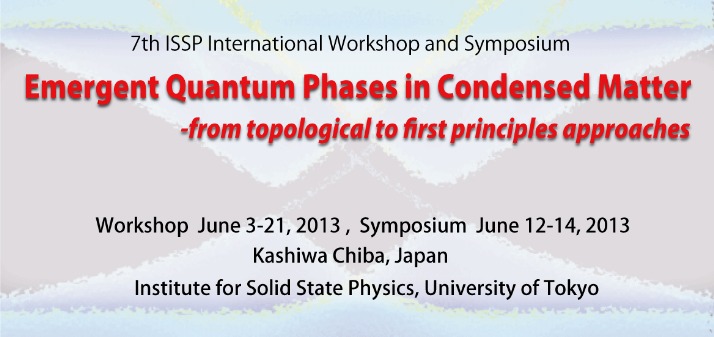


7th ISSP International Workshop and Symposium

Emergent Quantum Phases in Condensed Matter

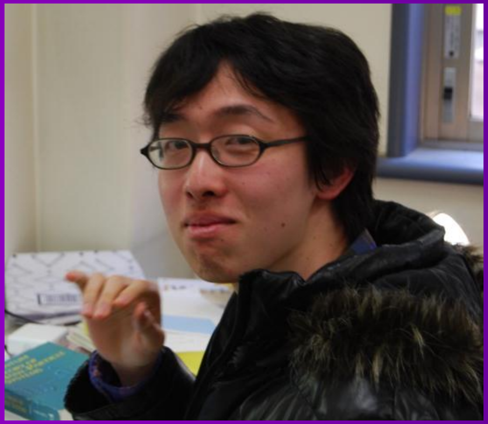
-from topological to first principles approaches

Workshop June 3-21, 2013 , Symposium June 12-14, 2013
Kashiwa Chiba, Japan
Institute for Solid State Physics, University of Tokyo

Effects of electron correlation on topological materials

June 13, 2013

Youhei Yamaji **Moyuru Kurita** **M. Imada**



⇒ P14, P24

Outline

1. Introduciton
2. Topological insulator indued by electron correlation = topological Mott insulator
3. Transitions between zero-gap semiconductors (semimetals) and topological-insulators
    - unusual universality
4. In case of pyrochlore
    - pyrochlore iridates; $R_2Ir_2O_7$
        - role of magnetic domain wall
        - fate of Weyl semimetal

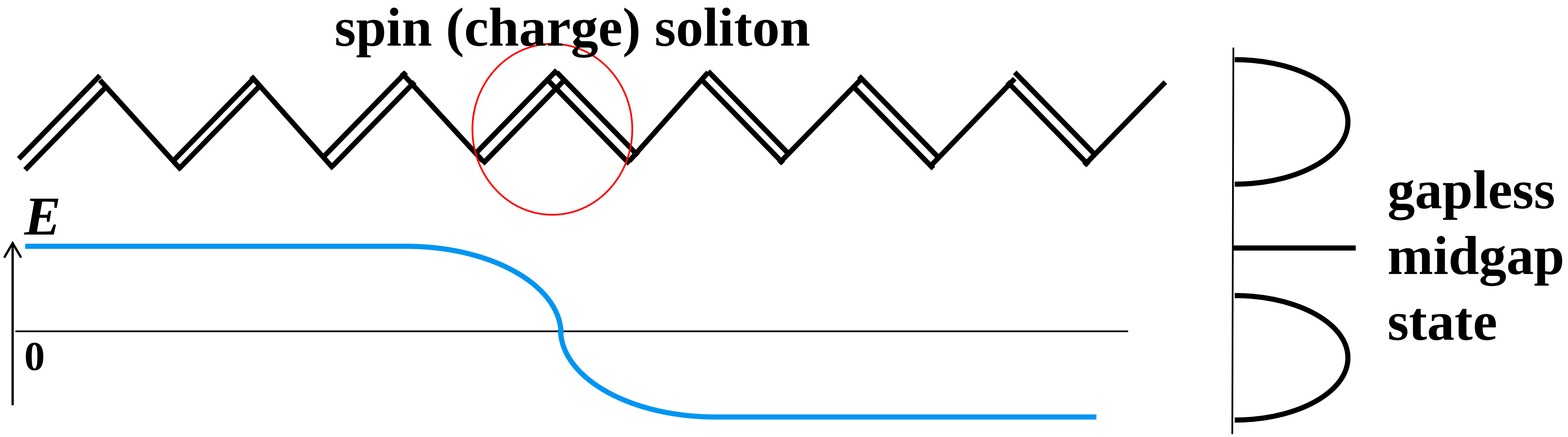
Introduction

topological insulator: bulk insulator, while robust surface (edge) gapless state

How does a gapless state emerge?

polyacetylene

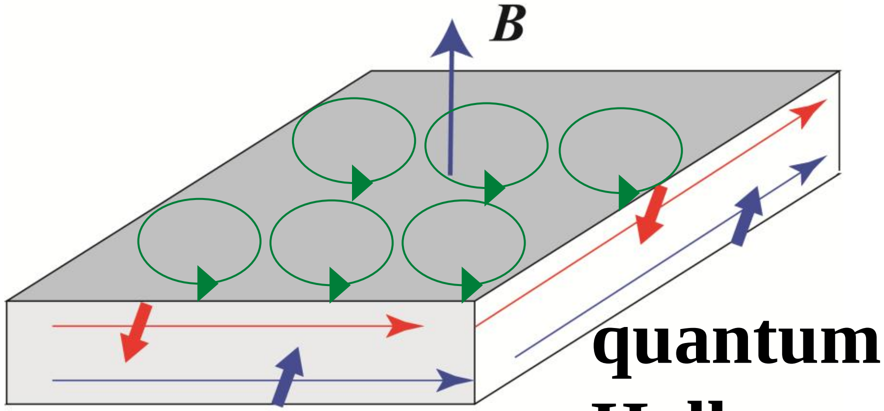
Su, Schrieffer, Heeger



When different topological gapful states are connected, a gapless state emerges

***cf.* edge of the Haldane gap state**

quantum (spin) Hall / topological insulator



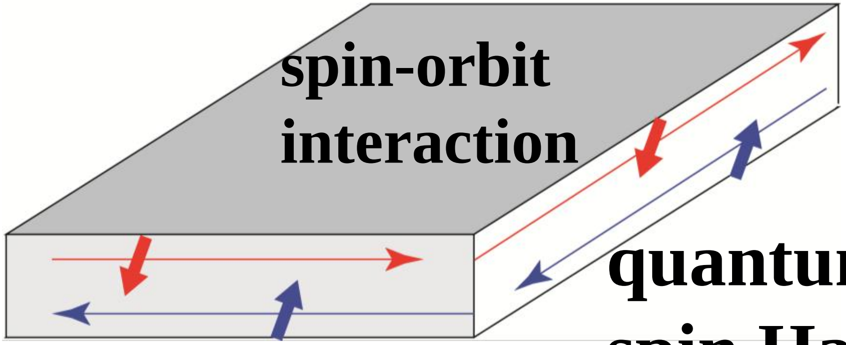
charge loop current

⇒ Chern ins.

spin loop current

⇒ topological ins.

