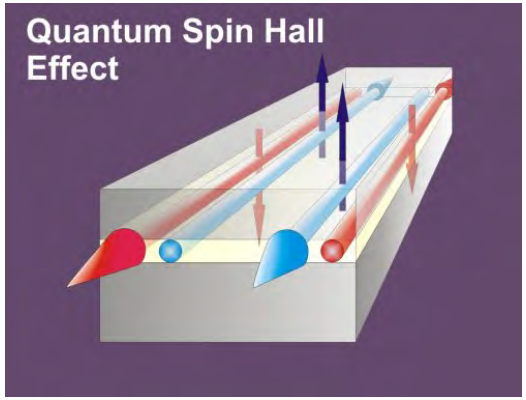
$$H = \begin{pmatrix} \xi_{\mathbf{p}}\hat{\sigma}_0 & \vec{\Delta}(\mathbf{p})\cdot\vec{\sigma} \\ \vec{\Delta}(\mathbf{p})\cdot\vec{\sigma} & -\xi_{\mathbf{p}}\hat{\sigma}_0 \end{pmatrix}$$



Idea

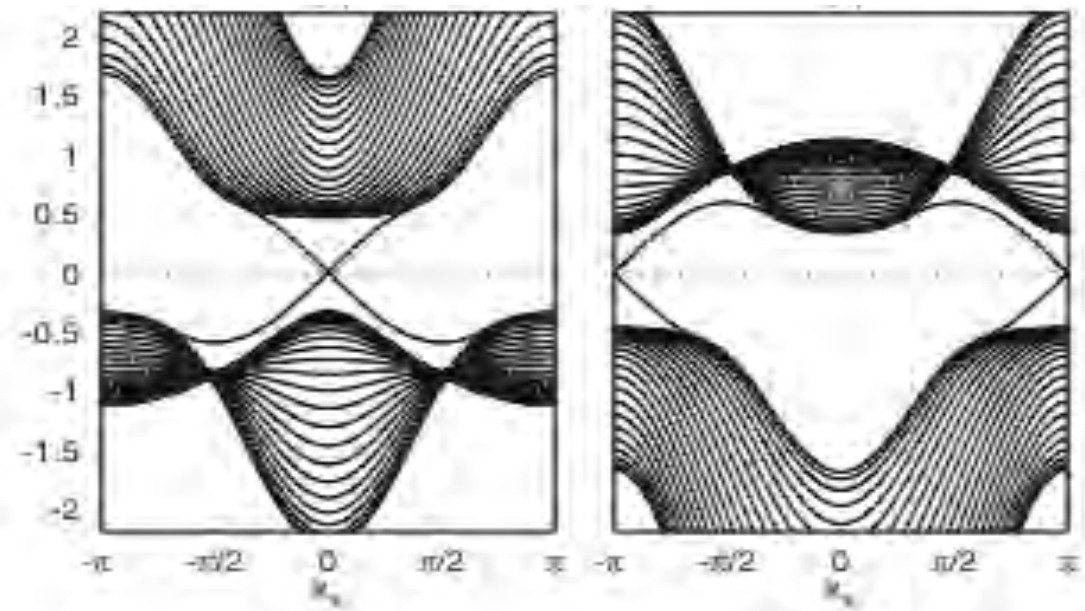
- Spin Hall effect (2D)

A. Bernevig, T. Hughes & S.-C. Zhang, Science 314, 1757 (2006)

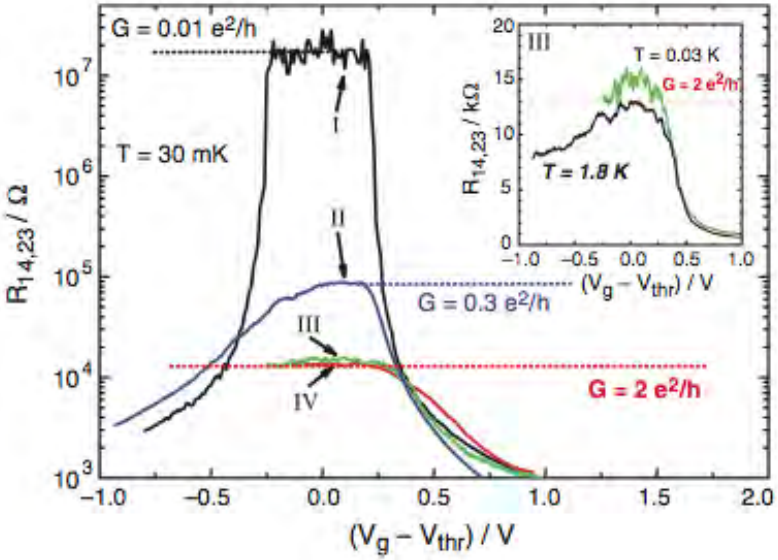


$$\mathcal{H}_0 = \sum_{\mathbf{k}} \psi^\dagger_{\mathbf{k}} \begin{bmatrix} H_{BHZ}(\mathbf{k}) & 0 \\ 0 & \overline{H}_{BHZ}(-\mathbf{k}) \end{bmatrix} \psi_{\mathbf{k}}$$

$$H_{BHZ}(\mathbf{k}) = (m - \cos k_x - \cos k_y)\sigma_z + \lambda(\sin k_x \sigma_x + \sin k_y \sigma_y)$$



Jan Werner and Fakher F. Assaad, PRB 88, 035113 (2013)



M. Konig et al. Science 318, 766 (2007)

Minimal model(s) for topological insulators

$$\mathcal{H} = \sum_{a=1,2} \sum_{\mathbf{k}\sigma} \varepsilon_a(\mathbf{k}) \hat{c}^\dagger_{\mathbf{k}\sigma a} \hat{c}_{\mathbf{k}\sigma a} + \lambda \sum_{\mathbf{k}} [\Phi_{\alpha\beta}(\mathbf{k}) \hat{c}^\dagger_{\mathbf{k}a\alpha} \hat{c}_{\mathbf{k}\bar{a}\beta} + \text{h.c.}]$$
$$+ \sum_{ia\sigma} U_{aa} \hat{n}_{ia\sigma} \hat{n}_{ia\bar{\sigma}}$$

- Special case will be discussed:

$$U_{11} \gg U_{22} > 0$$

$$D_1 \ll D_2$$

$$\Phi_{\alpha\beta}(-\mathbf{k}) = -\Phi_{\alpha\beta}(\mathbf{k})$$

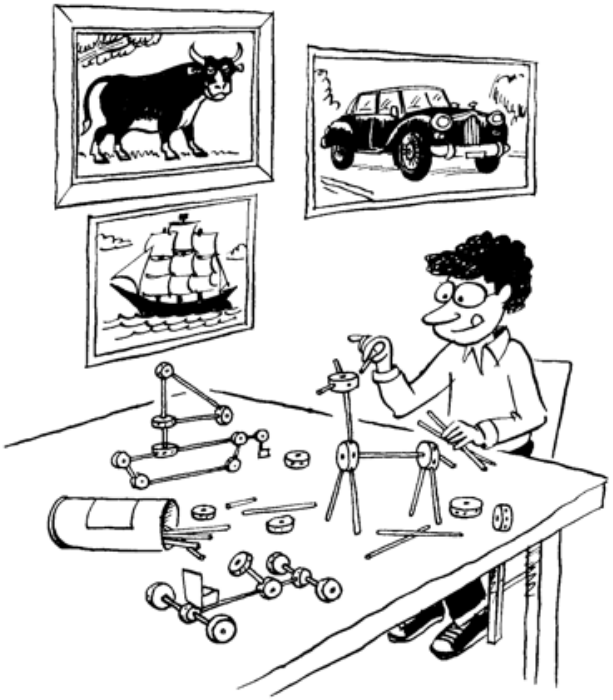
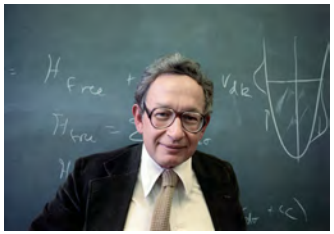


Illustration by Dick Codor.

Minimal model(s) for topological insulators

- Anderson lattice model: *U=0*



Philip W. Anderson

➢ basis $\psi^\dagger_{\mathbf{k}} = (c^\dagger_{\mathbf{k}\uparrow}\ c^\dagger_{\mathbf{k}\downarrow}\ f^\dagger_{\mathbf{k}+}\ f^\dagger_{\mathbf{k}-})$

➢ Hamiltonian (2D)

electrons

$$\mathcal{H}_0 = \sum_{\mathbf{k}} \psi^\dagger_{\mathbf{k}} \begin{bmatrix} \varepsilon_c(\mathbf{k})\hat{1} & V\vec{d}_{\mathbf{k}}\cdot\vec{\sigma} \\ \overline{V}\vec{d}_{\mathbf{k}}\cdot\vec{\sigma} & \varepsilon_f(\mathbf{k})\hat{1} \end{bmatrix} \psi_{\mathbf{k}}$$

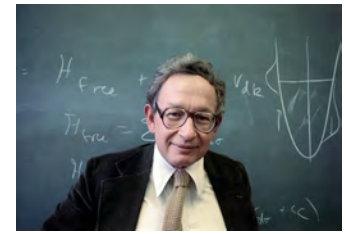
holes

c-f hybridization: $\vec{d}_{\mathbf{k}} = (\sin k_x, \sin k_y)$

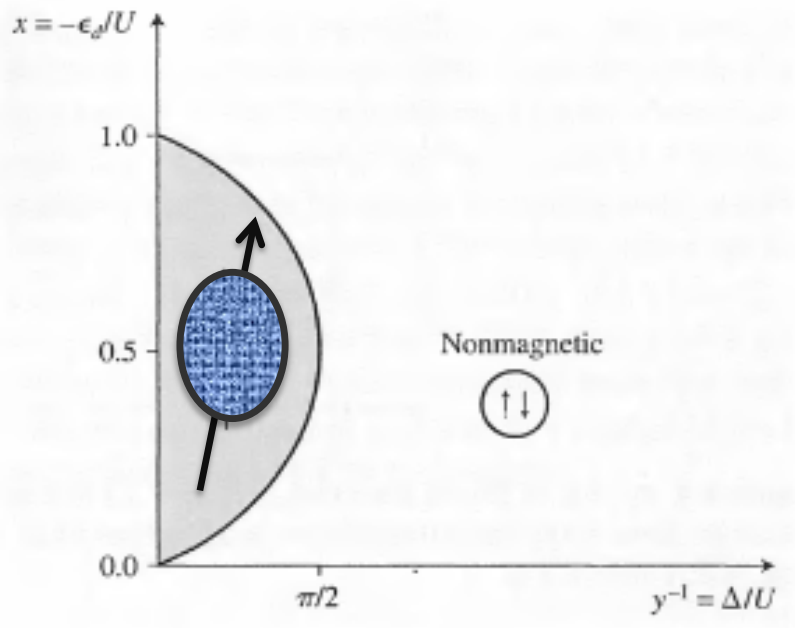
Equivalent to Bernevig-Hughes-Zhang (BHZ) model

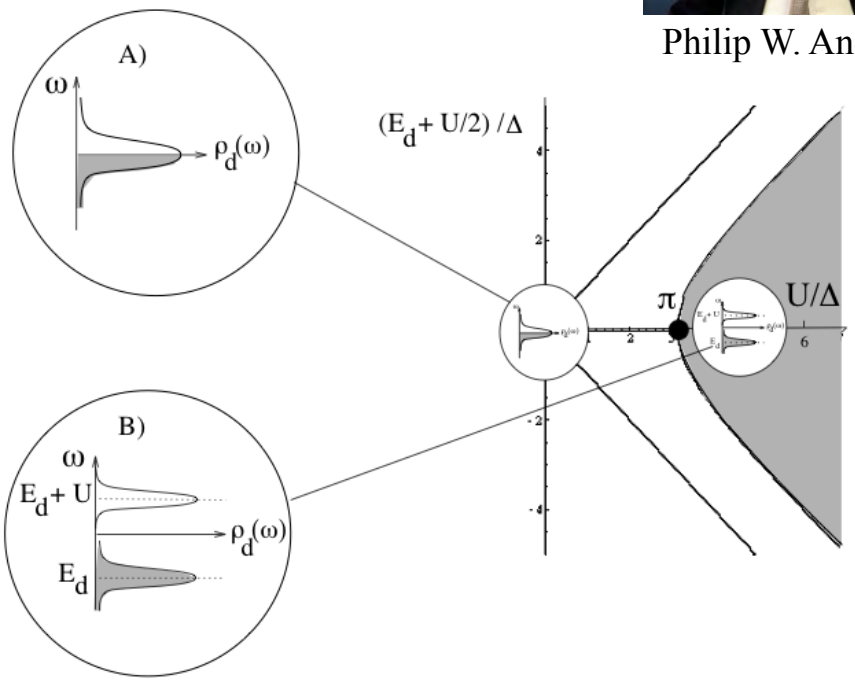
Finite-*U*: local moment formation

P. W. Anderson, Phys. Rev 124, 41, (1961)



Philip W. Anderson





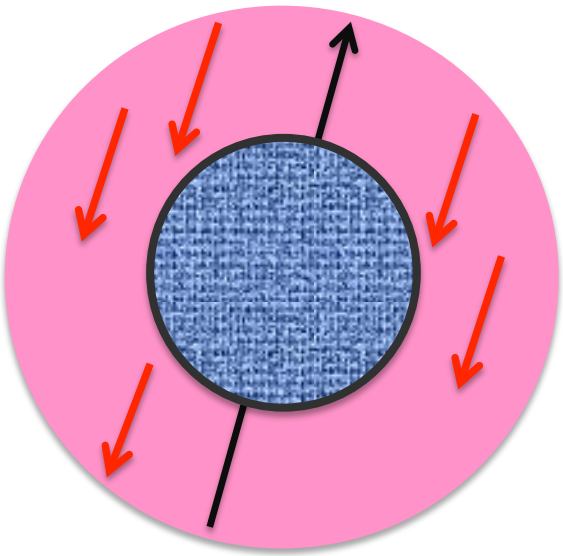
- local *d*- or *f*-electron resonance splits to form a local moment

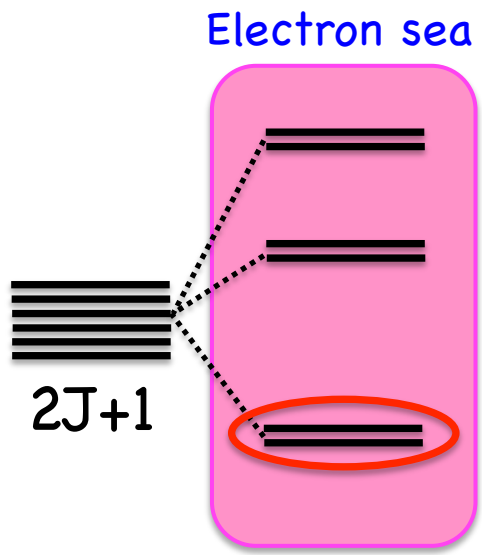
$$n_{d\uparrow} - n_{d\downarrow} \neq 0$$

