Topological Phases in Correlated Materials

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CANADIAN INSTITUTE for ADVANCED RESEARCH

Topological Phases of Matter

How can we characterize them ?

What are the "Topological Properties" ?

Where can we find them ?

Topological Phases of Matter

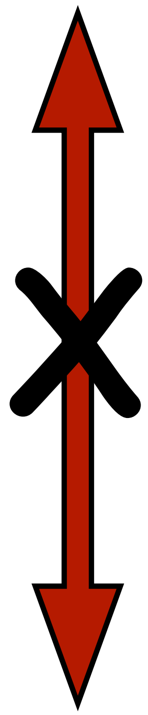
Cannot be fully characterized by
a local order parameter
such as magnetization in magnets

Cannot be transformed to "simple phases"
via local perturbations/operations
without going through phase transitions

Often characterized by a variety of
"Topological Properties" or "Non-local Properties"

Type I Topological Phases (Gapped Phases)

Topological Phases



No "Path"
(Local unitary transformations)
without closing the bulk gap

"simple phases" (fully characterized by local order parameter/information)

Quantum Hall States

Spin Liquids

(correlated quantum paramagnetic state)

Type-I Topological Phases (Gapped Phases)

Quantum Hall States

Non-trivial ground state degeneracy:

$\nu = 1/3$ quantum Hall state has "3" degenerate ground states on torus, but "1" on sphere

Non-trivial boundary states:

Edge state is a chiral Luttinger Liquid

Non-trivial topological invariant: $\sigma_{xy} = \frac{1}{3}\frac{e^2}{h}$

Non-trivial excitations:

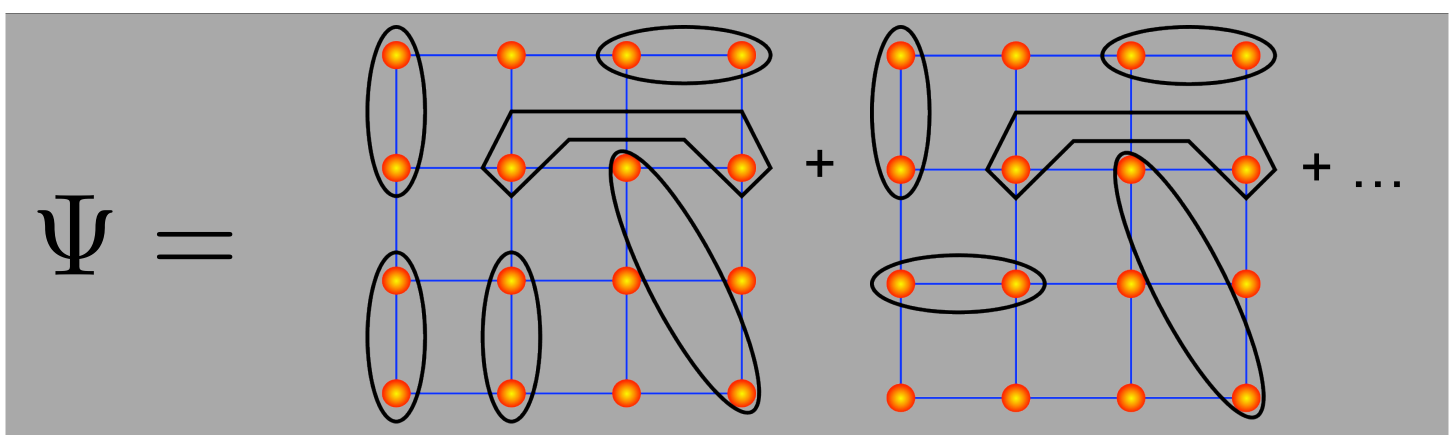
Fractionally charged e/3 Laughlin quasi-particles

Type-I Topological Phases (Gapped Phases)

Spin Liquids Quantum Paramagnet $\langle \mathbf{S} \rangle = 0$

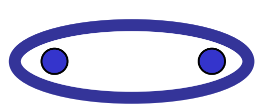
Correlated insulator with no broken translational symmetry

Resonating Valence Bond state (RVB);
Superposition of Valence Bond coverings



P.W.Anderson

Rokhsar-Kivelson



$$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

Valence Bond

Construction of a Spin Liquid

- BCS superconductor (L x L lattice)

average number of electrons per site = one (Half-filled)

$g(\mathbf{r}-\mathbf{r}') \Leftrightarrow$ Cooper pair wave function

BCS wave function $\quad |BCS\rangle \propto e^{\sum_{\mathbf{r},\mathbf{r}'} g(\mathbf{r}-\mathbf{r}') c^\dagger_{\mathbf{r}\uparrow} c^\dagger_{\mathbf{r}'\downarrow}} |0\rangle$

