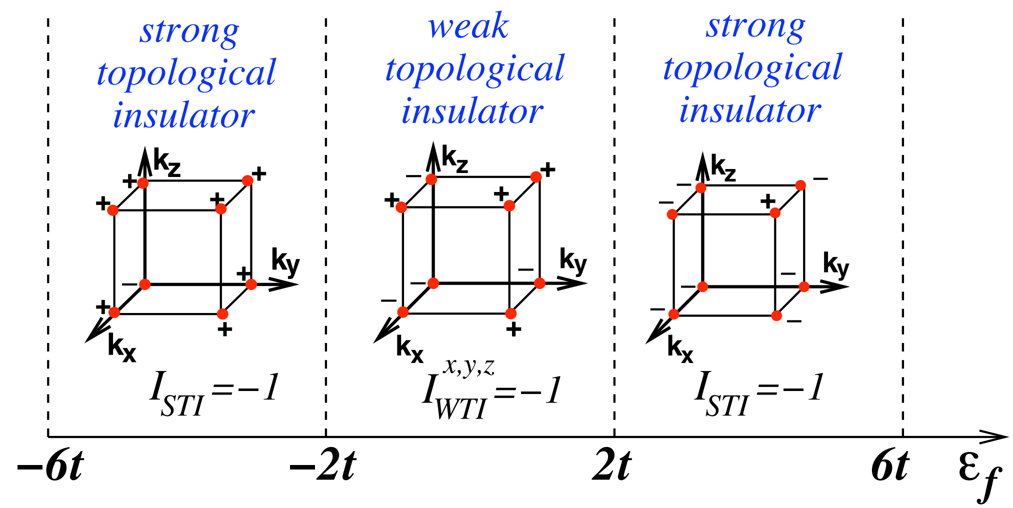
Topological Kondo Insulators

Maxim Dzero, University of Maryland

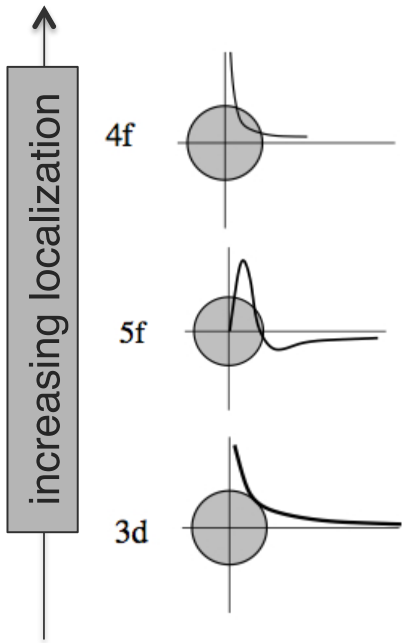
Collaborators:

Kai Sun, University of Maryland
Victor Galitski, University of Maryland
Piers Coleman, Rutgers University

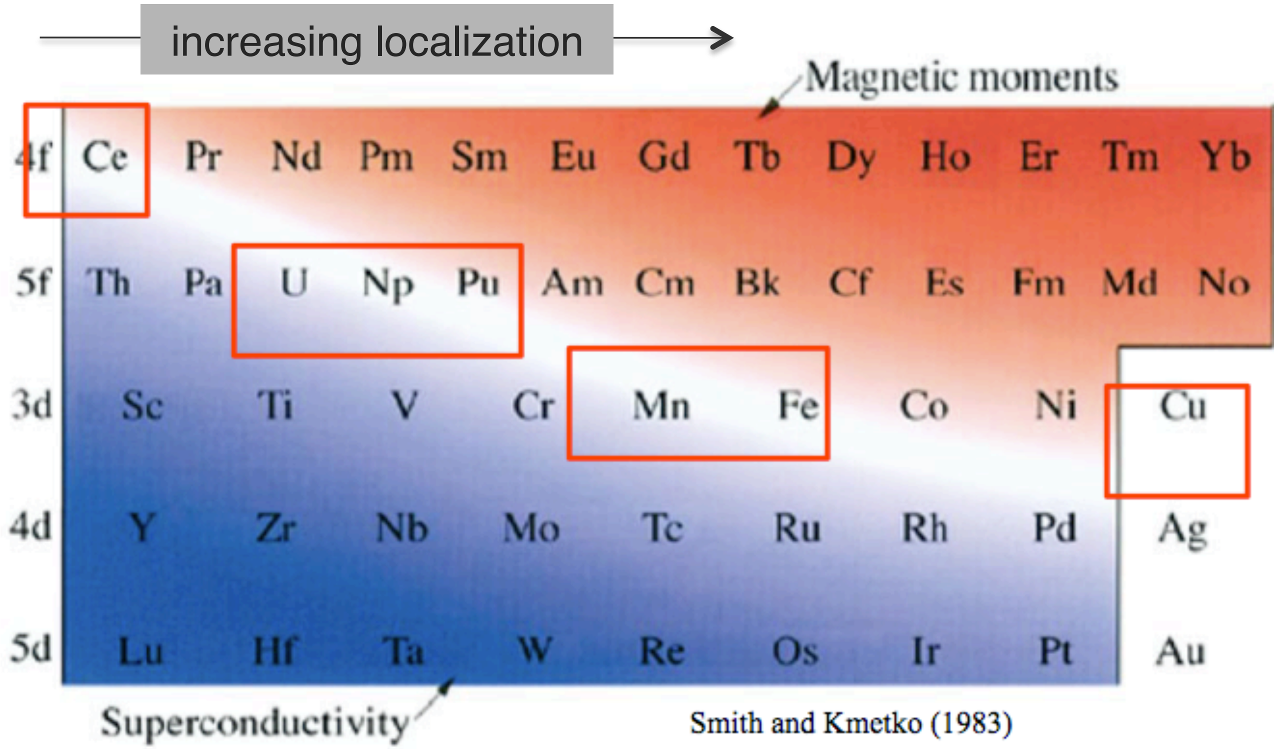
- Main idea
- Kondo Insulators
- Topological insulators
- Are Kondo insulators topological? Yes



jour-ref: Phys. Rev. Lett. **104**, 106408 (2010)



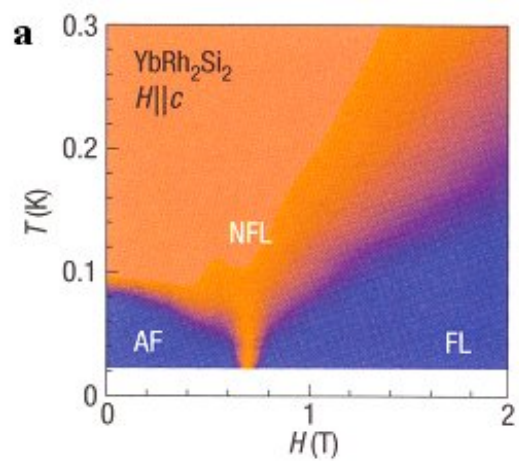
Coleman (2002)

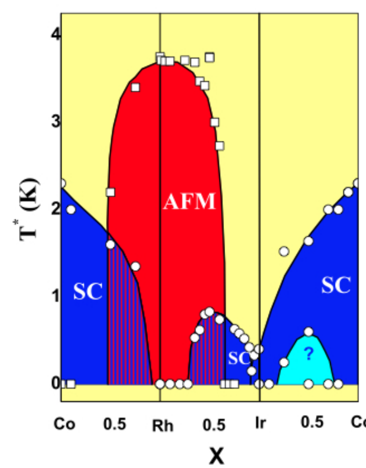


Smith and Kmetko (1983)