quantum Hall **Klitzing**

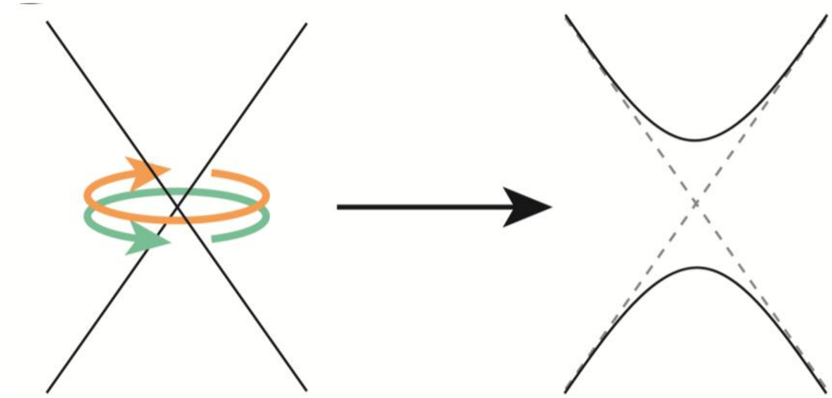


spin-orbit interaction

edge/surface gapless state

quantum spin Hall

Kane Mele 2005

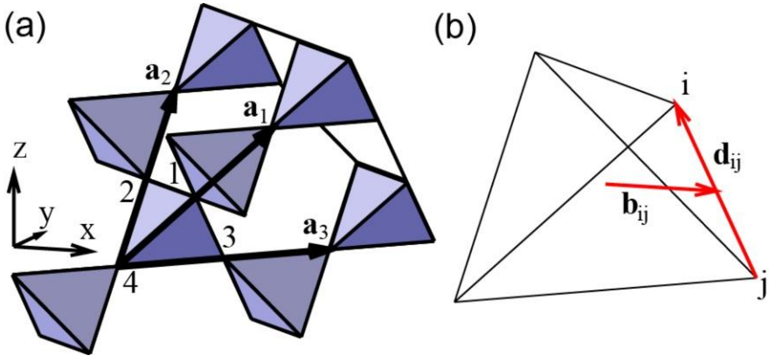


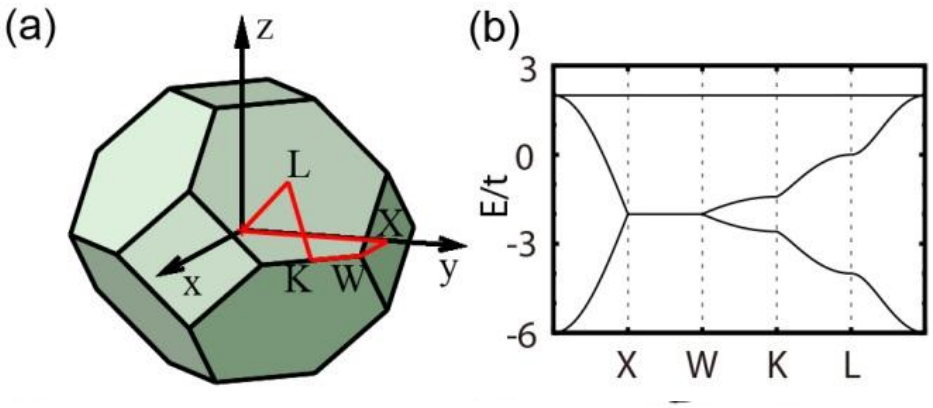
$$\varepsilon_{\pm} = \pm v_{\pm} k^{n} \rightarrow \pm\sqrt{v_{\pm}^{2} k^{2n} + m^{2}}$$

gap opening by clockwise or counterclockwise motion

Topological insulator on pyrochlore lattice

Kurita, Yamaji, Imada, J. Phys. Soc. Jpn. 80 (2011) 044708

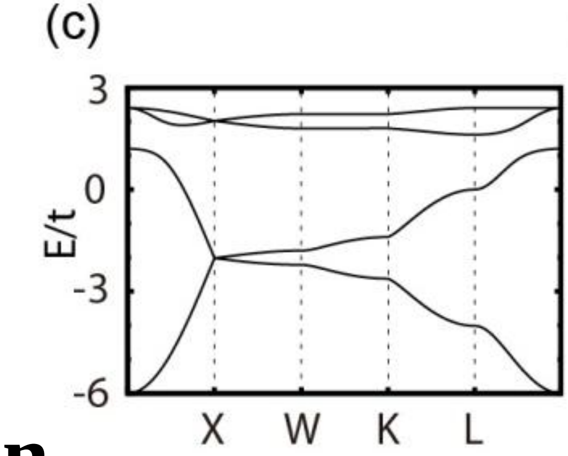




pyrochlore lattice

$$H_{SO} = -t \sum_{\langle i,j\rangle,\sigma} c_{i\sigma}^{\dagger} c_{j\sigma} + \mathrm{H.c.}$$

$$+ i\sqrt{2}\lambda \sum_{\langle i,j\rangle \alpha\beta} \nu_{ij} \cdot \sigma_{\alpha\beta} c_{i\alpha}^{\dagger} c_{j\beta} + \mathrm{H.c.}$$



$$\nu_{ij} = \frac{b_{ij} \times d_{ij}}{\left| b_{ij} \times d_{ij} \right|}$$

Spin-orbit interaction

nonzero λ > 0 opens a bulk gap

cf. **Guo & Franz (2009) for n.n.n hopping**

Electron correlation effects:

Topological insulators
even without
an explicit spin-orbit interaction?

Spontaneous symmetry breaking

intersite Coulomb *V* : Fock decoupling induces SOI

Raghu, Qi, Honerkamp, Zhang (2008)
Kurita, Yamaji, Imada (2011)

Kurita, poster P24

$$V\sum_{\langle i,j\rangle} n_i n_j \to$$

$$V\Big[-g\sum_{\langle i,j\rangle,\sigma} c_{i\sigma}{}^{\dagger} c_{j\sigma} + \text{H.c.}$$

$$+\sqrt{2}i\varsigma_s \sum_{\alpha\beta ij} c_{i\alpha}{}^{\dagger} c_{j\beta}\frac{b_{ij}\times d_{ij}}{|b_{ij}\times d_{ij}|}\cdot\sigma_{\alpha\beta}+\text{H.c.}$$