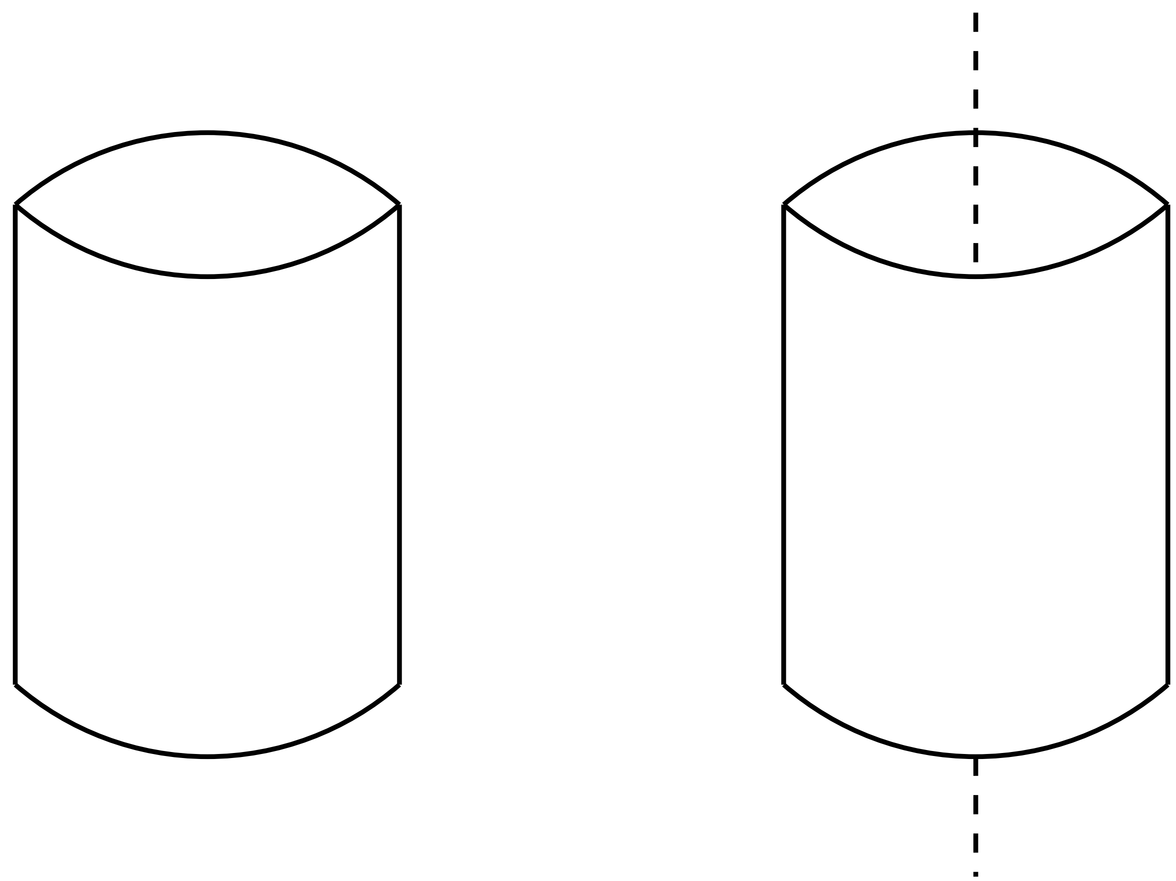
- RVB wave function $\quad |RVB\rangle = P_G |BCS\rangle \propto \sum_{vb} A_{vb} |vb\rangle$

P_G exactly one particle per site; freeze charge fluctuations

Hubbard $U \to \infty$ in $U n_{i\uparrow} n_{i\downarrow}$

$|vb\rangle$ valence bond covering $\quad A_{vb} = \prod_{\substack{\text{all valence} \\ \text{bond } (\mathbf{r},\mathbf{r}')}} g(\mathbf{r}-\mathbf{r}')$

