Correlation effects on topological insulators

-a dynamical mean field approach -

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T.Y., Satoshi Fujimoto, and Norio Kawakami Phys. Rev. B 85, 125113 (2012)

Outline

1. Introduction

- Topological phase in *d*- ,*f*- electron systems
- Several studies of correlated TBI

Mott vs. TBI

2. Purpose

3. Model and Method

4. Numerical Results

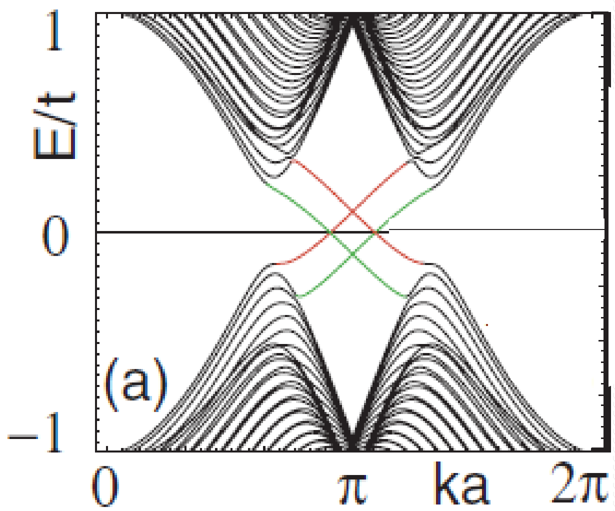
(DMFT study of BHZ+U model)

5. Summary

Related studies: (If time allows.)

1. Introduction

~Properties of topological insulators~



C. L. Kane *et al.* PRL **95** 146802

Topological insulators

Gapless edge states
(*robust against*
non-magnetic perturbations)

↕

Non-trivial band structure (Bulk)

Characteristic magnetoelectric response

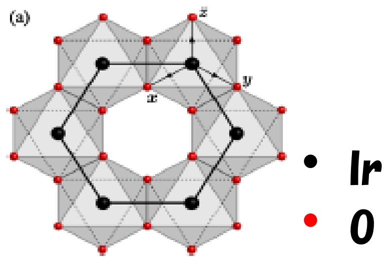
Quantized spin Hall conductivity. (QSH ins.)

Topological magnetoelectric effect. (3D strong-TBI)

$$\mathbf{P} = \frac{e^2}{2hc}\mathbf{B} \quad \mathbf{M} = -\frac{e^2}{2hc}\mathbf{E}$$

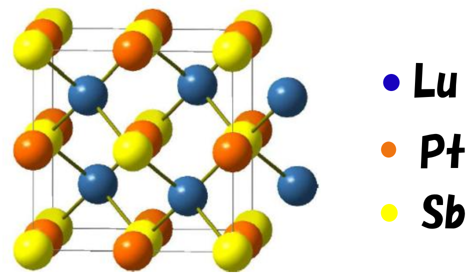
~Topological phase in d,f electron systems ~

Na_2IrO_3 (Iridium oxide)



A.Shitade *et al.* PRL. 102. 256403. (2009)

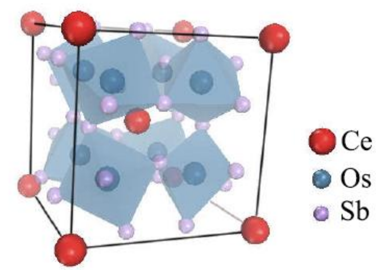
LuPtSb etc. (Heusler compounds)



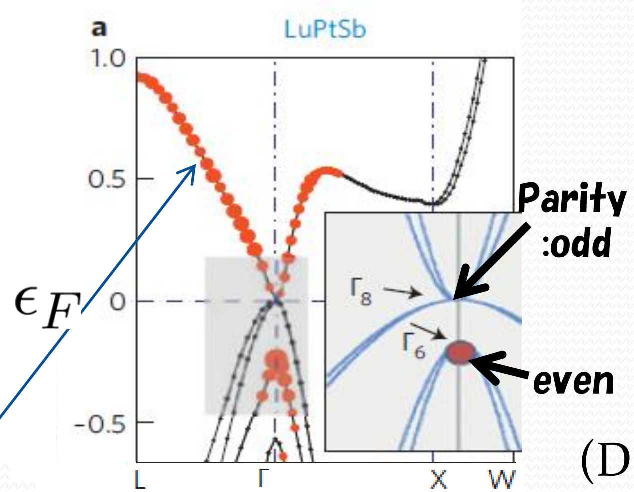
S. Chadov et al. Nature Materials 9, 541 (2010)

H. Lin et al. Nat. Mat. 9 546 (2010)

$CeOs_4Sb_{12}$ filled skutterudite



B. Yan *et al.* arXiv:1104.0641



(DFT)

● : probability of s-orbital occupation of Sb sites.

- Band inversion is observed *only* at the Γ point.
- Lattice distortion opens the bulk gap.

⇒ Heusler compounds (e.g. LuPtSb) can be topological insulator.

Correlated topological insulators

correlation + topological structure

Exotic phases !