$$+(24g^2+48\varsigma_s{}^2)L^3\Big]$$

order parameter

$$g=\left\langle c_{i\sigma}{}^{\dagger} c_{j\sigma}\right\rangle$$

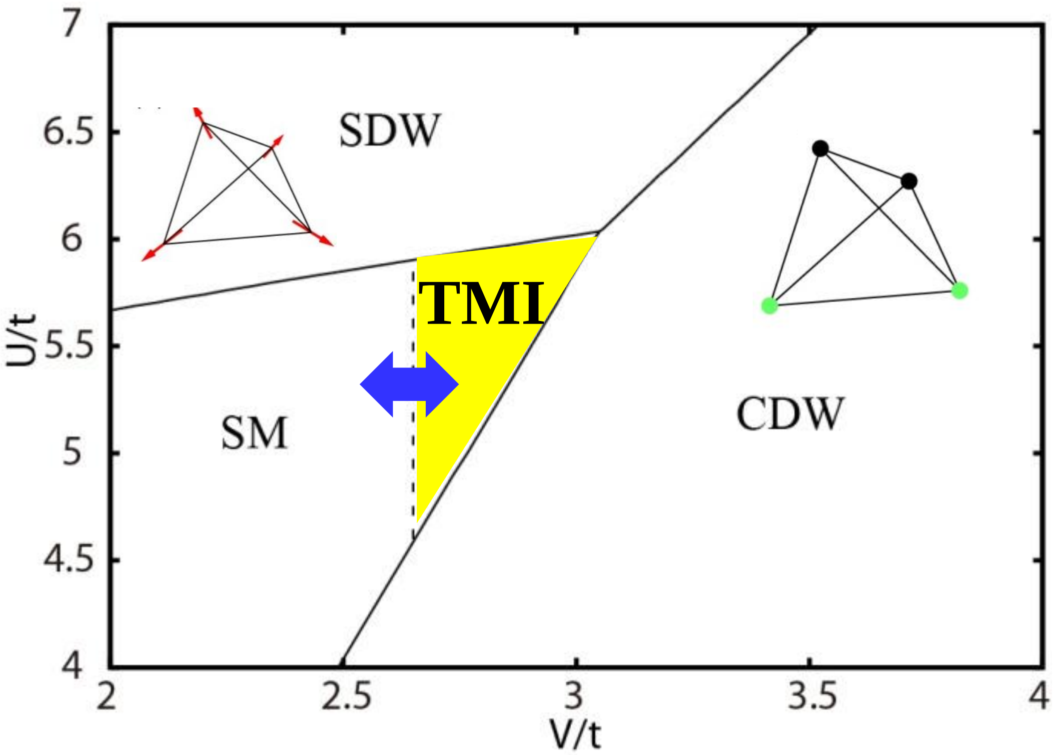
$$\varsigma_s=\frac{i}{2\sqrt{2}}\sum_{\alpha\beta}\left\langle c_{i\alpha}{}^{\dagger} c_{j\beta}\right\rangle\frac{b_{ij}\times d_{ij}}{|b_{ij}\times d_{ij}|}\cdot\sigma_{\alpha\beta}$$

Phase diagram of pyrochlore

Kurita, Yamaji, Imada
JPSJ 80 (2011) 044708

Kurita, poster P24

Hubbard model with *U* and *V* stabilizes a "topological Mott insulator" (TMI) without SO int.



★Topological and symmetry-breaking transitions occur simultaneously

★Electron correlation (intersite Coulomb) enhances the topological insulator

unconventional QCP

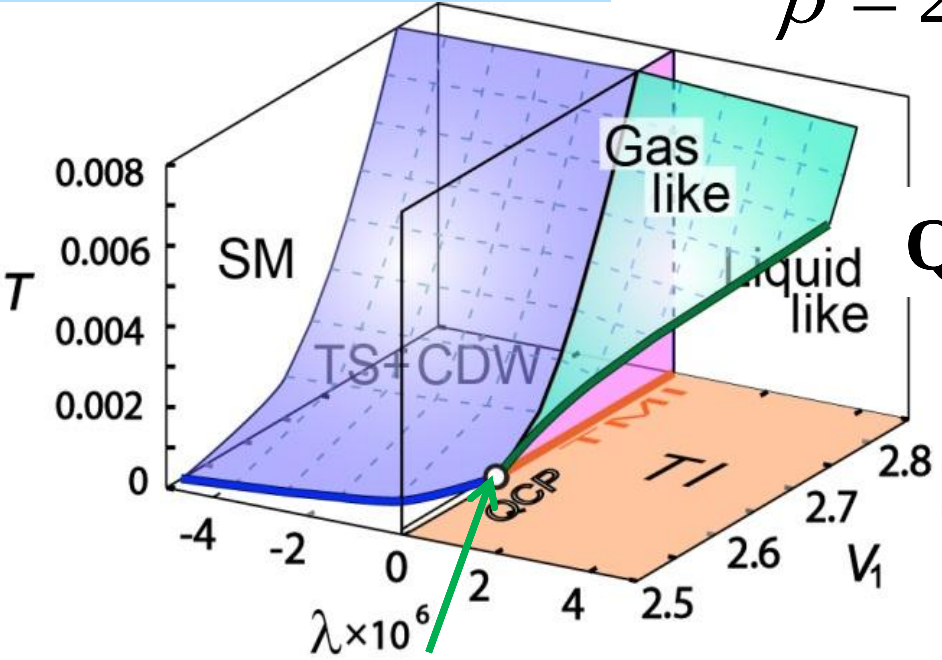
$$F(\varsigma)=\lambda\varsigma+a\varsigma^{2}+b\left|\varsigma\right|^{2.5}$$

$\beta=2,\ \gamma=1,\ \delta=3/2$ **at MQCP**

$\boldsymbol{\beta = 1 \quad \Rightarrow \quad 2 \quad \Rightarrow \quad 1/2}$

Quantum ⇒MQCP⇒Classical

$\boldsymbol{\delta = 1 \quad \Rightarrow \quad 3/2 \quad \Rightarrow \quad 3}$

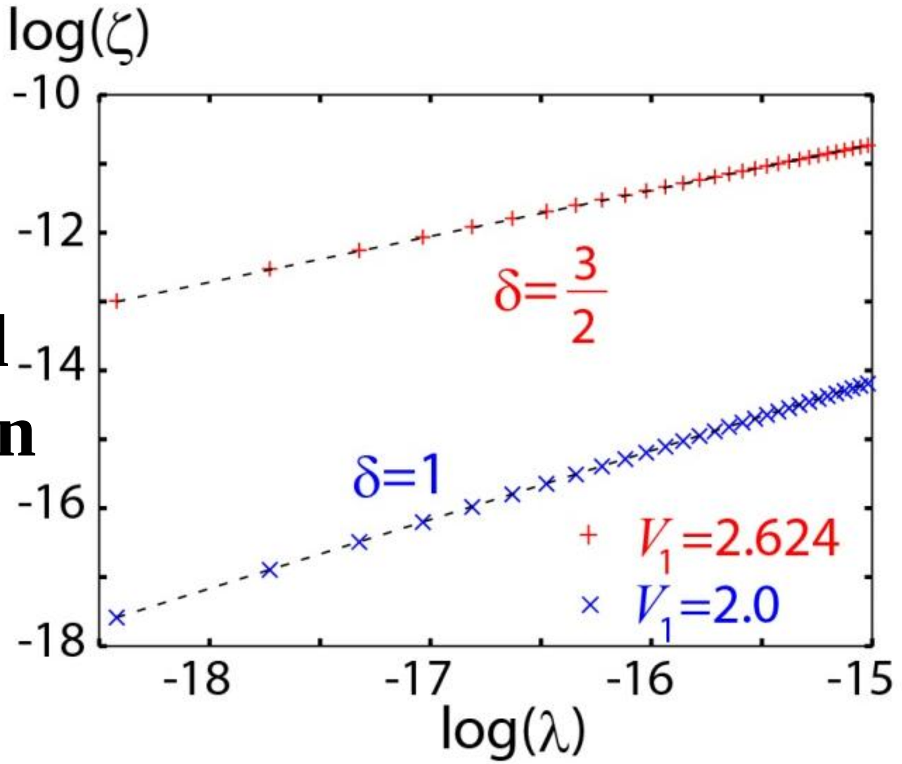


MQCP

simultaneous topological and symmetry breaking transition

Kurita et al. arXiv:1201.1395

Kurita poster P24



$$H_{SO} = -t \sum_{\langle i,j\rangle,\sigma} c_{i\sigma}{}^{\dagger} c_{j\sigma} + \mathrm{H.c.}$$

$$+ i\sqrt{2}\lambda \sum_{\langle i,j\rangle\alpha\beta} \nu_{ij} \cdot \sigma_{\alpha\beta} c_{i\alpha}{}^{\dagger} c_{j\beta} + \mathrm{H.c.}$$