Degenerate Ground States



$$|RVB\rangle = P_G|BCS\rangle \qquad |RVB'\rangle = P_G|BCS'\rangle$$

$\langle RVB|RVB'\rangle \rightarrow 0$ in the thermodynamic limit

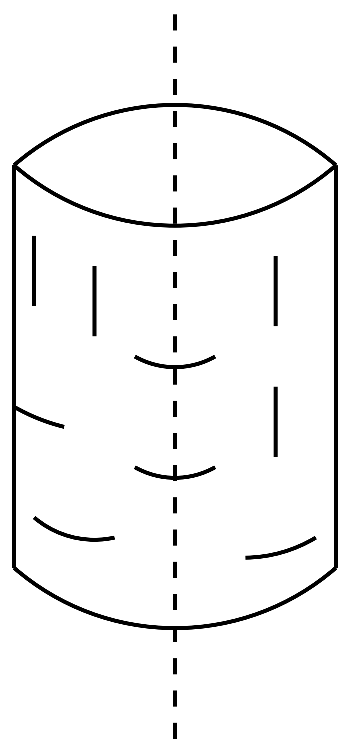
No local measurement can distinguish these phases

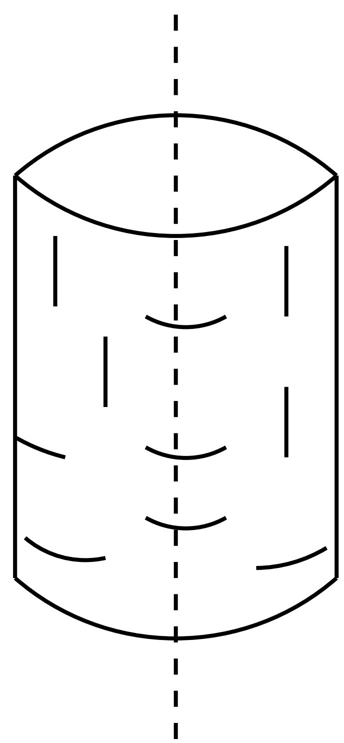
Short 'Coherence Length' Limit

$$|\text{even}\rangle = \frac{1}{2}(|RVB\rangle + |RVB'\rangle) \qquad |\text{odd}\rangle = \frac{1}{2}(|RVB\rangle - |RVB'\rangle)$$

TWO topologically distinct valence bond coverings

intersecting even number of dimers





intersecting odd number of dimers

Non-trivial ground state degeneracy

Elementary Excitations

- Elementary excitations in superconductors

  Bogoliubov quasiparticles (zero average charge, S=1/2)

- Elementary excitations in the spin liquid state

  P_G (Bogoliubov quasiparticles) = Spinons (Q=0,S=1/2)

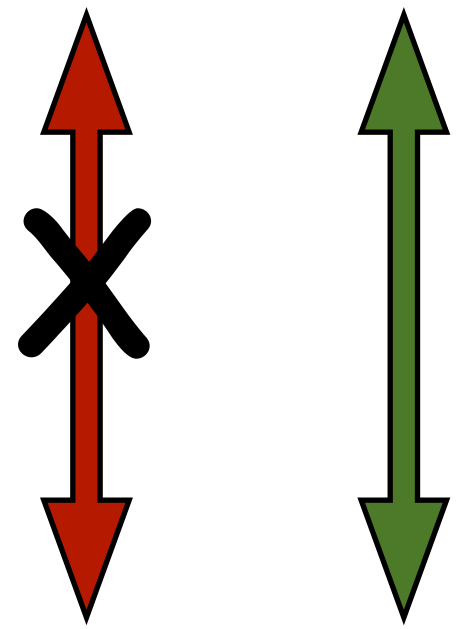
- Fractionalization of electrons !

Non-trivial excitations

Type II “Symmetry-Protected” Topological Phases (Gapped Phases)