- Intrinsic topological phase (FQHE etc.)
- Symmetry protected topological phase (Haldane phase in S=1 Heisenberg chain)

Symmetry protected phases

●Topological phases induced by Coulomb interaction

●Phase competition :
[Topological phase] vs. [ordered phases]

[magnetic phase,
charge density wave phase

etc…

●Topological phases induced by interactions

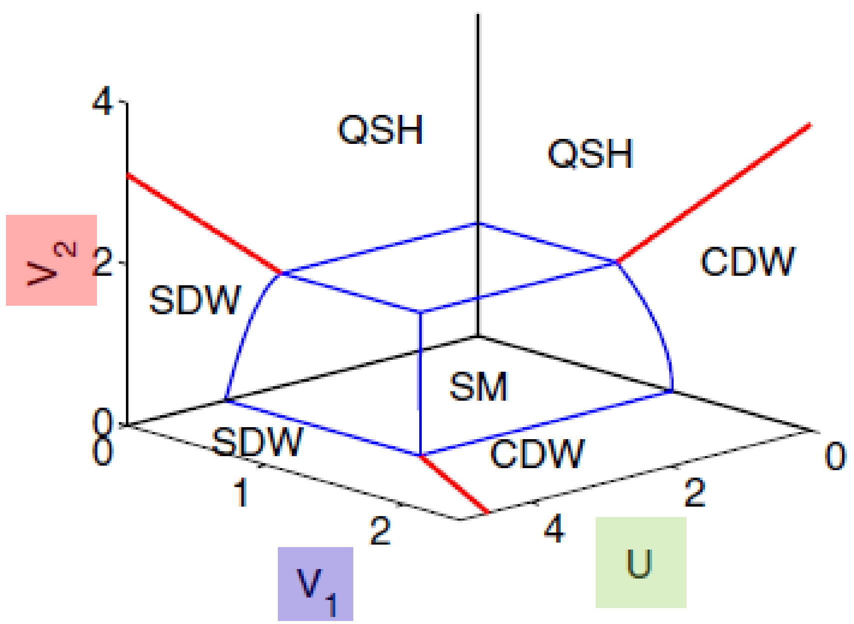
S. Raghu *et al.* PRL 100, 156401

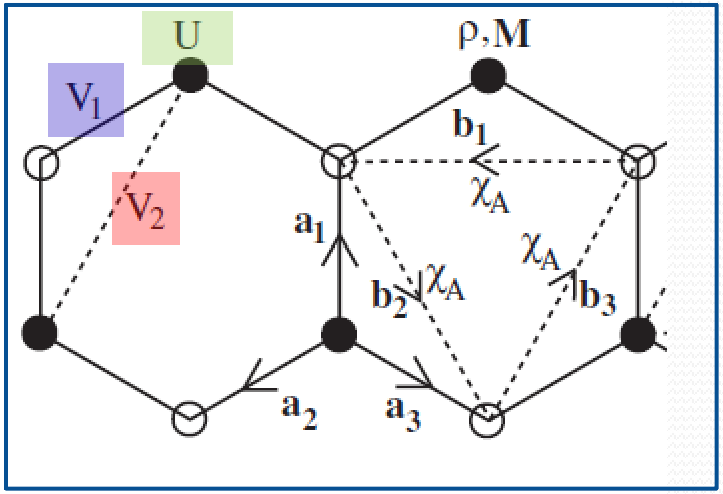
Coulomb interactions ⇒ Spin-orbit interaction

$$H = -\sum_{\langle ij\rangle\sigma} t(c_{i\sigma}^{\dagger}c_{j\sigma} + \mathrm{H.c.}) + U\sum_i n_{i\uparrow}n_{i\downarrow} + V_1\sum_{\langle i,j\rangle}(n_i-1)(n_j-1) + V_2\sum_{\langle\langle i,j\rangle\rangle}(n_i-1)(n_j-1)$$

$$\chi_{ij} = \chi_{ji}^{*} = \langle c_i^{\dagger}c_j\rangle$$

$$\chi_{i,i+\mathbf{b}_s} = \begin{cases}\chi_A = |\chi|e^{i\phi_A}, & i\in A\\ \chi_B = |\chi|e^{i\phi_B}, & i\in B\end{cases}$$



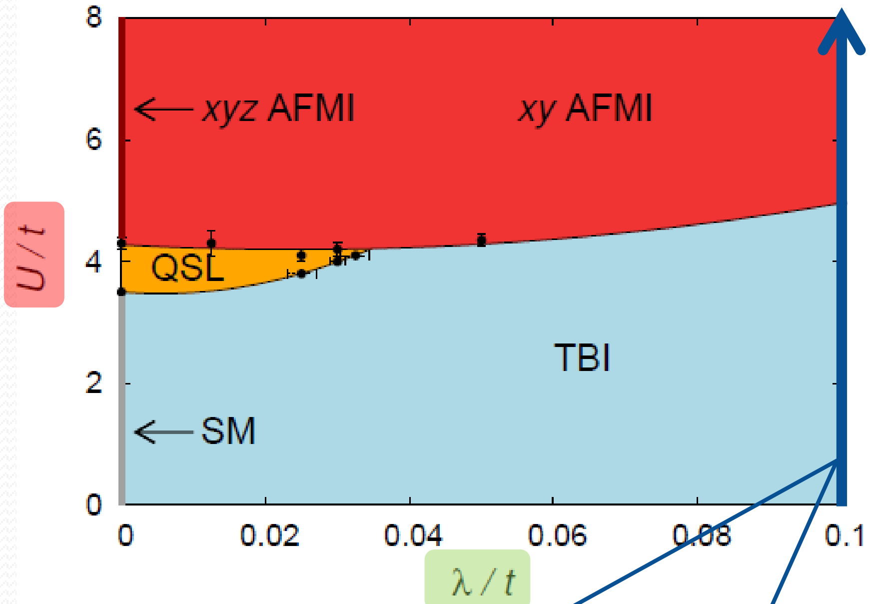


Such phases are also reported in pyrochlore and diamond lattice.

