# Quantum phase transitions in correlated topological insulators

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# Collaborators: Correlated Topological Insulators

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*ISSP*

Y. Tada

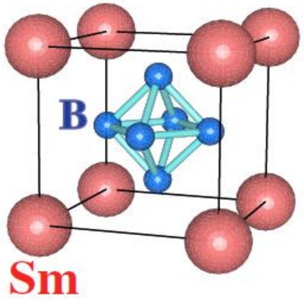
M. Oshikawa

*ETH*

M. Sigrist

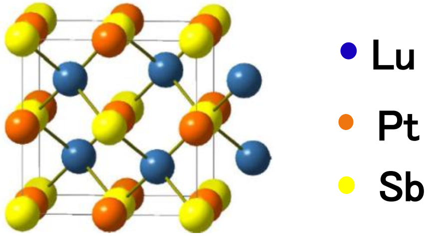
# ～Topological phases in correlated electron systems ～

**$SmB_6$ (Kondo insulator)**



Dzero *et al.* PRL (2010)

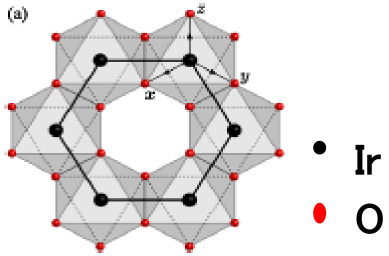
**LuPtBi (Heusler compound)**



Chadov et al. Nature Materials (2010)

Lin et al. Nat. Mat. (2010)

**$Na_2IrO_3$**



Shitade *et al.* PRL (2009)

## Electron correlations + SO coupling

# Correlation effects on Topological phases

Coulomb interaction + Topological nature

Exotic phenomena are expected.

- ◇ Interaction-driven topological insulators
- ◇ Competing phases :

[Topological phase] v.s. [ordered phases]

magnetic phase,
charge density wave phase

etc…

## *Interaction-driven TI*

- S. Raghu, Xl. L. Qi, C. Henerkampp, and S. C. Zhang, PRL 100, 156401 (2008).
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- M. Kurita, Y. Yamaji, and M. Imada, J. Phys. Soc. Jpn. 80 044708 (2011).
- G. A. Fiete, V. Chua, X. Hu, M. Kargarian, R. Lundgren, A. Ruegg, J. Wen and V. Zyuzin, arXiv:1106.0013

## *Correlation Effects on TI*

- Y. Yamaji and M. Imada, PRB 83, 205122 (2011).
- M. Hohenadler, T. C. Lang, and F. F. Assad. PRL 106, 100403 (2011).
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- S. L. Yu, X. C. Xie, and J. X. Li, PRL 107, 010401 (2011).
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- S. Rachel and K. L. Hur, PRB 82 075106 (2010).
- C. N. Varney, K. Sun, M. Rigol, and V. Galitski, PRB 82, 115125 (2010).
- L. Wang, H. Shi, S. Zhang, X. Wang, X Dai and X. C. Xie, arXiv. 1012.5163v1 (2011).
- T. Yoshida, S. Fujimoto, and N. Kawakami, PRB 85, 125113 (2012).
- Y. Tada, R. Peters, M. Oshikawa, A. Koga, N. Kawakami, and S. Fujimoto, PRB 85, 165138 (2012).

## *Topological AF*

- R. S. K. Mong, A. M. Essin, and J. E. Moore, PRB 81, 245209 (2010)
- A. M. Essin and V. Gurarie, arXiv:1112.6013v1 (2011)
- J. He, Y-H, Zong, S-P Kou, Y Liang, and S. Feng, PRB 84, 035127 (2011)
- J. He, B. Wang, and S-P Kou, arXiv:1204.4766 (2012)
- H. Guo, S. Feng, and S-Q Shen, PRB 83 045114 (2011)
- T. Yoshida, R. Peters, S. Fujimoto and N. Kawakami, PRB 87, 085134 (2013)

## *Topological Kondo Insulator*

- M. Dzero, K. Sun, V. Galitski, P. Coleman, PRL 104, 106408 (2010).
- T. Takimoto, J. Phys. Soc. Jpn 80, 123710 (2011).
- F. Lu, J. Zhao, H. Weng, Z. Fang, and X. Dai, arXiv:1211.5863
- T.Yoshida, R. Peters, S. Fujimoto and N. Kawakami, PRB 87, 165109 (2013)

***etc., etc***

# Contents

## Correlation Effects on Topological Insulators

### 1. Correlated TI at Finite $T$

Electron correlation
Strong renormalization effects
Edge states

### 2. Topological Kondo Insulator in a Metal

Collaboration, topology, ferromag, Kondo effect

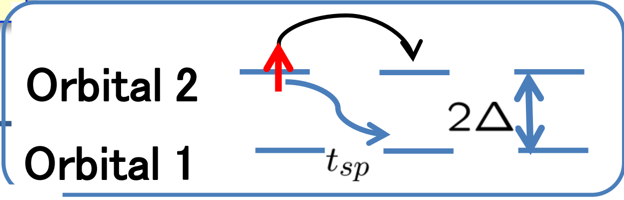
Nontrivial phase in a metal

# Correlated Topological Insulators at Finite Temperatures

T. Yoshida, S. Fujimoto, NK

# Bernevig-Hughes-Zhang model +U

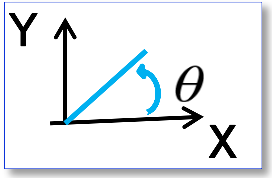
## Two-orbital system



$$H_{BHZ} = \Delta \sum_{i,\sigma} (n^2_{i,\sigma} - n^1_{i,\sigma}) - \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i,\alpha,\sigma} \hat{t}_{\sigma,\alpha,\alpha'} c_{i,\alpha',\sigma}$$

$$-\hat{t_\sigma} = \begin{pmatrix} -t & it_{so}e^{i\theta\sigma} \\ it_{so}e^{-i\theta\sigma} & t \end{pmatrix}$$