+ Hubbard *U*

$\lambda < 0$

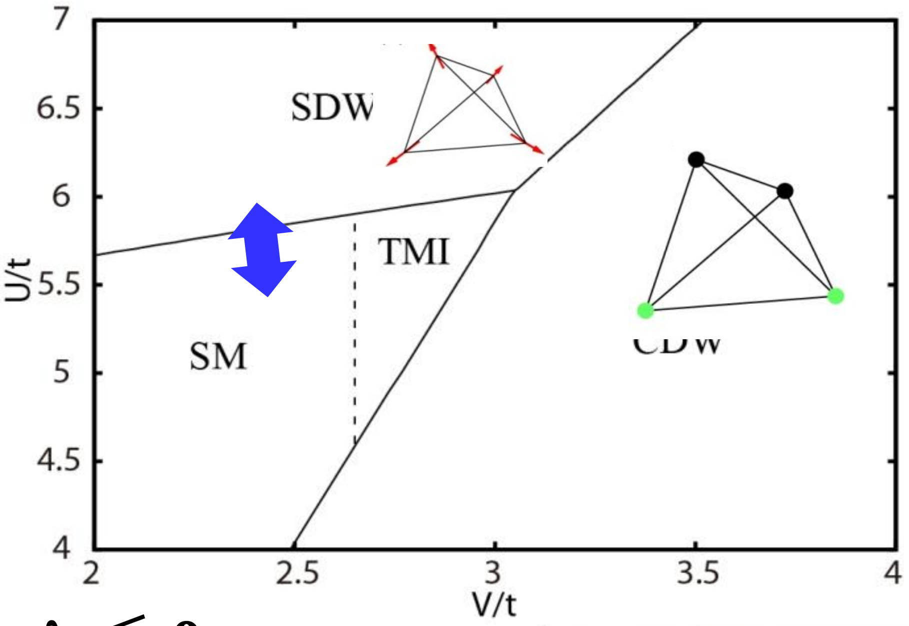
Metallic Interface Emerging at Magnetic Domain Wall of Antiferromagnetic Insulator

Yamaji, MI ;

arXiv:1306.2022
poster 14

TI and semimetal

Kurita et al. arXiv:1201.1395



Wan, Turner, Vishwanath & Savrasov PRB83(2011) 205101

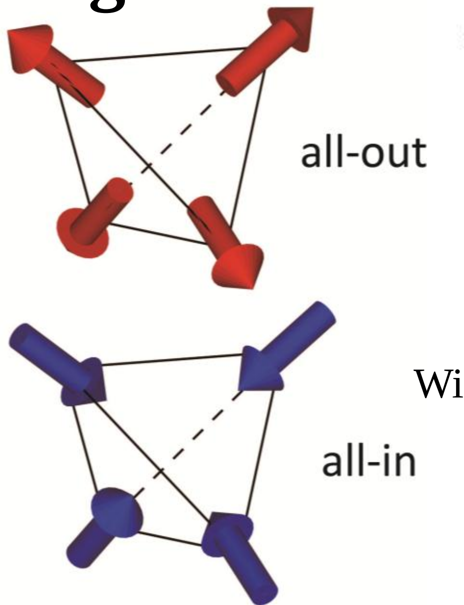
Kurita, poster P24

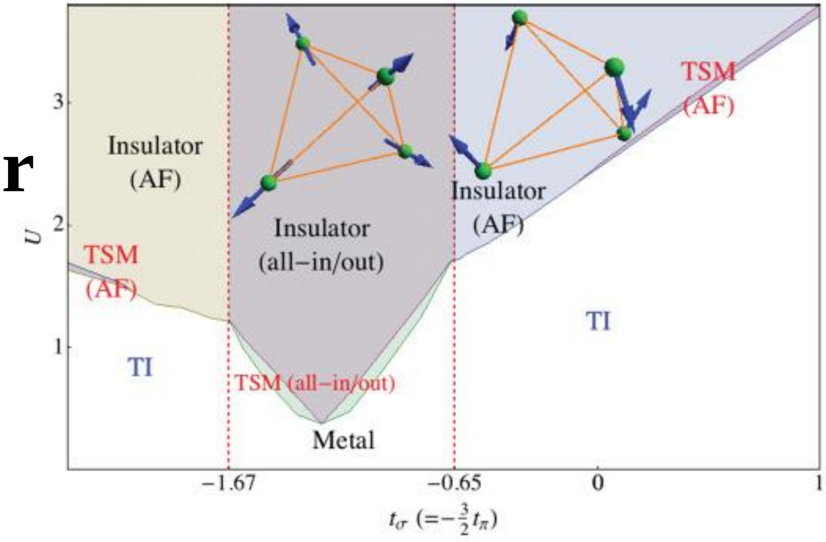
Witczak-Krempa, Chen, Y.-B. Kim, and Balents, arXiv:1305.2193v1

Weyl semimetal

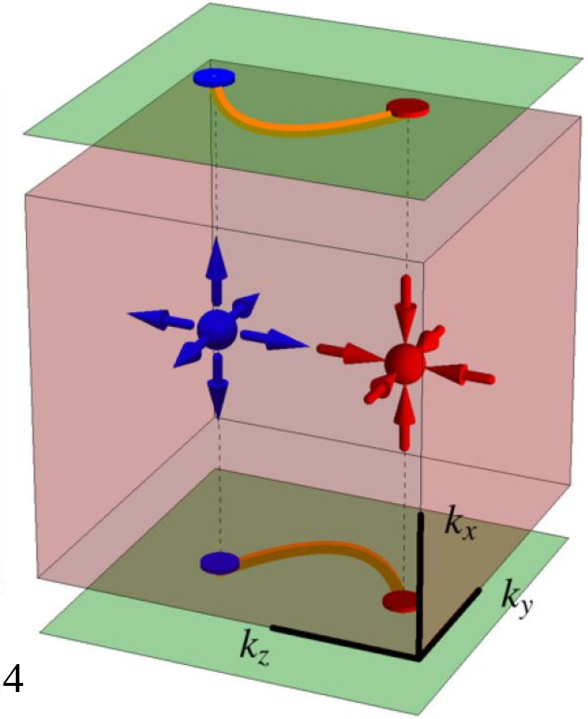
Fermi arc

λ ≦ 0
all-in/all-out magnetic order





Witczak-Krempa, Y.-B. Kim, PRB85(2012)045124



Weyl points are annihilated in pair
⇒ trivial AF insulator?