●Phase competition : Topological phase v.s. magnetic phase （Kane-Mele+U）

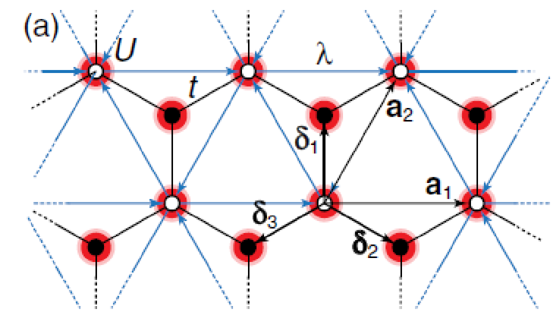
M. Hohenadler *et al.* PRL 106 100403

(Auxiliary field QMC)

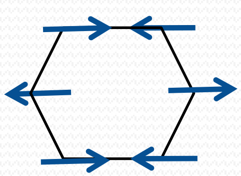


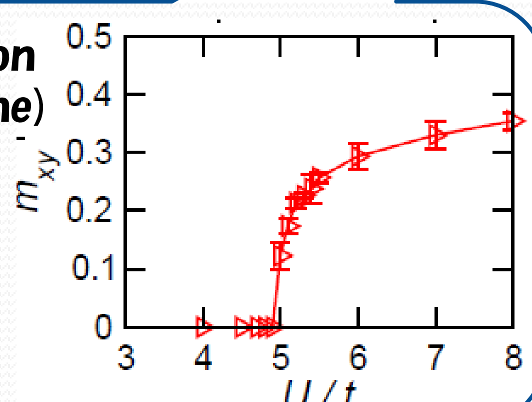
$$H_{\mathrm{KM}} = -t\sum_{\langle \mathbf{i},\mathbf{j}\rangle} c_{\mathbf{i}}^\dagger c_{\mathbf{j}} + i\lambda \sum_{\langle\langle \mathbf{i},\mathbf{j}\rangle\rangle} c_{\mathbf{i}}^\dagger \mathbf{e}_{\mathbf{i},\mathbf{j}}\cdot\boldsymbol{\sigma} c_{\mathbf{j}},$$

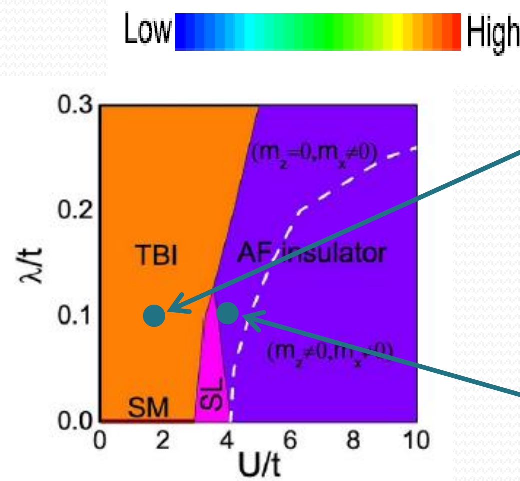
$$H_U = \frac{U}{2}\sum_{\mathbf{i}} (c_{\mathbf{i}}^\dagger c_{\mathbf{i}} - 1)^2.$$



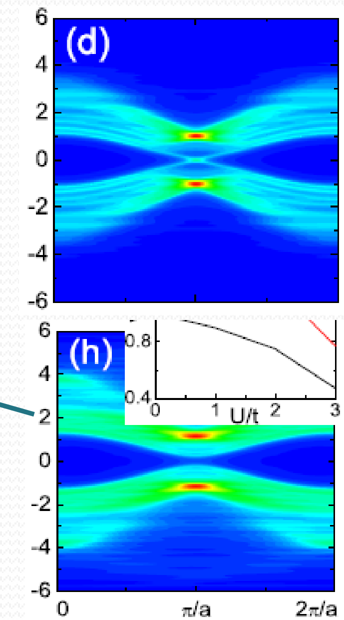
Spin configuration (in-plane)







(with VCA)



S. Yu *et al.* PRL 107, 010401

Outline

1. Introduction
2. **Purpose**
3. Model and Method
   - DMFT+CT-QMC
   - Relation between spin Hall conductivity and spin Chern number
4. Numerical Results
   - spin Hall conductivity,
   - spectral function,
   - magnetic instability
5. Summary and Outlook

2. Purpose

Correlated topological insulators

are extensively studied!

Weakly correlated

Strongly correlated

Topological ins.

Mott ins.

Understand the phase competition with non-perturbative method.

- Bernevig-Hughes-Zhang model+U
- Dynamical Mean field theory

+

Continuous Time-Quantum Monte Carlo simulation

1. Introduction

2. Purpose

3. Model and Method

- Model ～ BHZ+U model ～
- Method ～DMFT+CT-QMC ～
- How to detect the topological property

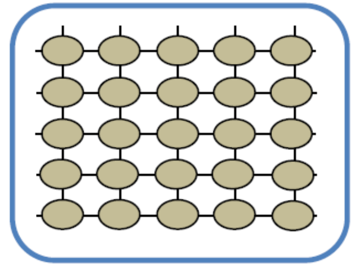
～Relation between spin Hall conductivity
and spin Chern number ～

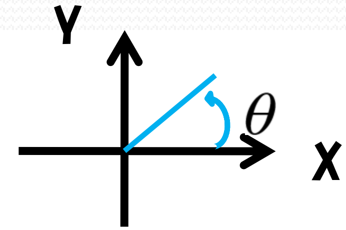
4. Numerical Results

5. Summary and Outlook

3. Model and Method

●Model (BHZ model + U)