SO-coupling

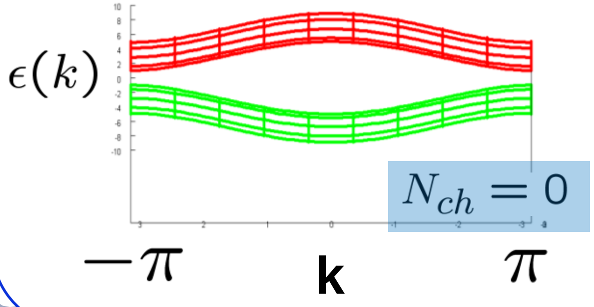


$$+U\sum_{i,\alpha} n_{i,\alpha,\uparrow} n_{i,\alpha,\downarrow}$$

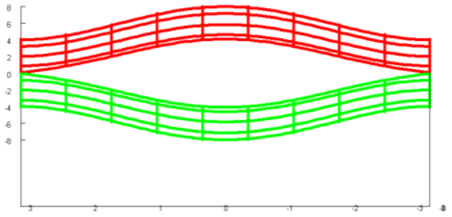
**BHZ+U ← DMFT**

## Non-interacting case

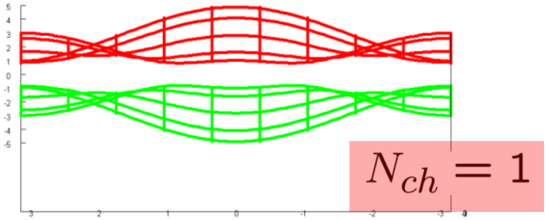
**Large Δ Trivial**



**gap-closing**

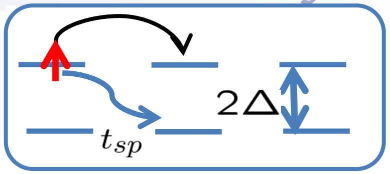


**SmallΔ Nontrivial**

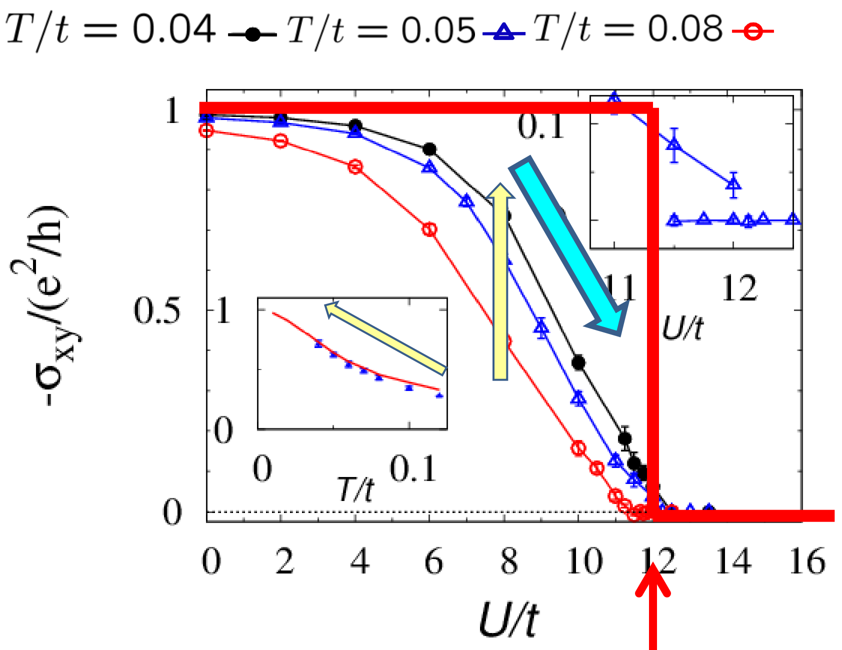


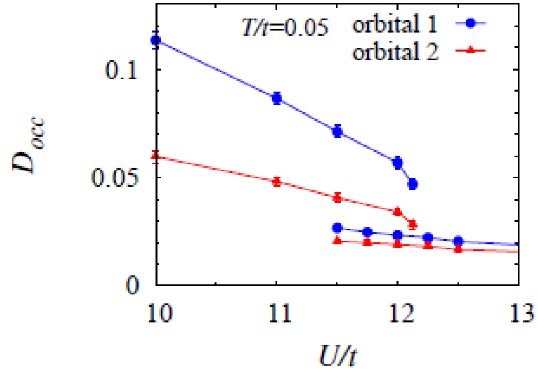
# Spin Hall conductivity

$\sigma_{xy}^{SH} = -\frac{e^2}{(2\pi)\hbar}N$ : Quantized at *T*=0



*Δ* = *t*
$t_{so} = 0.5t$



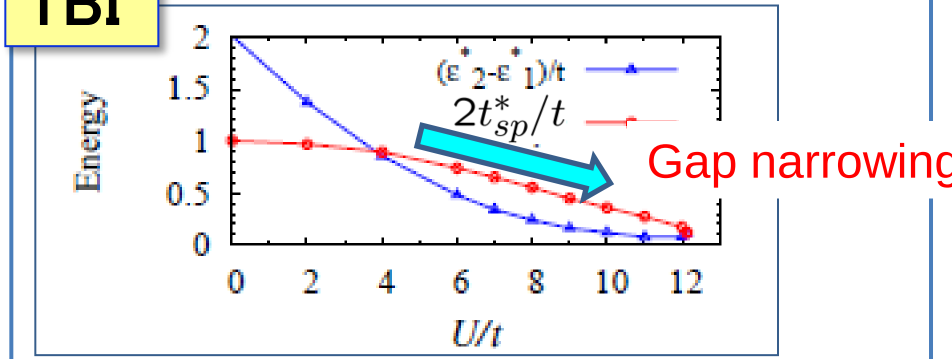


jump

hysteresis

**1st order transition**

## TBI

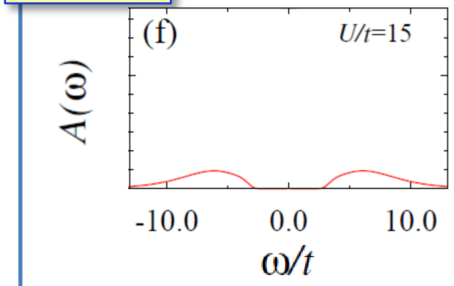


$\sigma_{xy}^{SH}$ **Gap narrowing**

⇩

**Increase of effective temperature ([Temp.]/[Gap size])**

## Mott



$\sigma_{xy}^{SH} = 0$

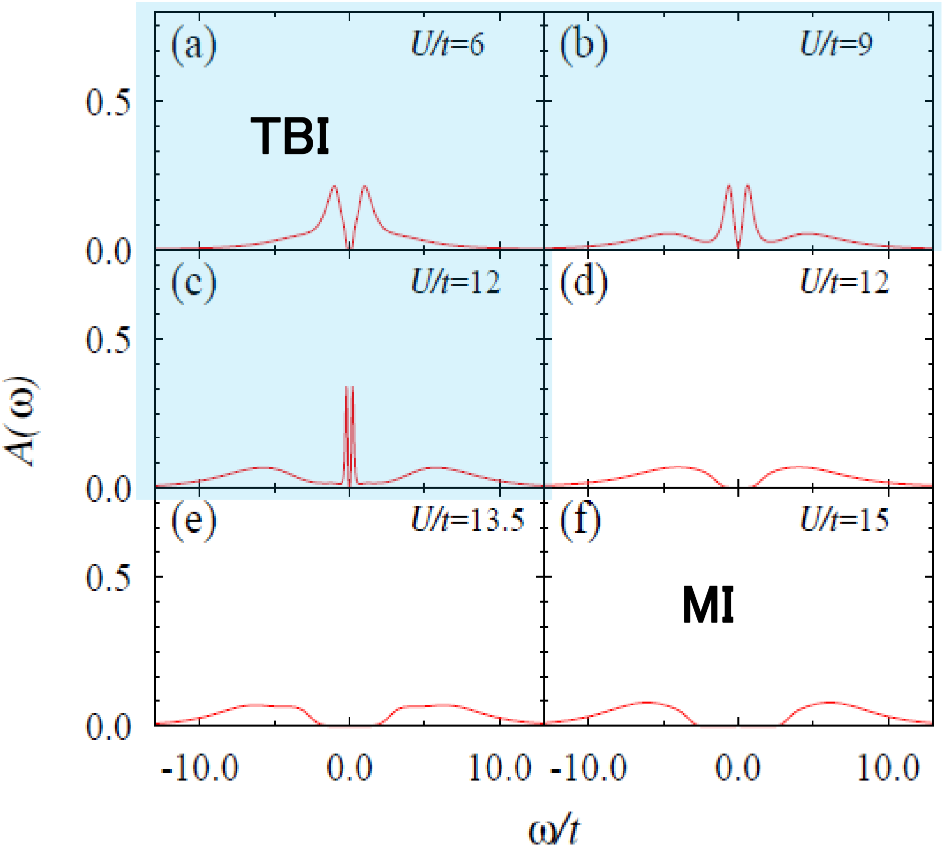
[gap size] $\sim U$

**Trivial Mott**

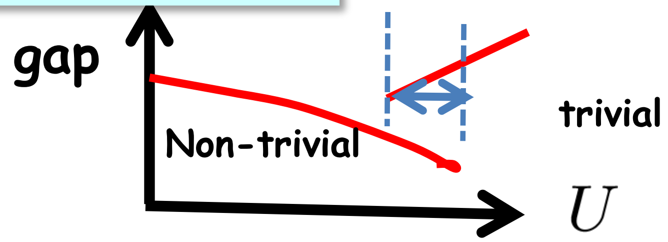
# Spectral function

$T = 0.05t$
$t_{so} = 0.5t$

🟦 :TBI
☐ :MI



## Mott transition



**Change of Topological structure without gap closing**

(1st order transition)

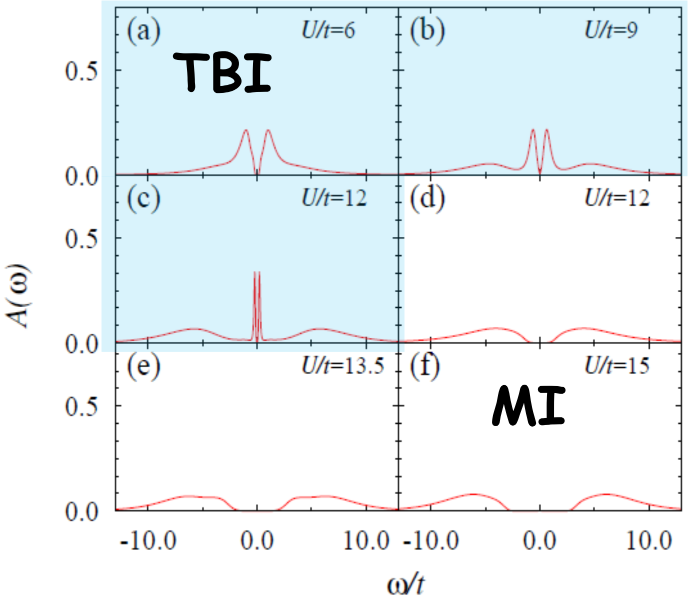
# Gap renormalization

**In generic band insulators**

⇨ gap renormalization depends on the origin of the gap at $U=0$.