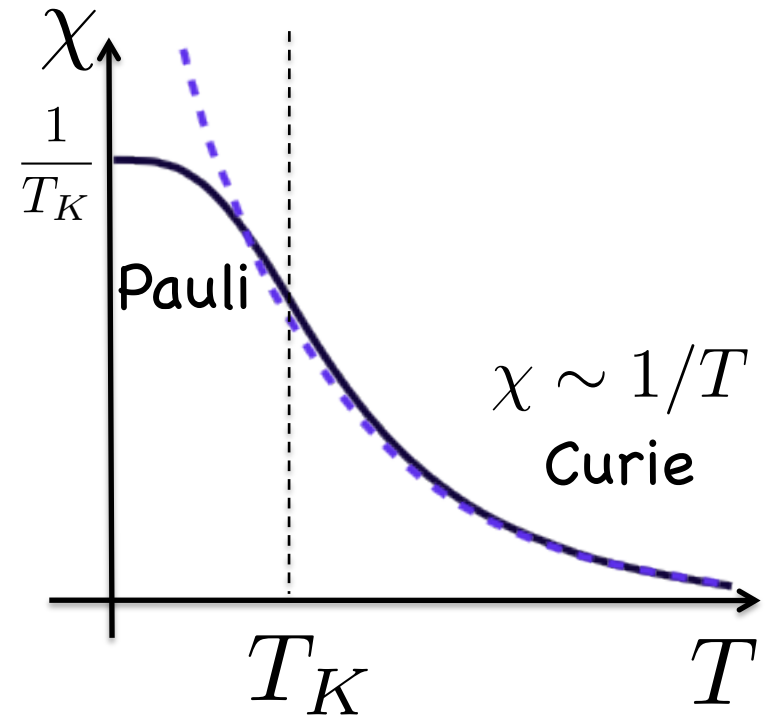
Heavy Fermion Primer: Kondo impurity

Ce or Sm impurity
total angular
momentum J=5/2

$S = 0$ ↓ $S \sim R \ln 2$ ↓





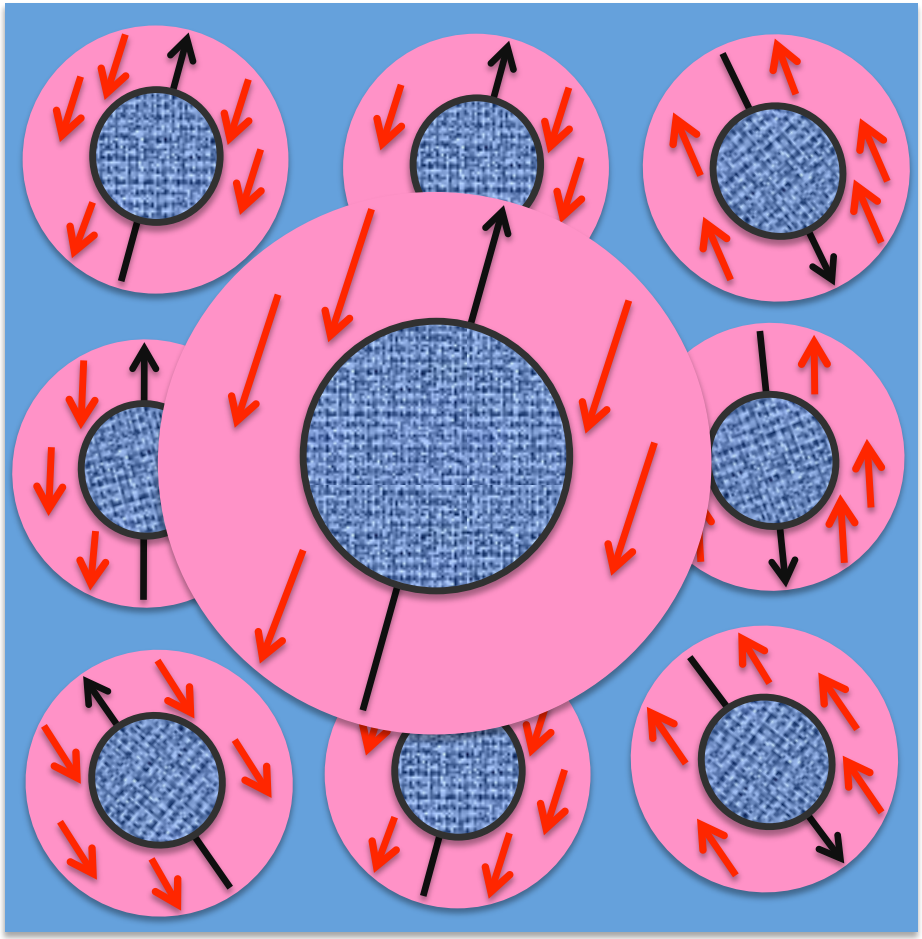


Kondo Temperature

Spin (4f,5f) screened by conduction electrons

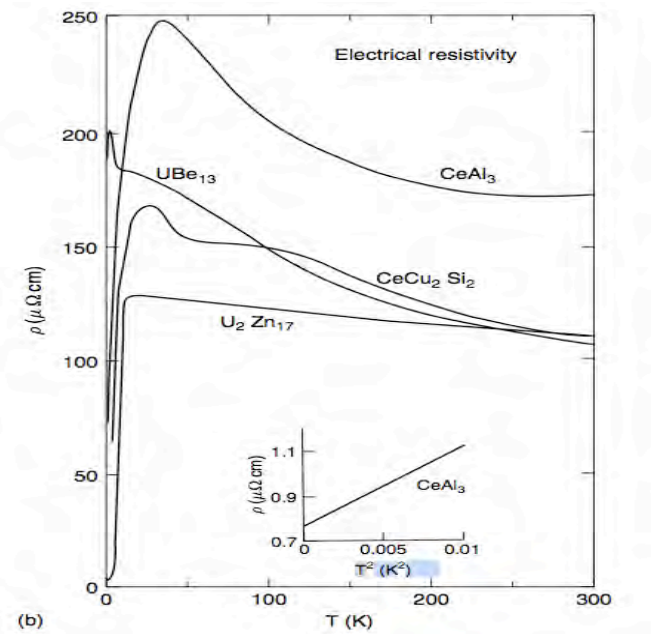
(4f,5f) basic fabric of heavy electron physics

Heavy Fermion Primer

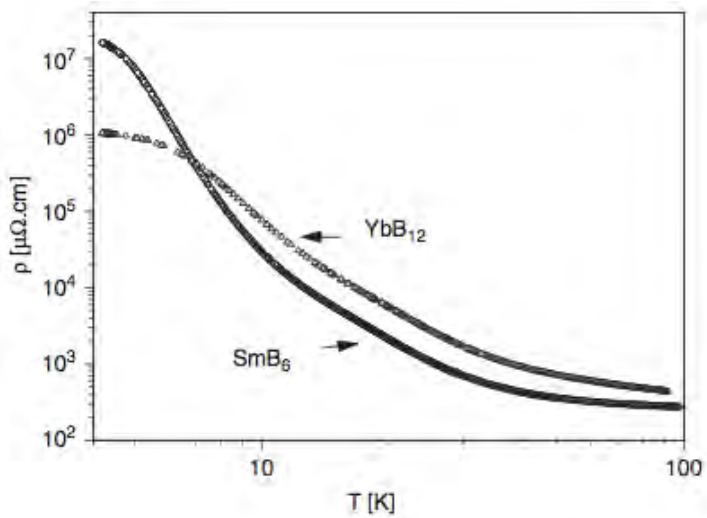


Kondo lattice

➢ coherent heavy fermions



➢ insulator



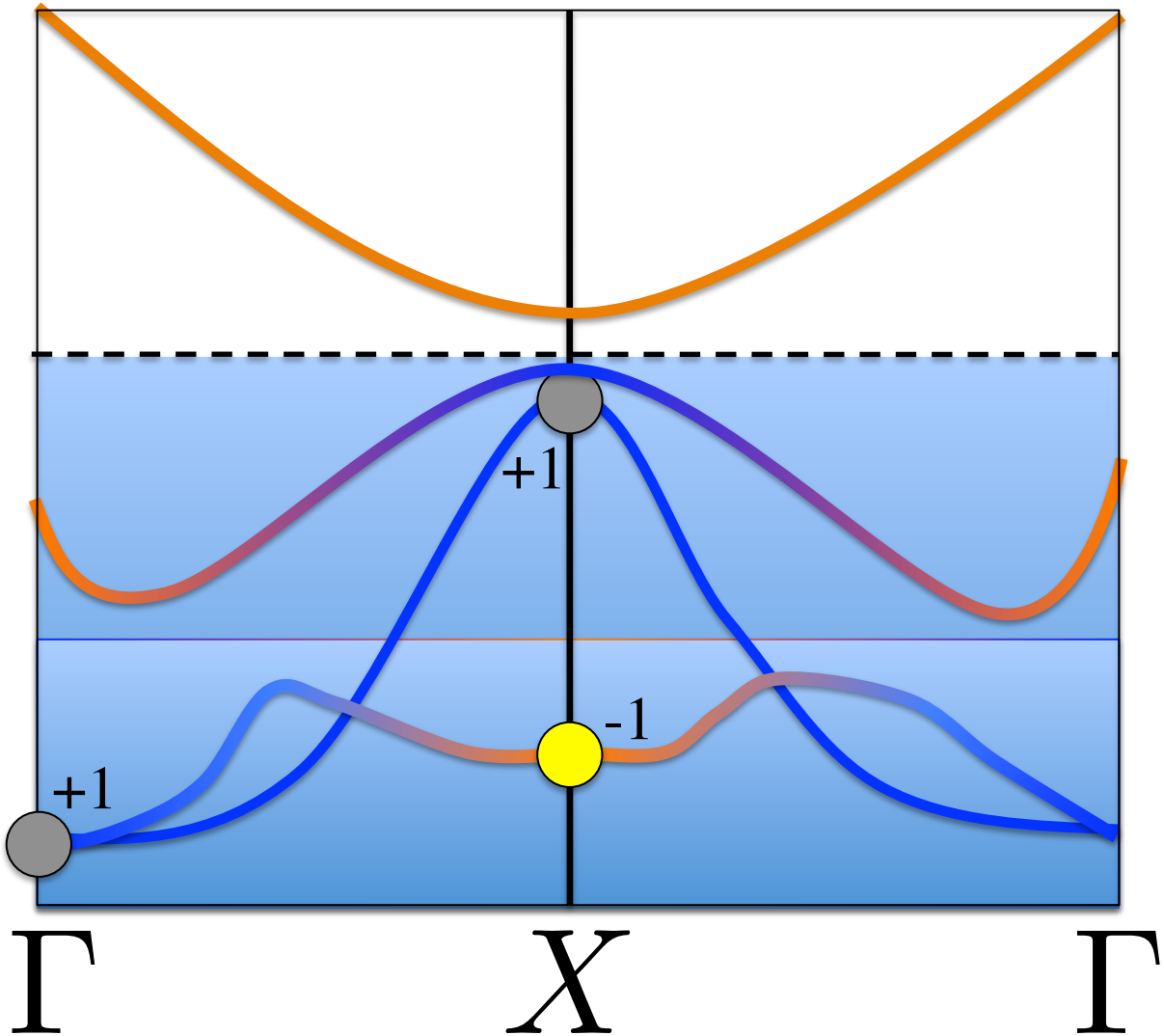
How do we know if an insulator is topological?

even and odd parity bands:

$$d^2 f^0 : \nu = 0$$

Band inversion near X

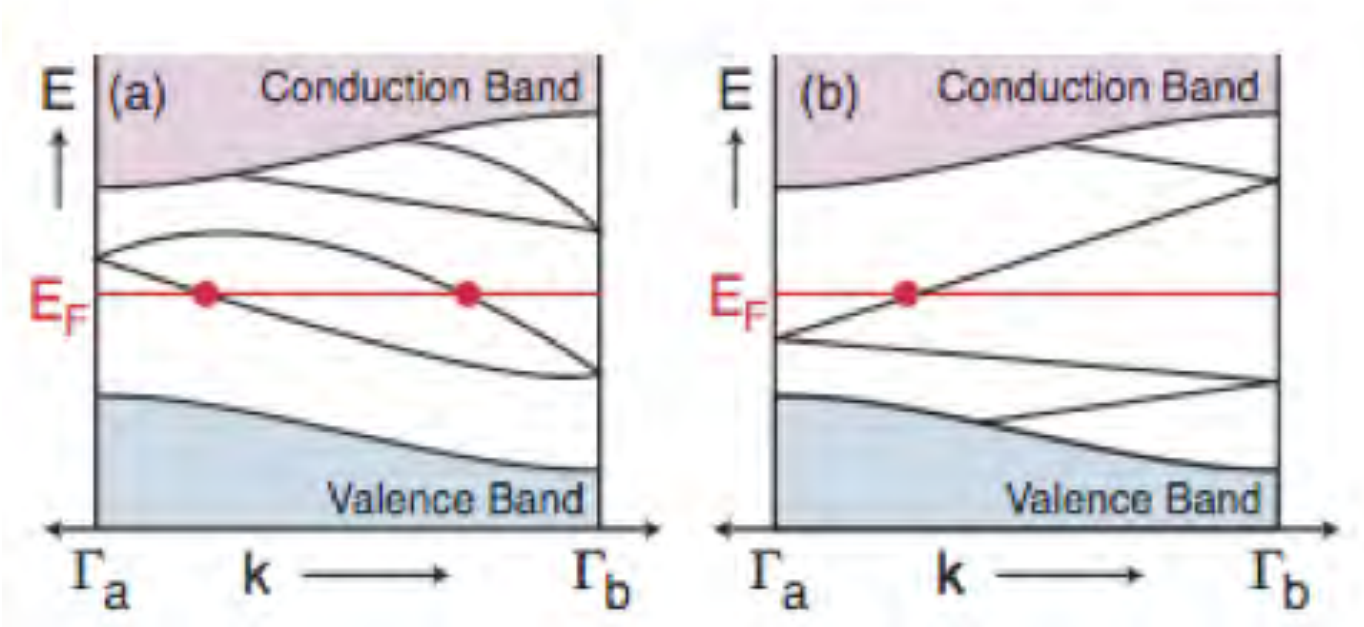
$$d^1 f^1 : \nu = 1$$



For strong TI one needs an odd number of band inversions!

Topological insulator: Z_2 invariant

- "Bulk + boundary" correspondence

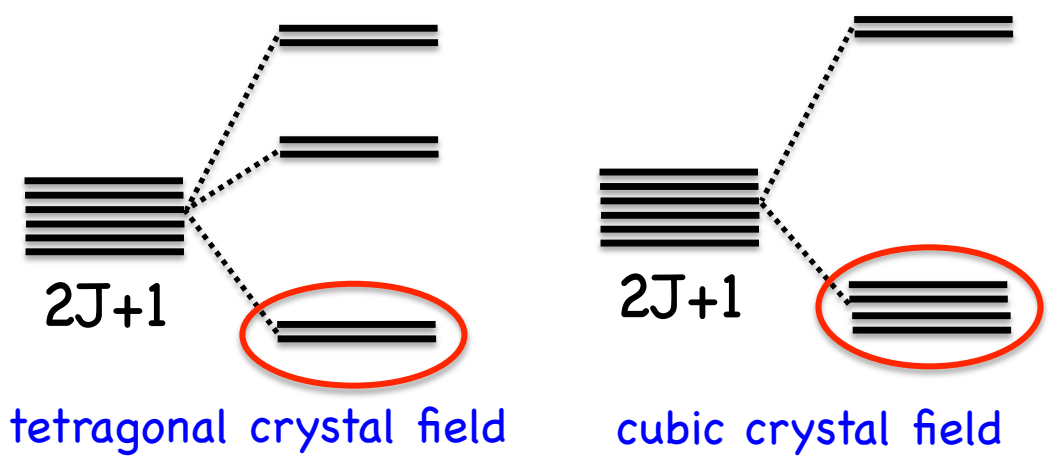


M. Z. Hasan & C. L. Kane, RMP **82,** 3045 (2010)

Two lines out of each Kramers point either connect with
the same Kramers point (even number of nodes)
or different Kramers points (odd number of nodes)

f-orbital insulators: Anderson lattice model

$$H = \underbrace{\sum_{\mathbf{k}\sigma a} \xi_{\mathbf{k}a} \hat{c}^{\dagger}_{\mathbf{k}\sigma a} \hat{c}_{\mathbf{k}\sigma a}}_{\text{conduction electrons (s,p,d orbitals)}} + \underbrace{\sum_{i\alpha} \varepsilon_f \hat{f}^{\dagger}_{i\alpha} \hat{f}_{i\alpha} + U \sum_{i\alpha\beta} \hat{n}_{f\alpha}(i) \hat{n}_{f\beta}(i)}_{f\text{-electrons}}$$



f-orbital insulators: Anderson lattice model

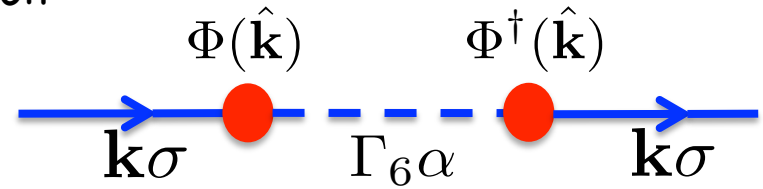
$$H = \underbrace{\sum_{\mathbf{k}\sigma a} \xi_{\mathbf{k}a} \hat{c}^{\dagger}_{\mathbf{k}\sigma a} \hat{c}_{\mathbf{k}\sigma a}}_{\text{conduction electrons (s,p,d orbitals)}} + \underbrace{\sum_{i\alpha} \varepsilon_f \hat{f}^{\dagger}_{i\alpha} \hat{f}_{i\alpha} + U \sum_{i\alpha\beta} \hat{n}_{f\alpha}(i) \hat{n}_{f\beta}(i)}_{f\text{-electrons}}$$

$$+ \underbrace{\sum_{\langle i,j \rangle} \sum_{a\sigma\alpha} \left(V_{i\sigma,j\alpha} \hat{c}^{\dagger}_{i\sigma a} \hat{f}_{j\alpha} + \text{h.c.} \right)}_{\text{Non-local hybridization}}$$