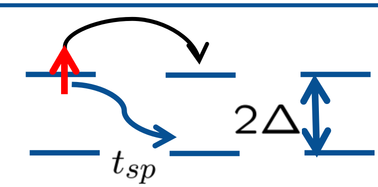




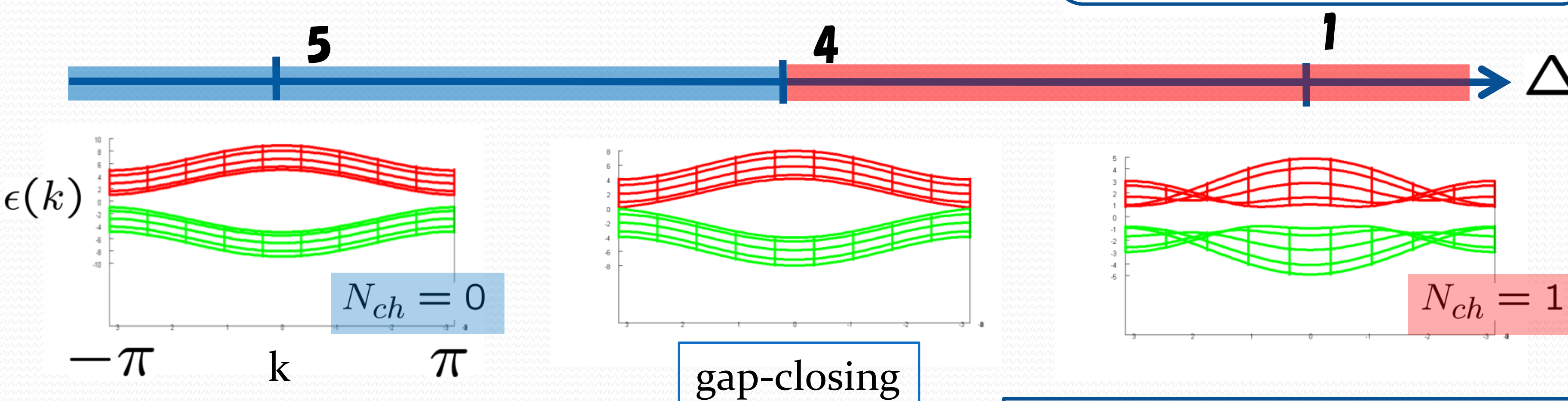
$$H = H_{BHZ} + U \sum_{i,\alpha} n_{i,\alpha,\uparrow} n_{i,\alpha,\downarrow}$$

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

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



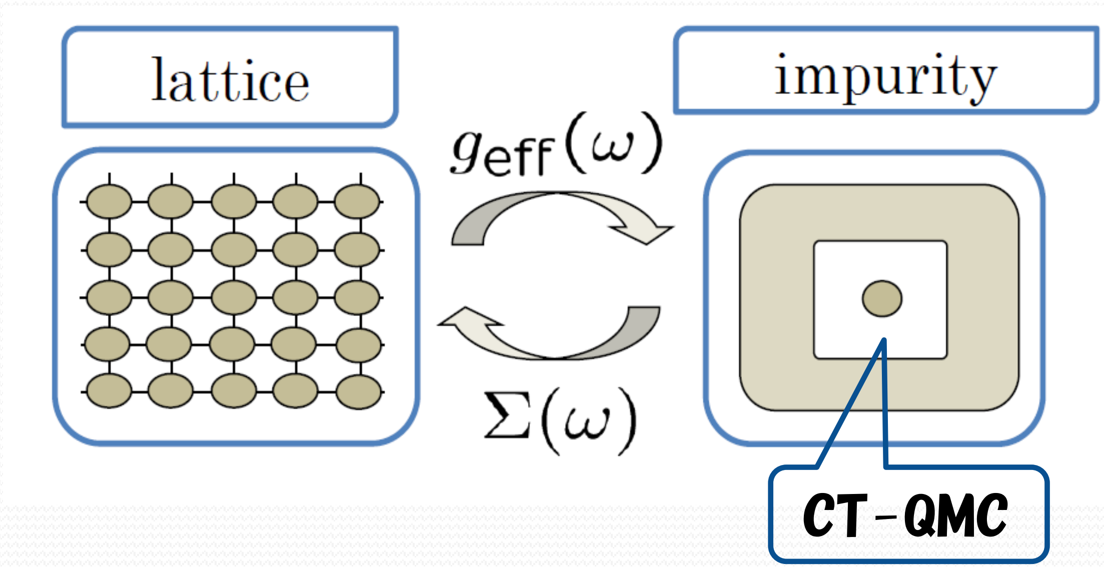
Non-interacting case



BHZ+U ⟵ DMFT+CT-QMC

Method : Dynamical Mean Field Theory (DMFT+CT-QMC)

schematic picture



Advantage

DMFT has had a great success describing Mott transitions

CT-QMC provides numerically exact solutions.

● ～ How to detect topological property ～

Even in $U \neq 0$: $\sigma_{xy}^{SH} = -\frac{e^2}{(2\pi)\hbar}N$

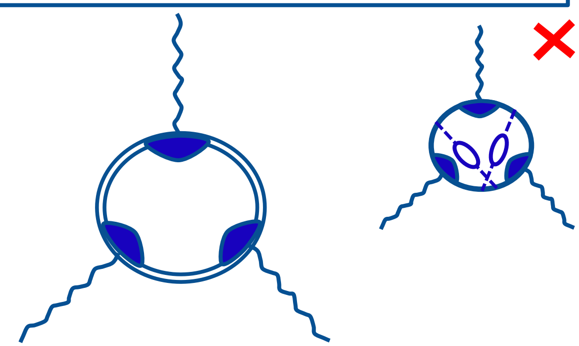
K. Ishikawa *et al.* Nucl. Phys. B **280 523**.