M. IMADA

Question

Does the all-in/all-out ordered state becomes a trivial good insulator at low *T* after the pair annhilations of Weyl points ?

example: $R_2Ir_2O_7$

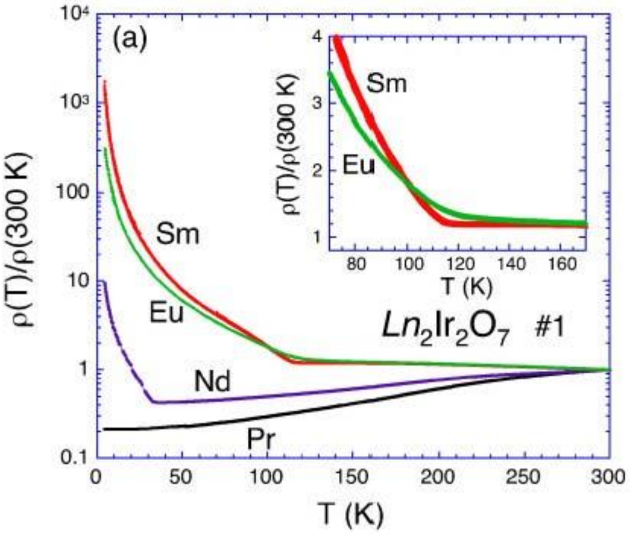
Experimental indications of pyrochlore iridates

Yanagishima Maeno JPSJ 70 (2001) 2880

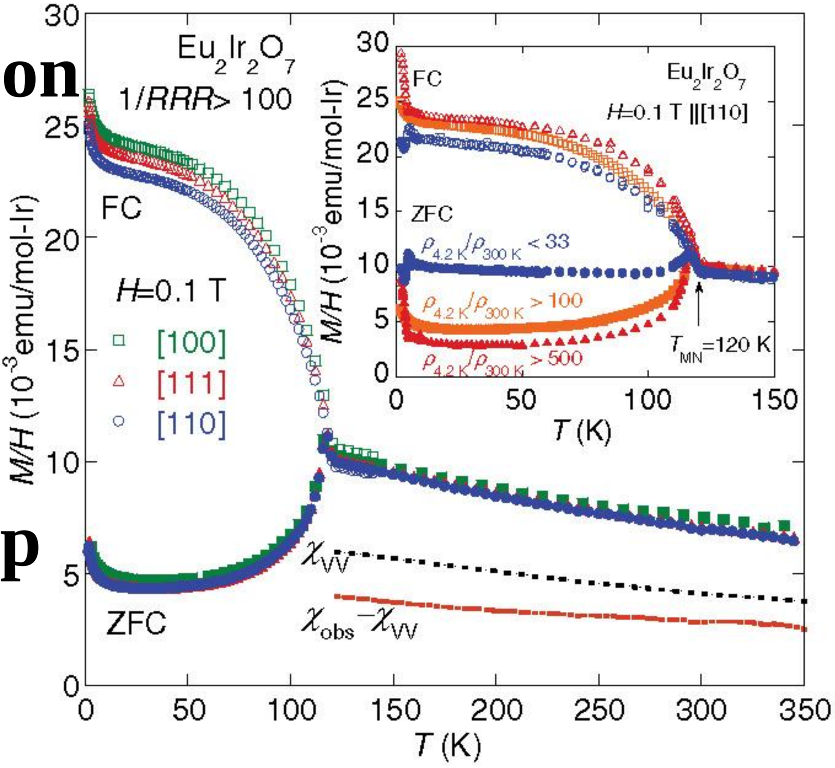
Matsuhira et al. JPSJ 76 (2007) 043706

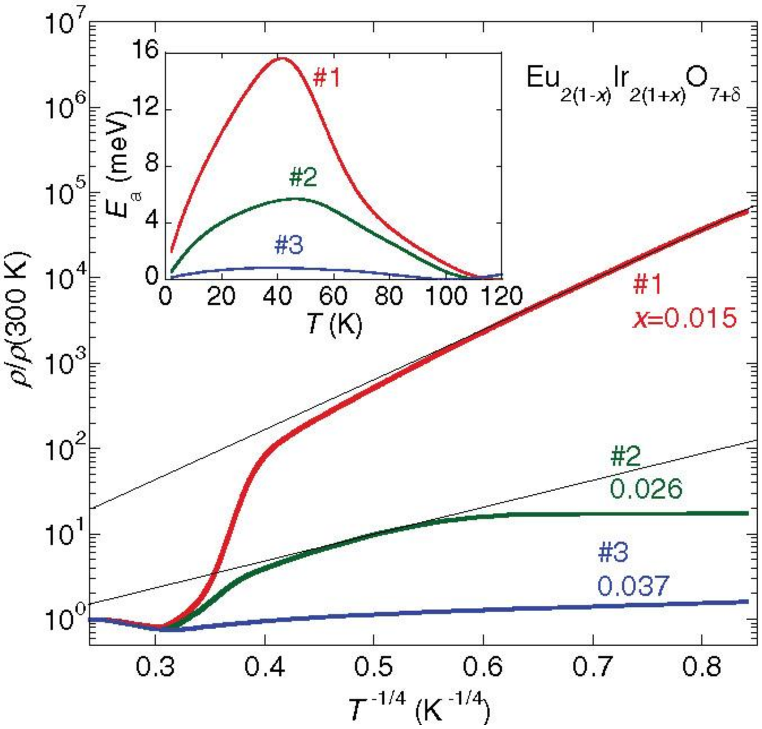
Ishikawa,O'Farrell, Nakatsuji, PRB 85 (2012) 245109