- hybridization: matrix element

$$V_{i\sigma,j\alpha} = \sum_{\mathbf{k}} [\Phi(\mathbf{k})]_{\sigma\alpha} \, e^{-i\mathbf{k}(\mathbf{R}_i - \mathbf{R}_j)}$$

odd functions of **k**



Strong spin-orbit coupling is encoded in hybridization

Interacting electrons: Kondo insulators

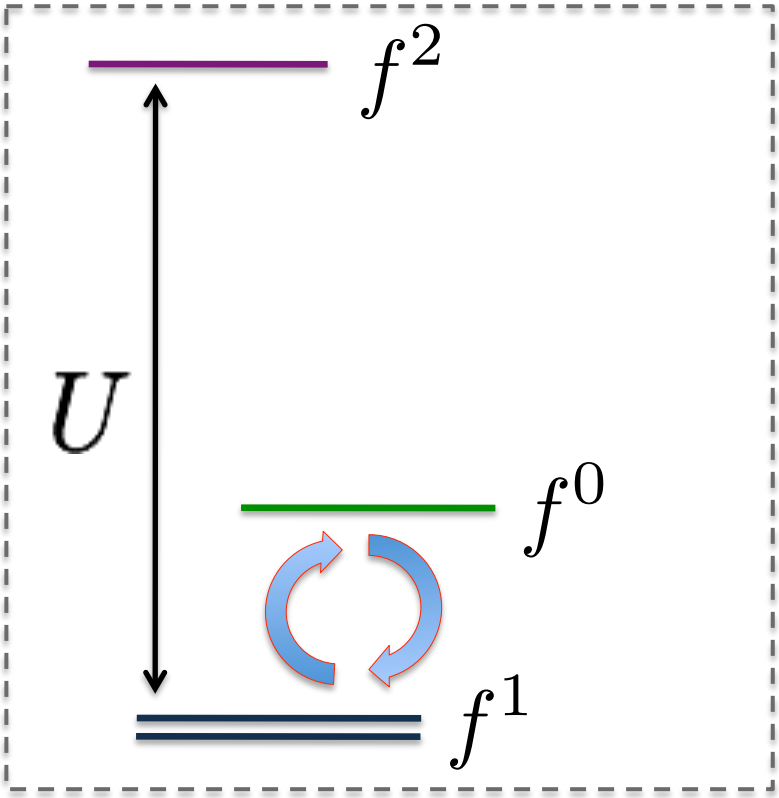
- Anderson model: infinite-*U* limit

Projection (slave-boson) operators:

$$\hat{f}^\dagger_{i\alpha} \rightarrow \hat{f}^\dagger_{i\alpha}\hat{b}_i$$

Constraint:

$$\sum_\alpha \hat{f}^\dagger_{i\alpha}\hat{f}_{i\alpha} + \hat{b}^\dagger_i\hat{b}_i = const.$$



- infinite-*U* limit: hamiltonian

$$\hat{H}_{U=\infty} = \sum_{\mathbf{k}\sigma a}\xi_{\mathbf{k}a}\hat{c}^\dagger_{\mathbf{k}\sigma a}\hat{c}_{\mathbf{k}\sigma a} + \sum_{\langle i,j\rangle}\sum_\alpha t^{(f)}_{ij}\hat{f}^\dagger_{i\alpha}\hat{b}_i\hat{b}^\dagger_j\hat{f}_{j\alpha} + \sum_{\langle i,j\rangle}\sum_{\sigma\alpha a}\left(V_{i\sigma,j\alpha}\hat{c}^\dagger_{i\sigma a}\hat{b}^\dagger_j\hat{f}_{j\alpha} + \text{h.c.}\right)$$

mean-field approximation: $\hat{b}_i \rightarrow \langle\hat{b}_i\rangle = b$

Kondo insulators: mean-field theory

- self-consistency equations:

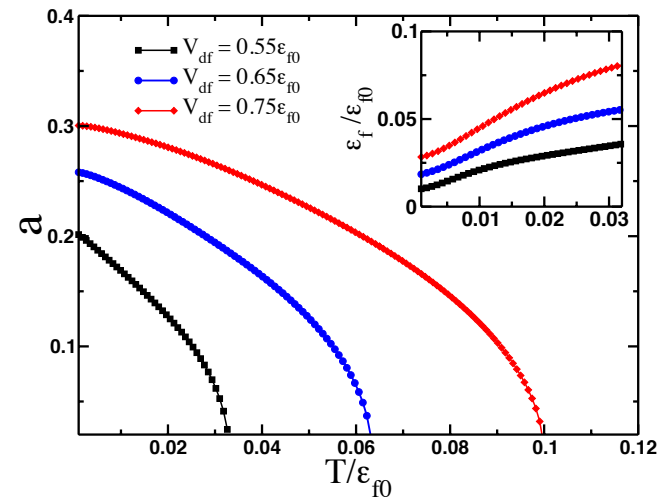
$$(\varepsilon_f - \varepsilon_f^{(0)})a + T\sum_{i\omega,\mathbf{k}}[Nah_{\mathbf{k}}A_{ff}(\mathbf{k},i\omega) + V\phi_{\mathbf{k}}A_{fc}(\mathbf{k},i\omega)] = 0$$

$$(a^2 - q_N) + T\sum_{i\omega}\sum_{\mathbf{k}} A_{ff}(i\omega,\mathbf{k}) = 0$$

$$(q_N - a^2) + T\sum_{i\omega}\sum_{\mathbf{k}} A_{cc}(\mathbf{k},i\omega) = 1$$

- mean-field Hamiltonian:

$$\mathcal{H}_{mf}(\mathbf{k}) = \begin{pmatrix} \xi_{\mathbf{k}}\underline{1} & \tilde{V}\Phi^\dagger_{\Gamma\mathbf{k}} \\ \tilde{V}\Phi_{\Gamma\mathbf{k}} & \underbrace{\varepsilon_f\underline{1}}_{\text{renormalized position of the f-level}} \end{pmatrix}$$



Kondo insulators: mean-field theory

- mean-field Hamiltonian:

L. Fu & C. Kane, PRB 76, 045302 (2007)

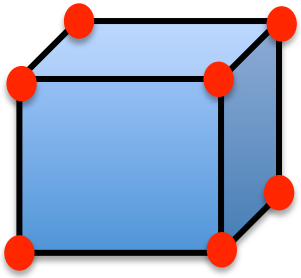
$$\mathcal{H}_{mf}(\mathbf{k}) = \begin{pmatrix} \xi_{\mathbf{k}}\underline{1} & \tilde{V}\Phi^{\dagger}_{\Gamma\mathbf{k}} \\ \tilde{V}\Phi_{\Gamma\mathbf{k}} & \underbrace{\varepsilon_f\underline{1}}_{\text{renormalized position of the f-level}} \end{pmatrix}$$

- parity $P = \begin{pmatrix} \underline{1} & 0 \\ 0 & -\underline{1} \end{pmatrix}$
- time-reversal $\mathcal{T} = \begin{pmatrix} i\sigma_y & 0 \\ 0 & i\sigma_y \end{pmatrix}$

✓ $H_{mf}(\mathbf{k}) = PH_{mf}(-\mathbf{k})P^{-1}$ ✓ $[H_{mf}(\mathbf{k})]^T = \mathcal{T}H_{mf}(-\mathbf{k})\mathcal{T}^{-1}$

P-inversion odd form factor vanishes @ high symmetry points of the Brillouin zone

$$H_{mf}(\mathbf{k}_m) = \frac{1}{2}(\xi_{\mathbf{k}_m} + \varepsilon_f)\underline{1} + \frac{1}{2}(\xi_{\mathbf{k}_m} - \varepsilon_f)P$$



Tetragonal Topological Kondo Insulators

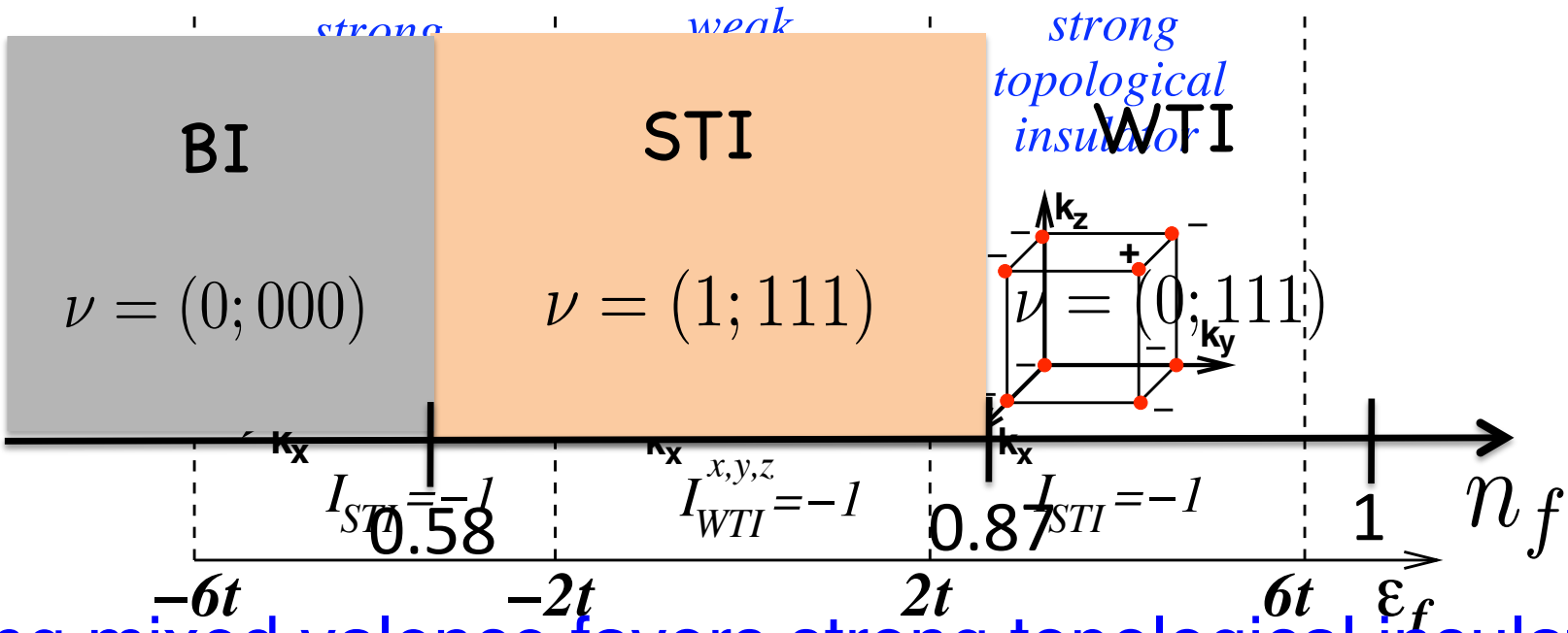
Z_2 invariants: $(\nu_0; \nu_1, \nu_2, \nu_3)$

$$\delta(\Gamma_m) = \mathrm{sign}(\xi_{\mathbf{k}_m} - \varepsilon_f)$$

"strong": $(-1)^{\nu_0} = \prod_{m=1}^{8} \delta_m = \pm 1$

3 "weak": $(-1)^{\nu_j} = \prod_{\mathbf{k}_m \in P_j} \delta_m = \pm 1$

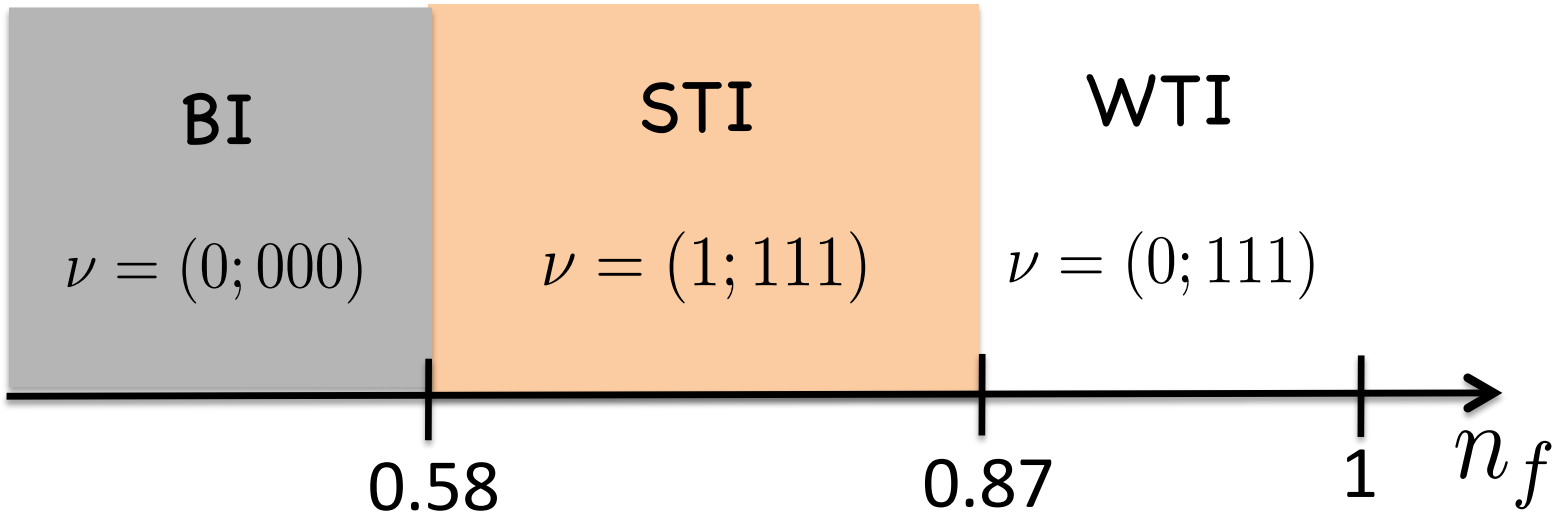
tetragonal symmetry: Kramers doublet



Strong mixed valence favors strong topological insulator!

jour ref: Phys. Rev. Lett. 104, 196403 (2010)

Strong Topological Kondo Insulators



Q: What factors are important for extending strong topological insulating state to the local moment regime ($n_f \approx 1$)?

