Topological Kondo Insulator SmB_6

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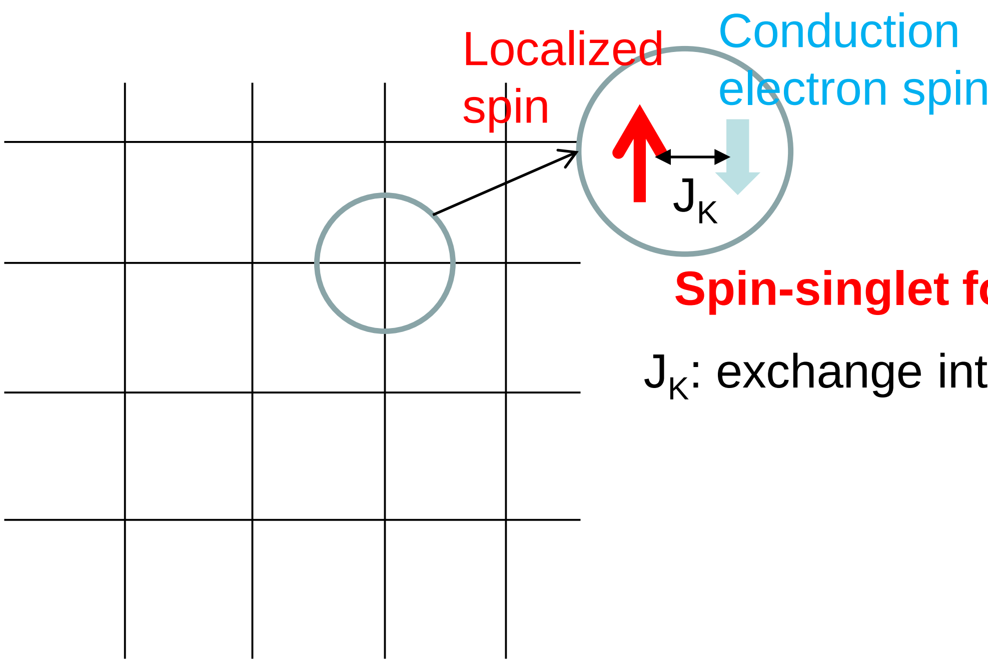
Content

Kondo effect

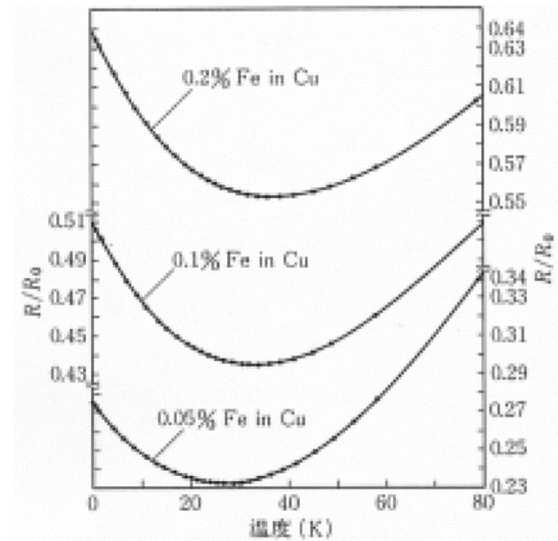
Kondo lattice (strong correlation):

Lattice of localized spin
+
Sea of conduction electrons



Spin-singlet for $T<T_K$

J_K: exchange interaction



Logarithmic increase of resistivity below T_K

Due to the coherence of Kondo states, heavy fermion are formed in the Kondo lattice

Heavy fermion system and Kondo insulator

Another picture from weak correlation (Anderson lattice)

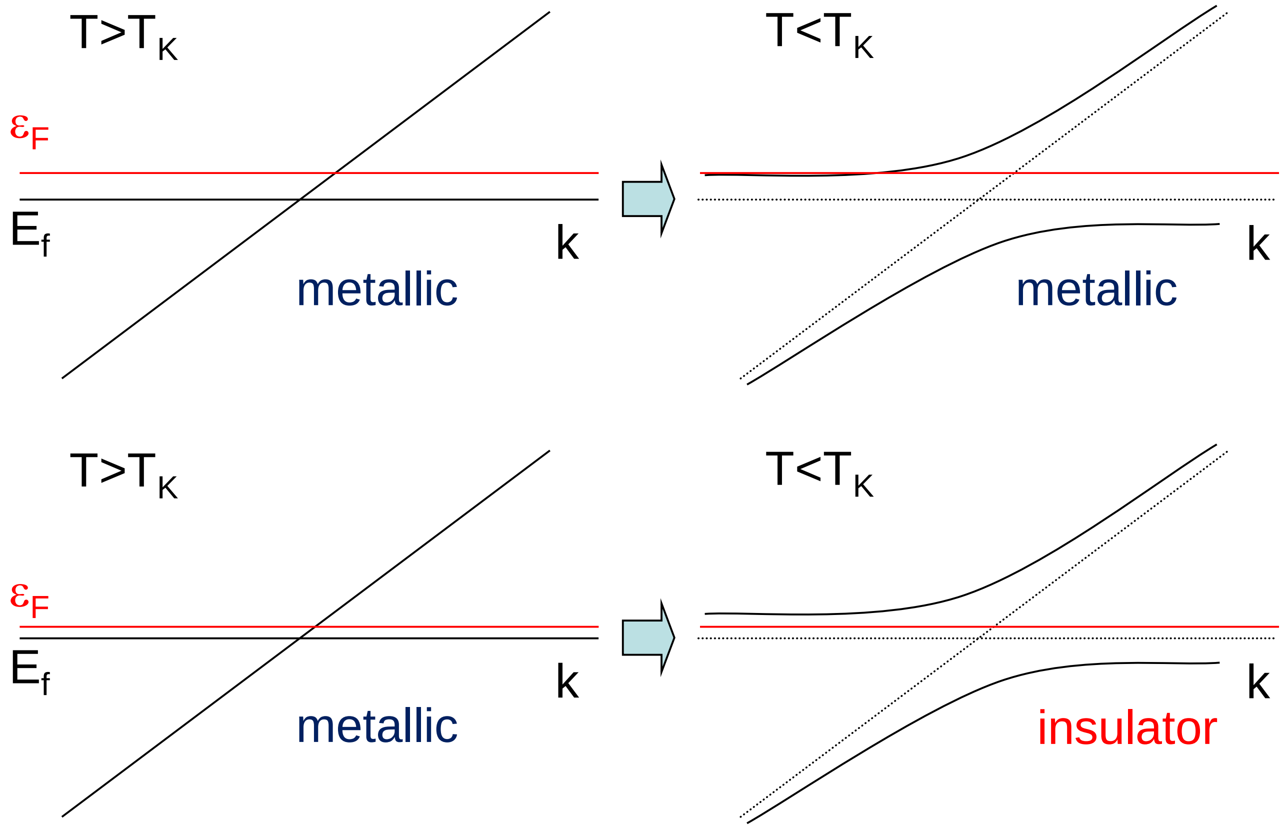
Renormalization of hybridization
between conduction and localized electrons