Topological Phases

No Symmetry-Preserving “Path” without closing the bulk gap



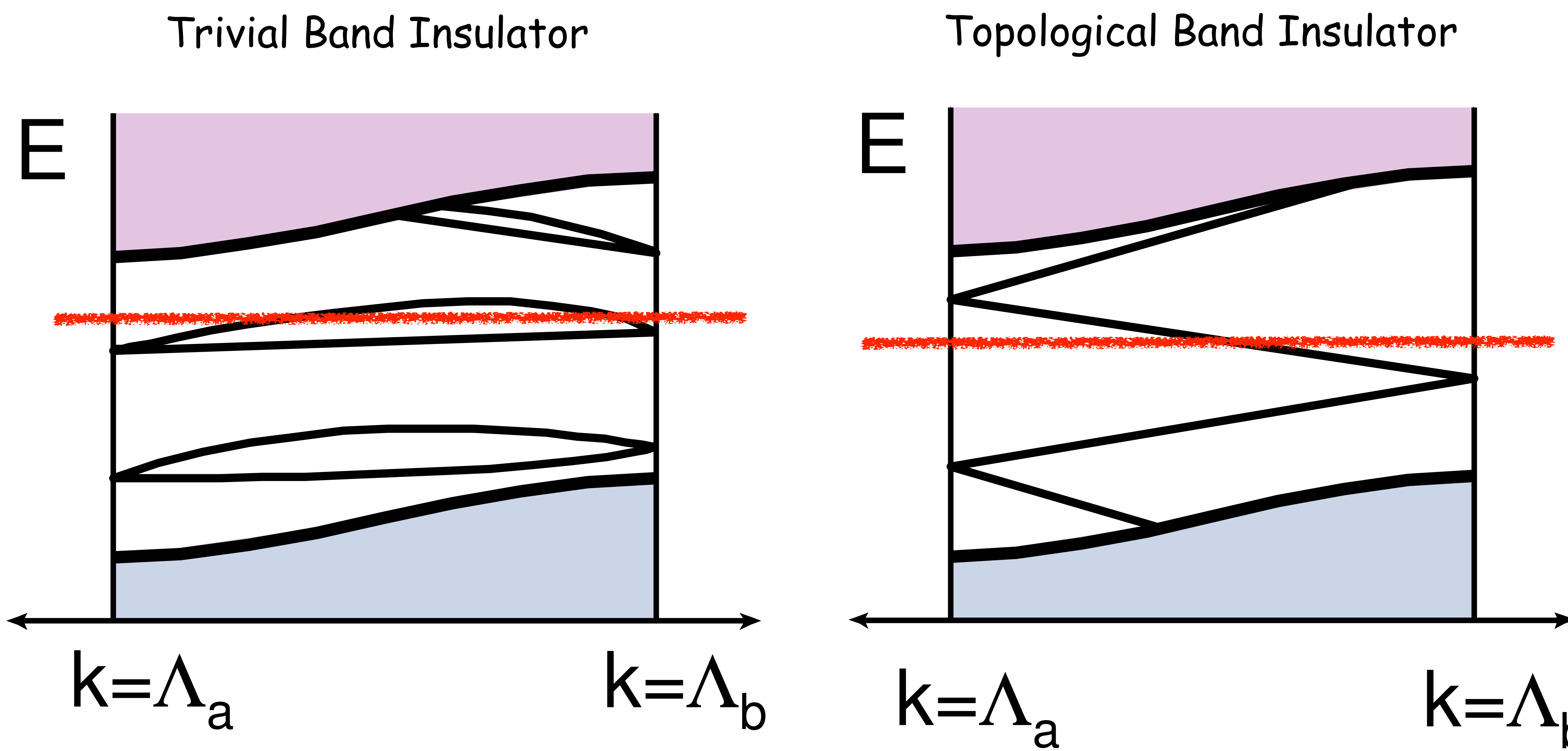
Symmetry-Breaking “Path” without closing the bulk gap

“simple phases”

Topological Band Insulator
(e.g. time-reversal symmetry)