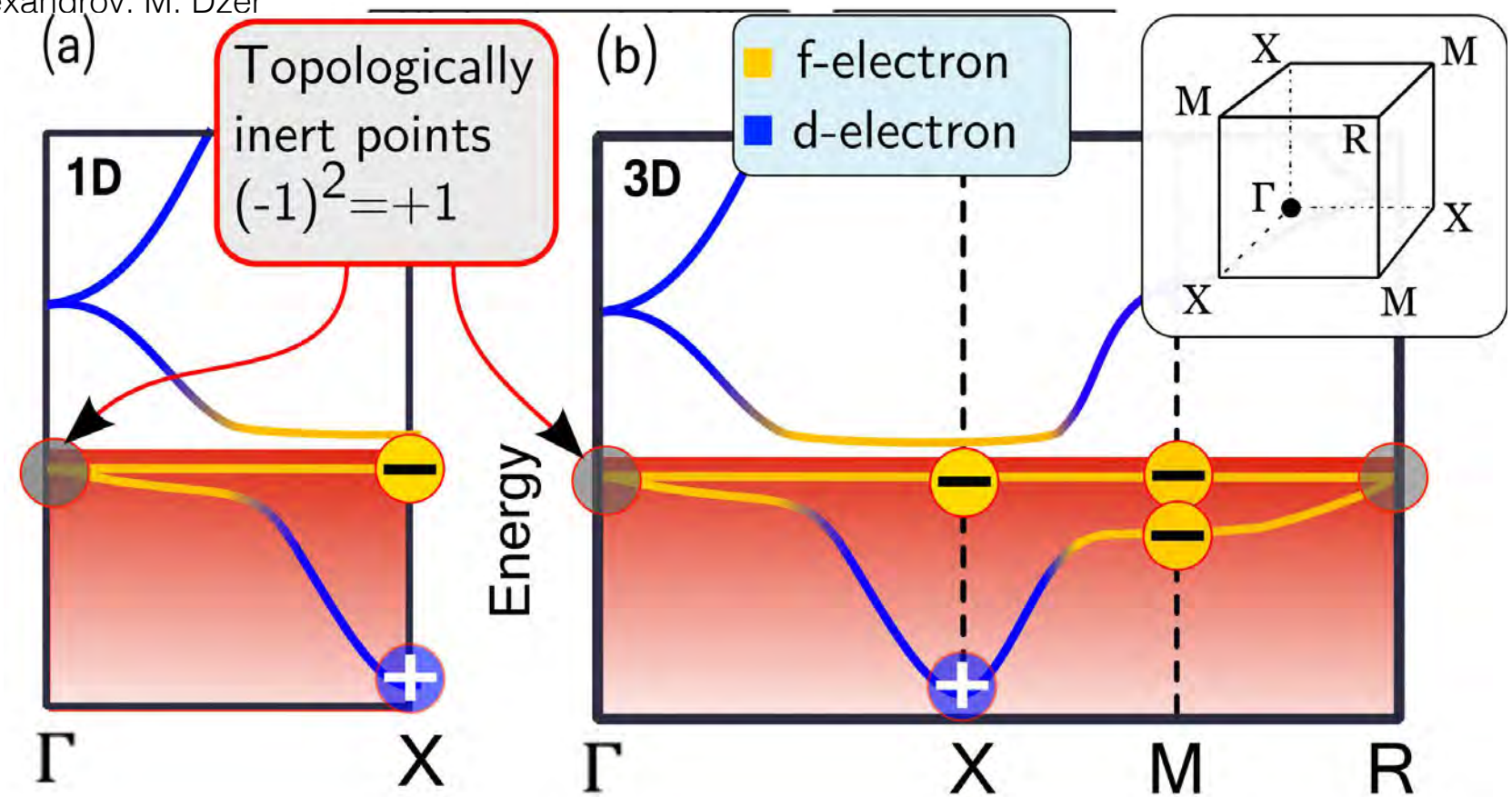
A: Degeneracy = high symmetry (cubic!)

M. Dzero, Europhys. Jour. B **85**, 297 (2012)

Cubic Topological Kondo Insulators

Cubic symmetry (quartet)

T. Takimoto, Jour. Phys. Soc. Jpn. **80**, 123710 (2011)
V. Alexandrov. M. Dzer



V. Alexandrov, M. Dzero, P. Coleman, Phys. Rev. Lett. 111, 206403 (2013)

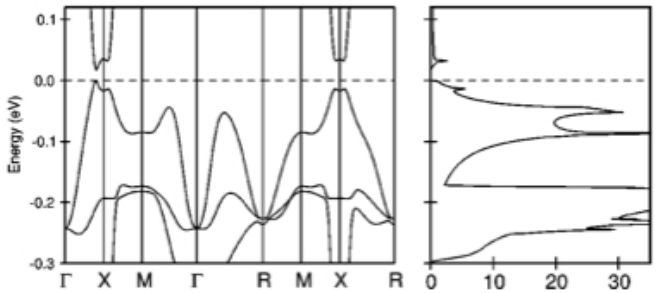
$$|\Gamma_{8(1)}\rangle = \pm\sqrt{\frac{5}{6}}|\pm 5/2\rangle \pm \sqrt{\frac{1}{6}}|\mp \frac{3}{2}\rangle$$

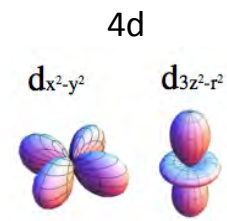
$$|\Gamma_{8(2)}\rangle = \pm|\pm 1/2\rangle$$

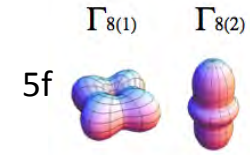
Bands must invert either @ X or M high symmetry points

Cubic Topological Kondo Insulators

Cubic symmetry (quartet)







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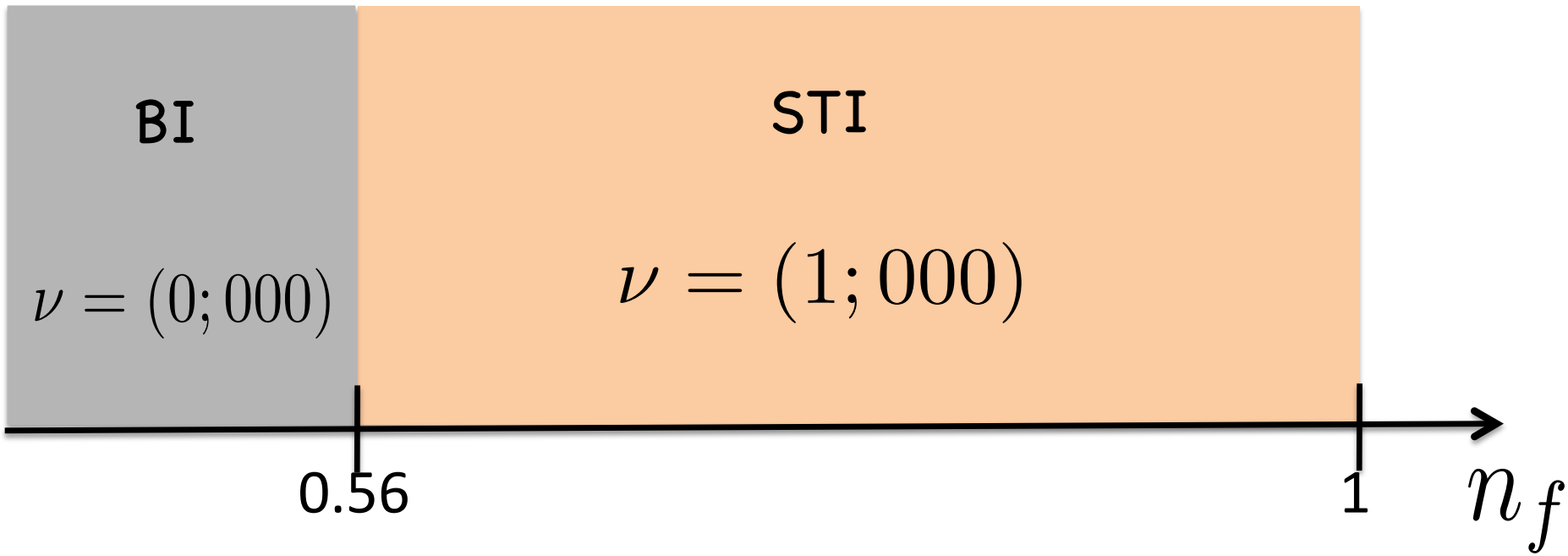


V. Alexandrov, M. Dzero, P. Coleman, Phys. Rev. Lett. 111, 206403 (2013))

Cubic symmetry protects strong topological insulator!

Cubic Topological Kondo Insulators: surface states

- Bulk Hamiltonian:

$$H_{bulk}(\mathbf{k}) = \begin{pmatrix} H_d(\mathbf{k}) & V_h(\mathbf{k}) \\ V_h^\dagger(\mathbf{k}) & H_f(\mathbf{k}) \end{pmatrix}$$

$$H_l(\mathbf{k}) = \epsilon^l \hat{\mathrm{I}}_4 + t^l \begin{pmatrix} \hat{\phi}_1(\mathbf{k}) + \eta_l \hat{\phi}_2(\mathbf{k}) & (1-\eta_l)\hat{\phi}_3(\mathbf{k}) \\ (1-\eta_l)\hat{\phi}_3(\mathbf{k}) & \eta_l \hat{\phi}_1(\mathbf{k}) + \hat{\phi}_2(\mathbf{k}) \end{pmatrix}$$

$$V_h(\mathbf{k}) = \frac{V}{4} \begin{pmatrix} 3(\bar{\sigma}_x - \bar{\sigma}_y) & \sqrt{3}(\bar{\sigma}_x + \bar{\sigma}_y) \\ \sqrt{3}(\bar{\sigma}_x + \bar{\sigma}_y) & \bar{\sigma}_x - \bar{\sigma}_y + 4\bar{\sigma}_z \end{pmatrix}$$

Assumption: boundary has little effect on the bulk parameters, i.e. mean-field theory in the bulk still holds with open boundaries

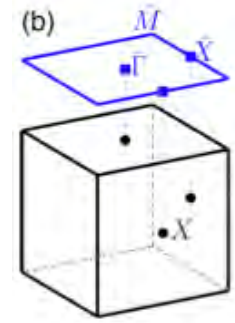
$$H_{bulk}(\delta k_z \to -i\partial_z)\Psi(z) = E_m \Psi(z).$$

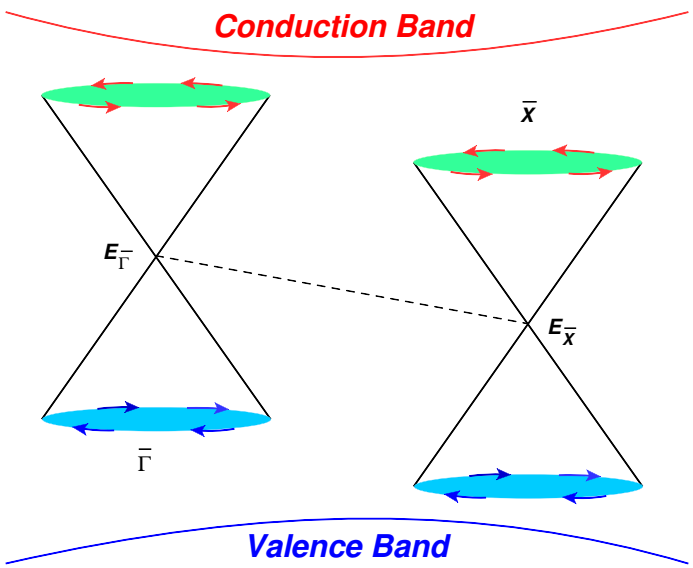
Cubic Topological Kondo Insulators: surface states

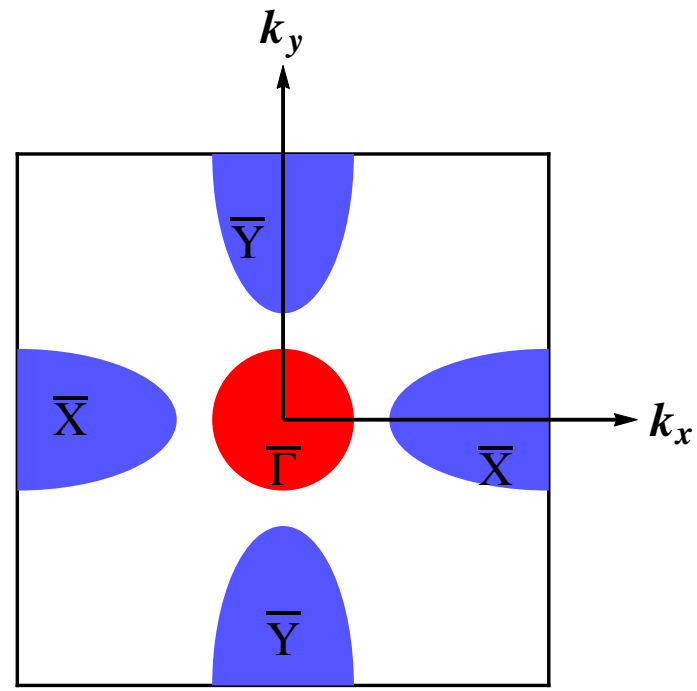
- effective surface Hamiltonian:

$$H^{\bar{\Gamma}}_{surf} = v^{\bar{\Gamma}}_F \left(\sigma_x k_x - \sigma_y k_y\right) \quad v^{\bar{\Gamma}}_F = 2V\sqrt{\frac{-2t^d t^f \eta_d \eta_f}{(\eta_d t^d - \eta_f t^f)^2}}.$$

$$H^j_{surf} = \left(v^j_x \sigma_x k_x - v^j_y \sigma_y k_y\right), j = \overline{X}, \overline{Y}$$