(instead of exchange interaction)

Anderson lattice
↓ Strong coupling limit
Kondo lattice

Heavy fermion system

Kondo insulator

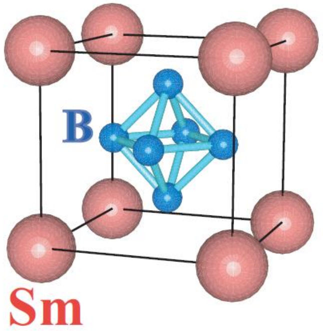


Introduction

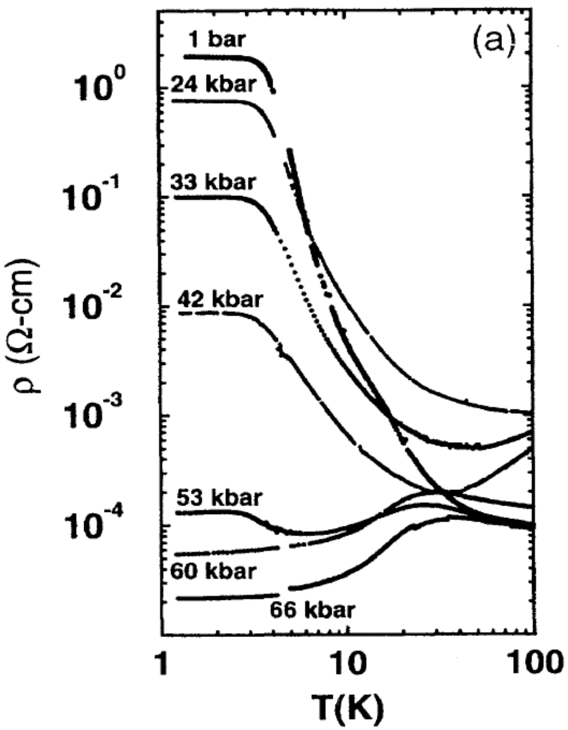
SmB_6: Kondo insulator

Δ_{gap}=15 meV

point group : O_h



in-gap state below 5K



Cooley et al. PRL 74 1629 (1995)

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Topological Kondo Insulators

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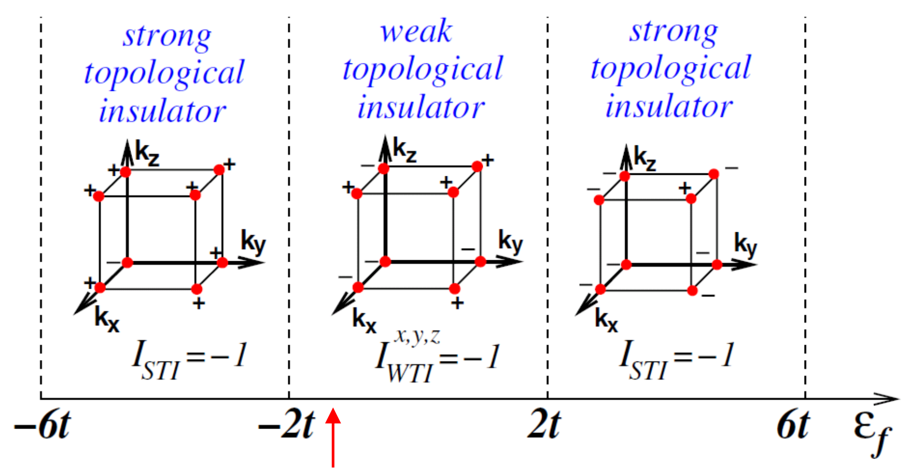
periodic Anderson model (s+f)

f: jz=-1/2 and +1/2 (Γ_8 of O_h)

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

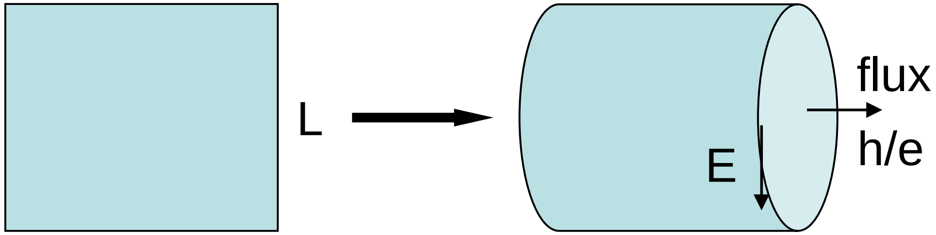


SmB6

Topological Insulator

- two copies of integer quantum Hall system
- time reversal invariant
- large spin-orbit coupling
- metallic edge (surface) state

two-dimensional case (Kane & Mele PRL **95**)



circumferential electric field E
can be induced by a threading flux

$k \longrightarrow k+2\pi/L$

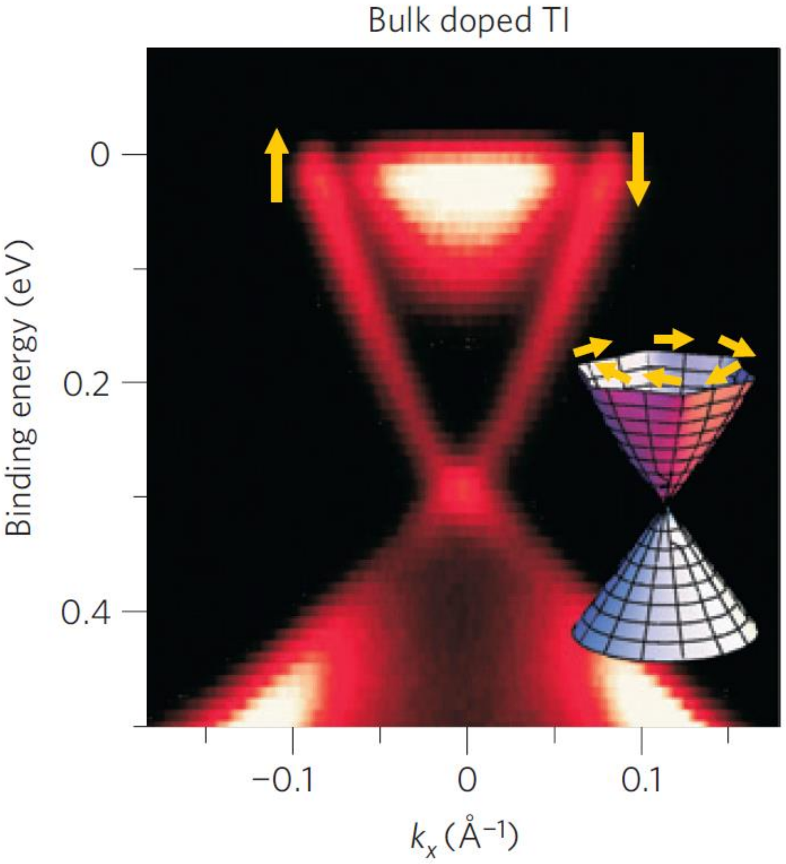
trivial insulator (ν_0=0) no effect

gapped around E_F

topological insulator (ν_0=1) spin Hall

particle-hole excitation around E_F on the edge

spin-direction is different between particle and hole



Dirac cone on a surface of Bi_2Se_3

Wray et al. Nature Phys. **7** 32

ref.