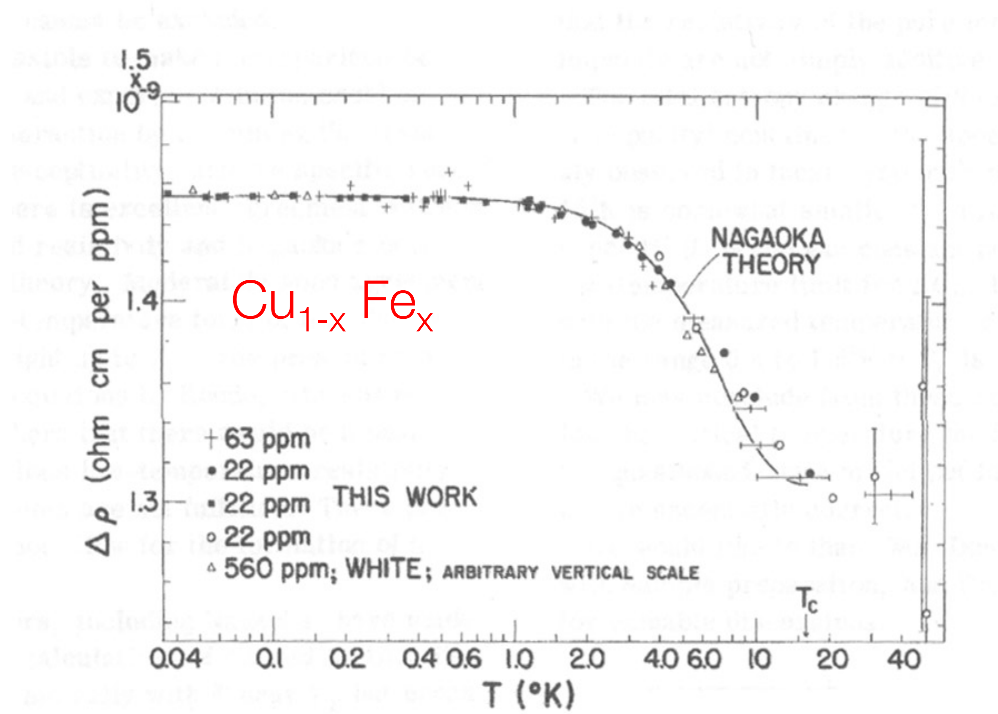
A lot of action takes place on the brink of localization!

- Non-Fermi Liquid phases
- Unconventional Superconductivity
- Hidden Order: URu_2Si_2
- Metal-Insulator transitions





Kondo Effect

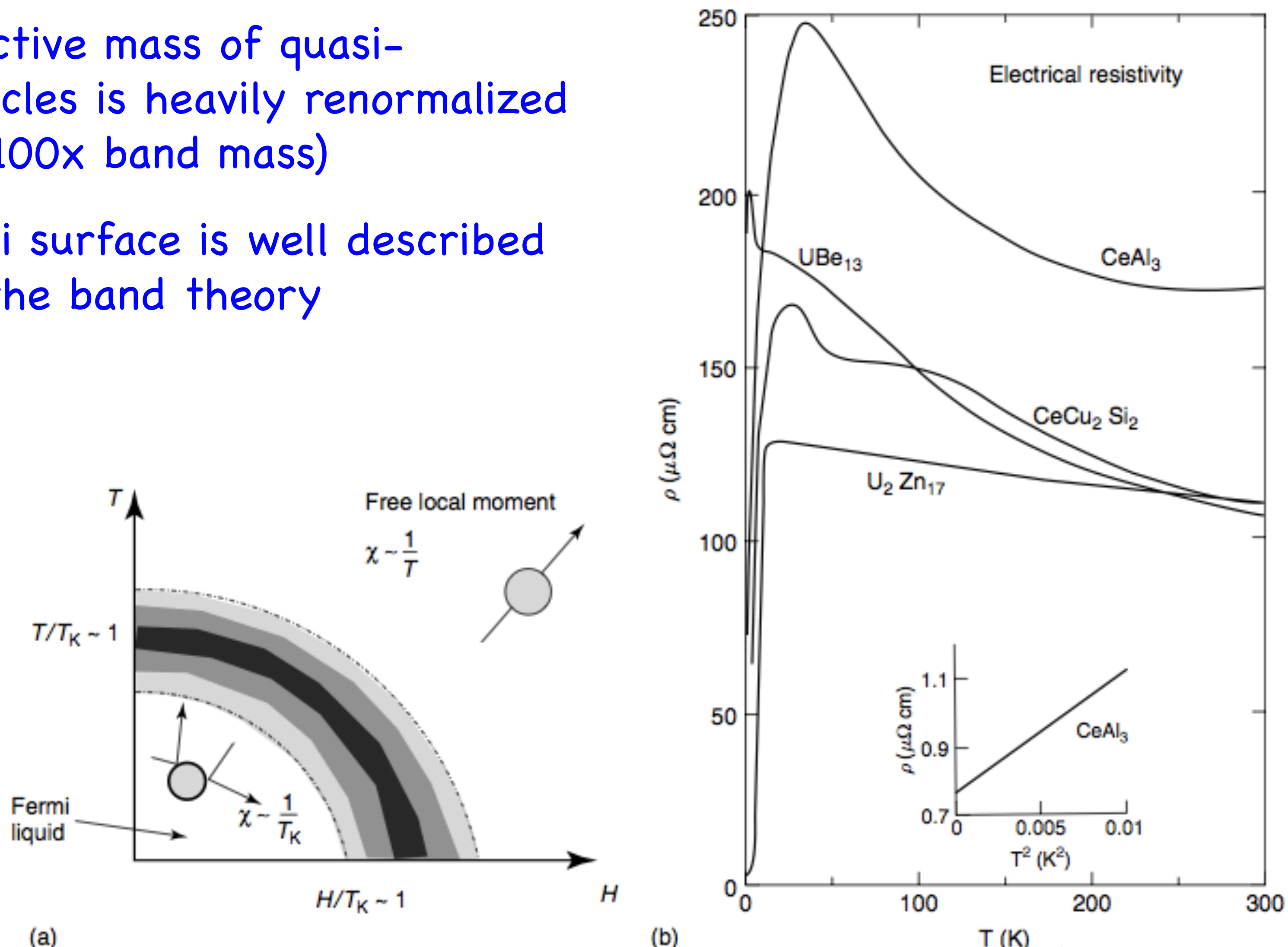


A. J. Heeger, in Solid State Physics vol 23 (1969)

- At high temperatures: free local moment $S \approx k_B \log 2$
- At low temperatures: moment is "quenched" $C \approx k_B \frac{T}{T_K}$

➡ single impurity Kondo effect

- Effective mass of quasi-particles is heavily renormalized (20-100x band mass)
- Fermi surface is well described by the band theory



Coleman (2002)

- At high temperatures: local moment metals
- At low temperatures: moments "quench" to form heavy fermions