$U\neq0$ case:

gets wider or narrower ?



**Gap Narrowing is generic behavior of TBIs.**

Gap ⇐ Spin orbit interaction (contributes to kinetic term)
(narrow the gap)

Renormalization due to correlations
=> $\sigma_{xy}^{SH}$ at $T\neq0$

**Important ! QPT**

# Finite-size effects on correlated TBI

Y. Tada, R. Peters, M. Oshikawa, A. Koga, NK, S. Fujimoto

# Finite-Size Effects

$$H = H_{\mathrm{BHZ}} + U\sum_{il} n_{il\uparrow}n_{il\downarrow}$$

**Bernevig-Hughes-Zhang model**

**Hubbard interaction**

$$H_{\mathrm{BHZ}} = \sum_{ij} C_i^\dagger \hat{H}_{ij} C_j, \qquad C_i = (c_{i1\uparrow}, c_{i2\uparrow}, c_{i1\downarrow}, c_{i2\downarrow})^t$$

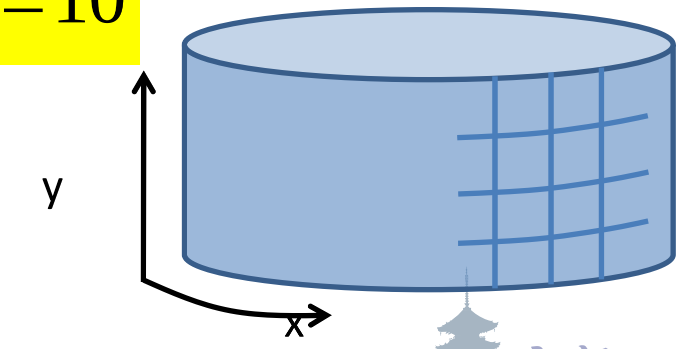
$$\hat{H}_{ij} = \begin{bmatrix} \mathcal{H}_{ij} & 0 \\ 0 & \mathcal{H}_{ij}^* \end{bmatrix},$$

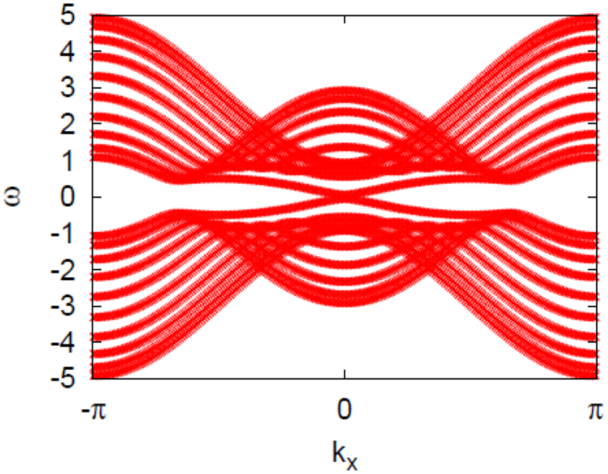
🡐 Spin-diagonal

$$\mathcal{H}_{ij} = \begin{bmatrix} M_0\delta_{ij} - t(\delta_{i,j\pm\hat{x}} + \delta_{i,j\pm\hat{y}}) & t'[i(\delta_{i,j+\hat{x}} - \delta_{i,j-\hat{x}}) + \delta_{i,j+\hat{y}} - \delta_{i,j-\hat{y}}] \\ t'[i(\delta_{i,j-\hat{x}} - \delta_{i,j+\hat{x}}) + \delta_{i,j-\hat{y}} - \delta_{i,j+\hat{y}}] & -M_0\delta_{ij} + t(\delta_{i,j\pm\hat{x}} + \delta_{i,j\pm\hat{y}}) \end{bmatrix}$$