Kubo formula

$$\sigma_{xy}^{SH} = \frac{e^2}{\hbar}\mathrm{Im}\frac{\partial}{\partial\omega}K^R(\omega+i\delta)$$

$$K(i\omega) = -\frac{1}{V\beta}\sum_{\mathbf{k},i\nu,\sigma}\frac{\mathrm{sign}(\sigma)}{2}\mathrm{tr}[\frac{\partial\hat{\Lambda}_\sigma}{\partial k_y}(k)\ \hat{G}_\sigma(\mathbf{k},i\omega+i\nu)\frac{\partial\hat{h}_\sigma}{\partial k_x}(\mathbf{k})\hat{G}_\sigma(\mathbf{k},i\nu)$$

Genetic diagram contributing to σ_{xy}^{SH}



※ **Three external lines.** ($\frac{\partial}{\partial\omega}$ **is included.**)

※ σ_{xy}^{SH} **is anti-symmetric tensor**

Periodic boundary condition.

Spin Chern number

$$\sigma_{xy}^{SH} = -\frac{e^2}{(2\pi)\hbar}N,$$

$$N = \frac{\epsilon_{\mu\nu\rho}}{48\pi^2}\int d^3p\sum_\sigma \mathrm{sign}(\sigma)\mathrm{tr}[\frac{\partial\hat{G}_\sigma^{-1}(p)}{\partial p_\mu}\hat{G}_\sigma(p)\frac{\partial\hat{G}_\sigma^{-1}(p)}{\partial p_\nu}\hat{G}_\sigma(p)\frac{\partial\hat{G}_\sigma^{-1}(p)}{\partial p_\rho}\hat{G}_\sigma(p)],$$

Ward-identity [Vertex] $= \frac{\partial\hat{G}_\sigma^{-1}(p)}{\partial p_\mu}$

1. Introduction
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4. Numerical Results

Phase competition

- Topological ins.
- Mott ins.

(i). Spin Hall conductivity
(ii). Spectral function
(iii). Magnetic instability

(at finite temperature)

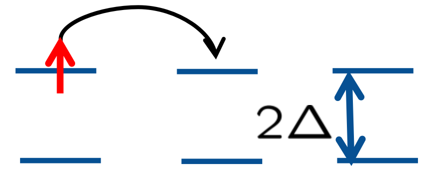
5. Summary and Outlook

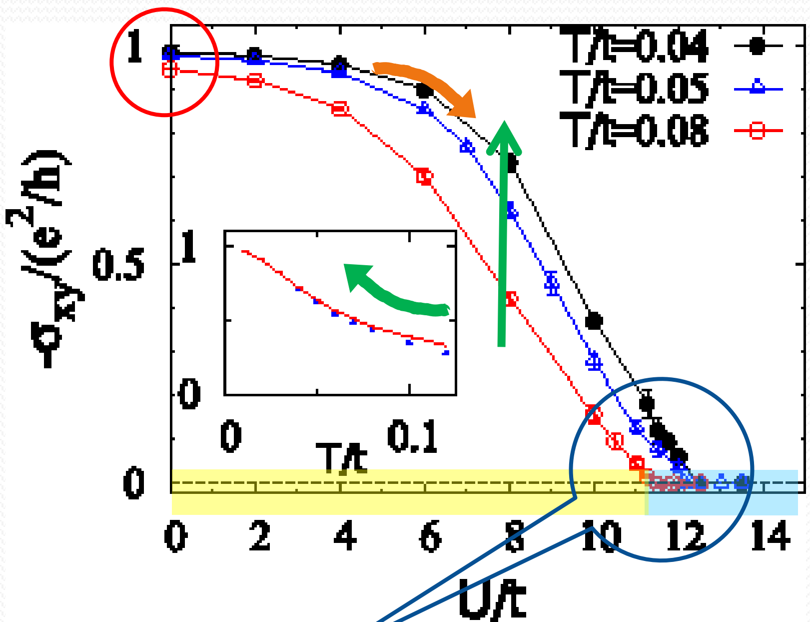
～(i) Spin Hall conductivity ～

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

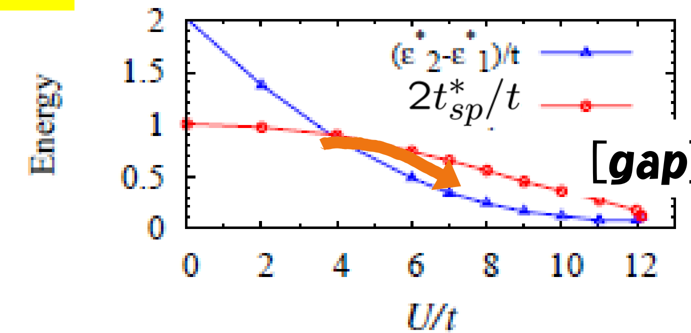
Orbital 2

Orbital 1





TBI



[gap]～$2t^*_{sp}/t$

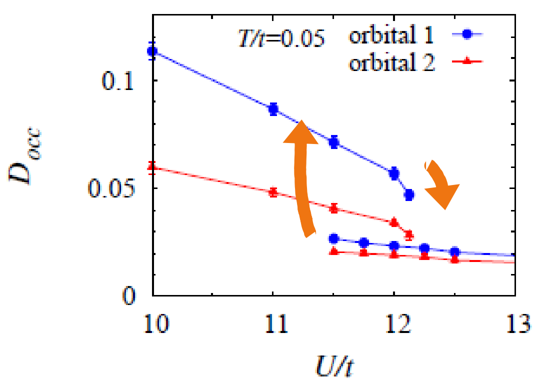
discrepancy of σ_{xy}^{SH} : Temp. effect

Gap renormalization

⇩

Increase of effective temperature

([Temp.]/[Gap size])