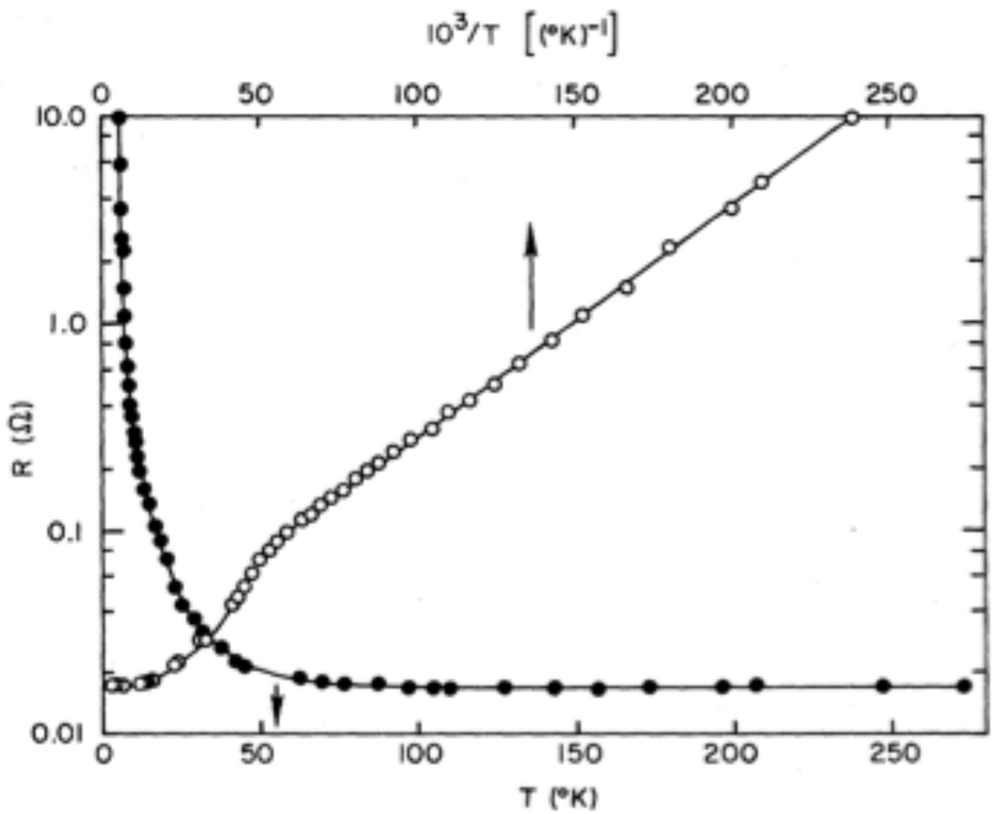
Kondo Insulators: SmB_6

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)



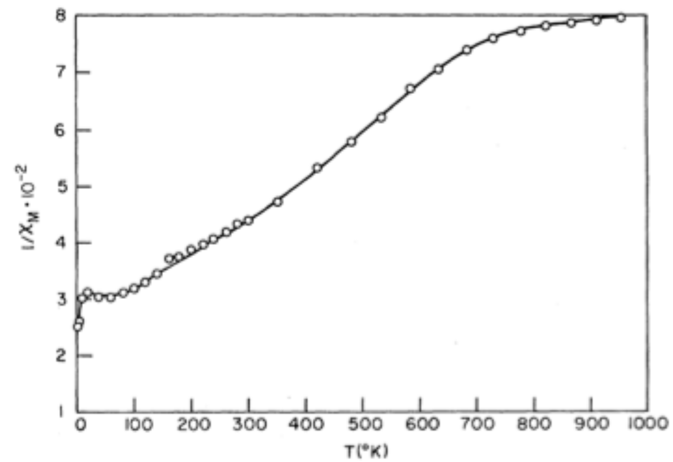


FIG. 2. Reciprocal molar susceptibility of SmB_6 as a function of temperature.

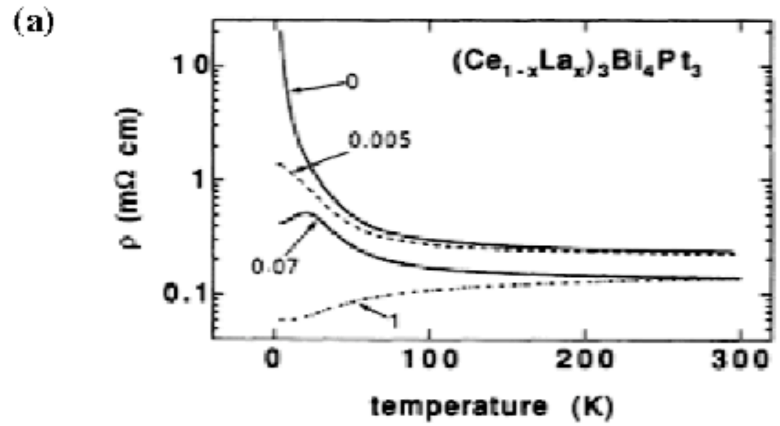
- Magnetic susceptibility flattens out below 100 K
- Band structure calculations: mixed valence behavior

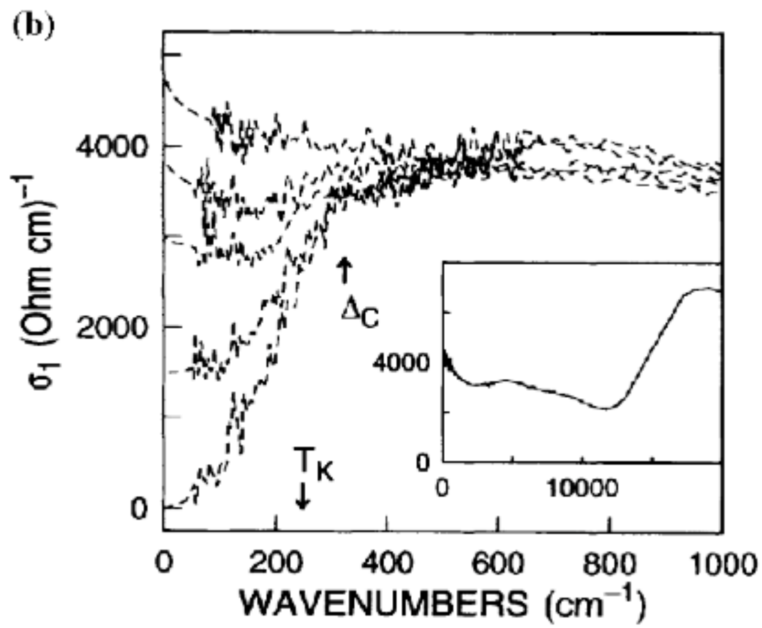
$$n_f \simeq 0.7$$

Kondo Insulators: $Ce_3Bi_4Pt_3$

- Hybridization gap arises due to interaction between 4f and conduction band electrons
- Gap is suppressed by doping: disordered Kondo Lattice
- Real part of the optical conductivity: disappearance of the spectral weight below 100 K.

Hundley et al. (1990)



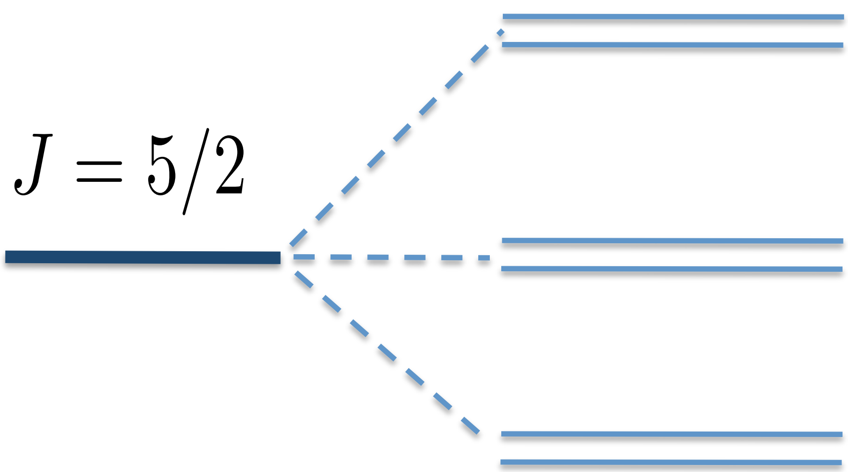


Bucher et al. (1994)