Hasan & Kane RMP 82

Qi & Zhang RMP

Topological number in noninteracting system

In TRI compound (2D square lattice)

Fu and Kane: PRB **74** 195312

gauge invariance (phase of wave function)

time reversal symmetry $H(-\mathbf{k})=\Theta H(\mathbf{k})\Theta^{-1}$ $(\Theta=\sigma_y K)$

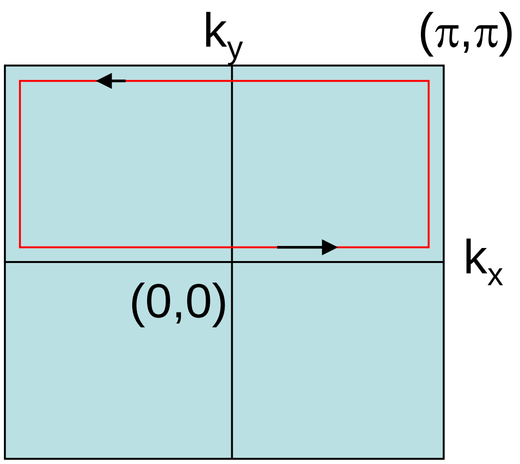
determine gauge potential $\mathcal{A}(k) = i\sum_n \langle u_{k,n}|\nabla_k|u_{k,n}\rangle$ ⟹ topological #

Chern # = 0 (cancellation in Kramers doublet)

topological # ν_0
calculated by choosing one from a doublet

$$\nu_0 = \frac{1}{2\pi}\left[\oint_{\partial\tau_{1/2}} d\ell\,\mathcal{A} - \int_{\tau_{1/2}} d\tau\,\mathcal{F}\right] \bmod 2$$

field strength
$\mathcal{F}=d\mathcal{A}$



trivial case

$\nu_0=0$
$\mathcal{A}$ is continuous
in Brillouin zone.

topological case

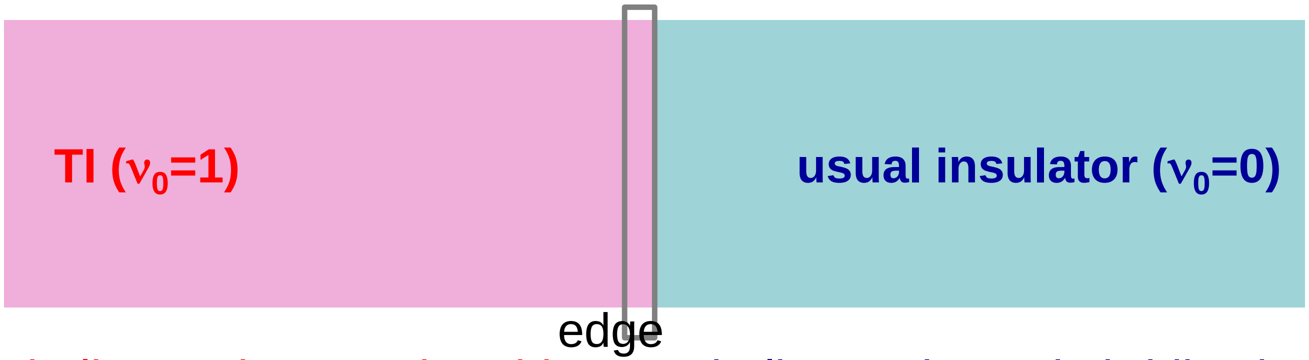
ν_0=odd #
$\mathcal{A}$ has one or three singular points
at (0,0), (π,0), (0,π), or (π,π).

Bulk-edge correspondence

electronic states in bulk ⇒ topological number ν_0

ν_0=1: topological
ν_0=0: trivial

a junction between TI and usual insulator in real space



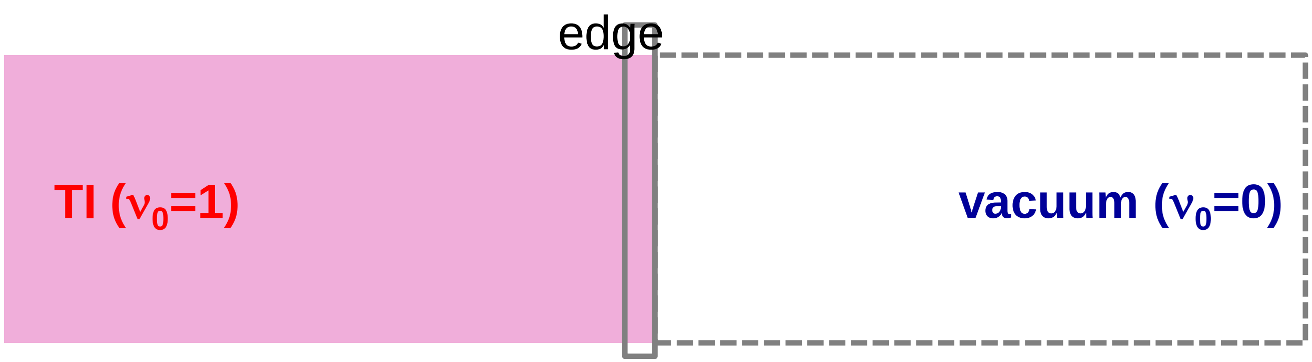
bulk gap due to spin-orbit

bulk gap due to hybridization between electrons with the same spin

different origin of bulk gap

necessary close the gap to move to the other side!

gapless states must appear on the edge



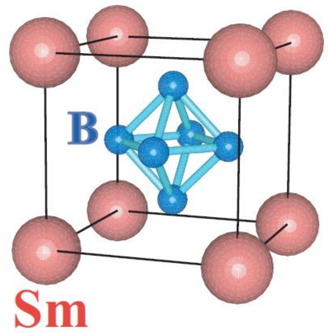
relevant orbitals

dominant electronic states

$(4f)^5(5d)^1$ and $(4f)^6$

band structure calculation

Yanase and Harima:
Prog. Theor. Phys. Suppl. **108** 19, (1992).
Antonov et al. : PRB **66** 165209, (2002).