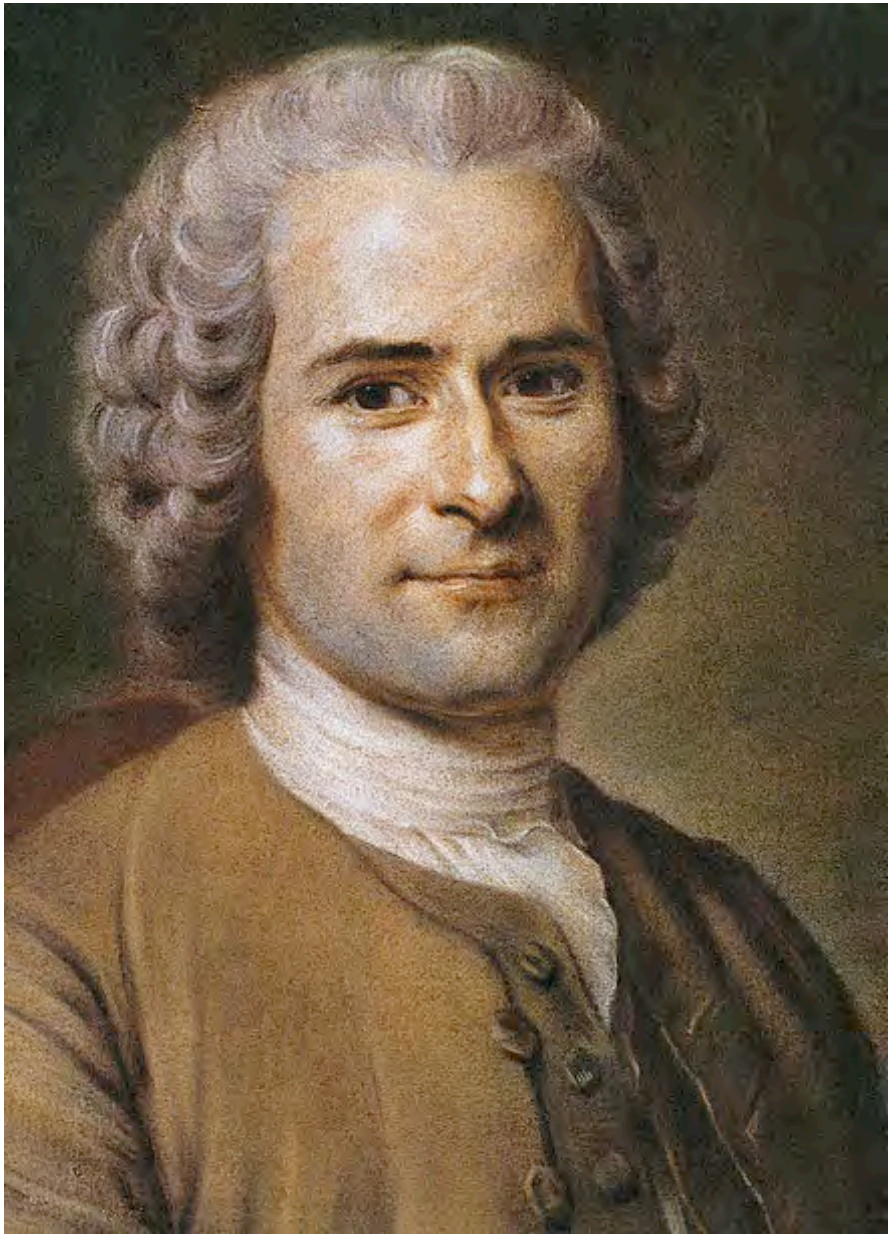




➢ Fermi velocities are small: surface electrons are heavy

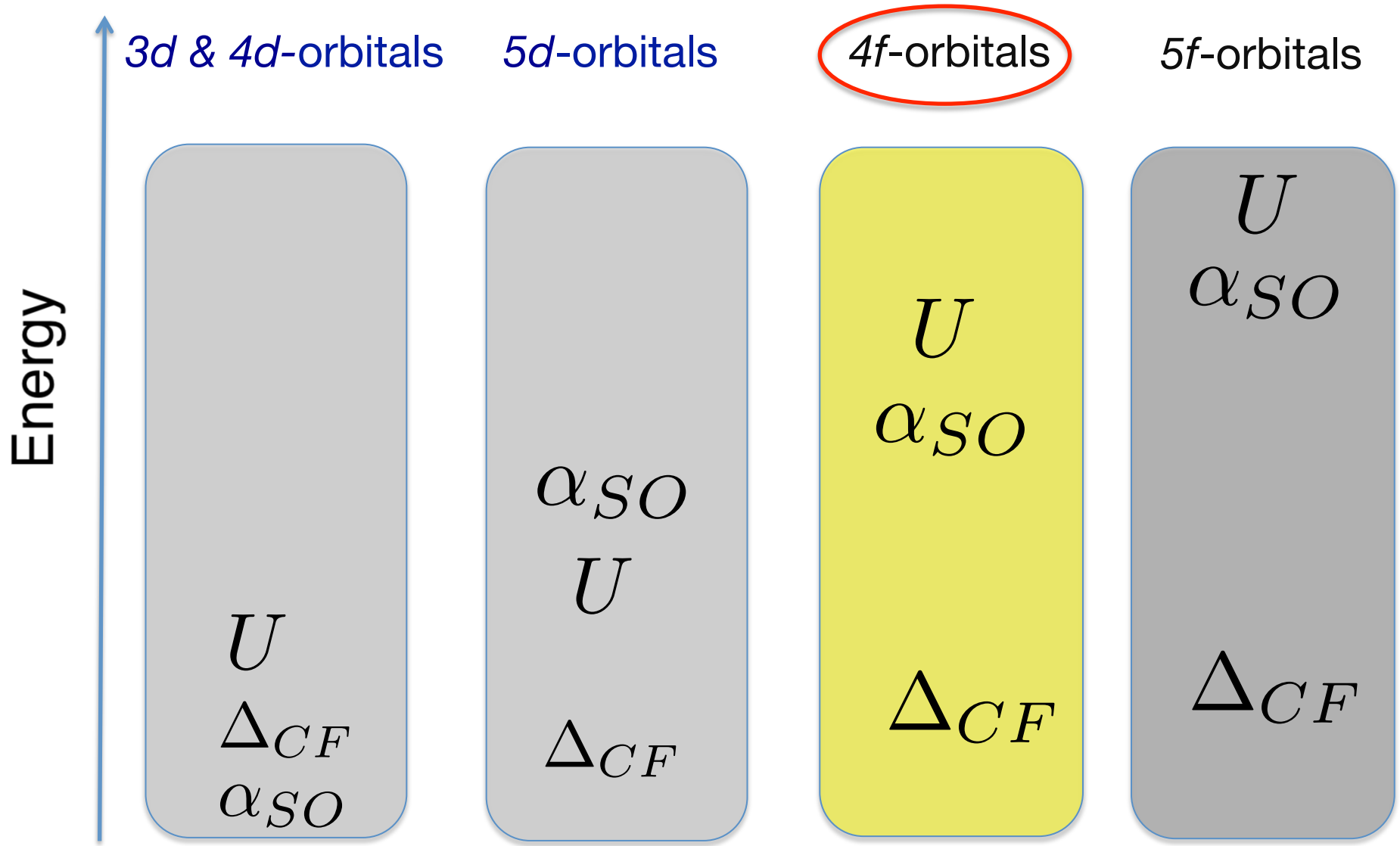
“The world of imagination is boundless. The world of reality has its limits.”

J. J. Rousseau



Quest for ideal topological insulators

- complex materials with *d*- & *f*-orbitals



Quest for ideal topological insulators

- complex materials with *d*- & *f*-orbitals

TABLE I: Strength of Hubbard interaction U and spin-orbit coupling λ depending on a type of orbital state

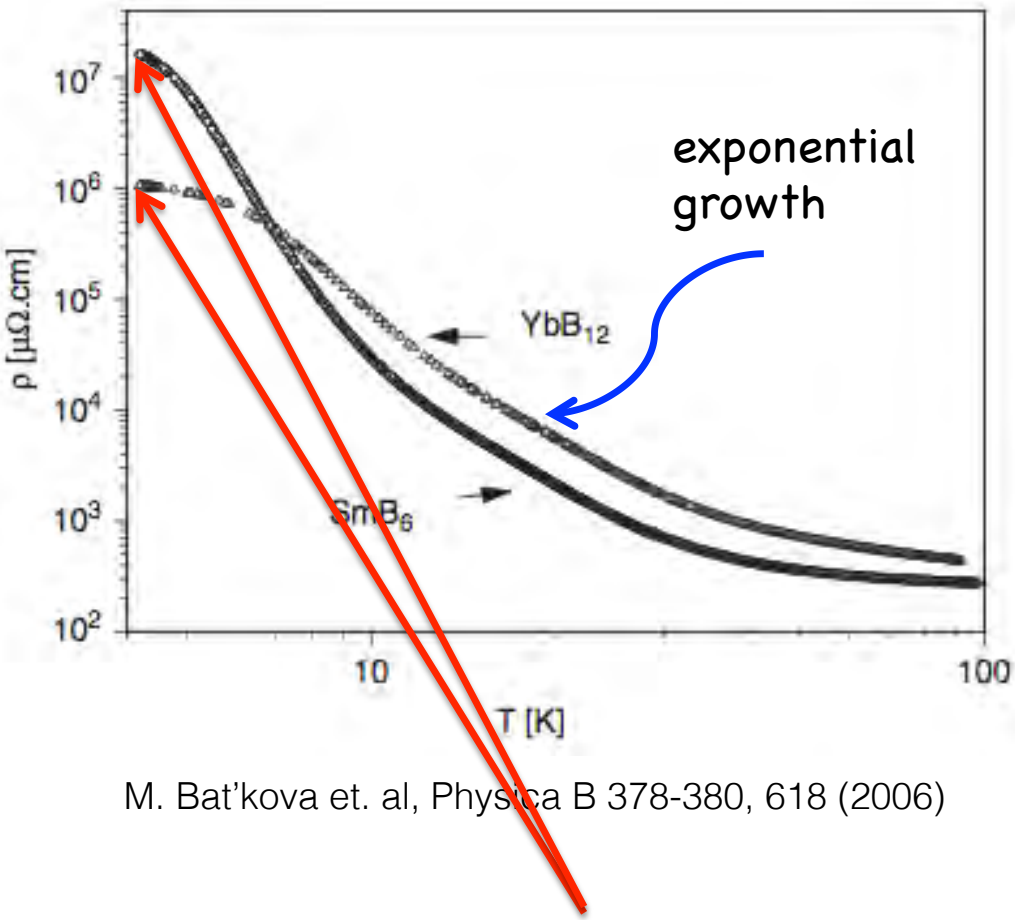
	$4d$	$5d$	$4f$	$5f$
U (eV)	1.5	1	1.7	2.1
α (eV)	$0.1 \div 0.2$	$0.4 \div 0.6$	$0.7 \div 1$	$1 \div 2$

- candidates for *f*-orbital topological insulators

$FeSb_2$, SmB_6, YbB_{12}, YbB_6 & $Ce_3Bi_4Pt_3$

Semiconductors with f-electrons

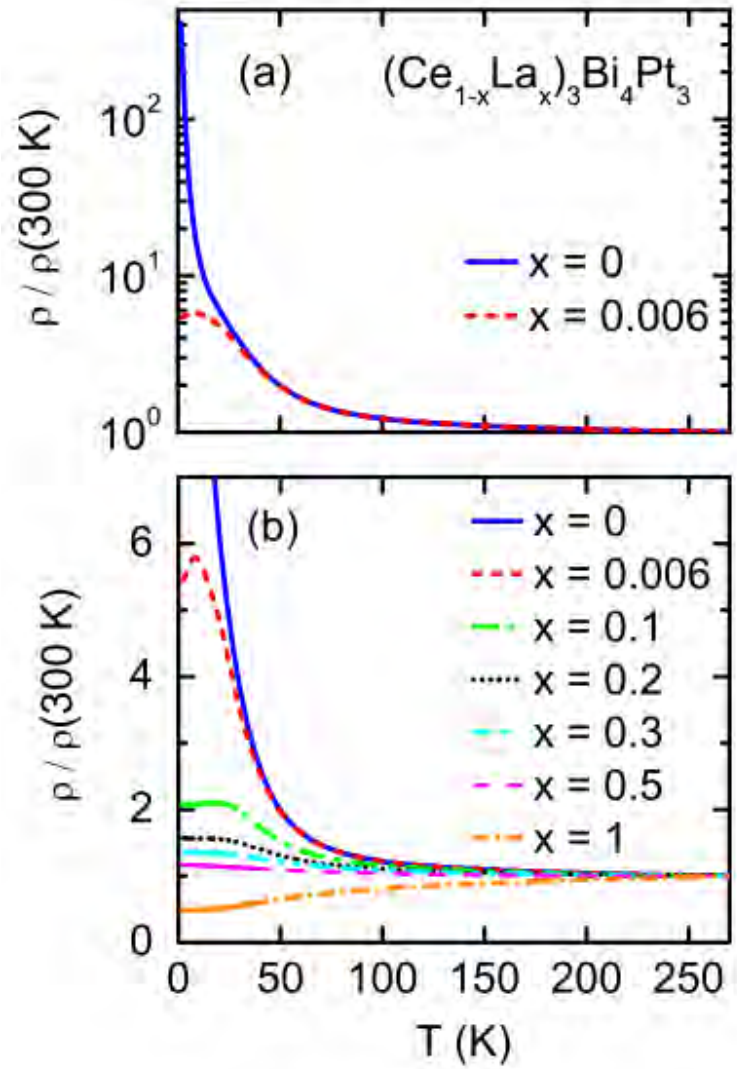
- canonical examples: SmB_6 & YbB_{12}



M. Bat'kova et. al, Physica B 378-380, 618 (2006)

Conductivity remains finite!

$Ce_3Bi_4Pt_3$



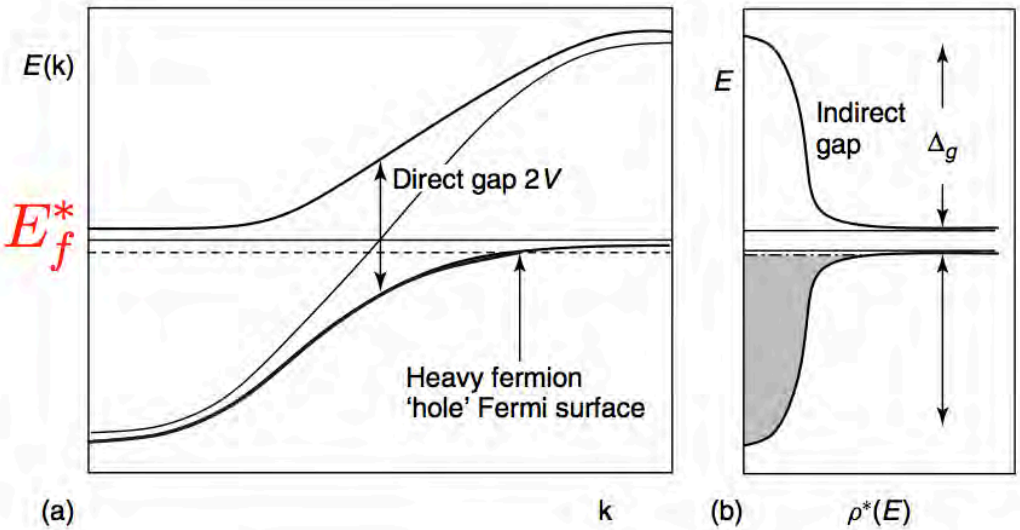
P. Canfield et. al, (2003)

Mott's Hybridization picture

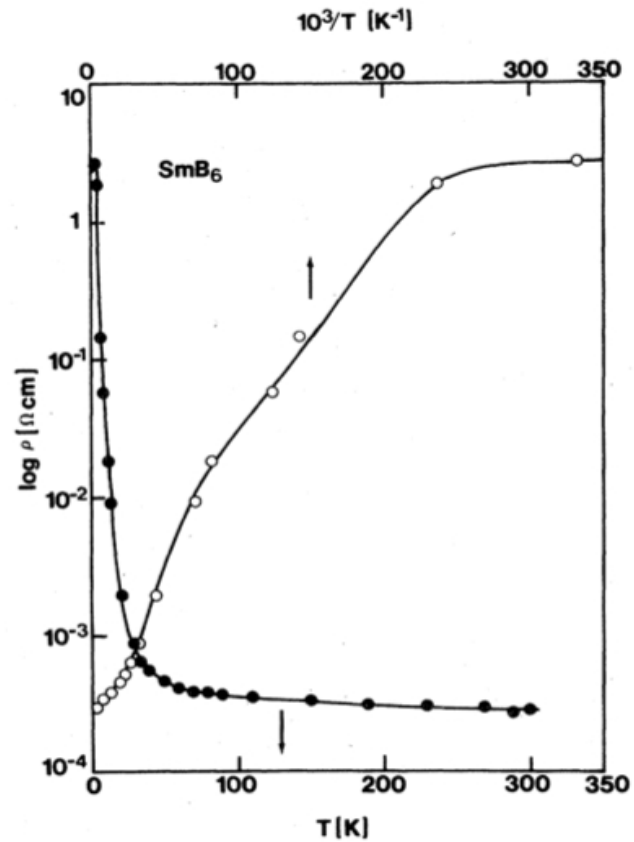
N. Mott, Phil. Mag. 30, 403 (1974)

Formation of heavy-fermion insulator

$n_c + n_f = 2 \times integer$



- Focus of this talk: SmB_6



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

SmB_6: potential candidate for correlated TI

nature International weekly journal of science

Despite being insulators inside, samarium hexaboride crystals can conduct electricity on their surface.

CONDENSED-MATTER PHYSICS

Hopes surface for exotic insulator

Findings by three teams may solve a 40-year-old mystery.

SmB_6: experiments

Q: Can we establish that SmB_6 hosts helical surface states with Dirac spectrum while relying on <u>experimental data only</u>?