Ce (f^1) in tetragonal crystal field environment

- strong spin-orbit coupling

f^1: $S = 1/2, \; L = 3, \; J = L - S = 5/2$



$$f^\dagger_{\Gamma_7^+ \pm} = \cos\beta |\mp 3/2\rangle + \sin\beta |\pm 5/2\rangle$$

$$f^\dagger_{\Gamma_7^- \pm} = \sin\beta |\mp 3/2\rangle - \cos\beta |\pm 5/2\rangle$$

$$f^\dagger_{\Gamma_6 \pm} = |\pm 1/2\rangle$$

Actual position of the Kramers doublets is determined experimentally (XAFS)

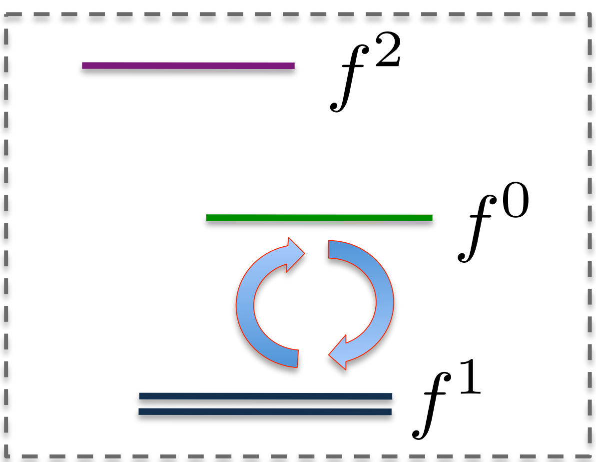
Kondo insulators: theory

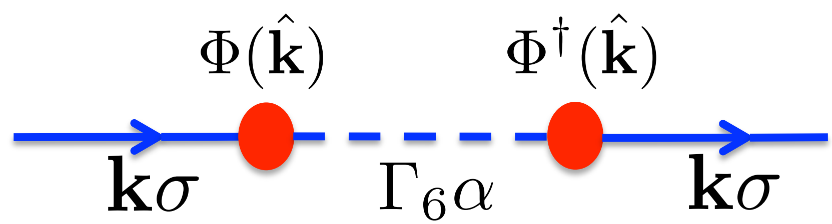
- Anderson model:

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

$$\psi_{j\alpha} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \underbrace{\Phi_{\alpha\sigma}(\hat{\mathbf{k}})}_{\text{f-electron form factor}} e^{-i\mathbf{k}\cdot\mathbf{x}_j} c_{\mathbf{k}\sigma}$$

- Hybridization





Strong spin-orbit coupling is present on the level of interaction between *c*- and *f*-electrons

Kondo insulators: theory

- Anderson model:

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

$$\psi_{j\alpha} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \underbrace{\Phi_{\alpha\sigma}(\hat{\mathbf{k}})}_{\text{f-electron form factor}} e^{-i\mathbf{k}\cdot\mathbf{x}_j} c_{\mathbf{k}\sigma}$$

- form factors: $$[\Phi_{\Gamma\mathbf{k}}]_{\alpha\sigma} = \sum_m \langle \Gamma\alpha | jm \rangle \underbrace{\langle jm | \mathbf{k}\sigma \rangle}_{\text{Matrix element between the Bloch and Wannier states}}$$

tight-binding $$[\Phi_{\Gamma\mathbf{k}}]_{\alpha\sigma} = \sum_{m\in[-3,3]} \left\langle \Gamma\alpha \middle| 3m, \frac{1}{2}\sigma \right\rangle \frac{1}{Z} \sum_{\mathbf{R}\neq 0} Y^3_M(\hat{\mathbf{R}}) e^{i\mathbf{k}\cdot\mathbf{R}}$$

Spin-orbit coupling is present on the level of Interaction between *c*- and *f*-electrons

Kondo insulators: theory

- 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-U interaction

- approximations:

  - neglect self-energy dispersion: Kondo limit
  - ignore the physics at high Matsubara frequencies

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

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

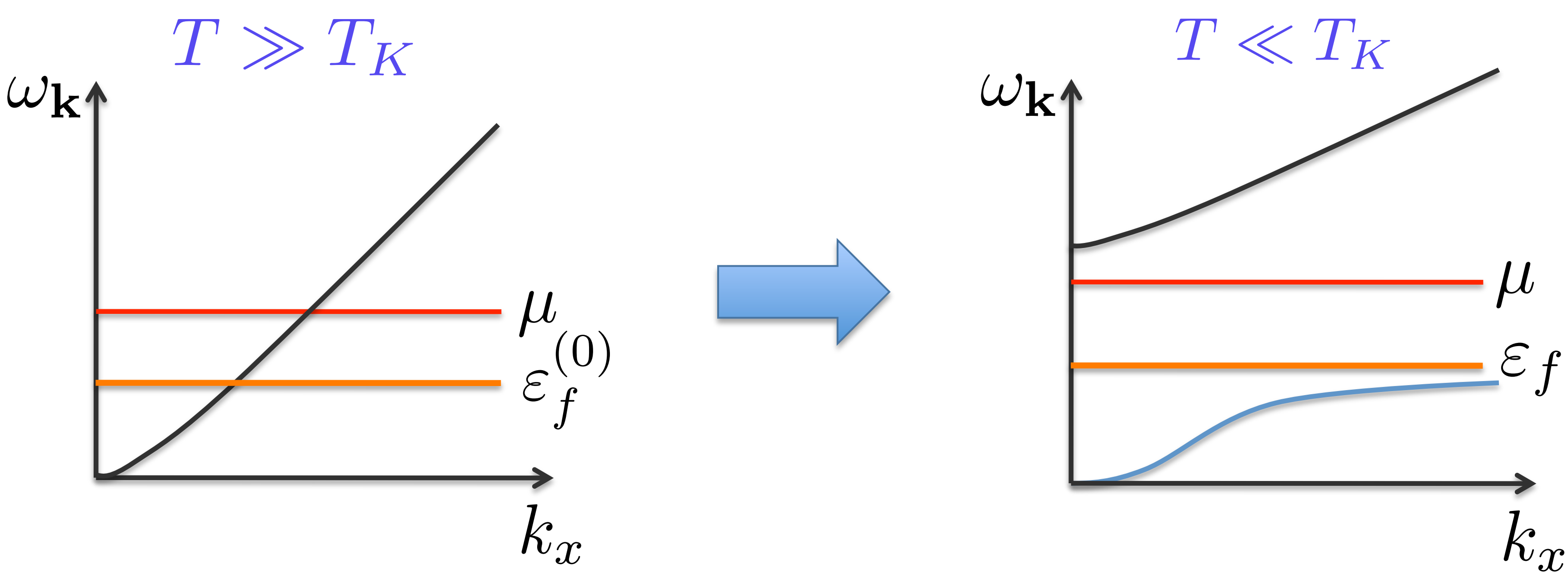
- hybridization amplitude $\tilde{V}(\mathbf{k}) = \sqrt{Z} V(\mathbf{k})$