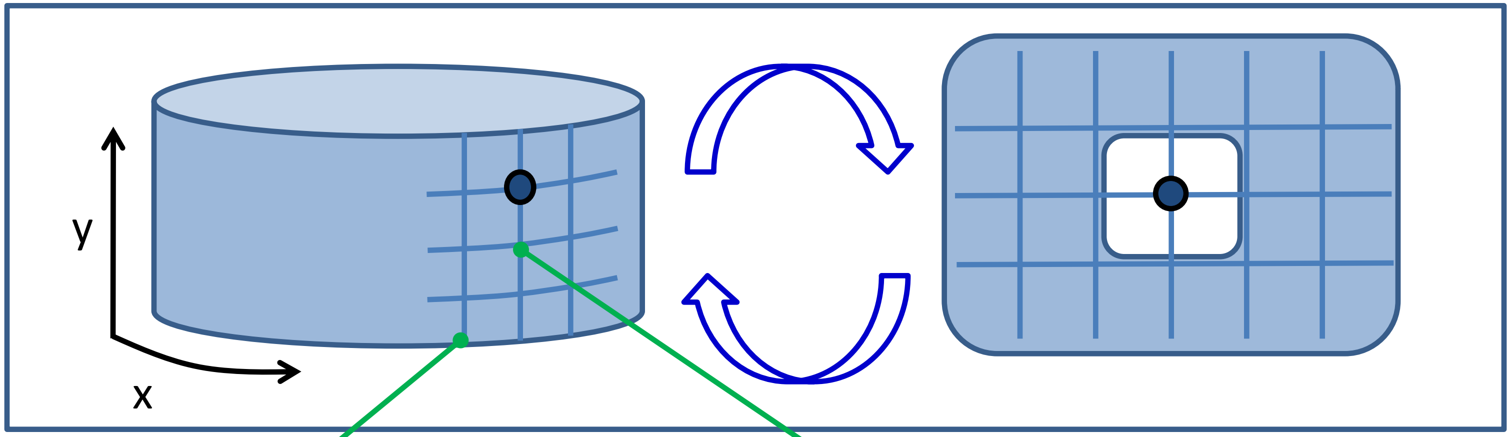
$t' = 0.25, \quad M_0 = -1.0$

$L_y = 10$

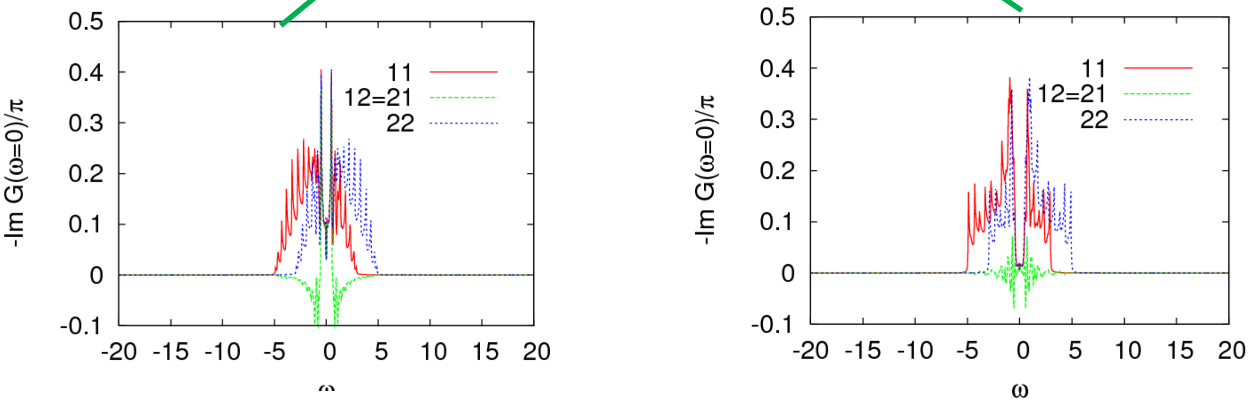




# Inhomogeneous DMFT



*Site dependent LDOS*



Successful application to
heterostructures,
optical lattices

***Advantage:***

Applicable for geometries with edges

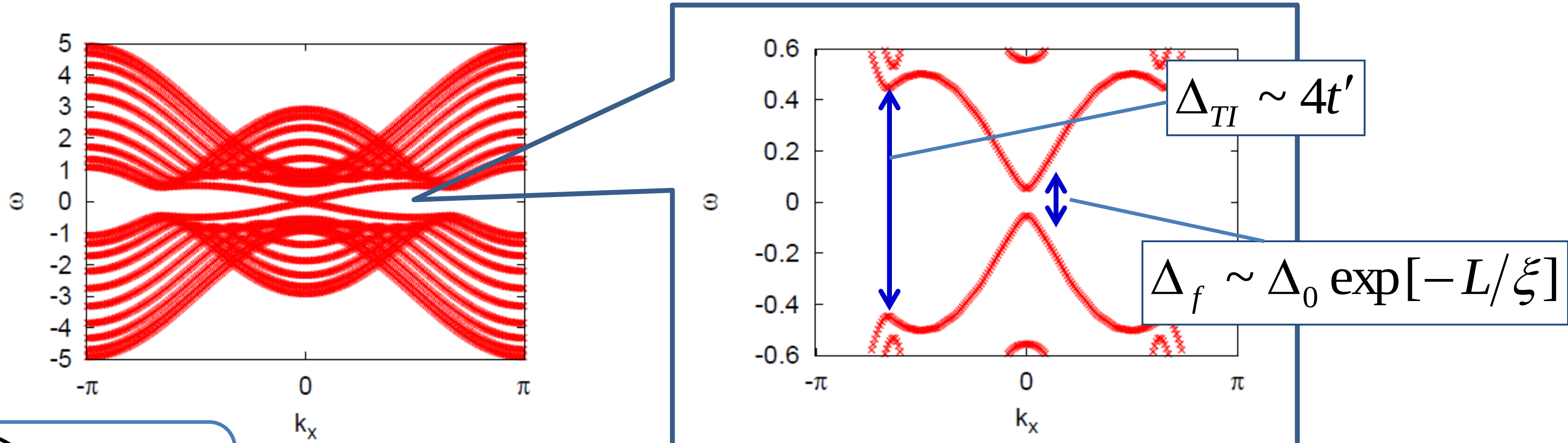
Extension to higher dimension is easy

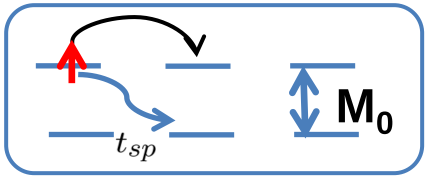
***Disadvantage:***

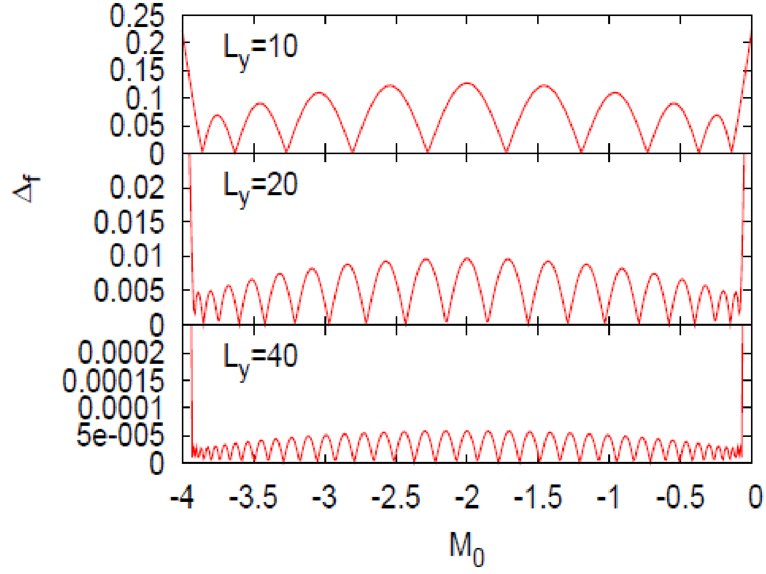
Spatial correlation is not incorporated

➔ cluster extensions will improve

# Finite size effects







◆Oscillations due to lattices

◆$L_y = 10, \quad \Delta_f \sim 0.1\Delta_{TI}$

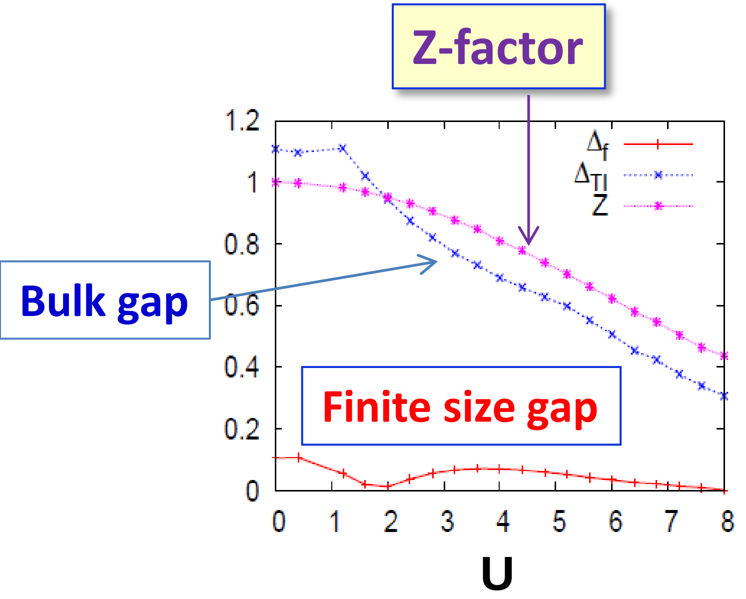
**Edge states = massive**

➔renormalized massive Dirac

➔Bulk = *gapped Fermi liquid*

# Finite size effects with interaction

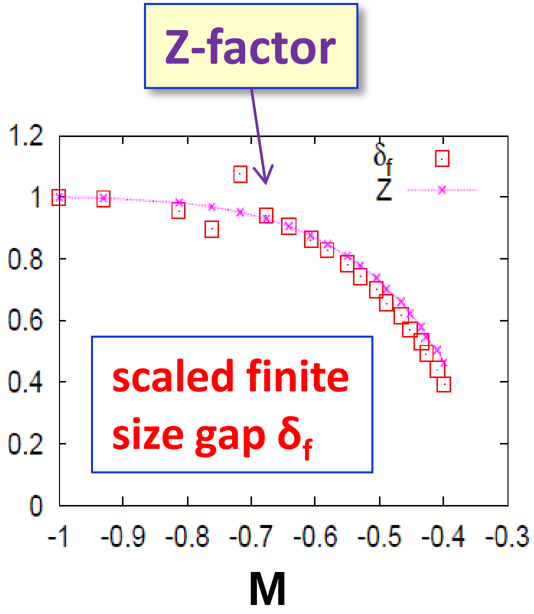
**DMFT + IPT**



**Z-factor**

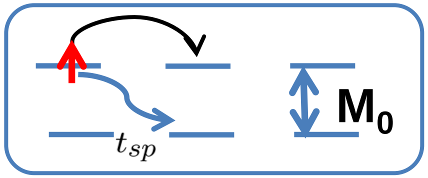
**Bulk gap**

**Finite size gap**



**Z-factor**

**scaled finite size gap $\delta_f$**



$$\mathcal{Z} = (1/L_y)\sum_y z(y)$$ *Renormalization factor*

$$\boxed{\begin{aligned} \mathcal{M}(U) &= \mathcal{M}_0 + \frac{1}{2L_y}\sum_y [\mathrm{Re}\Sigma_{11}(\omega=0,y) - \mathrm{Re}\Sigma_{22}(\omega=0,y)], \\ \delta_{\mathrm{f}}(\mathcal{M}) &= \Delta_{\mathrm{f}}(\mathcal{M}(U))/\Delta_{\mathrm{f}}(M_0;U=0)|_{M_0=\mathcal{M}}, \end{aligned}}$$