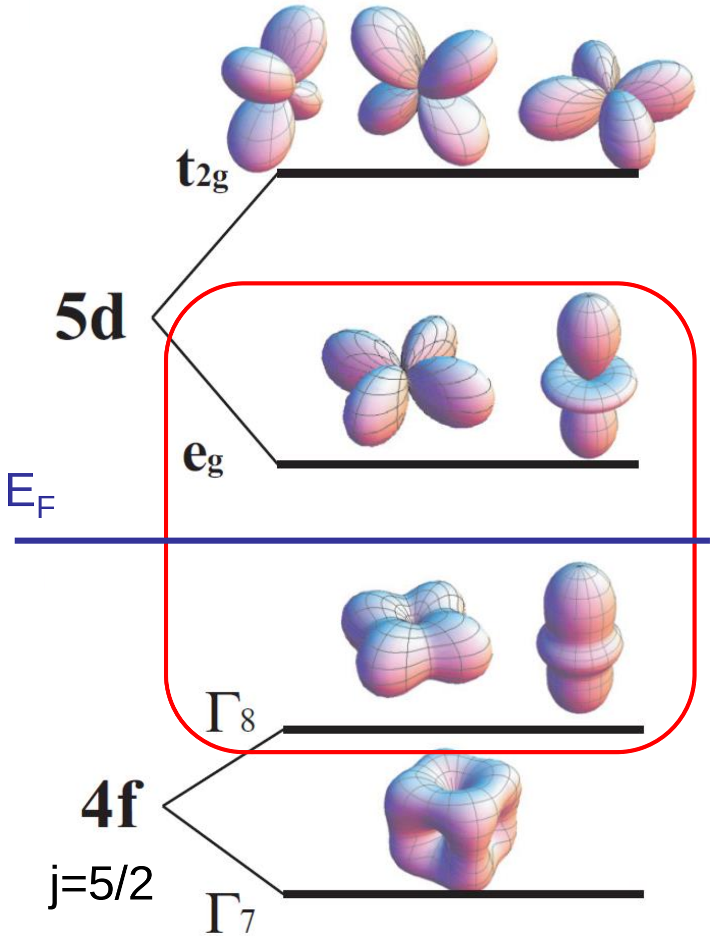


4f and 5d electrons are from Sm.

Sm^{3+}: $(4f)^5$

angular momentum: J=5/2
CEF ground state: Γ_8

~ one hole in Γ_8 states
in j-j coupling scheme



effective model

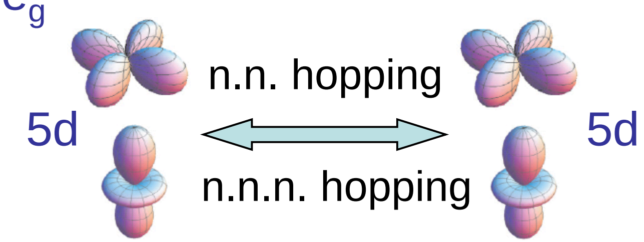
tight-binding

5d-electron term (NN+NNN)

$$H_c = \sum_{\mathbf{k}} \sum_{\xi,\xi'} \sum_{\sigma} \varepsilon^d_{\xi\xi'}(\mathbf{k}) c^\dagger_{\mathbf{k}\xi\sigma} c_{\mathbf{k}\xi'\sigma}$$

$$\hat{\varepsilon}^d(\mathbf{k}) = d^d_0(\mathbf{k})\hat{\tau}_0 + d^d_1(\mathbf{k})\hat{\tau}_z + d^d_2(\mathbf{k})\hat{\tau}_x$$

ξ : orbital in e_g
σ : real spin



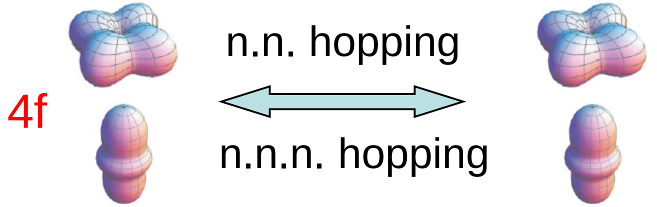
4f-electron term (NN+NNN)

$$H^0_f = \sum_{\mathbf{k}} \sum_{\gamma,\gamma'} \sum_{\tau,\tau'} \varepsilon^f_{\gamma\tau,\gamma'\tau'}(\mathbf{k}) f^\dagger_{\mathbf{k}\gamma\tau} f_{\mathbf{k}\gamma'\tau'}$$

$$\hat{\varepsilon}^f(\mathbf{k}) = d^f_0(\mathbf{k})\hat{\tau}_0\hat{\sigma}_0 + \sum_{n=1}^{5} d^f_n(\mathbf{k})\Gamma^n$$

$$\Gamma^{1,2,3,4,5} = (\hat{\tau}_z\hat{\sigma}_0, \hat{\tau}_x\hat{\sigma}_0, \hat{\tau}_y\hat{\sigma}_x, \hat{\tau}_y\hat{\sigma}_y, \hat{\tau}_y\hat{\sigma}_z)$$

γ : orbital in Γ_8
τ : pseudo spin in a Kramers doublet



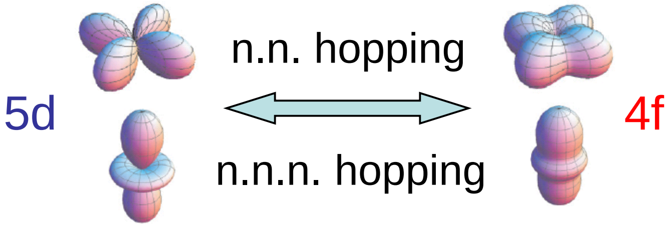
hybridization term (NN+NNN)

H_{hyb} The seed of singularity for $\mathcal{A}$

$$= \sum_{\mathbf{k}} \sum_{\xi,\gamma} \begin{bmatrix} c^\dagger_{\mathbf{k}\xi\uparrow} & c^\dagger_{\mathbf{k}\xi\downarrow} \end{bmatrix} \mathrm{i}\mathbf{V}_{\xi\gamma}(\mathbf{k}) \cdot \hat{\sigma} \begin{bmatrix} f_{\mathbf{k}\gamma+} \\ f_{\mathbf{k}\gamma-} \end{bmatrix}$$

$$+h.c.,$$

$$\hat{V}^\alpha(\mathbf{k}) = V^\alpha_0(\mathbf{k})\hat{\tau}_0 + V^\alpha_1(\mathbf{k})\hat{\tau}_z + V^\alpha_2(\mathbf{k})\hat{\tau}_x$$



renormalization of interaction term

interactions between 4f

interactions between 5d

interactions between 4f and 5d

localization character of 4f-electron

renormalization of interactions between 4f

- Gutzwiller projection
- slave boson

$$f_{\mathbf{k}\gamma\tau} \rightarrow \sqrt{z_{\mathbf{k}\gamma}}\,\tilde{f}_{\mathbf{k}\gamma\tau}$$

$$\varepsilon^{f}_{\gamma\tau,\gamma'\tau'}(\mathbf{k}) \longrightarrow z\,\tilde{\varepsilon}^{f}_{\gamma\tau,\gamma'\tau'}(\mathbf{k})$$