Mean-field theory: effective Hamiltonian

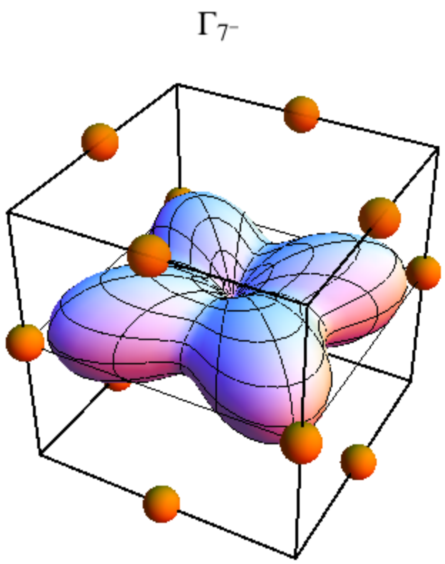
$$\mathcal{H}_{mf}(\mathbf{k}) = \begin{pmatrix} \xi_{\mathbf{k}}\underline{1} & \tilde{V}\Phi^{\dagger}_{\Gamma\mathbf{k}} \\ \tilde{V}\Phi_{\Gamma\mathbf{k}} & \underbrace{\varepsilon_f \underline{1}} \end{pmatrix}$$

renormalized position of the f-level

- Qualitative description

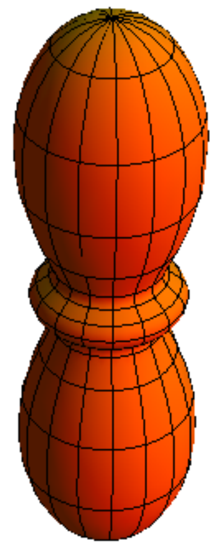


Hybridization gap: momentum dependence $\mathrm{Tr}\left[\hat{\Phi}^{\dagger}_{\Gamma\mathbf{k}}\hat{\Phi}_{\Gamma\mathbf{k}}\right]$



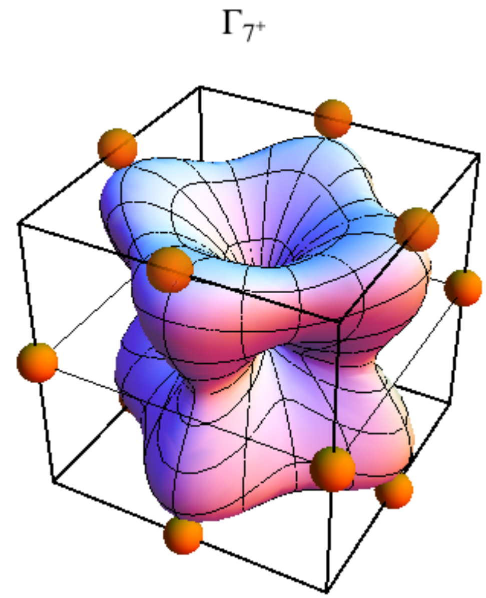
$|\Gamma_7^-\rangle \sim |M_J = \pm 3/2\rangle$

Nodes along k_z



$|\Gamma_6\rangle \sim |M_J = \pm 1/2\rangle$

Fully gapped!



$|\Gamma_7^+\rangle \sim |M_J = \pm 5/2\rangle$

Nodes along k_z

- Linear combination of any of two gapless shapes with the fully gaped one yields non-vanishing hybridization gap. TKI with nodes?

Quantum Hall Kondo insulators

P. Ghaemi & T. Senthil (2007); M. Dzero et al. (2010)

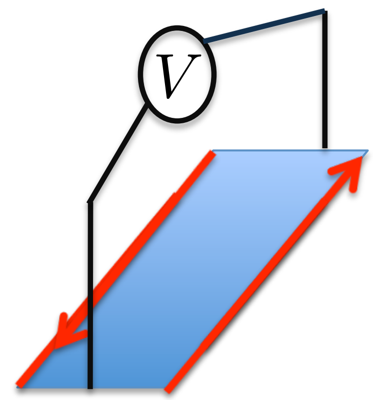
- 2D model of the Kondo insulator

$$H = \sum_{\mathbf{k}} \left[\frac{1}{2}(\epsilon_{\mathbf{k}} + \varepsilon_f) + \vec{m}_{\mathbf{k}} \cdot \vec{\tau} \right]$$

➢ $\mathbf{m_k} = \left(-\alpha V \hat{k}_x, \alpha V \hat{k}_y, \frac{1}{2}(\epsilon_{\mathbf{k}} - \varepsilon_f) \right)$ maps torus (BZ) to a sphere

➢ current operator $j_\mu = \frac{\partial}{\partial k_\mu} H$

$$\sigma_{xy} = \frac{e^2}{4\pi h} \int d^2k \frac{\vec{m} \cdot (\partial_x \vec{m} \times \partial_y \vec{m})}{|\vec{m}|^3}$$



chiral mode exists even in the absence of external magnetic field

2D Kondo insulator has a quantized Hall conductivity

Topological insulators

M. Z. Hasan & C. L. Kane,
“Topological Insulators”, RMP (2010).

Four bulk Z_2 invariants determine whether the surface states are protected (even or odd # of points)

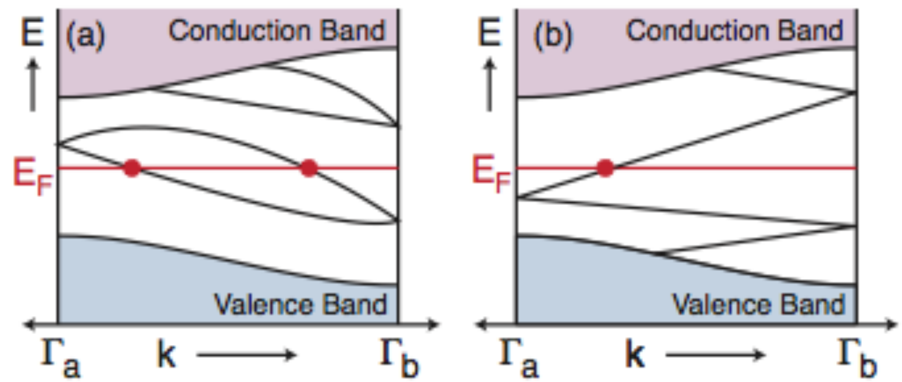
- Simplest 3D TI: stack of layers

$\{x, y, z\}$

three indices (Miller indices:
orientation of the layers)

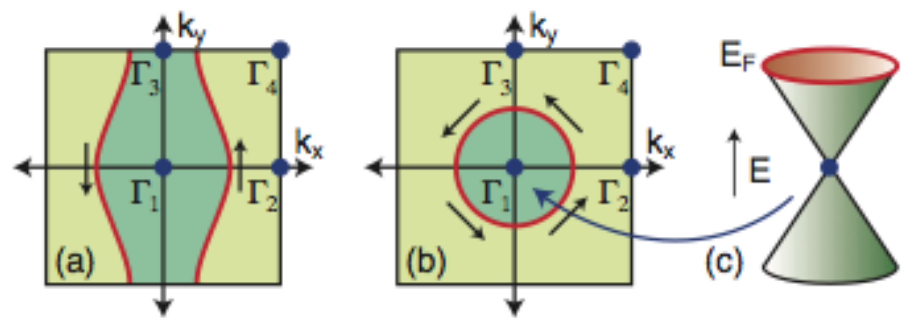
- Strong TI: odd number of Dirac points enclosed by the FS