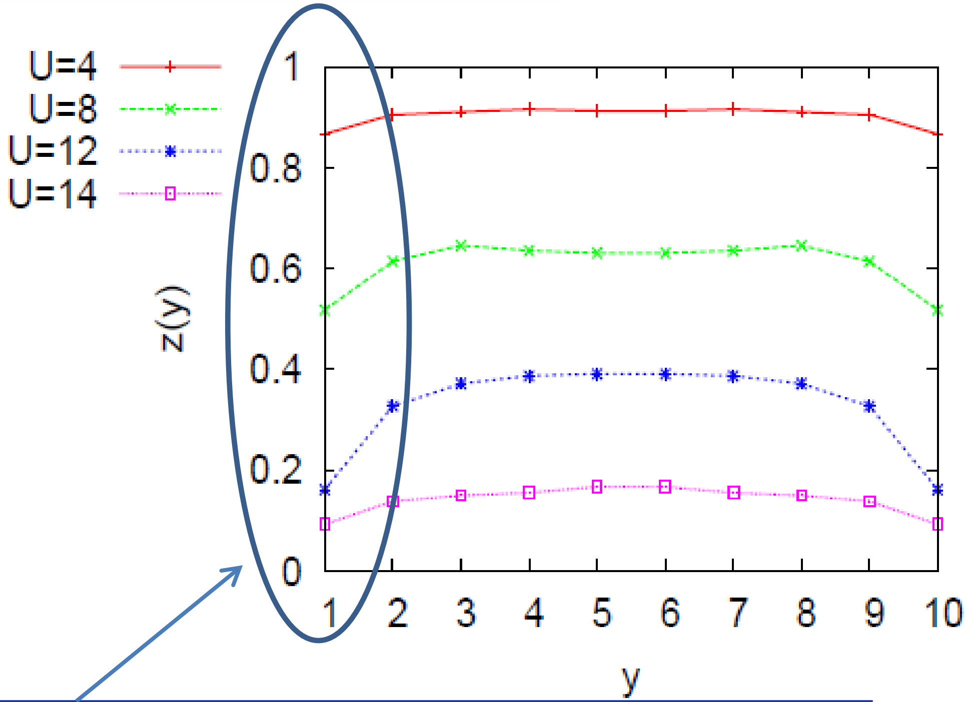
*Finite size gap is simply renormalized*

*➔ Consistent with gapped Fermi liquid picture*

# Site-dependence

**Renormalization factor**

$$z(y) = [1 - \partial\Sigma(y)/\partial\omega]^{-1}_{\omega=0}$$

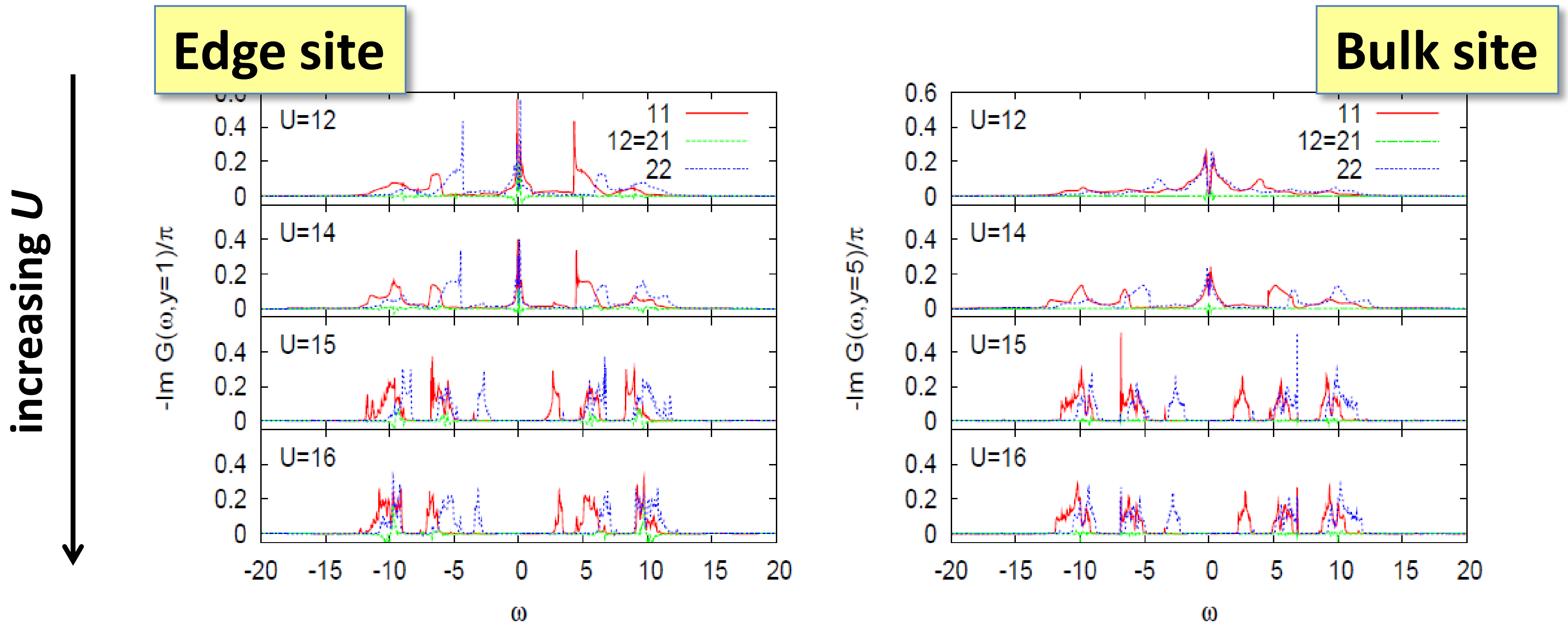


*Strong renormalization at the edges due to reduction of coordinate number*

✔**Strong site dependence:**

$z$ (edge) << $z$ (bulk)

# Local density of states

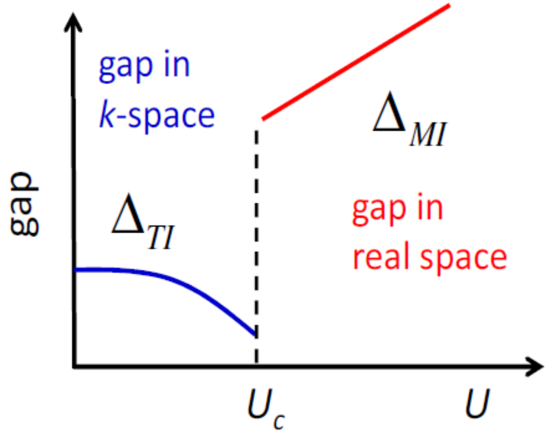


✔ $U<U_c$: renormalized gap around ω~0

✔ $U>U_c$: Mott insulating gap $\Delta_{MI}$~ $U$ for all the sites

Generally, discontinuous transitions

➔ Gap closing is not required



# Summary of Part I

Competition between TBI and MI
BHZ model + U

**Mott transition**

**Topological insulator**

↕ 1st order

**(Topologically trivial) Mott phase**

no gap-closing

**Strong renormalization: near Mott transition**

**Finite size effects at T=0**

- ✔renormalization of finite size gap
- ✔simple Mott transition

# Spin-selective Topological insulator

## *hidden **in a metallic phase***

<u>T.Yoshida,</u> R. Peters, S. Fujimoto, NK

# Correlation effects on Topological phases

Coulomb interaction + Topological nature

⇨ Exotic phenomena

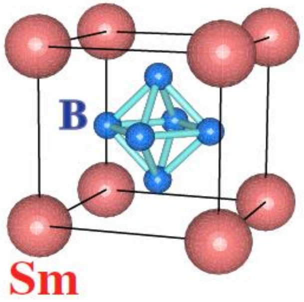
- **Topological Kondo Insulator** at half filling

  M. Dzero *et al.* PRL (2010), PRB (2012).

  M.T. Tran *et al.* PRB (2012), T. Takimoto, JSPS (2011)

- **SmB6** midgap state -> edges state

  S. Wolgast *et al*, cond-mat 1211.5104 (2012) resistivity
  J. Botimer *et al*, cond-mat 1211.6769 (2012) Hall effect
  X. Zhang *et al*, cond-mat-1211.5532 (2012) tunneling

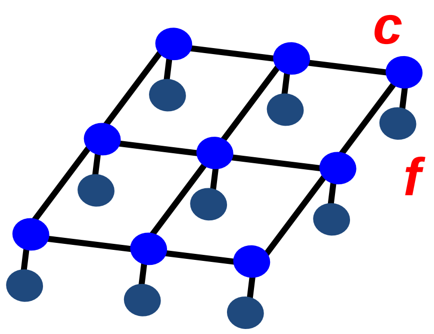


**Topological Kondo Insulator** in a metallic phase !?

# Heavy fermion systems

Ce, Yb, Sm…

**Correlated *f*-electrons**
**+ *c*-electrons**



⇒ **Intriguing phenomena**

**At half-filling**

**Kondo insulator**
**Antiferromagnetic insulator**

*SO coupling* →

SmB$_6$ ?