Ueda. Fujioka et al. PRL 109 (2012) 136402



uniform magnetization under FC





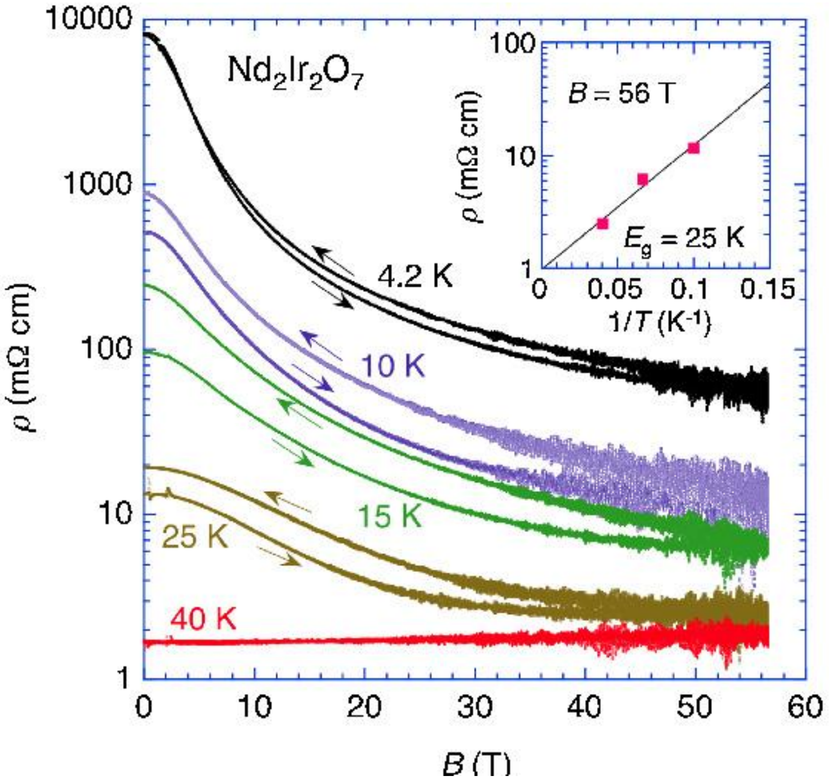
VRH and/or small gap

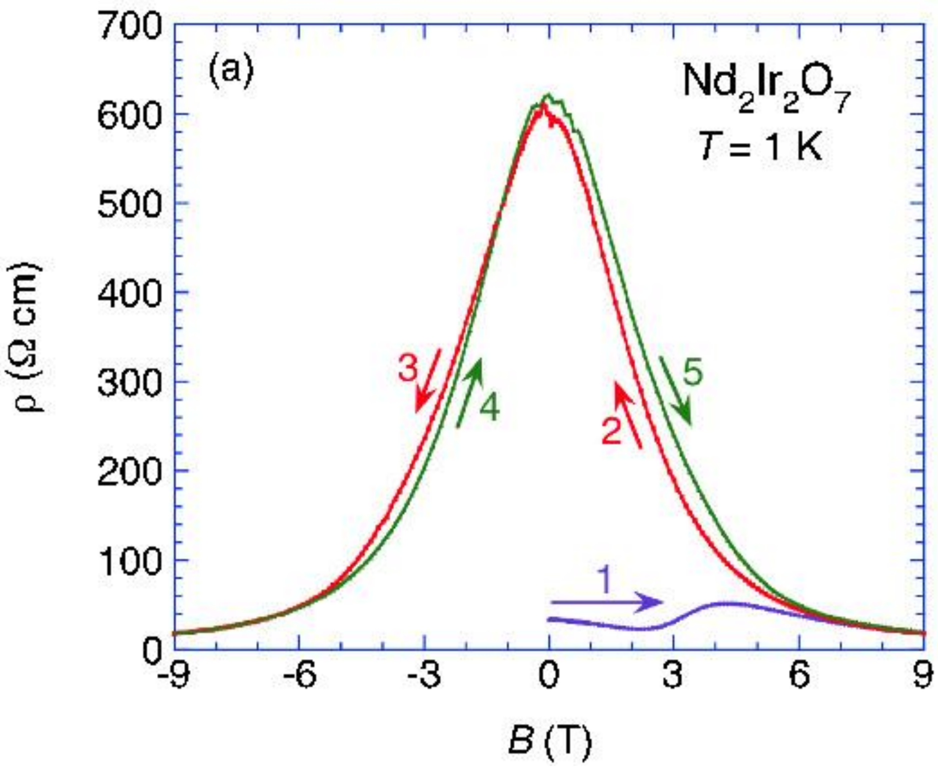
"bad insulator" weak ferromagnet

Experimental indications II

large negative magnetoresistance & hysteresis for Gd/Nd

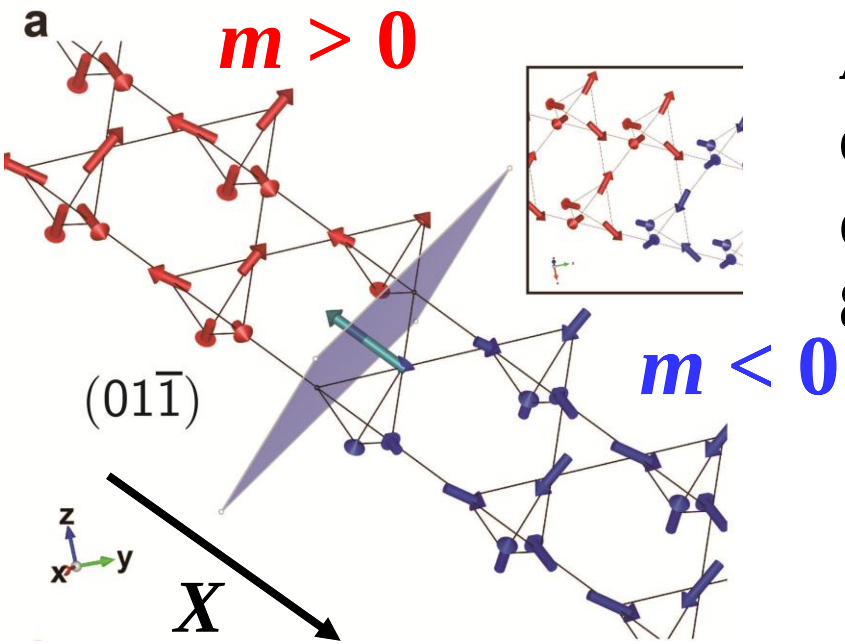
Matsuhira *et al.* JPSJ 82 (2013) 023706





Domain wall

Yamaji, Imada,
arXiv:1306.2022



Around each Weyl point,
extract two degenerate zero modes out of
8-component spin-orbit +Hubbard
J=1/2 manifold

⇒ Dirac equation

simplified model

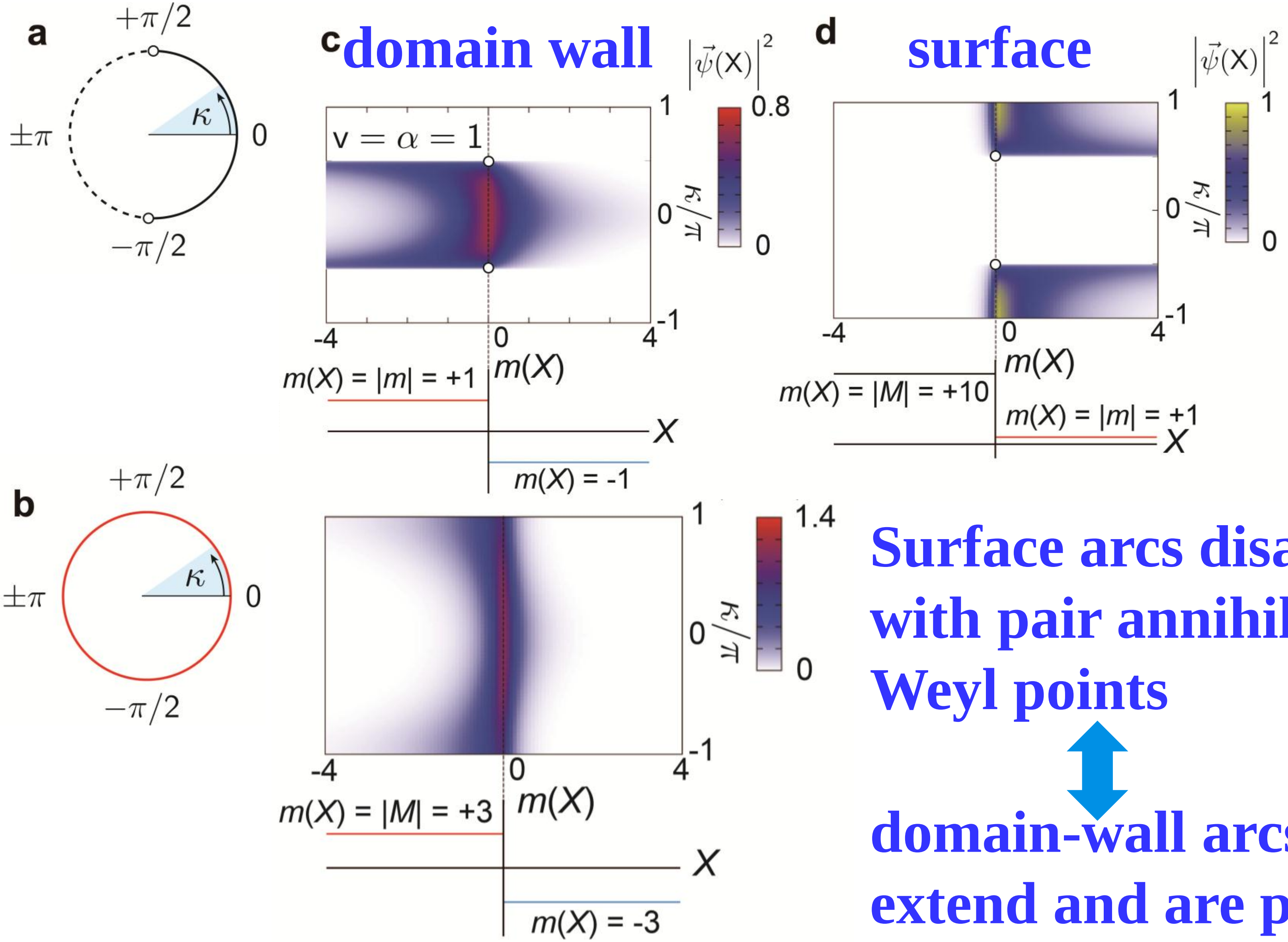
$$\left\{\left[\alpha(1-\cos\kappa)-m(X)\right]\hat{\sigma}_z+vi\hat{\sigma}_y\partial_X\right\}\vec{\psi}(\vec{X})=E\vec{\psi}(\vec{X})$$