- surface states as a function of surface crystal momentum



Surface states can be pushed outside the gap

Surface state is topologically protected



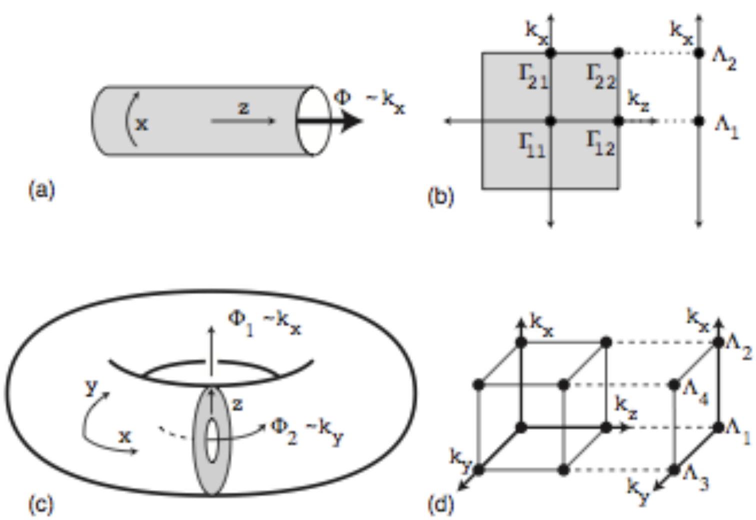
“weak” TI

“strong” TI

Topological insulators

L. Fu & C. Kane, “Topological Insulators with Inversion Symmetry”, PRB 76, 45302 (2007).

Response to a fictitious applied magnetic field



- 2D: Flux plays the role of the edge crystal momentum k_x
- 3D: two fluxes corresponding to two components of the surface crystal momentum

Z_2 invariants are computed from the parity of the occupied bands: change in time reversal polarization due to changes in bulk Hamiltonian

$$w[\Gamma_i]_{mn} = \langle u_{m-k}|\Theta|u_{nk}\rangle \qquad \delta_i = \frac{\sqrt{\det[w(\Gamma_i)]}}{\mathrm{Pf}[w(\Gamma_i)]} = \pm 1$$

Topological insulators: invariants

L. Fu & C. Kane, "Topological Insulators with Inversion Symmetry", PRB 76, 45302 (2007).

- topological structure is determined by parity at high symmetry points

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

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

P-inversion odd form factor vanishes @ high symmetry points

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

- Z_2 invariants are characterized by the parity eigenvalues:

$$\delta_m = \mathrm{sgn}(\xi_{\mathbf{k}^*_m} - \varepsilon_f)$$

Topological Kondo insulators

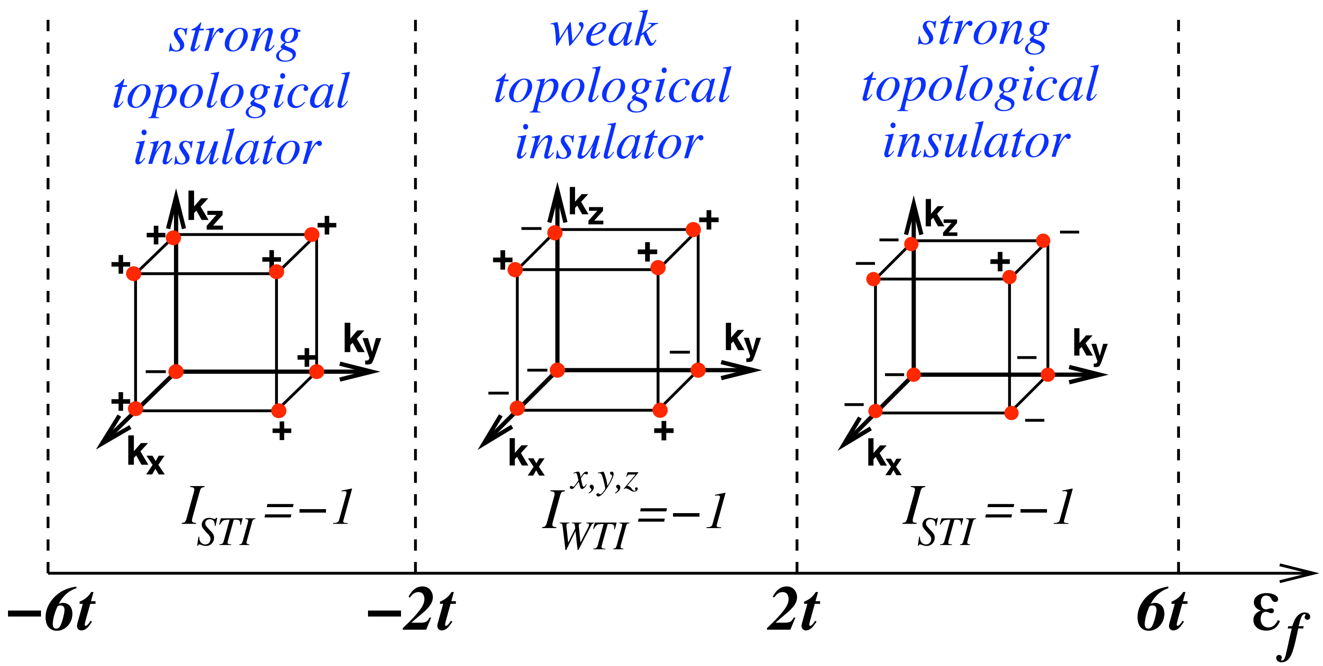
$\delta_m = \mathrm{sgn}(\xi_{\mathbf{k}^*_m} - \varepsilon_f)$

primitive unit cell (EASY!)

Z_2 invariants: 1 "strong" $I_{\mathrm{STI}} = \prod_{m=1}^{8} \delta_m = \pm 1$

3 "weak" $I^j_{\mathrm{WTI}} = \prod_{\mathbf{k}_m \in P_j} \delta_m = \pm 1$

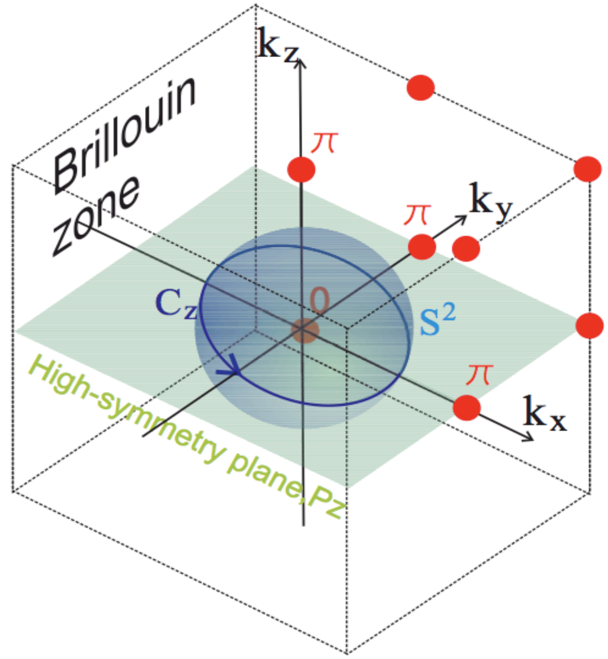
"phase diagram": tight binding $\xi_{\mathbf{k}} = -2t(\cos k_x + \cos k_y + \cos k_z)$



jour-ref: Phys. Rev. Lett. **104**, 106408 (2010)