**Topological**
**Kondo insulator**

**Away from half-filling**

**Paramagnetic metal**
**Ferromagnetic metal**
**Unconventional superconductor**

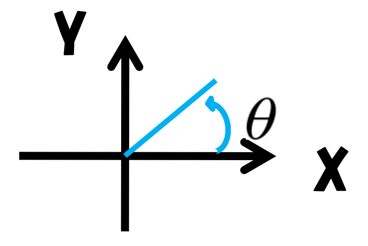
*SO coupling* →

**Spin-selective**
**Topological**
**Kondo insulator**

*New phase*

# Spin-selective topological Kondo insulator

～Topological ins. in a metallic phase～



$$H = H_{topological-PAM} + U n_{i,f,\uparrow} n_{i,f,\downarrow}$$

$$H_{topological-PAM} = \epsilon_f \sum_{i,\sigma} (n_{i,f,\sigma}) - \sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\alpha,\sigma} \hat{t}_{\sigma,\alpha,\alpha'} c_{i,\alpha',\sigma}$$

$$-\hat{t_\sigma} = \begin{pmatrix} -t_f & i t_{so} e^{i\theta\sigma} \\ i t_{so} e^{-i\theta\sigma} & t_c \end{pmatrix}$$

***c-f mixing (SO coupling)***

**Ferromagnetic metallic phase: spin-selective Kondo insulator**

**(half-metallic, half-insulating)**

***Topologically nontrivial phase***

*DMFT calculation*

# Phase Diagram: Topological PAM

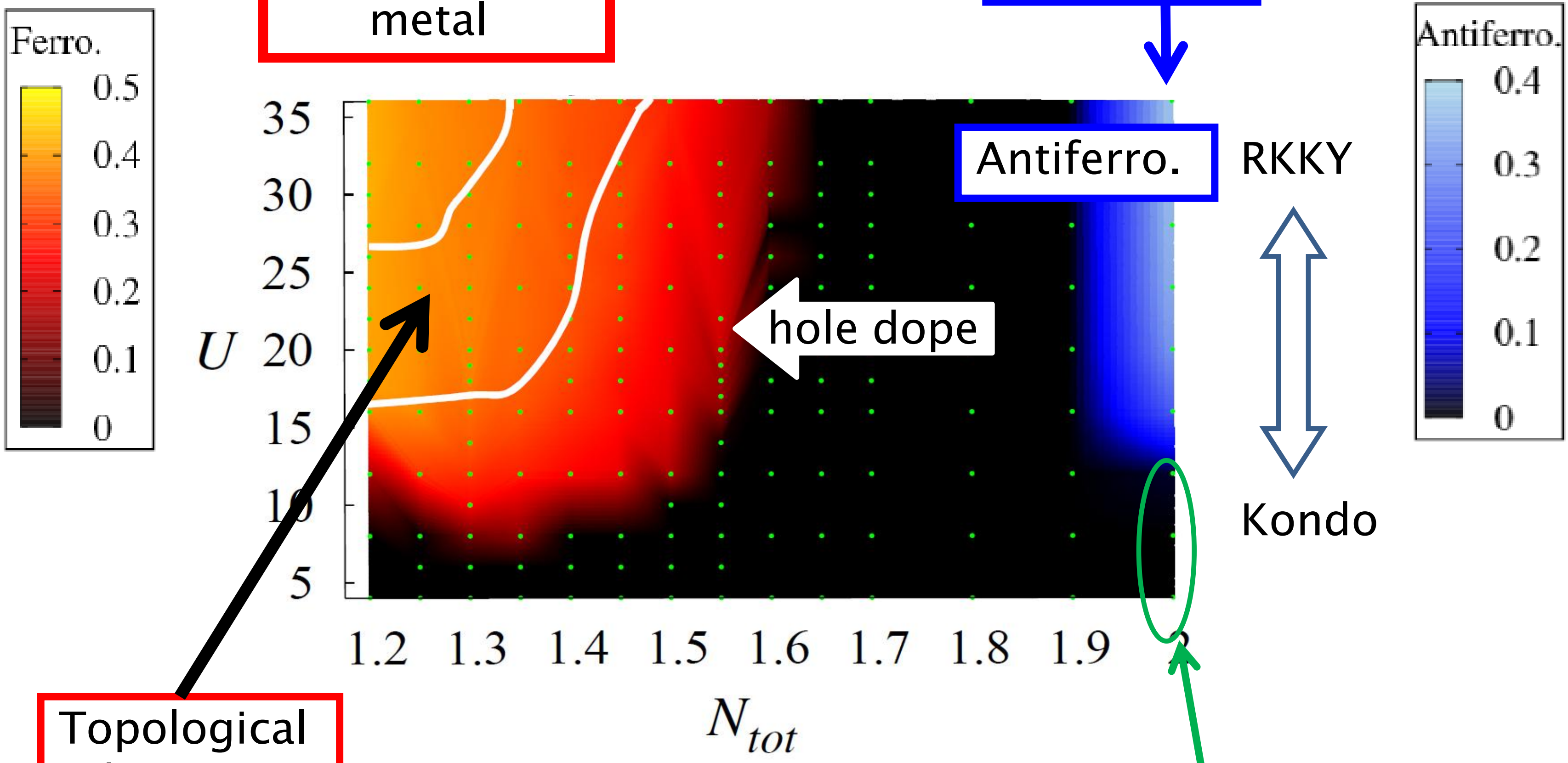
$t_{cc} = 1$

$\epsilon_c - \epsilon_f = 8$

[conduction band width] = 8

Ferromagnetic metal

Half-filling



Antiferro.