⇒ Weyl point and Fermi arc if |*m*| is small

Arcs of domain wall and surface

simplified model

$$\left\{\left[\alpha(1-\cos\kappa)-m(X)\right]\hat{\sigma}_z+vi\hat{\sigma}_y\partial_X\right\}\vec{\psi}(\vec{X})=E\vec{\psi}(\vec{X})$$



domain wall

surface

Surface arcs disappear with pair annihilation of Weyl points

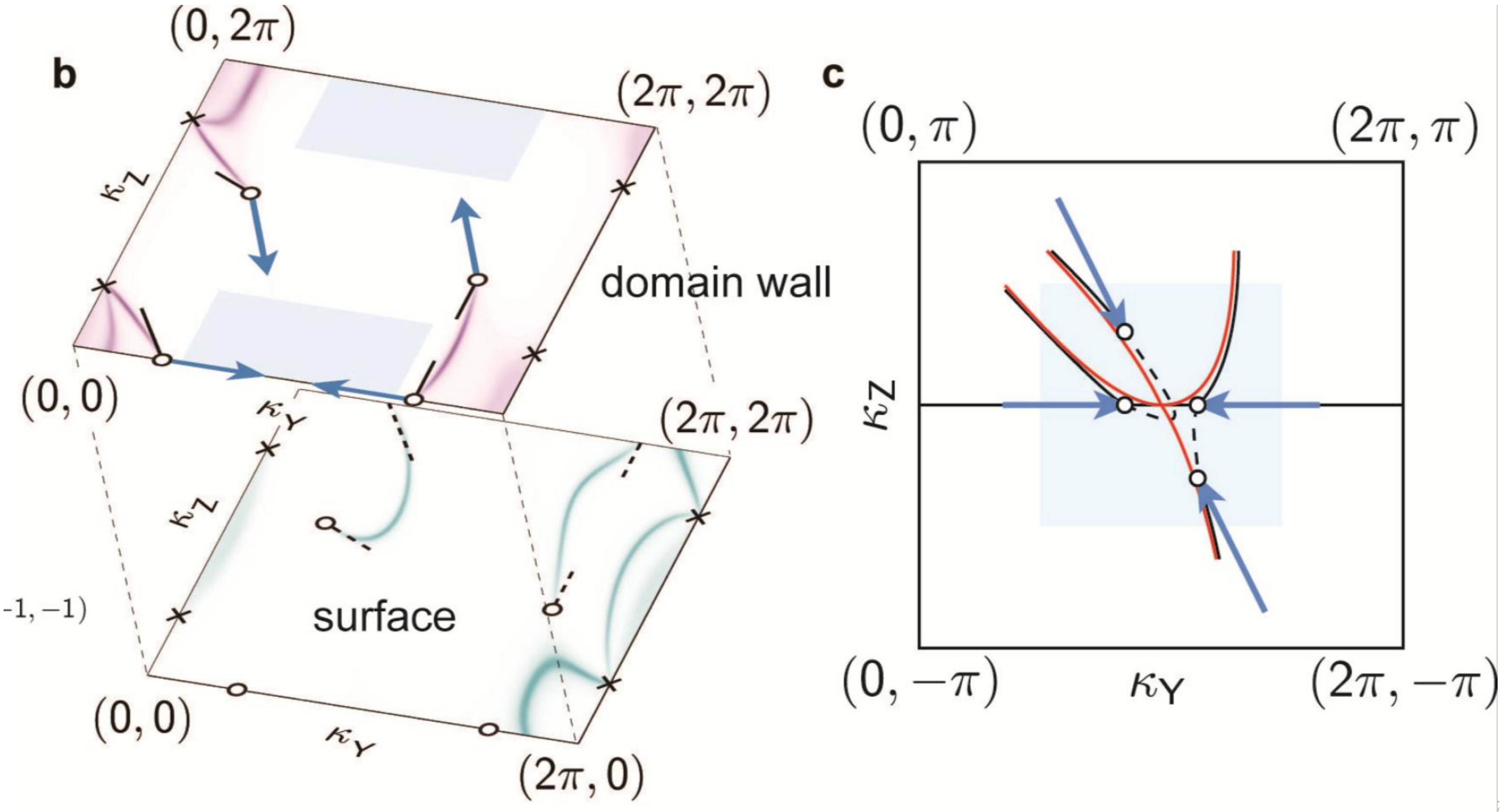
↕

domain-wall arcs extend and are protected

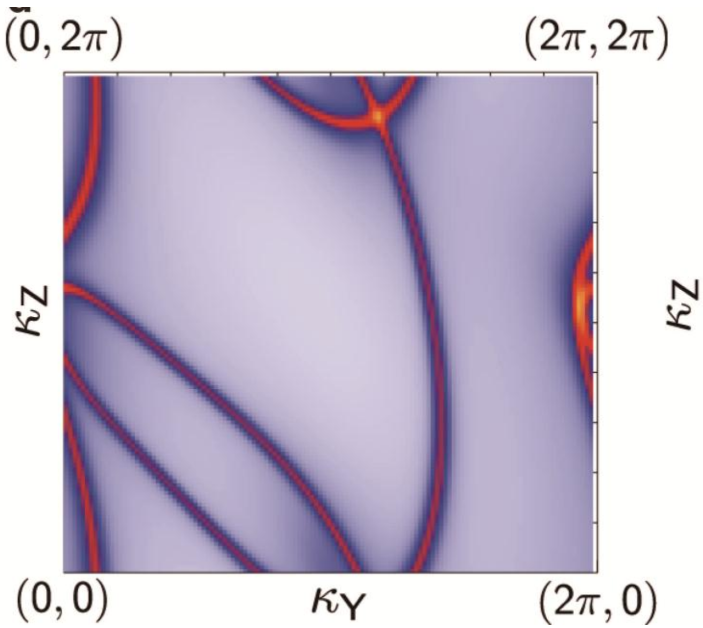
Arcs of domain wall and surface: full solution

$$H = -t\sum_{\langle i,j\rangle,\sigma} c_{i\sigma}{}^{\dagger}c_{j\sigma} + \text{H.c.} + i\sqrt{2}\lambda \sum_{\langle i,j\rangle\alpha\beta} \nu_{ij}\cdot\sigma_{\alpha\beta}c_{i\alpha}{}^{\dagger}c_{j\beta} + \text{H.c.}$$