Topological Kondo insulators

bcc unit cell

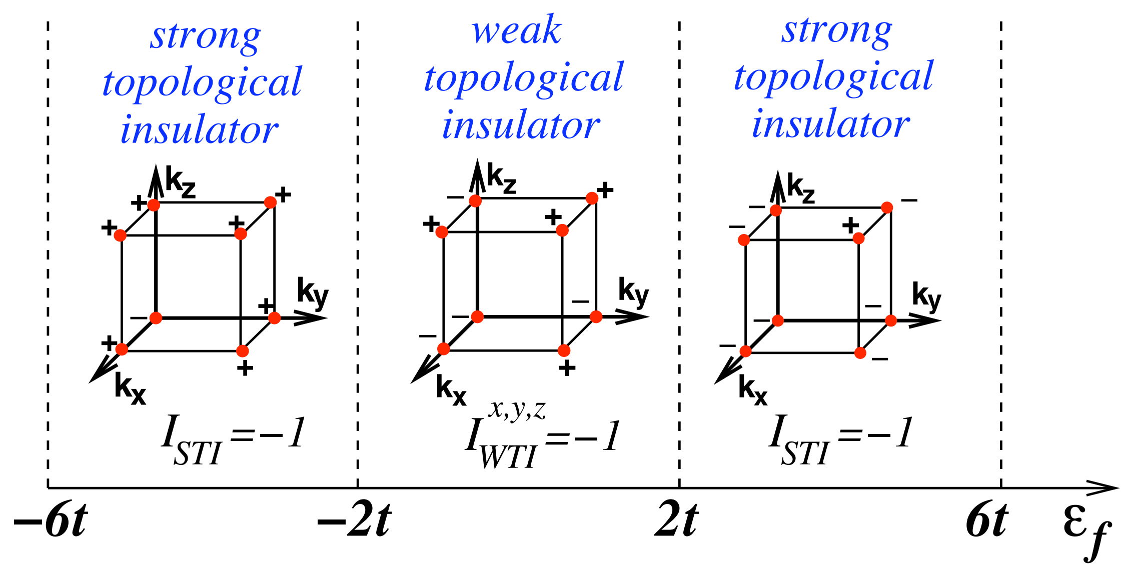


Z_2 invariants:

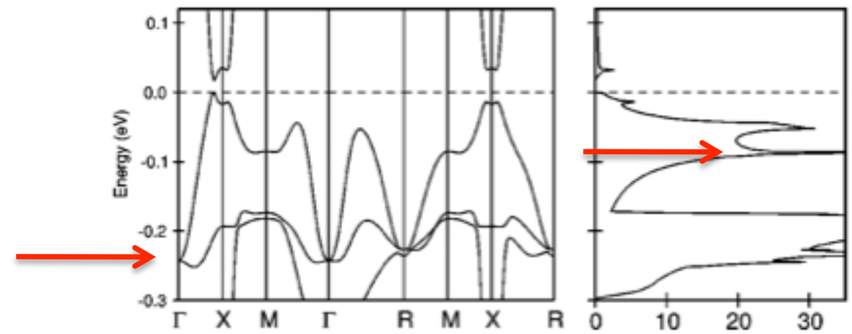
1 "strong" $I_{STI} = (-1)^{w_{P_j} + w_{P'_j}}$

3 "weak" $I^{(j)}_{WTI} = (-1)^{w_{P_j}}$

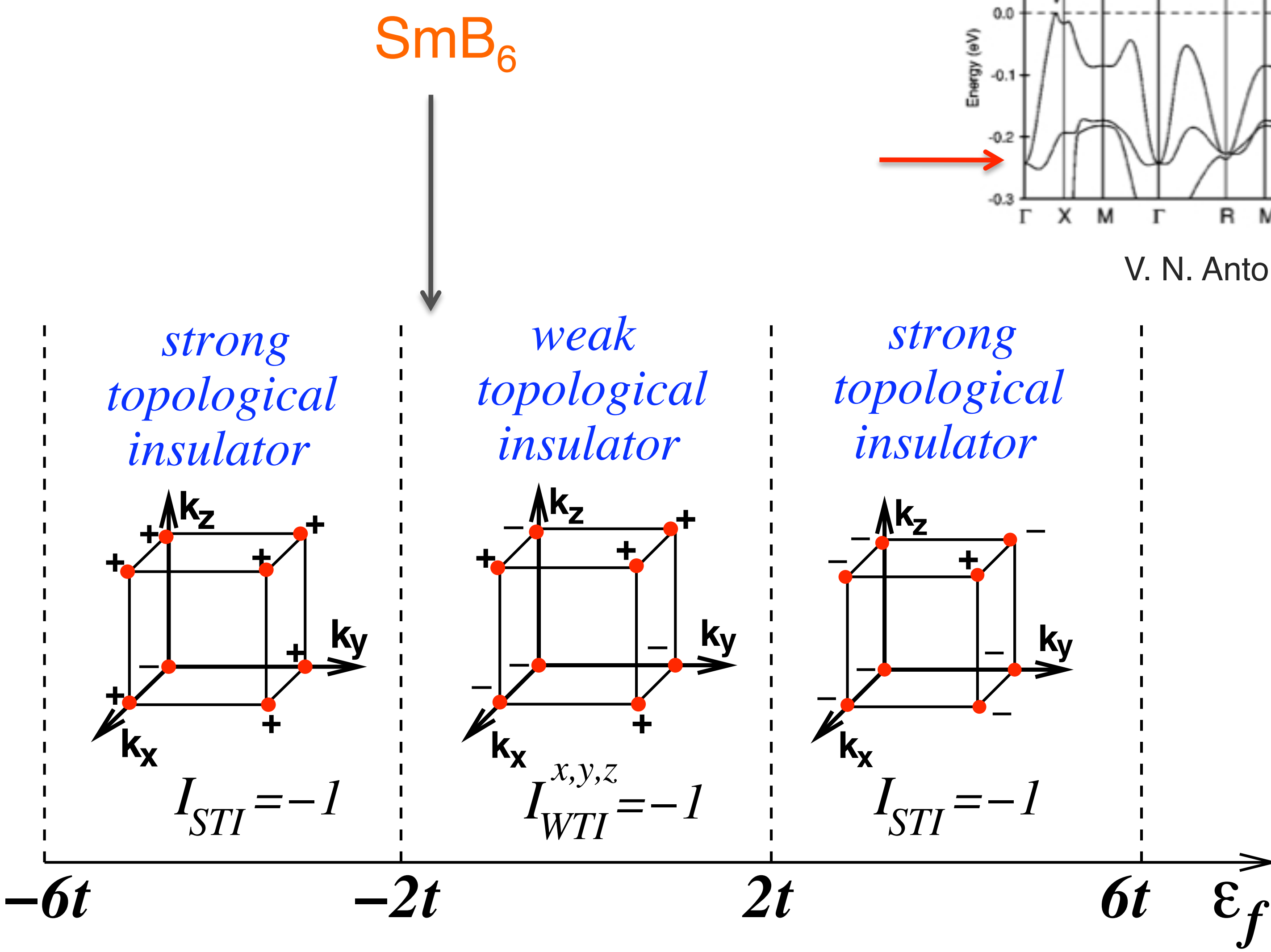
"phase diagram" does not depend on the underlying type of the unit cell



Are existing Kondo insulators weak or strong TI?