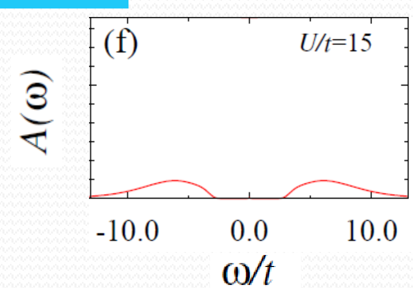


Discontinuous change

hysteresis

1st order transition

Mott



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

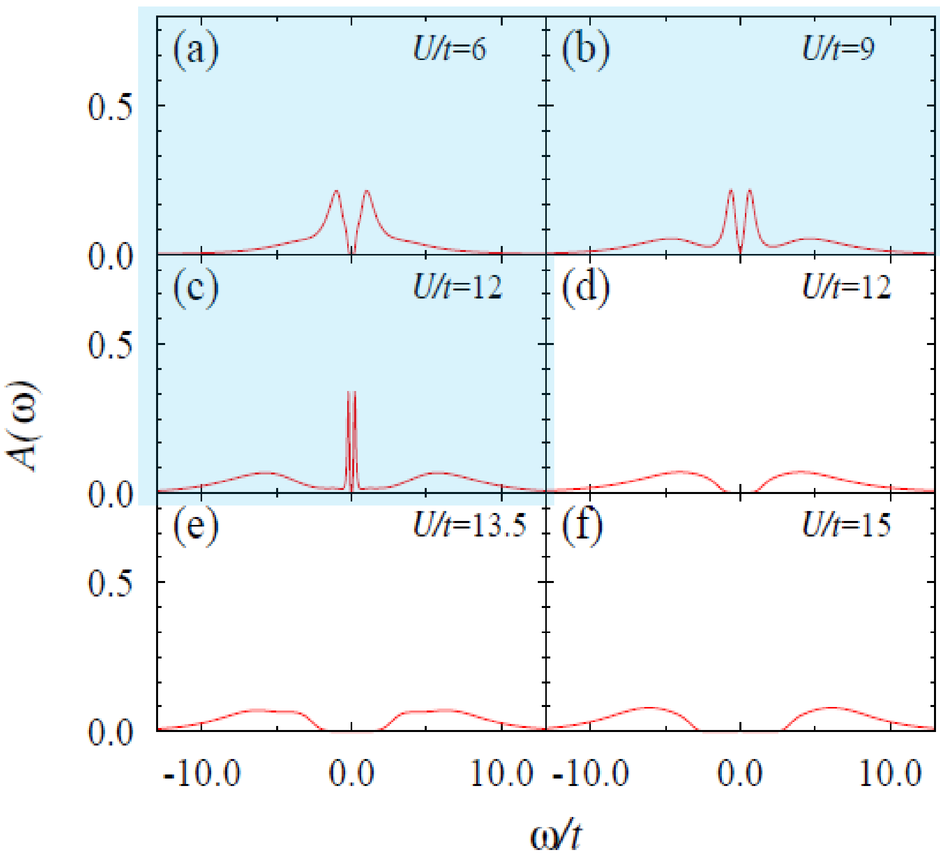
[gap size] $\sim U$

Trivial Mott ins.

～(ii) Spectral function ～

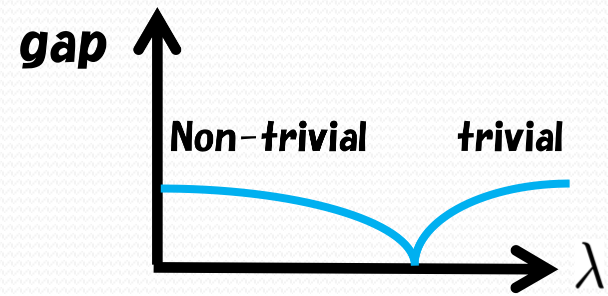
$T = 0.05t$
$t_{so} = 0.5t$

:TBI
:MI

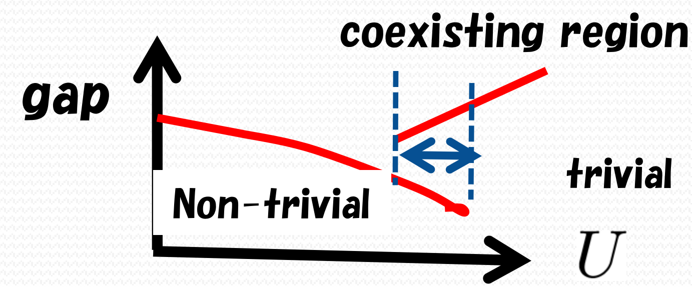


Behavior of the gap and Topological structure

non-interacting case



Mott transition



Change of Topological structure without gap closing

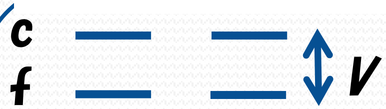
(Mott trans. is 1st order)

~The gap renormalization~

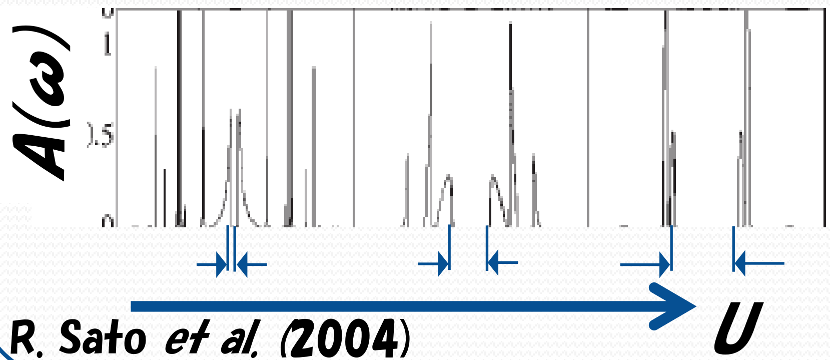
the renormalization depends on origin of the gap in U=0.