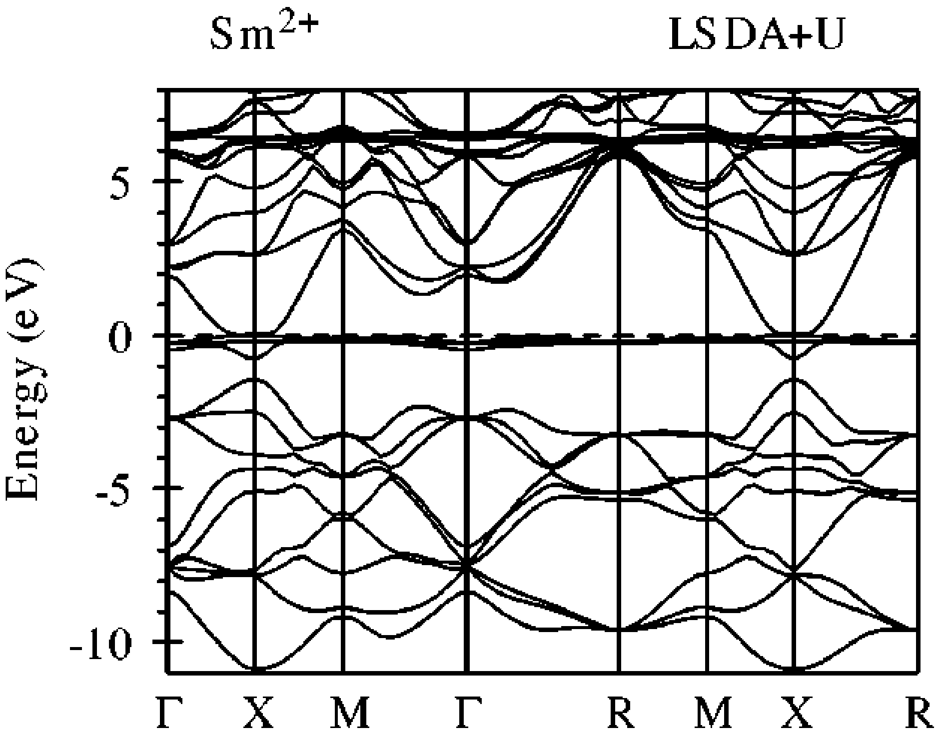
$$\mathbf{V}_{\xi\gamma}(\mathbf{k}) \longrightarrow \sqrt{z}\,\mathbf{V}_{\xi\gamma}(\mathbf{k})$$

map into effective Hamiltonian

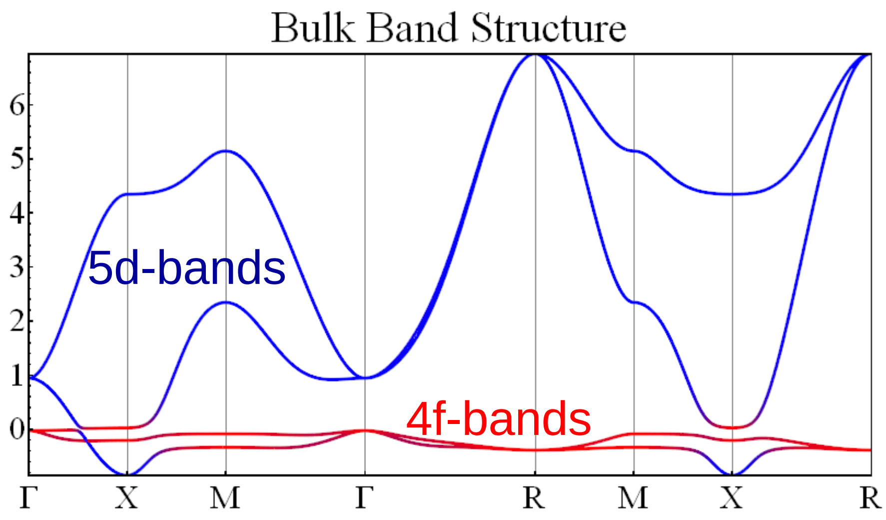
z : renormalization factor in Fermi liquid theory

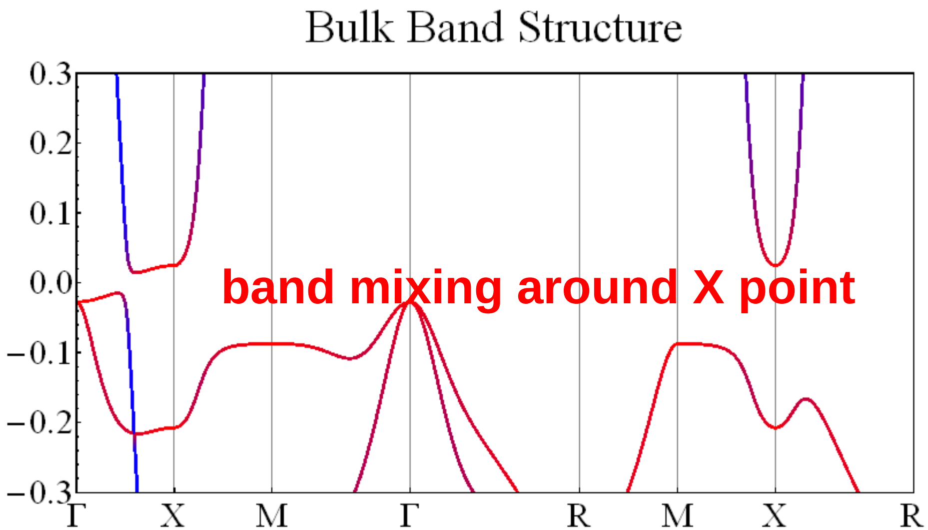
electronic structure

Antonov et al.: PRB **66** 165209, (2002).



half-filling case provides insulator





topological index

(ν_0: ν_1,ν_2,ν_3)

$$(-1)^{\nu_0} = \prod_m \delta_m$$

ν_0=0 WTI
ν_0=1 STI

$$(-1)^{\nu_k} = \prod_{n_k=1;n_{j\neq k}=0,1} \delta_{m=(n_1,n_2,n_3)}$$

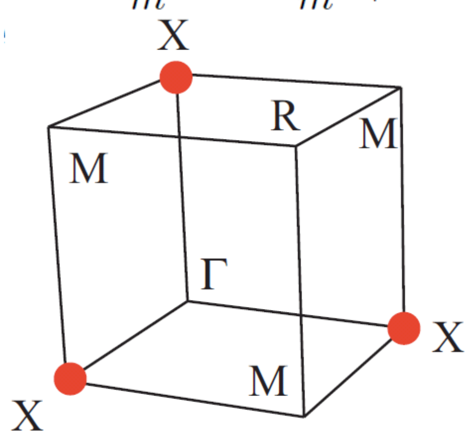
$$\delta_m = \prod_{E_n<\varepsilon_F} \delta_{n,m}$$

$\delta_{n,m}$: parity eigenvalue of n-th two-fold degenerate band at $\mathbf{k}_m^*$