RKKY

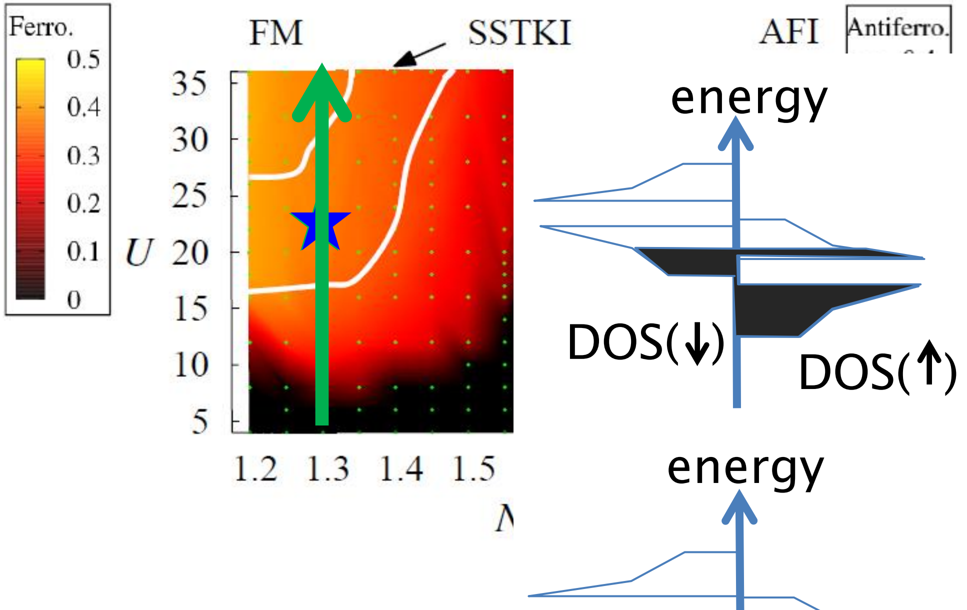
hole dope

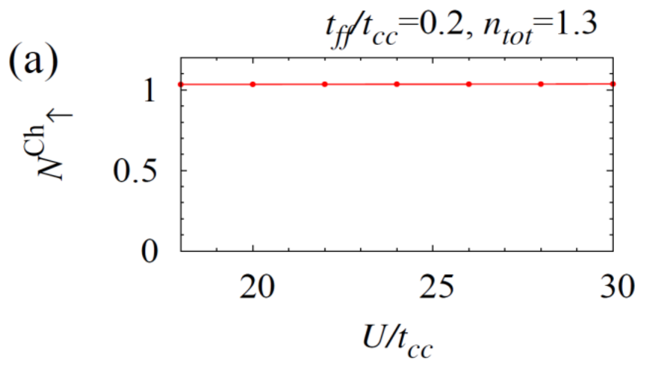
Kondo

Topological Chern # = 1

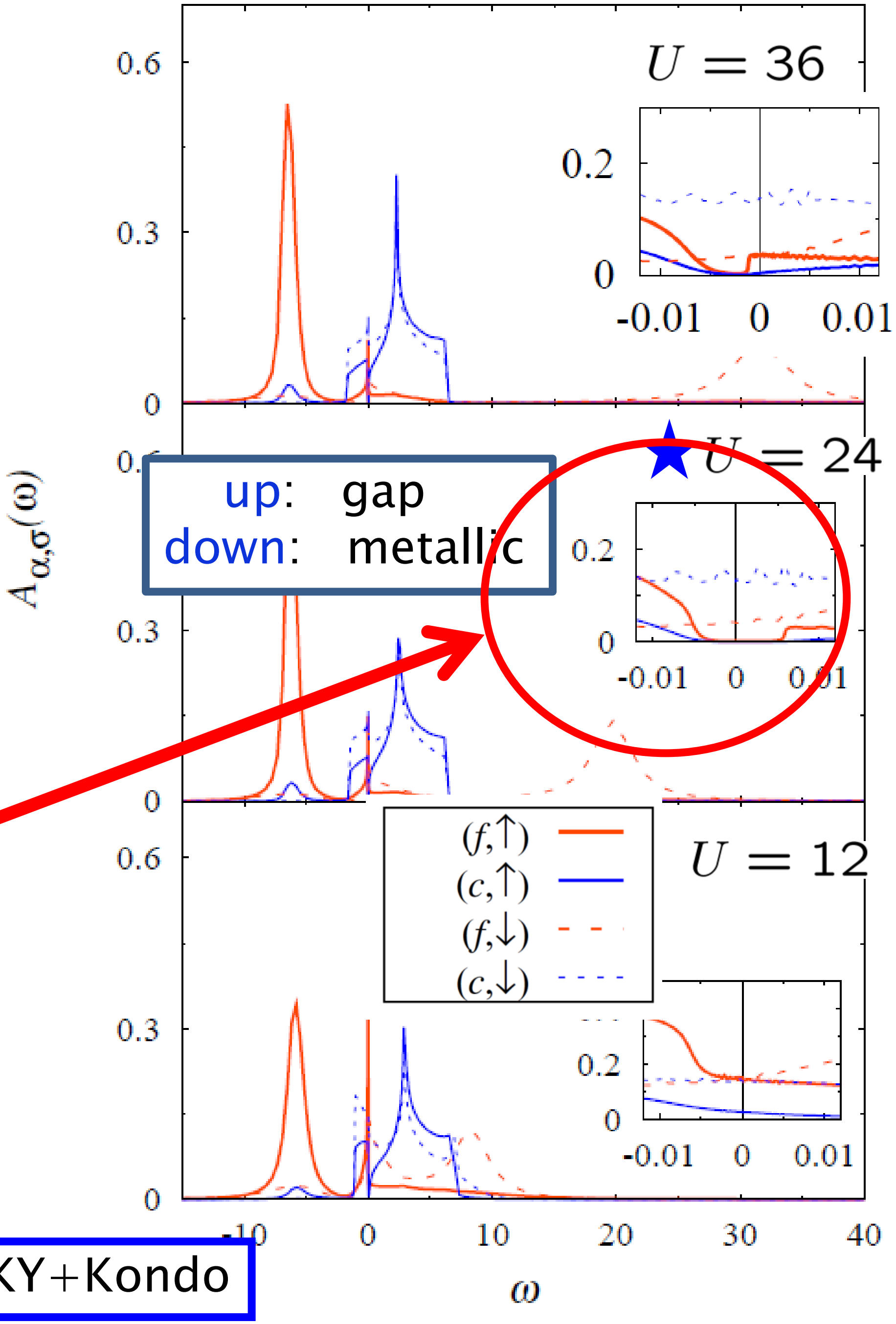
Spin-selective
Topological Kondo insulator

Topological Kondo insulator
(spin Chern # = 1)
(M. Dzero *et al.*) possibly $\mathrm{SmB}_6$





$$N^{ch}_{\uparrow} = \frac{\epsilon^{\mu\nu\rho}}{24\pi^2}\int d^3p\, \mathrm{tr}[\hat{G}_\sigma(p)^{-1}\frac{\partial \hat{G}_\sigma(p)}{\partial p_\mu}\hat{G}_\sigma(p)^{-1}\frac{\partial \hat{G}_\sigma(p)}{\partial p_\nu}\hat{G}_\sigma(p)^{-1}\frac{\partial \hat{G}_\sigma(p)}{\partial p_\rho}].$$

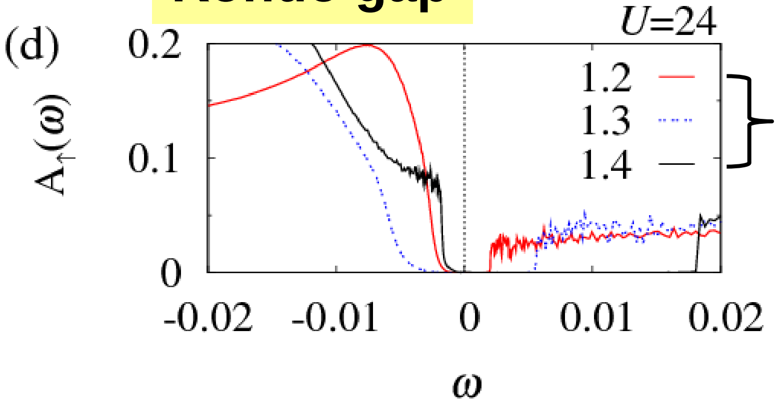


up: gap
down: metallic

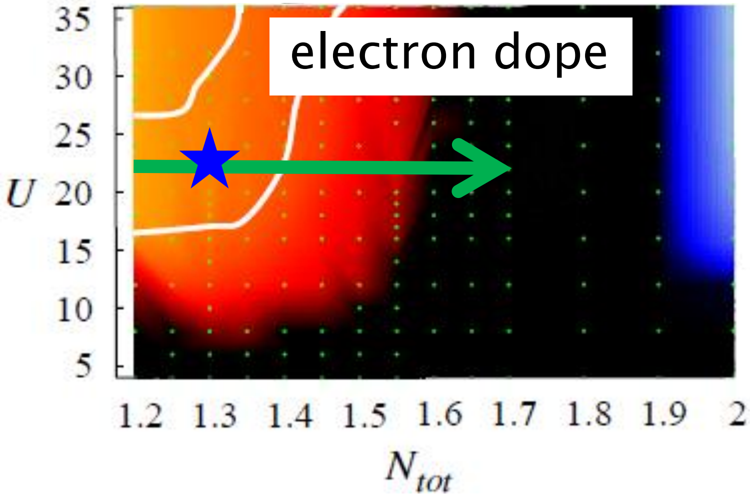
RKKY+Kondo

topological insulator
hidden in metallic phase!