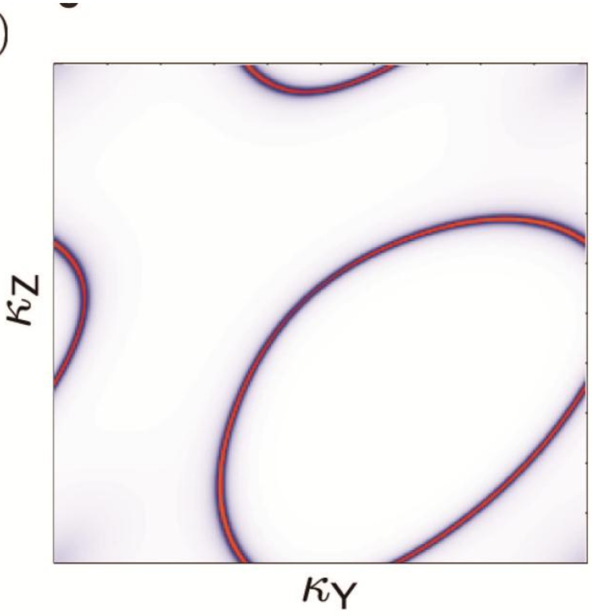
$$+\text{Hubbard } U$$



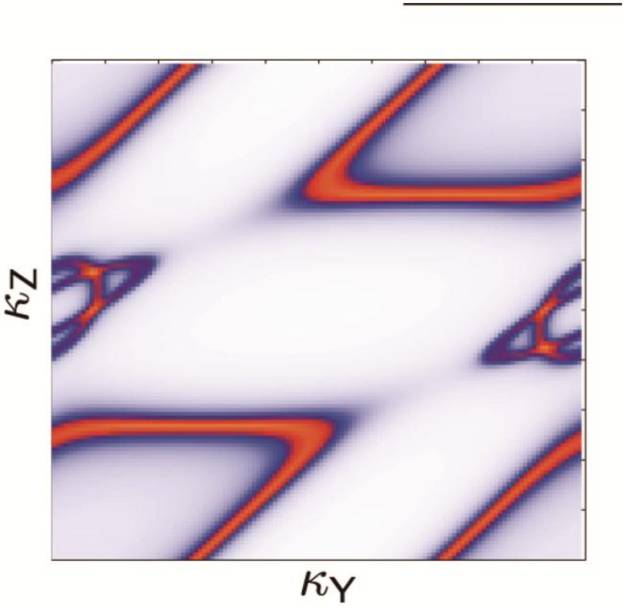
Closed Fermi surface on domain walls at low *T*



$(01\bar{1})$



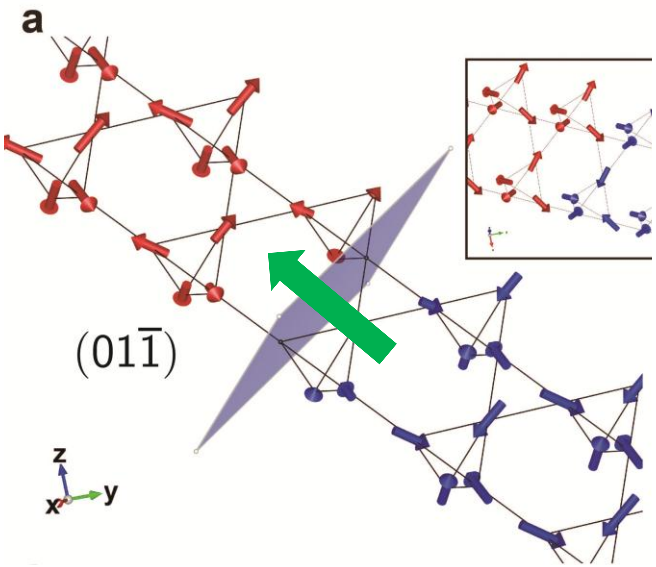
(111)

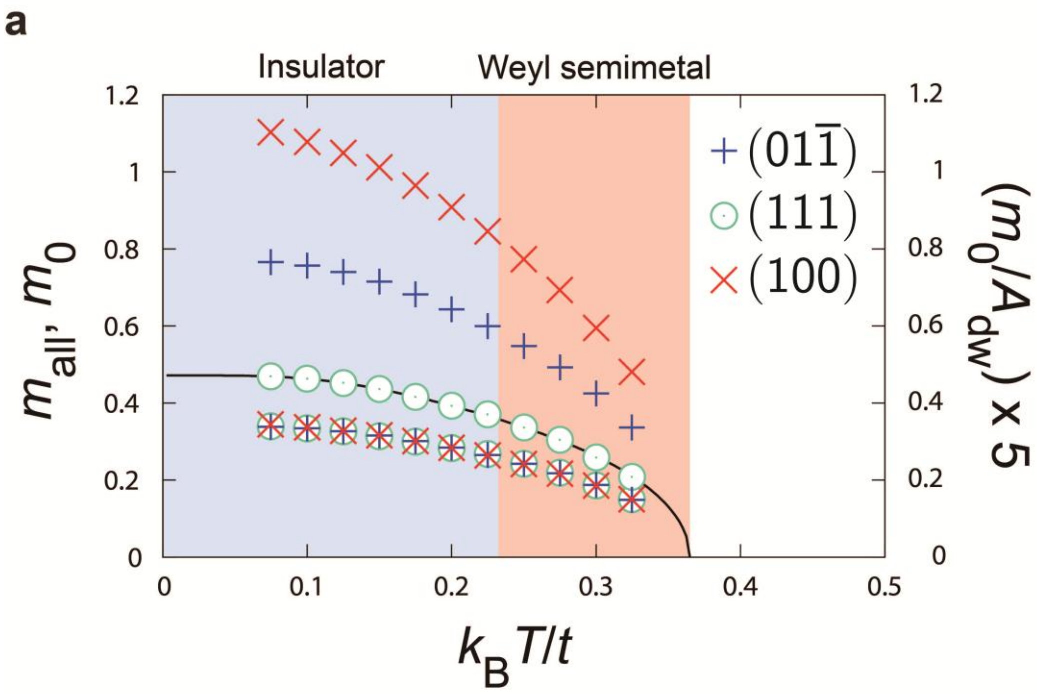


(100)

★metallicity on the domain walls survives

Magnetization





★**constant uniform magnetization per area**
⇒ cancellation of magnetization
⇒ incomplete cancellation by impurities/doping

Consistency with experiments

★ "bad insulator" ⇔ conduction at domain wall with Anderson localization

★magnetization under field cool, strong sample dependence

⇔ domain wall magnetization adjusted by impurities/disorder/self-doping

domain size ~10^3 unit cells ⇔ $10^{-3}\mu_B$/unit cell

smaller magnetization for polycrystals

⇔ domain walls are wiped out

★large negative magnetoresistance for Nd/Gd

⇔ fluctuating Nd/Gd moment at zero field

⇒ "double exchange" under the field

Summary and outlook

Unconventional quantum criticality of topological Mott transition from semimetal to topological insulator

Weyl points are easily annihilated at low *T* of all-in/all-out order, leading to a “trivial insulator” in bulk and surface.

However, ingap states are protected at domain walls generating Fermi surface/metallicity and weak ferromagnetism.

It explains “bad insulators” and weak ferromagnetism, together with negative MR for Nd/Gd compounds.

Future issue
Magnetic control of conduction at domain walls