V. N. Antonov et al. PRB (2006)

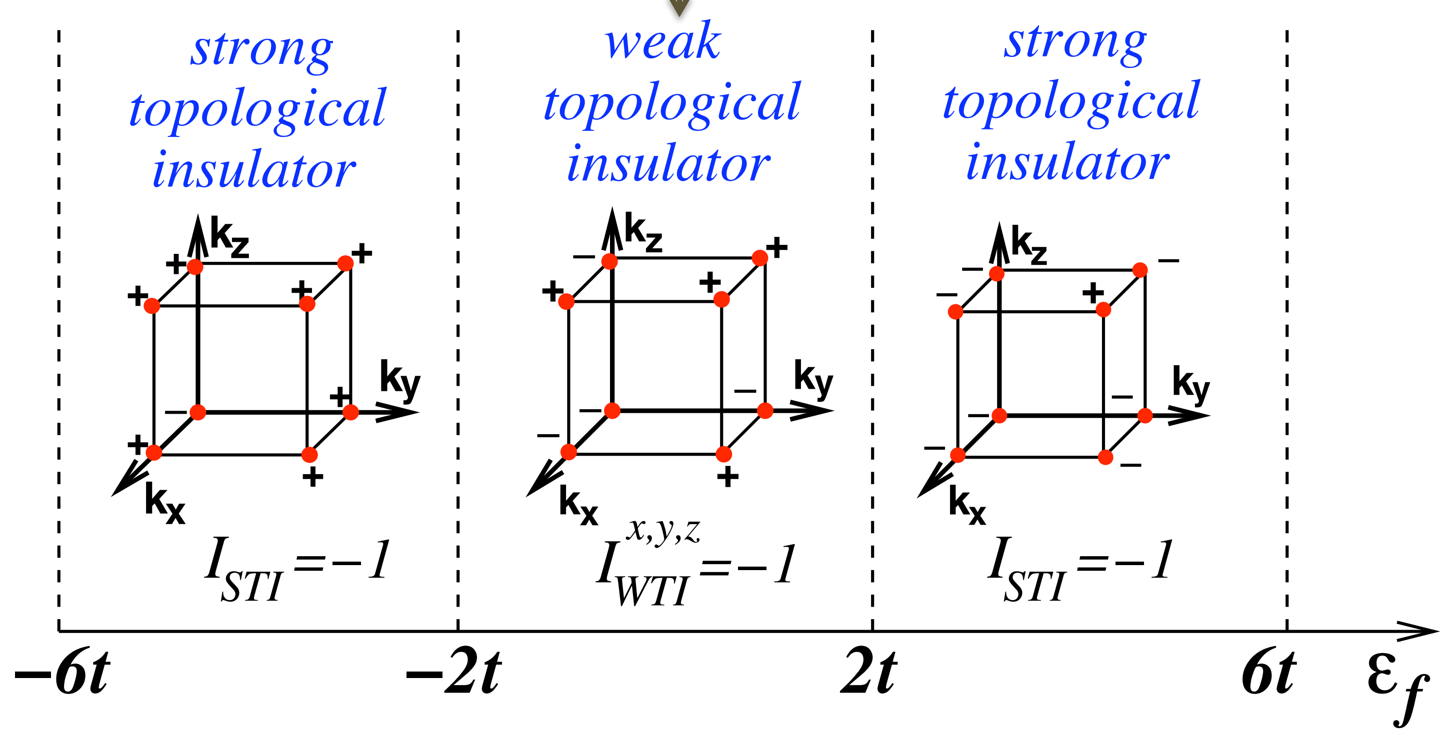


Are existing Kondo insulators weak or strong TI?

- Ce-based Kondo insulators: localized moment $n_f=1$
- Nodes in the gap (CeNiSn)?

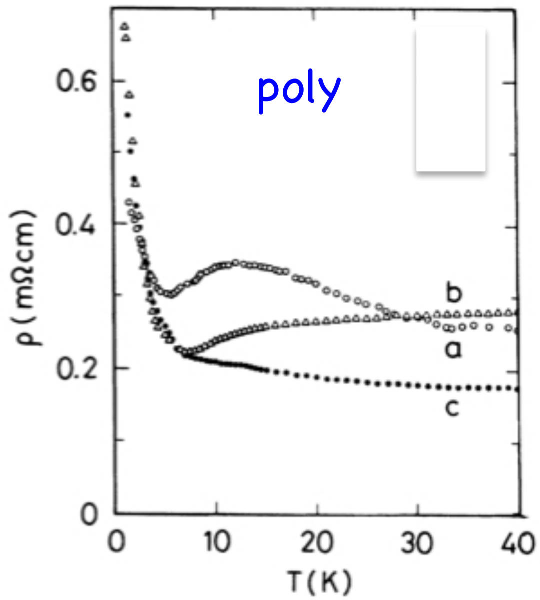
CeNiSn
CeRhSb
$Ce_3Bi_4Pt_3$

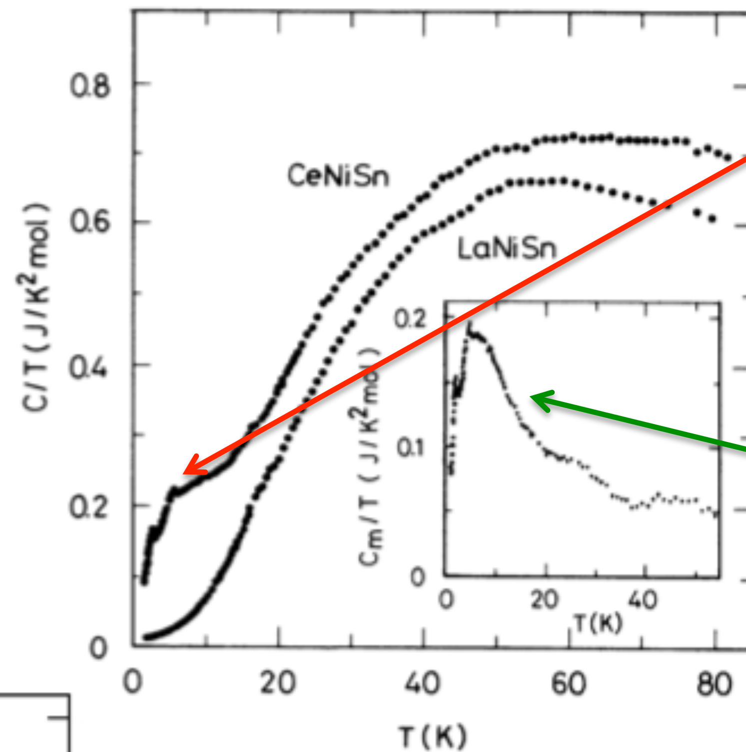
J. N. Chazalviel et al. PRB (1976)
T. Terashima et al. PRB (2002)



CeNiSn: weak topological insulator?

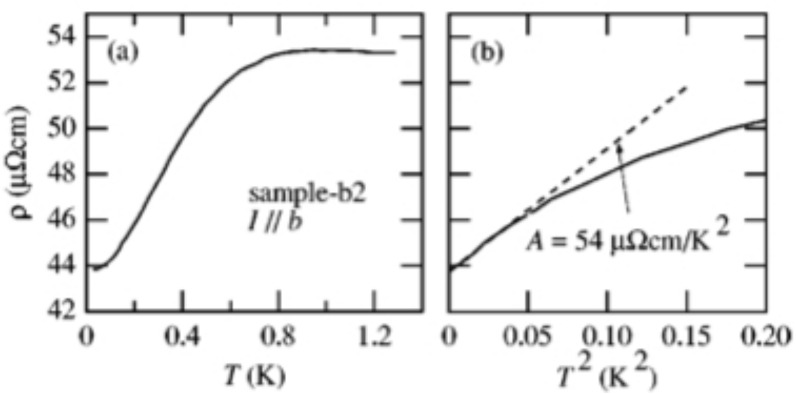
T. Takabatake et al. PRB (1990)





Depletion in the density of states below 10 K

Formation of heavy fermions



T. Terashima et al. PRB (2002)

- polycrystalline samples: insulators
- single crystal samples: metallic

Summary

- Ce-based Kondo insulators are weak topological insulators: unstable to disorder

- Strong Topological Insulators in f-electron systems are most likely to be observed in mixed-valence ($n_f \approx 30\%$) materials

- Strong spin-orbit coupling due to hybridization of conduction electrons with f-electrons

- We expect fundamentally novel type of metallic states on the surface of the STI