(1) transport is limited to the surface
(2) time-reversal symmetry breaking leads to localization
(3) strong spin-orbit coupling = helicity
(4) Dirac spectrum

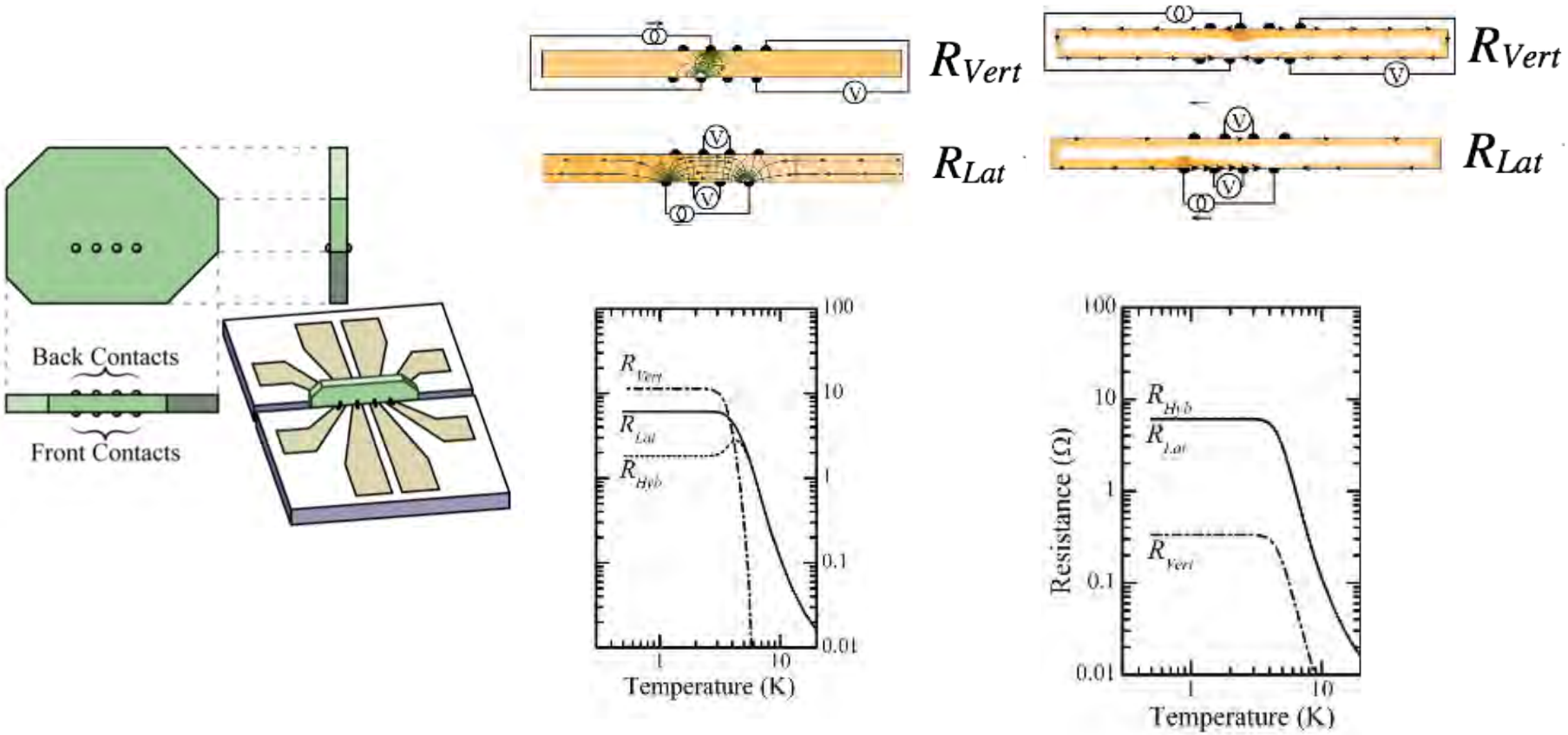
arXiv.org > cond-mat > arXiv:1211.5104

Condensed Matter > Strongly Correlated Electrons

Discovery of the First Topological Kondo Insulator: Samarium Hexaboride

Steven Wolgast, Cagliyan Kurdak, Kai Sun, J. W. Allen, Dae-Jeong Kim, Zachary Fisk

(Submitted on 21 Nov 2012 (v1), last revised 27 Nov 2012 (this version, v2))



➢ @ T < 5K transport comes from the surface ONLY!

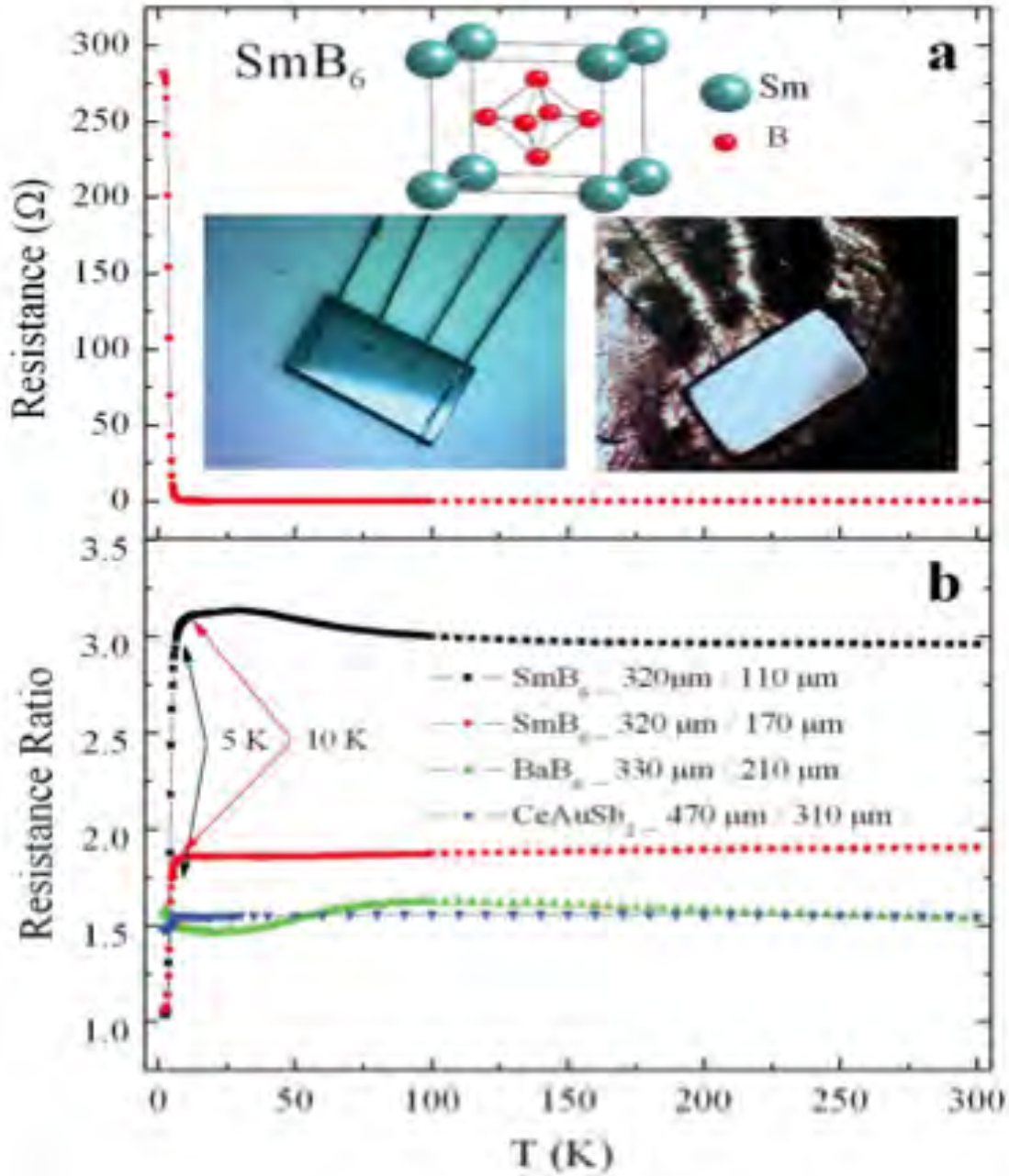
- Idea: Ohm's law

$$\rho = \frac{A}{L} R$$

in ideal topo insultor resistivity is independent of sample's thickness: surface transport

- Resistivity ratio

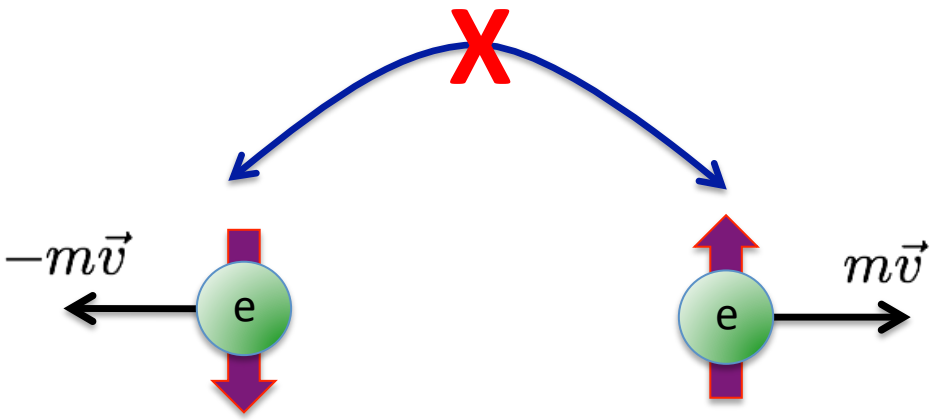
$$\frac{R_{thick}}{R_{thin}}$$



D. J. Kim, J. Xia & Z. Fisk, Nat. Comm. (2014)

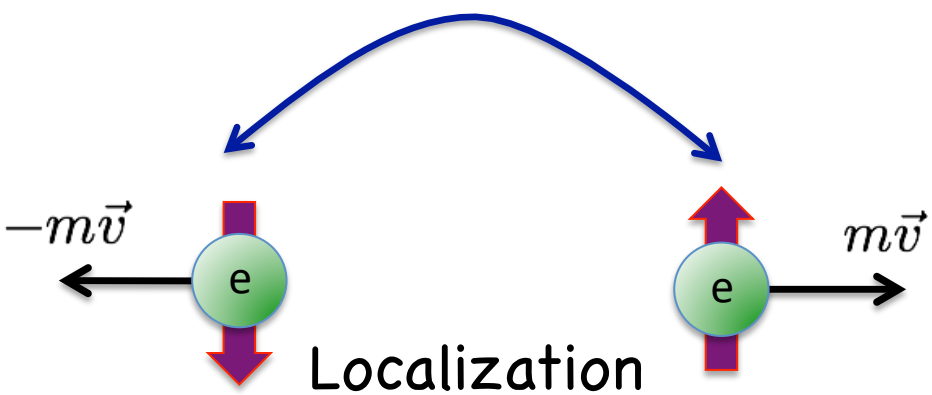
SmB_6: transport experiments

- Non-magnetic ions (Y) on the surface: time-reversal symmetry is preserved

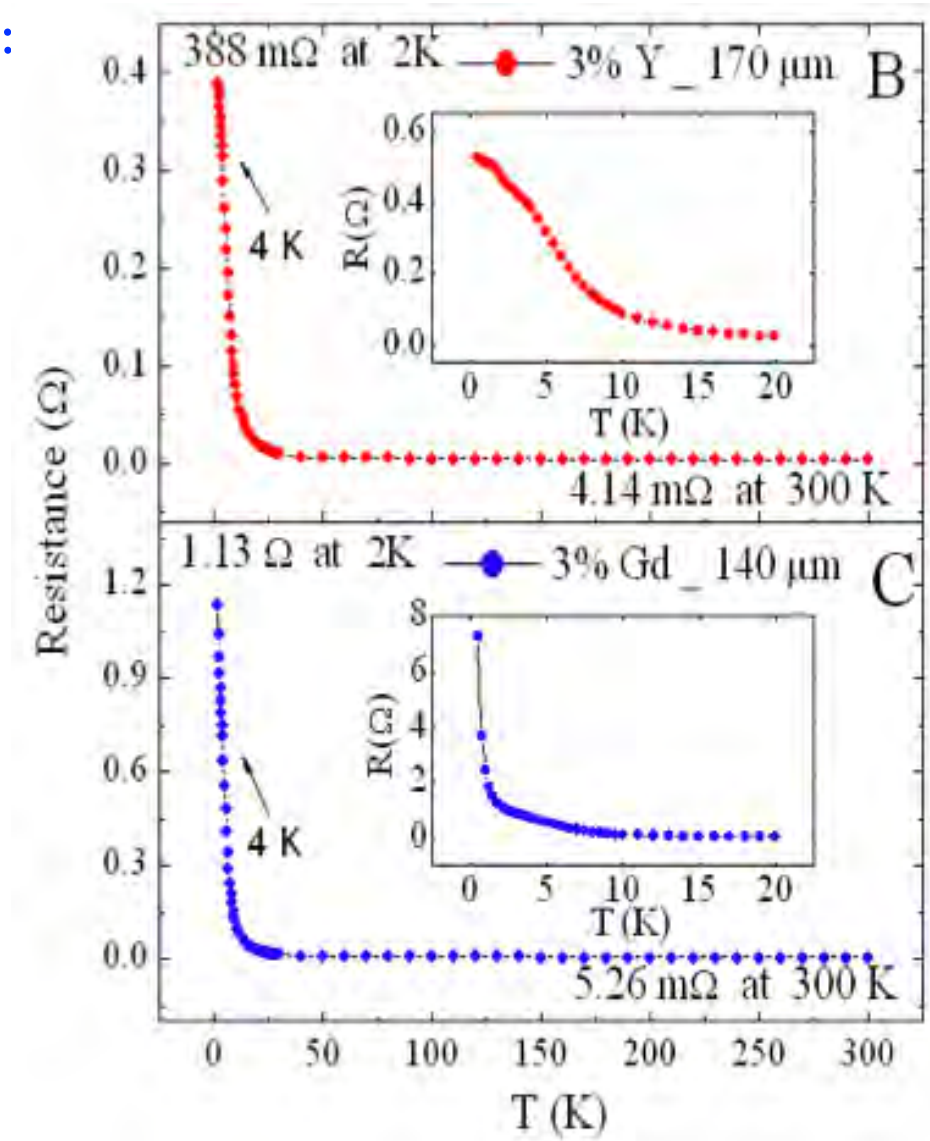


No backscattering

- Magnetic ions (Gd) on the surface: time-reversal symmetry is broken



Localization

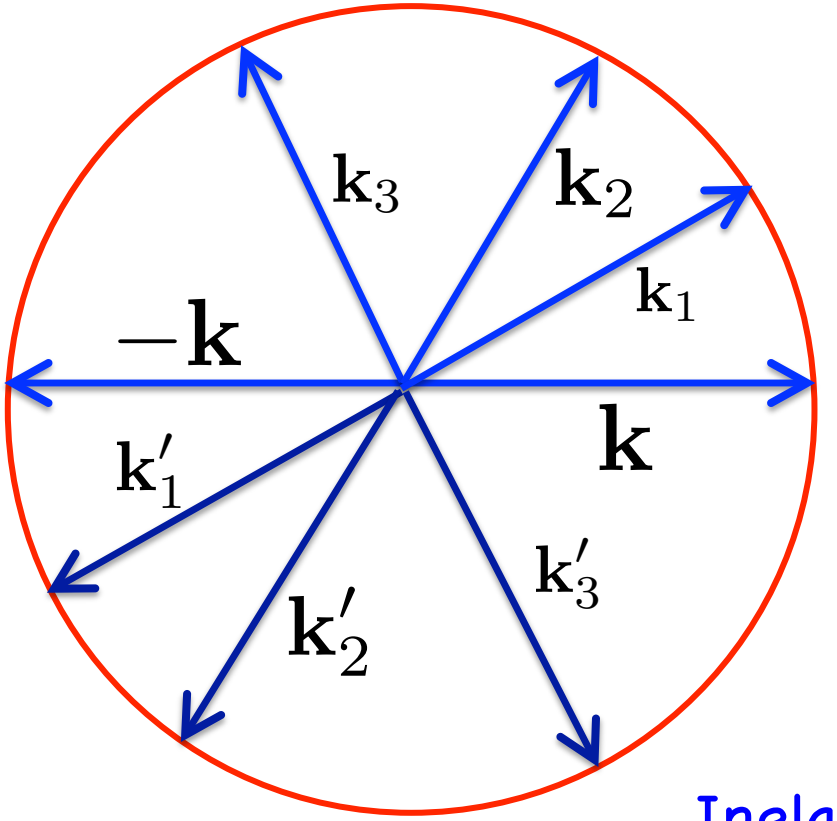


Kim, Xia & Fisk, arXiv:1307.0448

Quantum correction to conductivity (2D)