Fu and Kane: PRB 74 195312 (2006)
PRB 76 045302 (2007)

time reversal invariant point

$$-\mathbf{k}_m^* = \mathbf{k}_m^* + \mathbf{G}$$



parity operator

$$\hat{P} = \hat{s}_z\hat{\tau}_0\hat{\sigma}_0$$

$\hat{s}_\alpha$: 2X2 matrix between d- and f-electronic states

$$\left[\hat{H}(\mathbf{k}_m^*), \hat{P}\right] = 0$$

hybridization term is formed by s_x and s_y

$$\hat{P}\hat{s}_{x,y}\hat{P}^{-1} = -\hat{s}_{x,y}$$

hybridization term is irrelevant at **k*** for $\delta_{n,m}$

$E_\pm^d(\mathbf{k}_m^*)$ with even parity

$E_\pm^f(\mathbf{k}_m^*)$ with odd parity

$E_+^d(\mathbf{k}_m^*)$ is the highest energy

our model
(1: 1,1,1)

ε_F ↓

$$E_-^d(\mathbf{k}_m^*) > E_+^f(\mathbf{k}_m^*) > E_-^f(\mathbf{k}_m^*) \qquad \delta_m = +1$$

$$E_+^f(\mathbf{k}_m^*) > E_-^f(\mathbf{k}_m^*) > E_-^d(\mathbf{k}_m^*) \qquad \delta_m = -1$$

Necessary and sufficient conditions for TKI

$$H_{hyb} = \sum_{\mathbf{k}} \sum_{\xi,\gamma} \left[c^{\dagger}_{\mathbf{k}\xi\uparrow} \;\; c^{\dagger}_{\mathbf{k}\xi\downarrow} \right] \underline{\mathrm{i}\mathbf{V}_{\xi\gamma}(\mathbf{k}) \cdot \hat{\sigma}} \begin{bmatrix} f_{\mathbf{k}\gamma+} \\ f_{\mathbf{k}\gamma-} \end{bmatrix} + h.c.,$$

$$\hat{V}^{\alpha}(\mathbf{k}) = V_0^{\alpha}(\mathbf{k})\hat{\tau}_0 + V_1^{\alpha}(\mathbf{k})\hat{\tau}_z + V_2^{\alpha}(\mathbf{k})\hat{\tau}_x$$

n	$V_n^x(\mathbf{k})$	$V_n^y(\mathbf{k})$	$V_n^z(\mathbf{k})$
0	$4V_{df}S_x$	$-4V_{df}S_y$	$4V_{df}S_z$
1	$2V_{df}S_x$	$-2V_{df}S_y$	$-4V_{df}S_z$
2	$-2\sqrt{3}V_{df}S_x$	$-2\sqrt{3}V_{df}S_y$	0

$\mathbf{V}_{\xi\gamma}(\mathbf{k}) \cdot \hat{\sigma}$ ~ **k'.σ** at **k**=**k***+**k'** (|**k'**|<<π)

The seed of singularity for $\mathcal{A}$ at **k***

k'-linear: different parities
σ: large spin-orbit coupling

Necessary condition for TKI

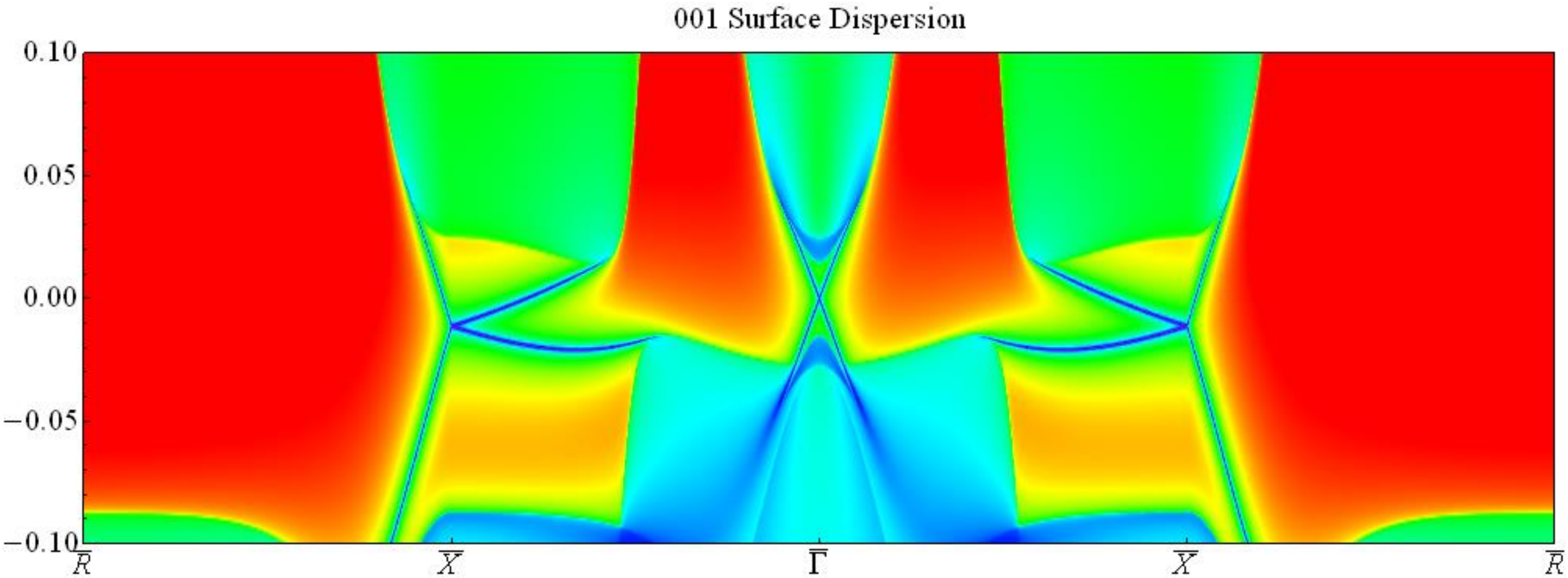
hybridization gap between d- and f-bands around **k**=**k***

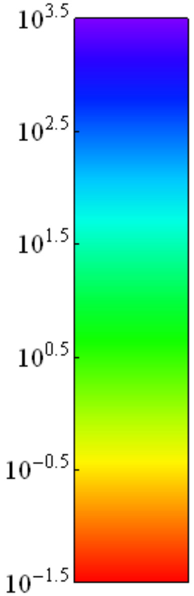
⇩

Nontrivial topological #
Determined by Hamiltonian without H_{hyb}

Sufficient condition for TKI

Spectral function of (001)-surface

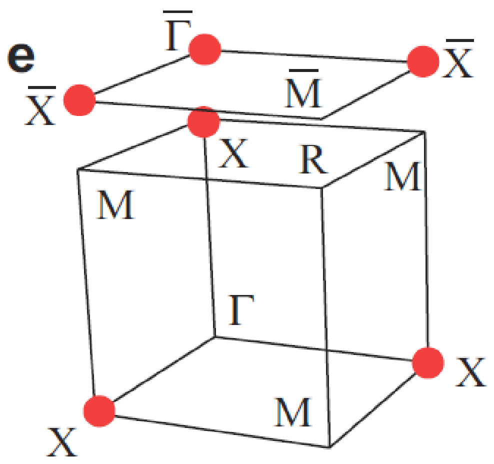




There are Dirac cones at Γ and X points.