**Kondo gap**

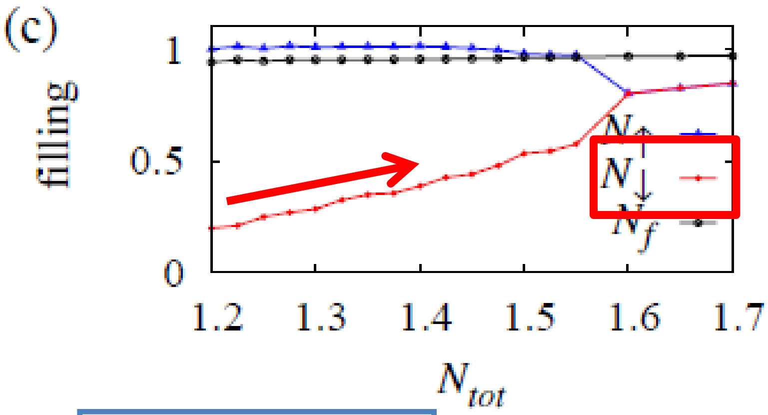


filling



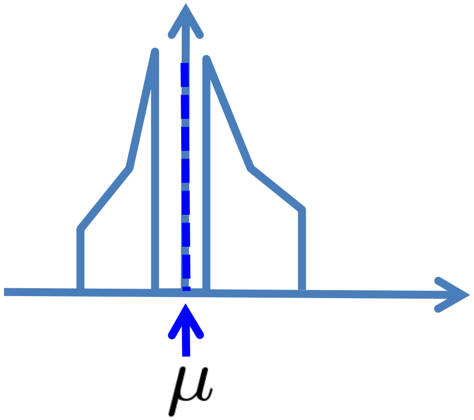
electron dope

**Electron filling**



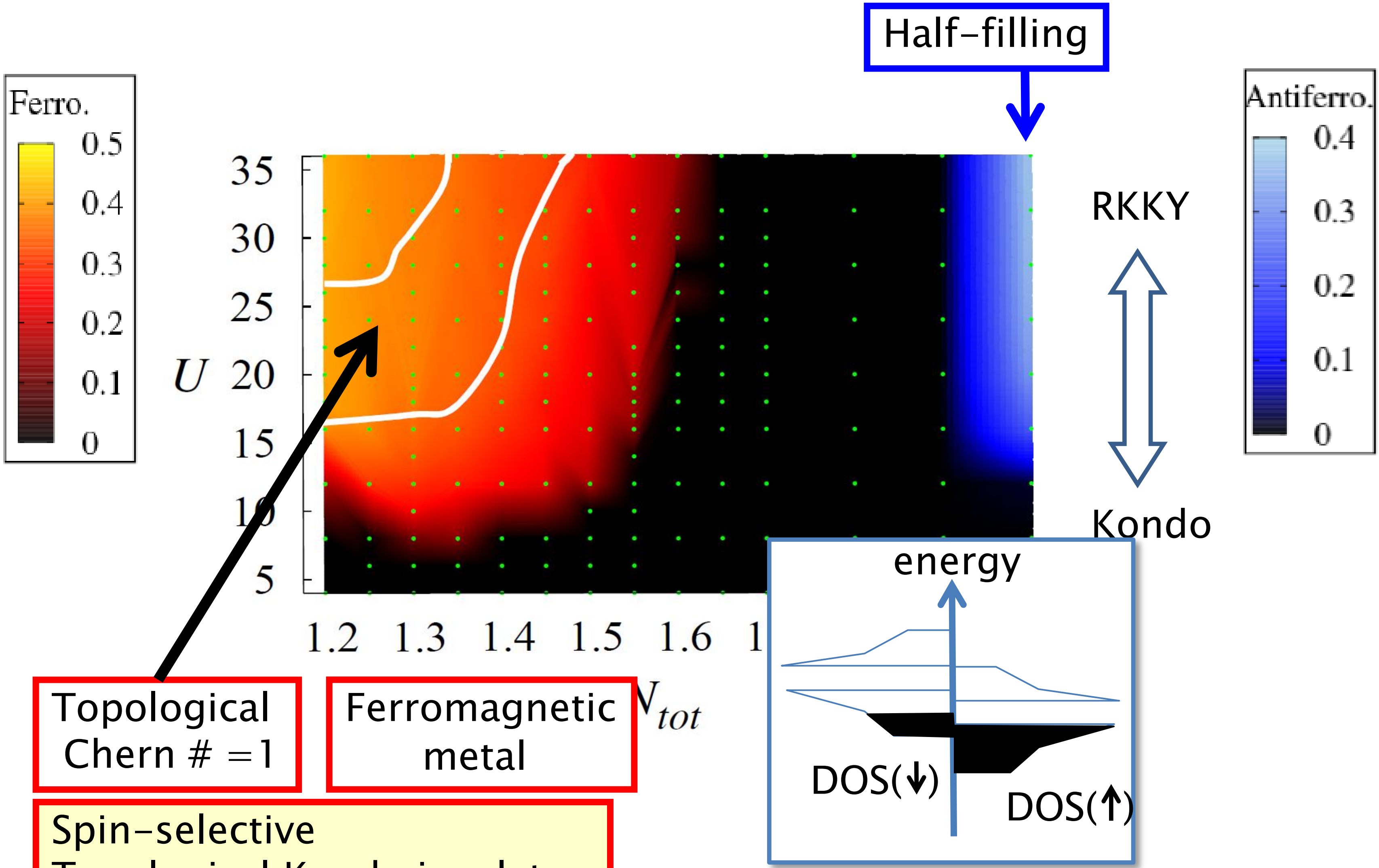
Only $N_\downarrow$
is changed

DOS (up-spin)



RKKY and Kondo effect
reconstruct the gap and
restore topological properties!

# Phase Diagram: Topological PAM



Half-filling

RKKY

Kondo

energy

DOS(↓)

DOS(↑)

Topological
Chern # =1

Ferromagnetic
metal

Spin-selective
Topological Kondo insulator

# Edge states

Chiral edge mode (up spin)
+ 2D ferromag. fluctuations

$$S = S_{edge} + S_c + S_{mag}$$

$$S_{edge} = \sum_k \phi(k) \frac{4\pi}{-k(i\omega_n - vk)} \phi(-k)$$

Tomonaga boson $\phi(k) \quad (= \quad \phi(i\omega, k_x))$

$$S_{mag} = \sum_k \psi(k)\chi'(k)\psi(-k)$$

$$\chi'(k) = \frac{1}{\xi^{-2} + (k_x^2 + k_y^2) + |\omega_n|/(\Gamma\sqrt{k_x^2 + k_y^2})}$$

Bulk spin- fluctuations $\psi(k) = \psi(i\omega_n, k_x, k_y)$

$$S_c = -g \sum_k ik_x \phi(k)\psi(-k)$$

# Non-Tomonaga-Luttinger (dissipative behavior)

$$G^R(k_x,\omega) = \frac{2\pi k_x^2}{k_x(\omega + i\delta - v k_x) + \pi g^2 k_x^2 \sum_{k_y} \chi'(k)^R}$$

$$(\chi'^R(k))^{-1} = \xi^{-2} + (k_x^2 + k_y^2) - i\omega/(\Gamma\sqrt{k_x^2 + k_y^2})$$

# NMR relaxation rate

$$\begin{aligned} \frac{1}{T_1 T} &= CA^2 \lim_{\omega\to 0} \sum_{k_x} \frac{1}{\omega} \mathrm{Im}\chi^{zz}(k_x, \omega + i\delta) \\ &\sim \frac{CA^2 2\pi^2 g^2}{\xi^{-4} v'^2}, \end{aligned}$$

$$1/(T_1 T) \sim T^{-4/3} e^{8bT}$$

*cf* 2D systems

$$1/(T_1 T) \sim \xi^3$$

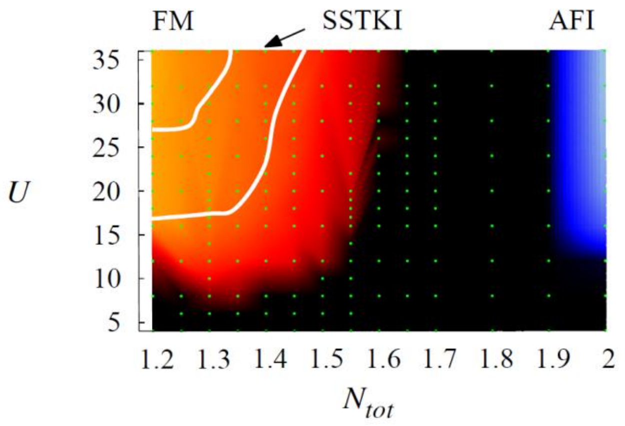
Spin fluctuations become stronger

⇒ Edge contribution becomes dominant

# Summary of Part II

**Correlated Topological insulator**

**Topological Kondo insulator**



**Even in a metallic phase**

**bulk gap is induced by interaction.**

**⇒ Kondo insulator in Ferromagnetic metal**

**Spin-selective Topological Kondo insulator**

*half-metallic, half insulating*

**Collaboration: Topology & Correlation**

# Summary

## Correlation Effects on Topological Insulators

### 1. Correlated TI: Mott transition

Electron correlation
Strong renormalization effects
Edge states

### 2. Topological Kondo Insulator in a Metal

Collaboration, topology, ferromag, Kondo effect

Nontrivial phase in a metal