- incoming wave **k** is split into two complimentary waves

  [G. Bergmann (1975)]



waves propagate independently and interfere in the final state **-k**

Interference correction to conductance:

$$\Delta G = -\frac{\Delta R}{R^2} = -\frac{e^2}{2\pi^2\hbar}\log\left(\frac{\tau_\phi(T)}{\tau_{tr}}\right)$$

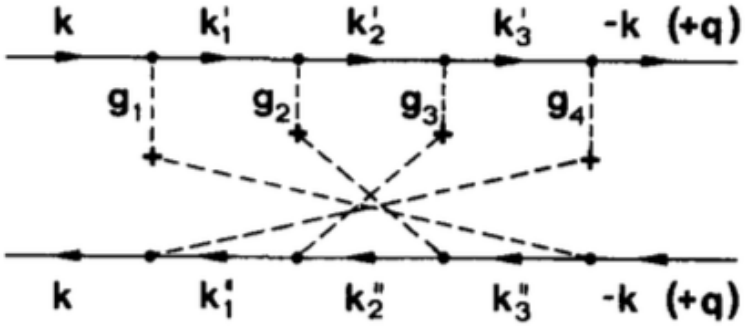
[E. Abrahams et al. (1979); L. P. Gor'kov et al (1979)]

Inelastic scattering time $\tau_\phi(T) \sim T^{-p}$

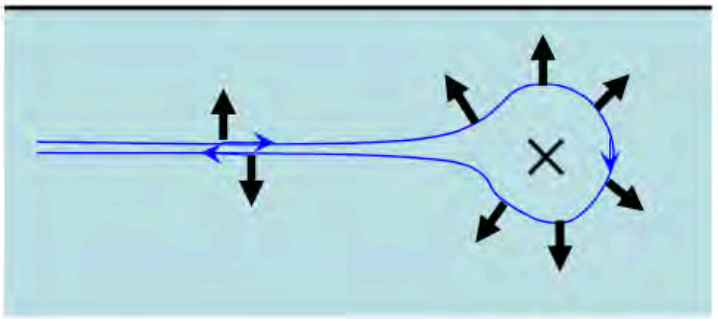
Weak localization

Quantum correction to conductivity (2D)

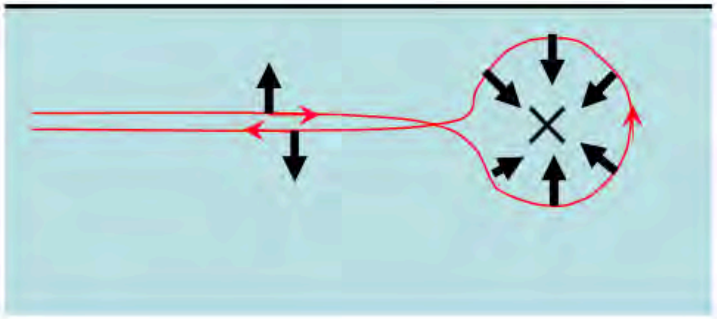
- quantum interference in topological insulators



Electron spin rotates adiabatically by π or $-\pi$



In topological insulators two waves always interfere destructively: weak anti-localization

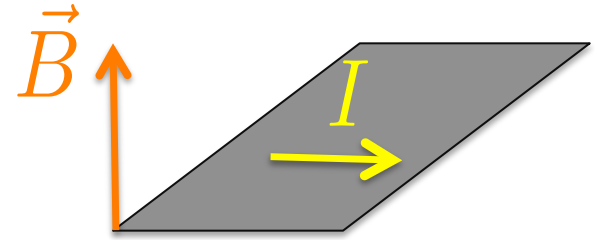


$$\frac{\Delta G}{\Delta T} < 0$$

[Qi & Zhang (2010)]

Quantum correction to conductivity (2D)

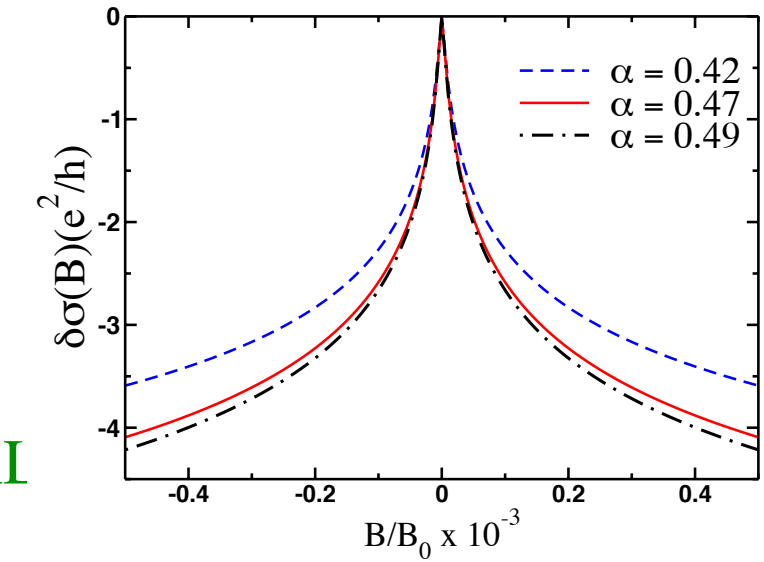
- weak anti-localization (WAL) in a perpendicular magnetic field.



Hikami-Larkin-Nagaoka formula

$$\Delta G(B) = -\alpha \frac{e^2}{2\pi^2\hbar} F(B)$$

$$F(B) = \psi\left(\frac{1}{2} + \frac{\hbar c}{4eBL_\phi^2}\right) + \ln\left(\frac{4eBL_\phi^2}{\hbar c}\right)$$



[MD et al. (2015)]

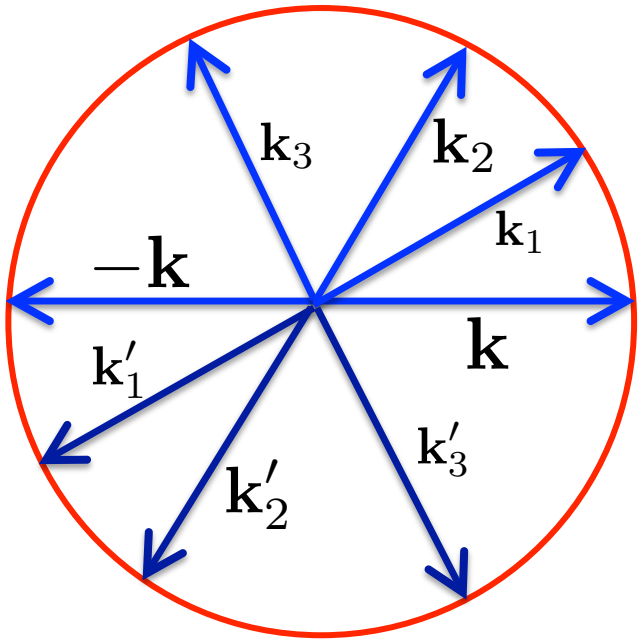
Interference correction in a field is negative: WAI

$$\alpha > 0$$

No effect in a parallel field

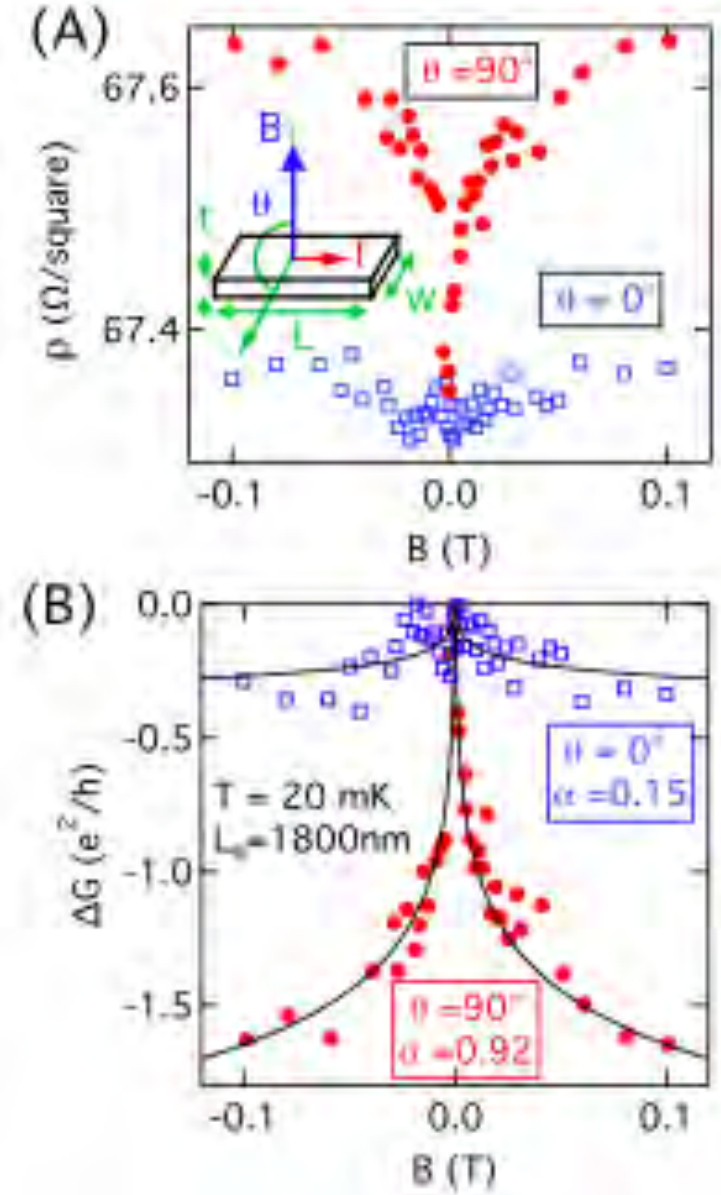
SmB_6: transport experiments

- weak anti-localization (WAL) in SmB_6



$$\Delta\sigma(H) = \delta\sigma(H) - \delta\sigma(0)$$

*diffusion (classical) conductivity is field-independent



S. Thomas et al. arXiv:1307.4133

SmB_6: quantum oscillations experiments

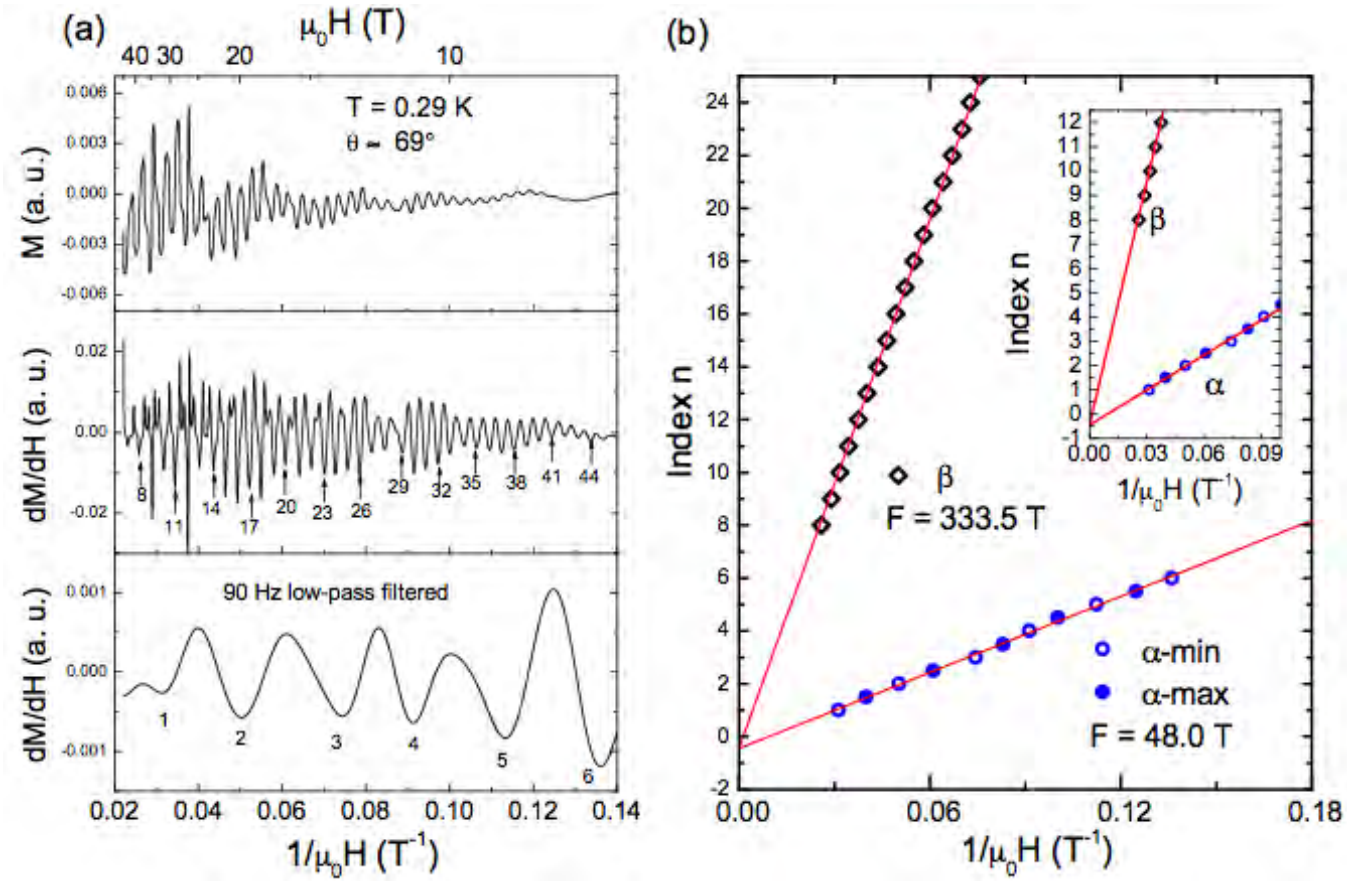
Idea: zero-energy Landau level exists for Dirac electrons:

$$E_n = \mathrm{sign}(n)\sqrt{2e\hbar v_F^2|n|B}$$

Experimental consequence: shift in Landau index *n* must be observed – only E_0=0 contributes at infinite magnetic field!

- very light effective mass: 0.07–0.1m_e

Strong surface potential!