:TBI
:MI

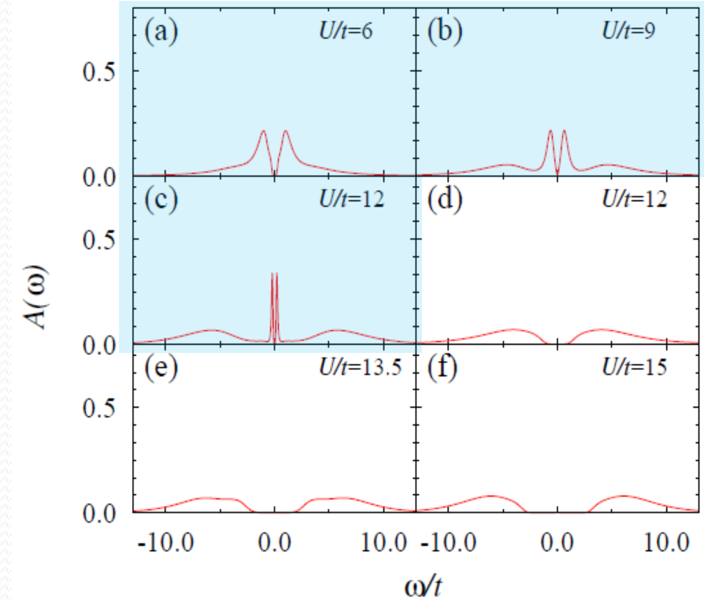
Two orbitals +U+ local hybridization V



V (gap) is enhanced !



R. Sato *et al.* (2004)



However, the gap renormalization is generic behavior of TBIs.

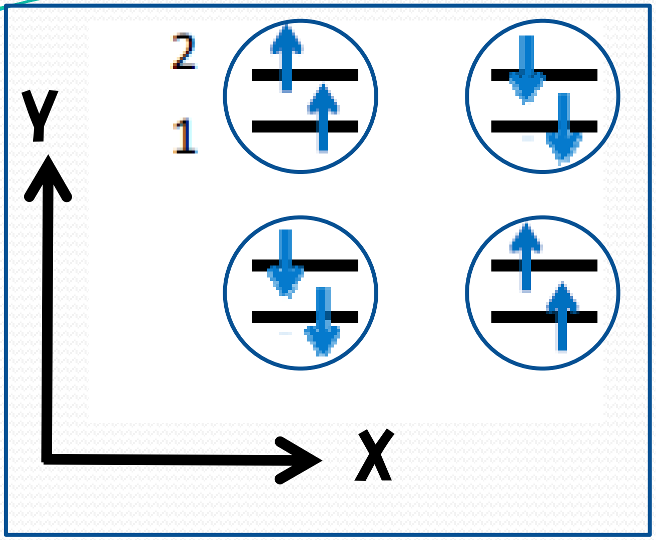
Gap ⟸ Spin orbit interaction (contributes to kinetic term)

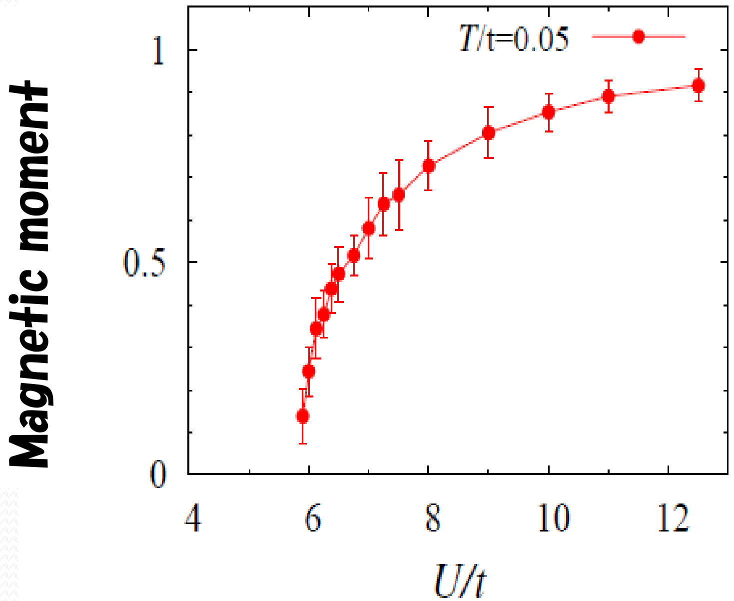
(should be renormalized)

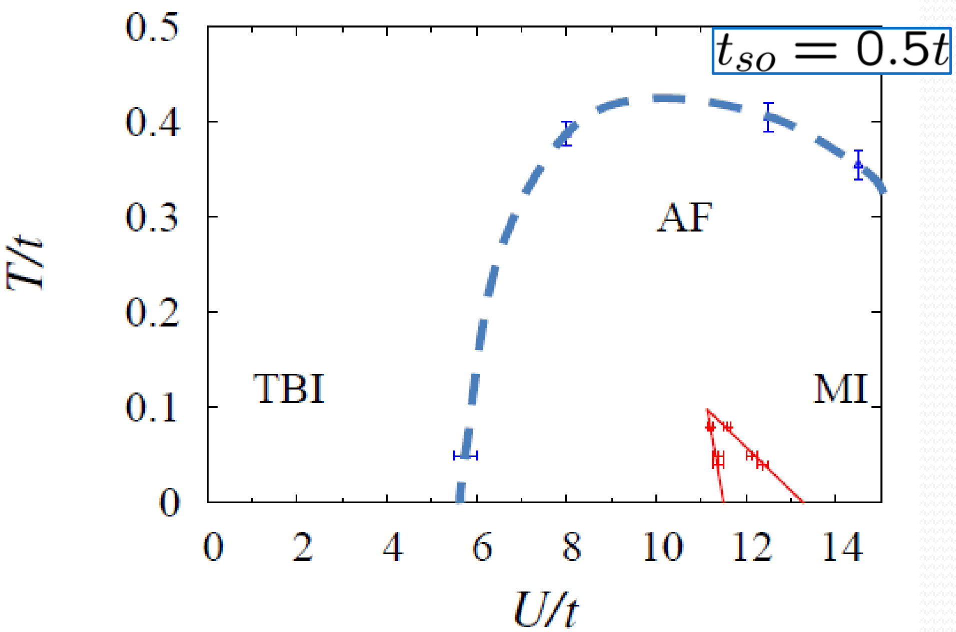
Renormalization of [the gap; σ_{xy}^{SH} at $T \neq 0$]