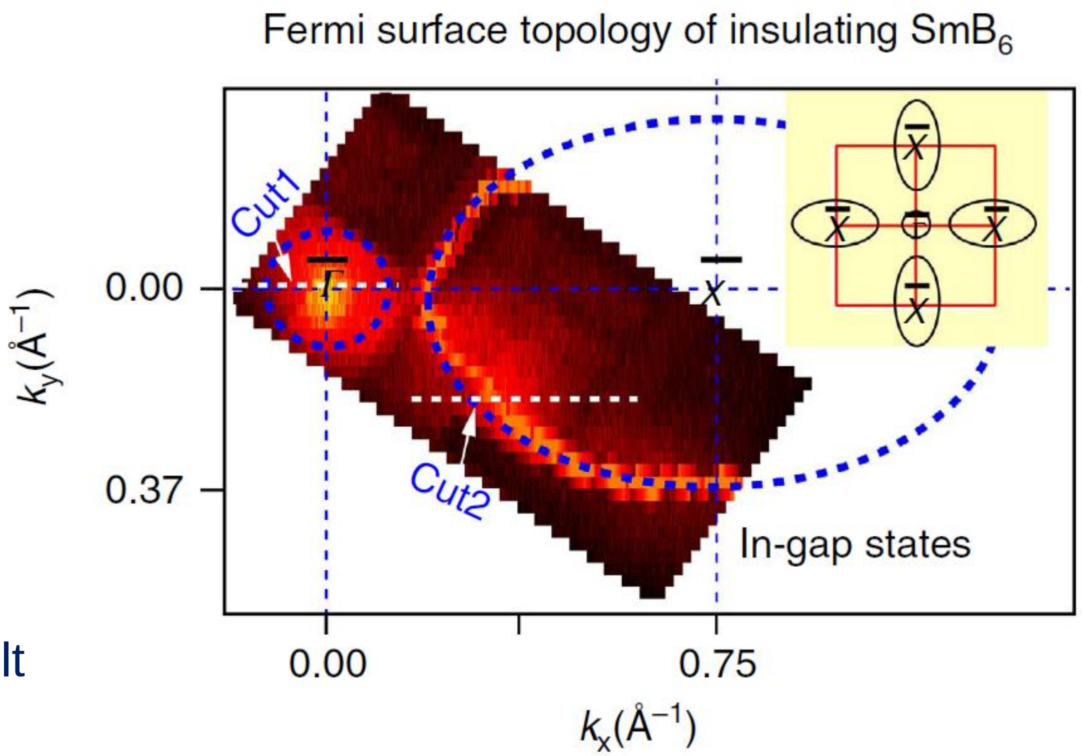
Intensity around X is stronger than that around Γ

There is a v.-H. singularity along Γ-X.



Recent ARPES measurement for (001) surface

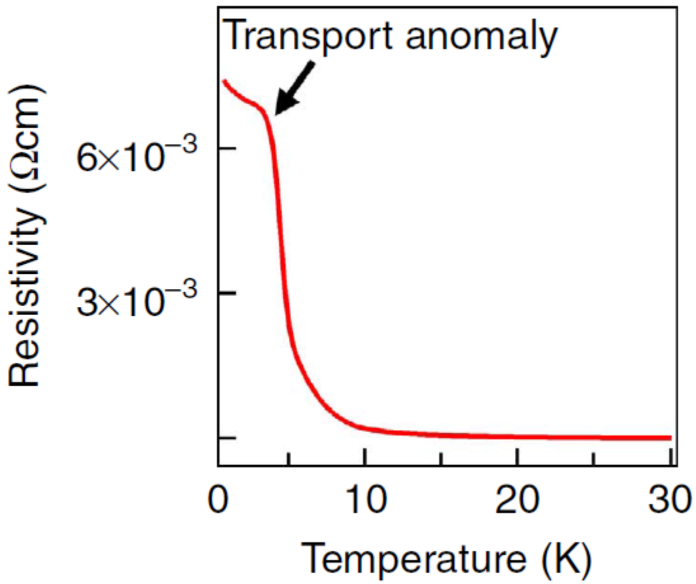
M. Neupane et al. (M.Z.Hasan)
Nat. Commun. 4, 2991 (2013).