G. Li et al. (Li Lu group Ann Arbor) **Science** (2015)

SmB_6: quantum oscillations experiments … BUT

- Key results:
  - Samples are bulk insulators
  - Rapid quantum oscillations corresponding to 50% the volume of the BZ
  - Large mean-free path (~ few microns)

Scien

Unconventic
insulating st

B. S. Tan,[1] Y.-T. Hs
Harrison,[4] Z. Zhu,[4]
Srivastava,[1] M. D. J
Balicas,[2] G. G. Lonz
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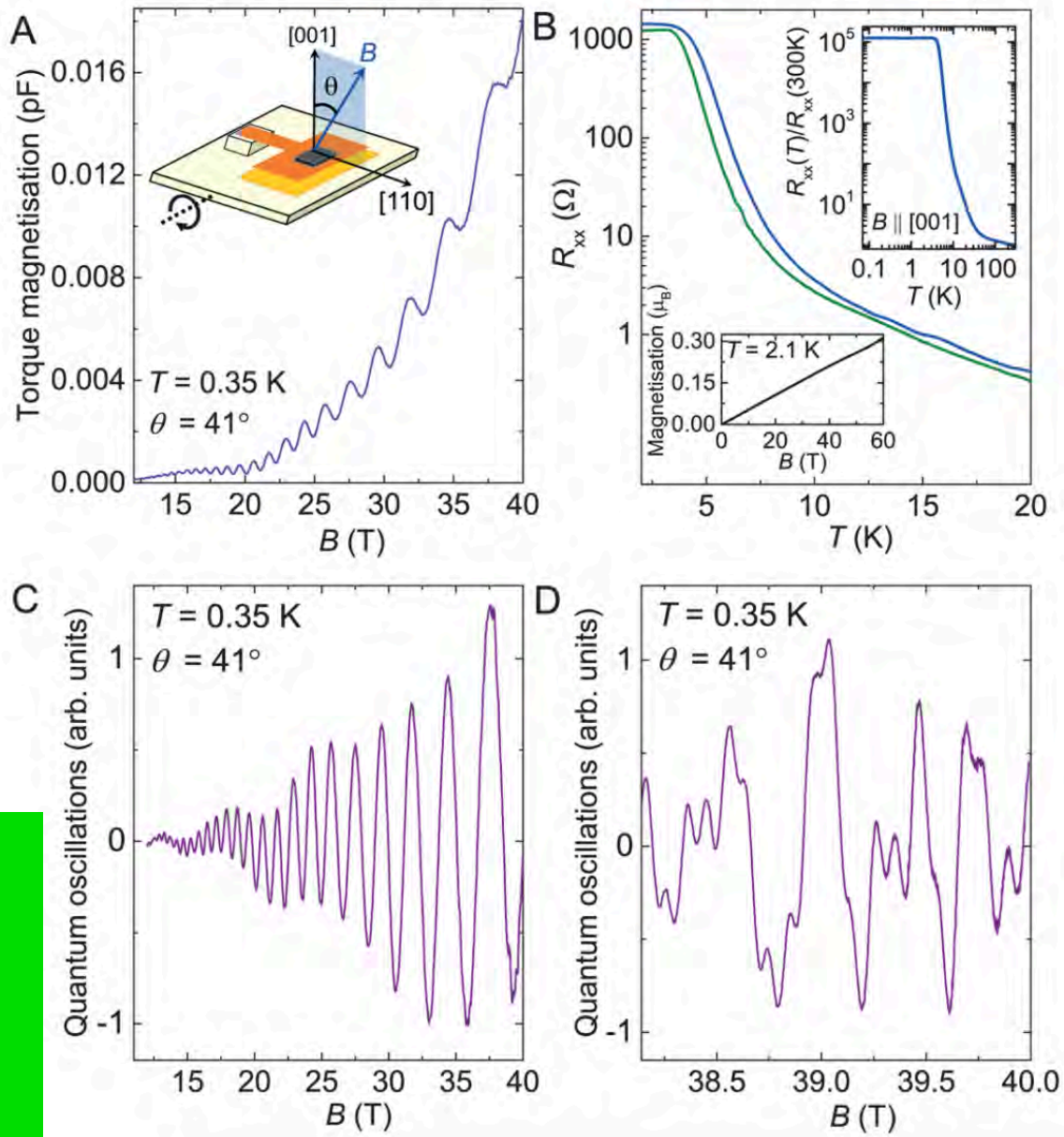
Science, Naval Research Laborator
*Corresponding author. E-mail: su

Insulators occur in mo
topological insulators
insulating bulk. Here



Contradicts earlier quantum oscillation experiments (Science'14)!

Collaborators:

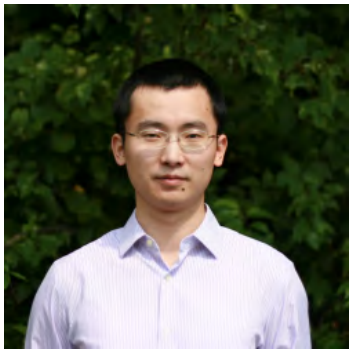
Kai Sun, U. Michigan

Piers Coleman, Rutgers U.

Victor Galitski, U. of Maryland

Victor A.

Victor G.



Kai

Bitan Roy, U. of Maryland

Jay Deep Sau, U. of Maryland

Maxim Vavilov, U. of Wisconsin

Victor Alexandrov, Rutgers U.

Kostya Kechedzhi, NASA-Ames

Jay Deep

Piers

Conclusion & open questions

➢ Role of correlations?

- Many-body instabilities on the surface of TKI driven by both long-range Coulomb and short range interaction.
- Why all Kondo insulators have cubic symmetry?
  [Kondo semimetals have tetragonal symmetry]

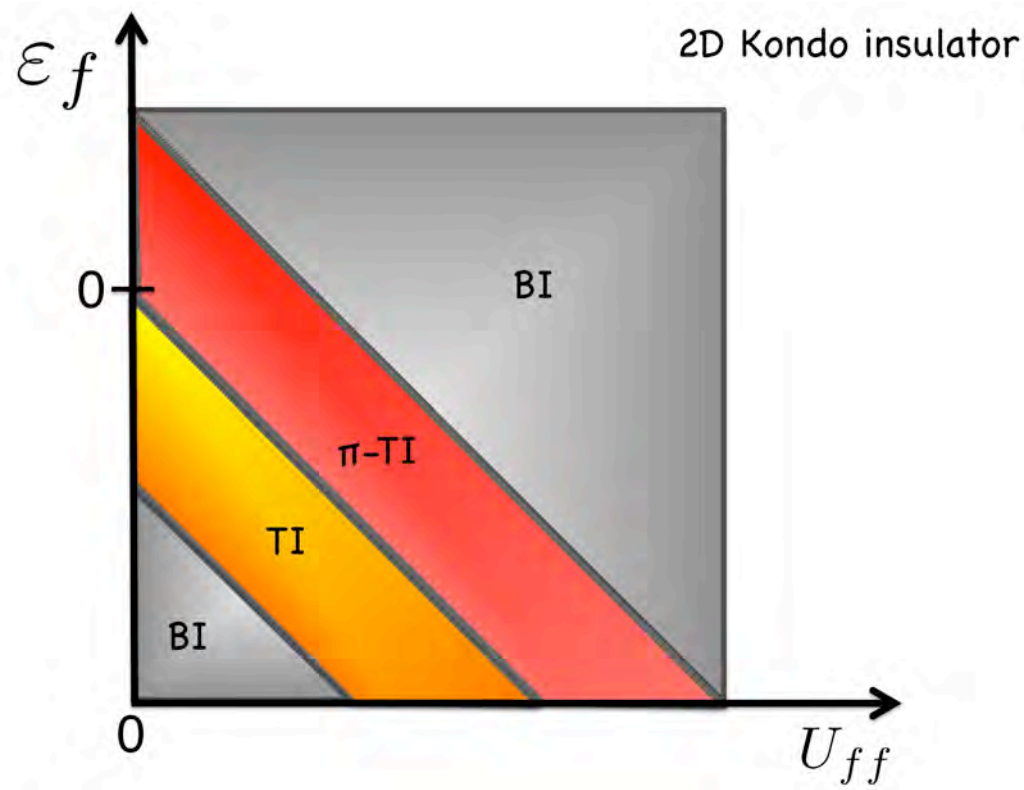
- effect magnetic vs. non-magnetic doping on the magnitude of surface conductivity
- surface conductance & insulating bulk below 5K
- quantum oscillations experiments confirm Dirac Dirac spectrum of surface electrons
- weak anti-localization: strong SO coupling

} SmB_6 is a correlated topological insulator

What makes topological Kondo insulators special?

Q: Are topological Kondo insulators adiabatically connected to topological band insulators?

A: NO! Gap closes as the strength of U gradually increases

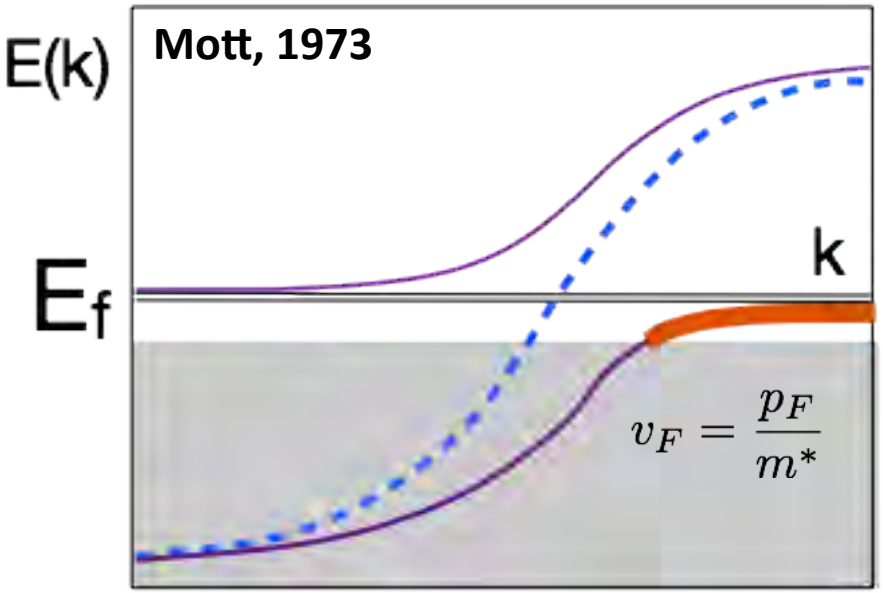


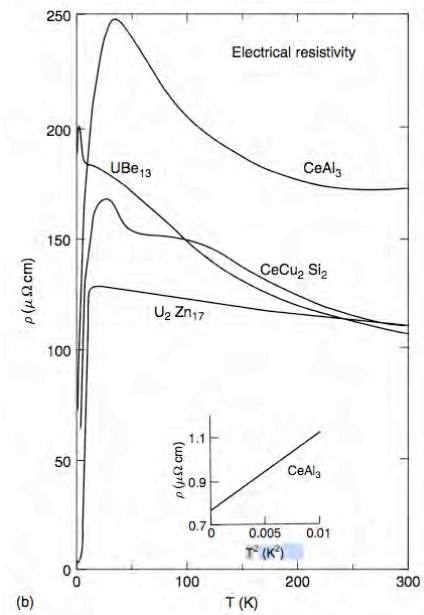
Jan Werner and Fakher F. Assaad, PRB 88, 035113 (2013)

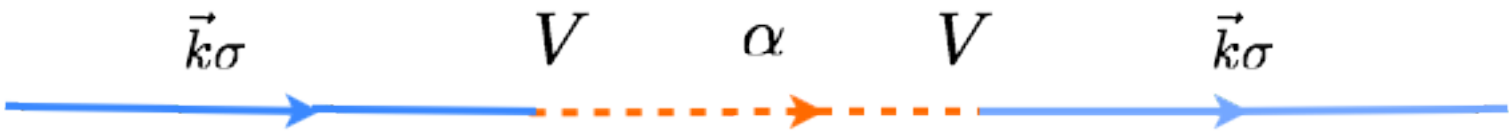
Mott's Hybridization picture

N. Mott, Phil. Mag. 30, 403 (1974)

Formation of Heavy f-bands: electrons $|\mathbf{k}\sigma\rangle$ and localized f doublets hybridize, possibly due to Kondo effect



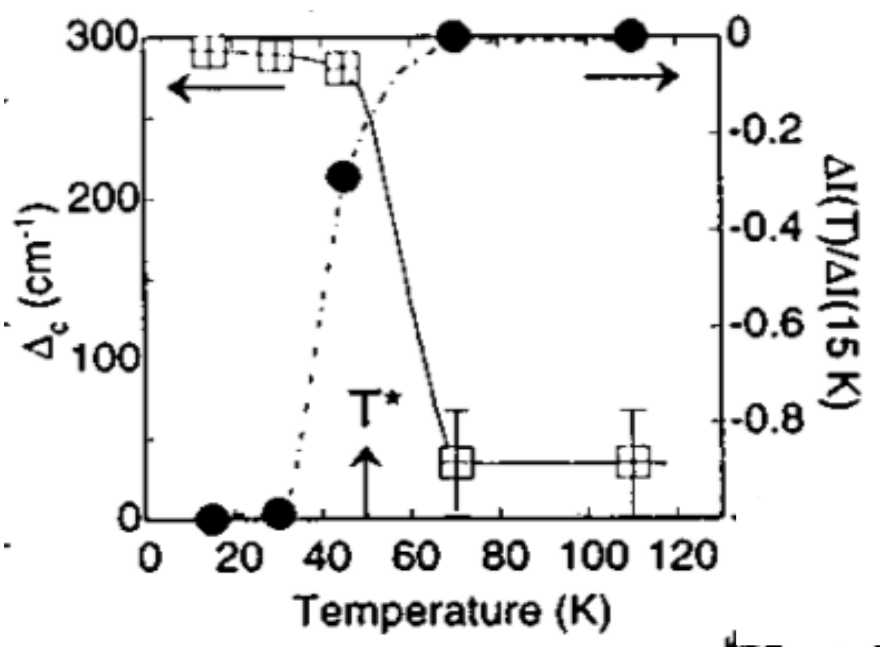




$$\mathcal{H} = (|\mathbf{k}\sigma\rangle V_{\sigma\alpha}(\mathbf{k})\langle\alpha| + \text{h.c.}) \qquad |\alpha\rangle \equiv |\pm\rangle$$

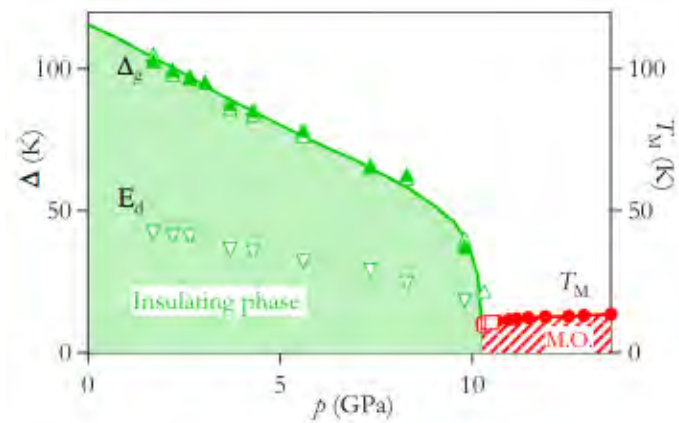
Mean-field theory for SmB_6: is *N=1/4* small enough?

- integrated spectral weight of the gap: T-dependence

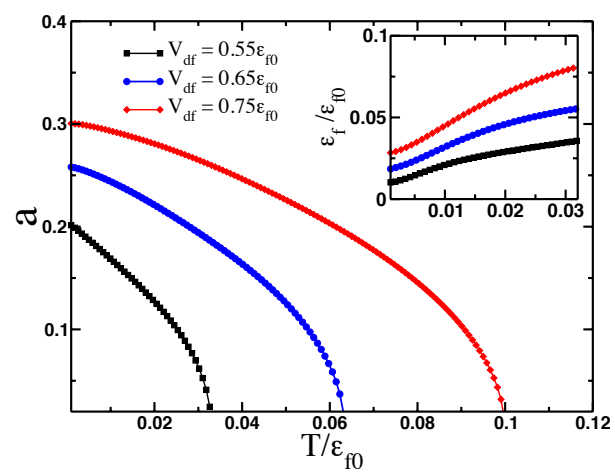


Nyhus, Cooper, Fisk, Sarrao, PRB **55**, 12488 (1997)

- full insulating gap: dependence on pressure



Derr et al. PRB **77**, 193107 (2008)



Mean-field-like onset of the insulating gap!