generic behavior of TBIs.

～(iii) Magnetic instability ～







Mott transition is masked by AF.

Observation of Mott trans. in geometrically frustrated TBI

Summary

•Phase competition between TBI and MI are studied.
(in BHZ+U with DMFT+CT-QMC)

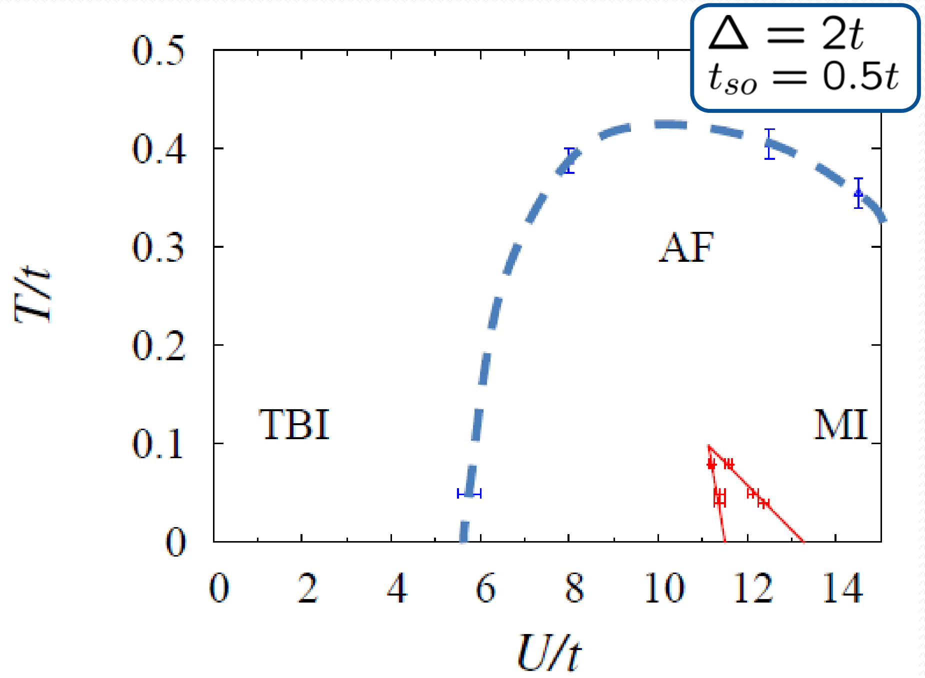
•Spin Hall conductivity
•Double occupancy

Topological ins.

1st order transition

(topologically trivial)
Mott ins.

Change of Top. # without gap-closing



Magnetic instability

AF phase masks the Mott transition

geometrically frustrated topological insulators

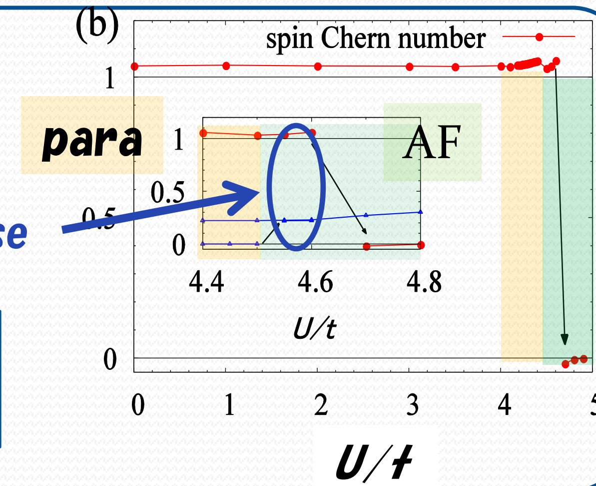
$A_2Ir_2O_7$ $(A = Pr, Eu)$: pyrochlore lattice

D.A. Pesin *et al.* Nat. Phys. 6 376

Related studies

Topological antiferromagnetic insulators

topological antiferromagnetic phase



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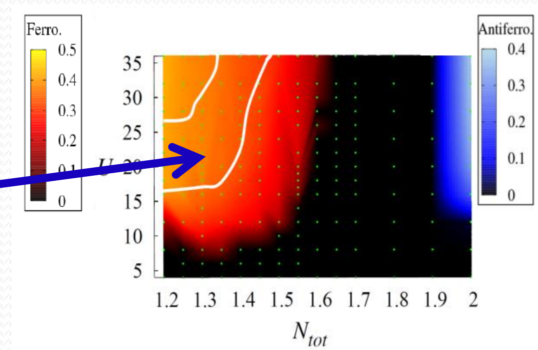
Topological Kondo insulators

-RKKY and Kondo effect in TBI -

topological phase in metal



T.Y, R. Peters, S. Fujimoto, and N. Kawakami PRB **87**, 165109 (2013)

Thank you for
your attention!