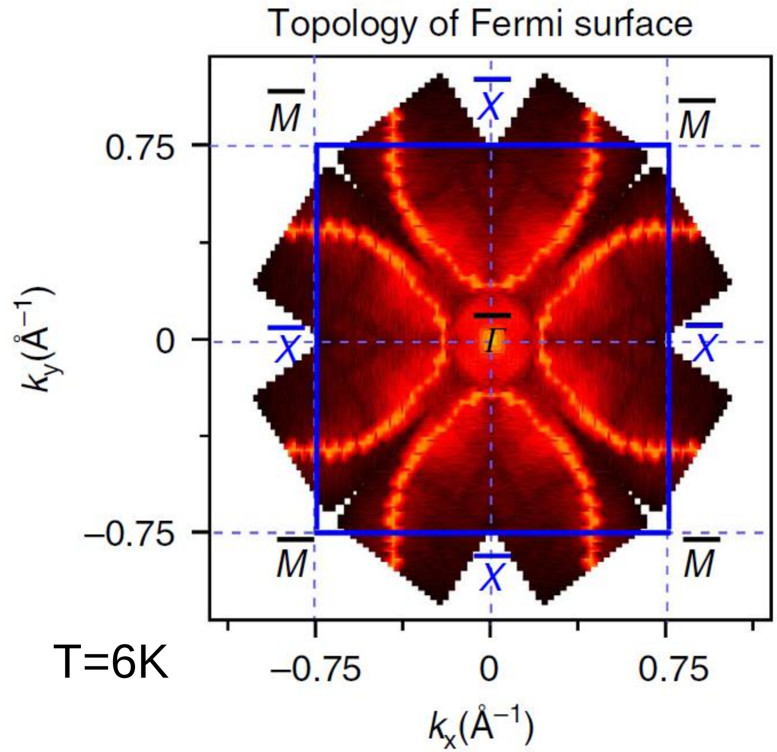


T=6K

Fermi surface around Γ and X

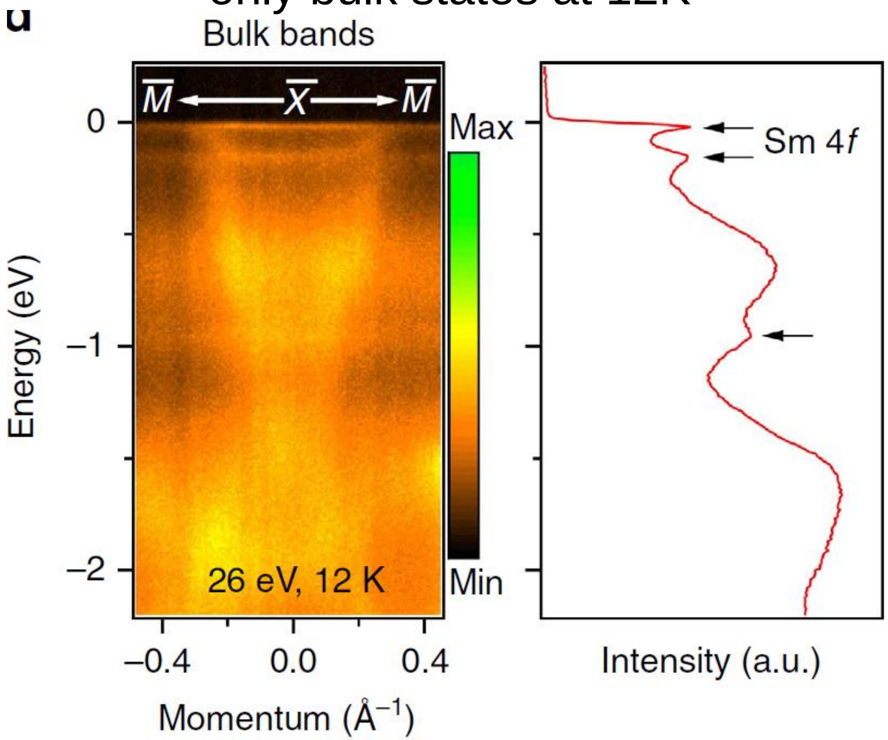
topology of Fermi surface
is the same as the theoretical result



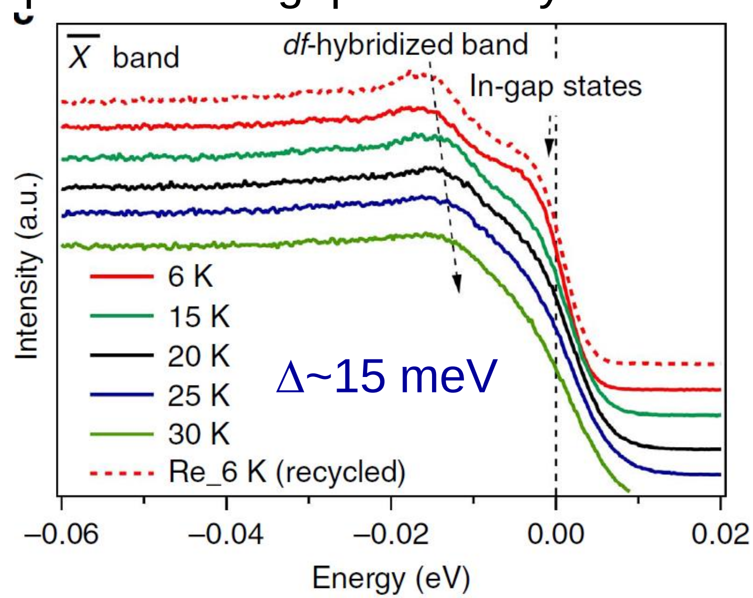


T=6K

only bulk states at 12K



development of in-gap states by decreasing T

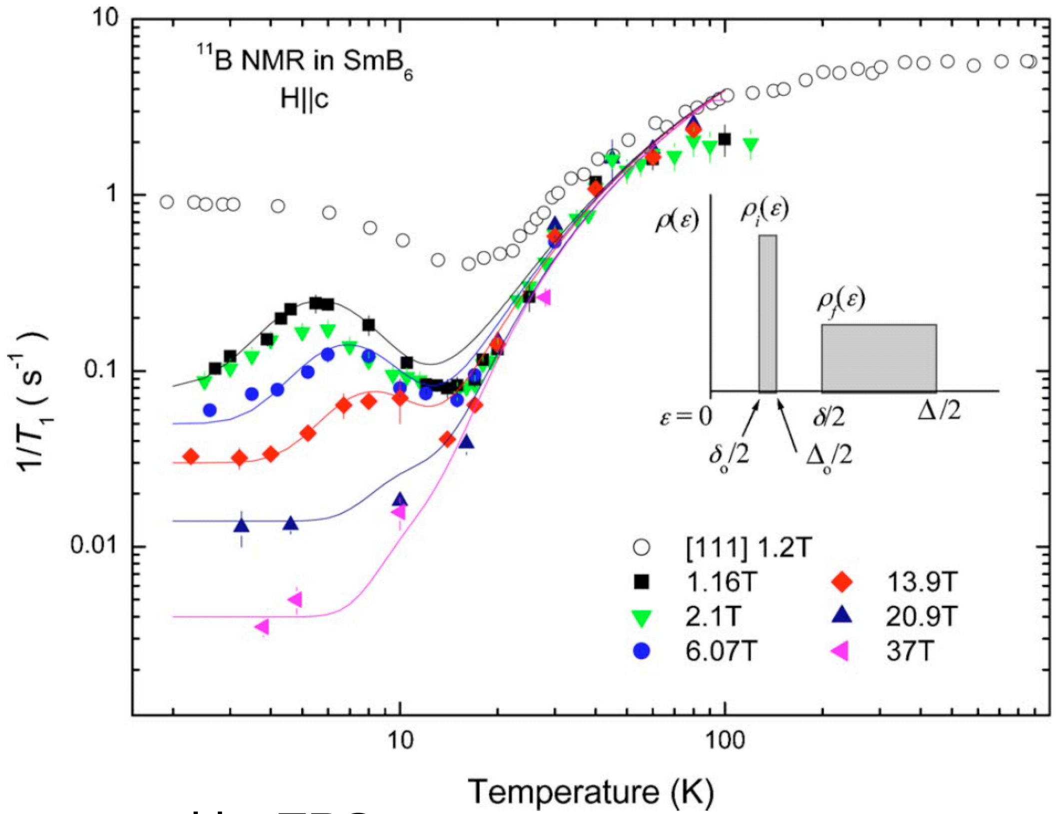


NMR in SmB_6

$$\frac{1}{T_1} = \frac{\hbar k_B T}{\omega_n} \sum_q A^2 F(q) \chi''_{q,\omega_n}$$

- insulator behavior down to ~20K
- contribution from the in-gap state below 20K
- magnetic field suppresses the in-gap state

Caldwell et al. PRB **75** 075106 (2007)



The magnetic field breaks TRS.

The metallic surface states of TI is protected by TRS.
The surface states should be gapped by the magnetic field

in-gap state~surface state of topological insulator

Why the value of $1/T_1T$ is so large at the low temperature limit?

Summary

We study the possibility of the topological insulator for SmB_6, calculating the topological index and spectral function of [001] surface, based on a realistic model.

The topological index is (1: 1,1,1).

In the spectral function, surface states appear with odd number of Dirac cones.

Based on the calculation, SmB_6 is a topological Kondo insulator.

Recent ARPES measurements show Fermi surfaces surrounding the Dirac points consistent with theoretical suggestions.

next step

experiment: measurements of Dirac points, spin texture

theory: clarification of electron correlation in the surface states