Topological Band Insulator

2D time reversal invariant band structure has
a Z2 topological invariant



C. L. Kane, E. Mele, L. Fu   B. A. Bernevig, T. L. Hughes, X.-L. Qi, S. C. Zhang ....

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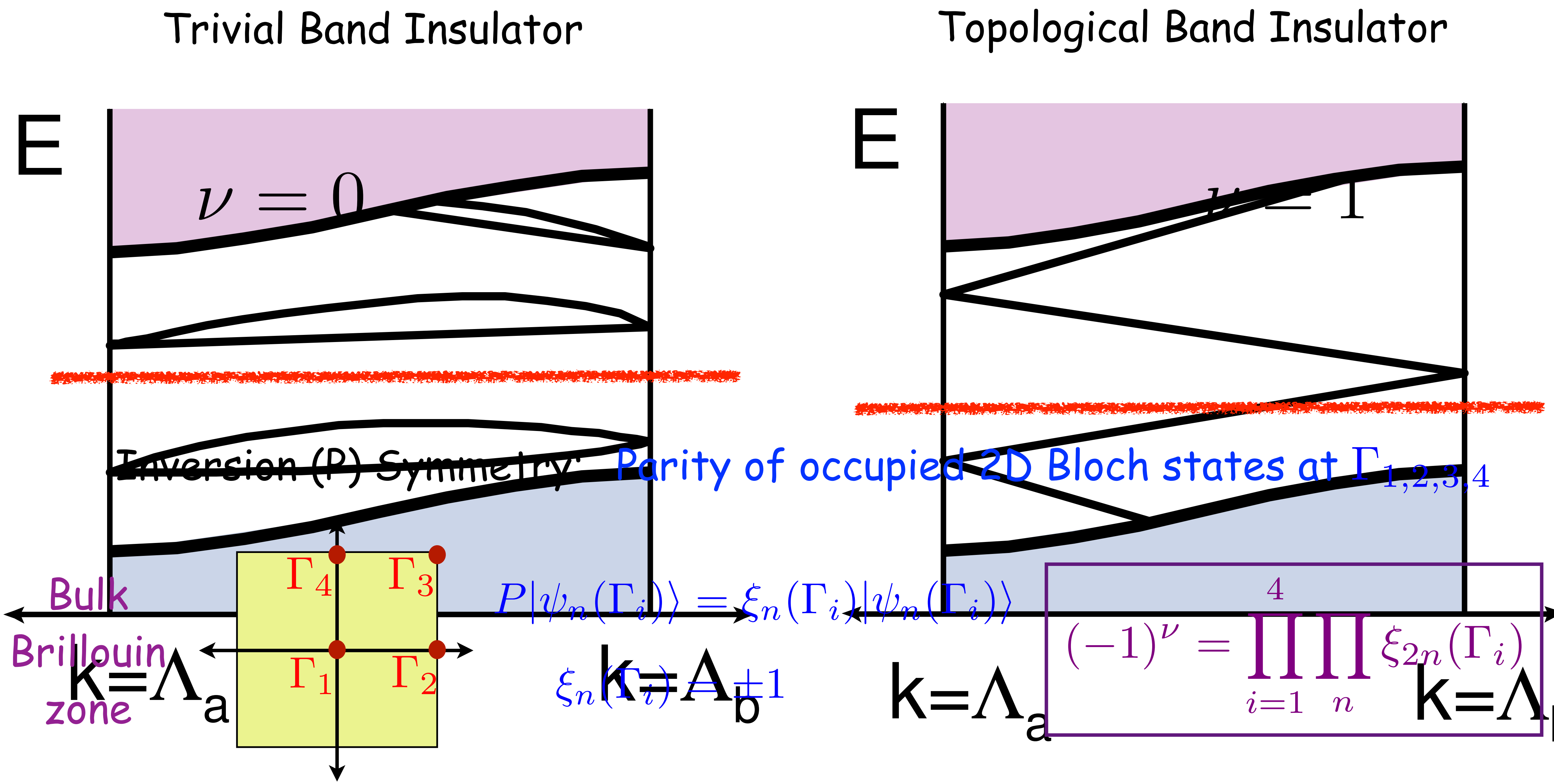


Inversion (P) Symmetry: Parity of occupied 2D Bloch states at $\Gamma_{1,2,3,4}$

$$P|\psi_n(\Gamma_i)\rangle = \xi_n(\Gamma_i)|\psi_n(\Gamma_i)\rangle$$

$$\xi_n(\Gamma_i) = \pm 1$$

$$\boxed{(-1)^\nu = \prod_{i=1}^{4} \prod_n \xi_{2n}(\Gamma_i)}$$

Spin-Orbit driven inversion of two bands with opposite parity

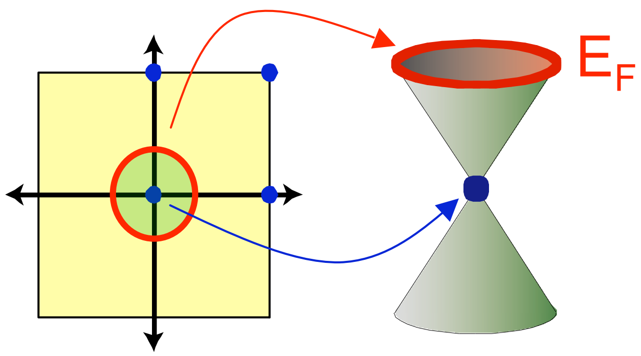
C. L. Kane, E. Mele, L. Fu B. A. Bernevig, T. L. Hughes, X.-L. Qi, S. C. Zhang ..

3D Topological Band Insulator

In 3D there are four Z_2 invariants: $(\nu;\nu_1\nu_2\nu_3)$
characterizing the bulk.
These determine how surface states connect.

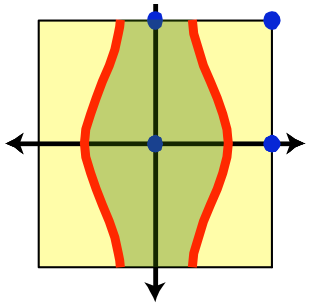
$\nu = 1$: Strong Topological Insulator

Fermi surface encloses odd number of Dirac points



$\nu = 0$: Weak Topological Insulator

Fermi surface encloses even number of Dirac points



L. Fu, C. L. Kane
J. E. Moore, L. Balents
R. Roy

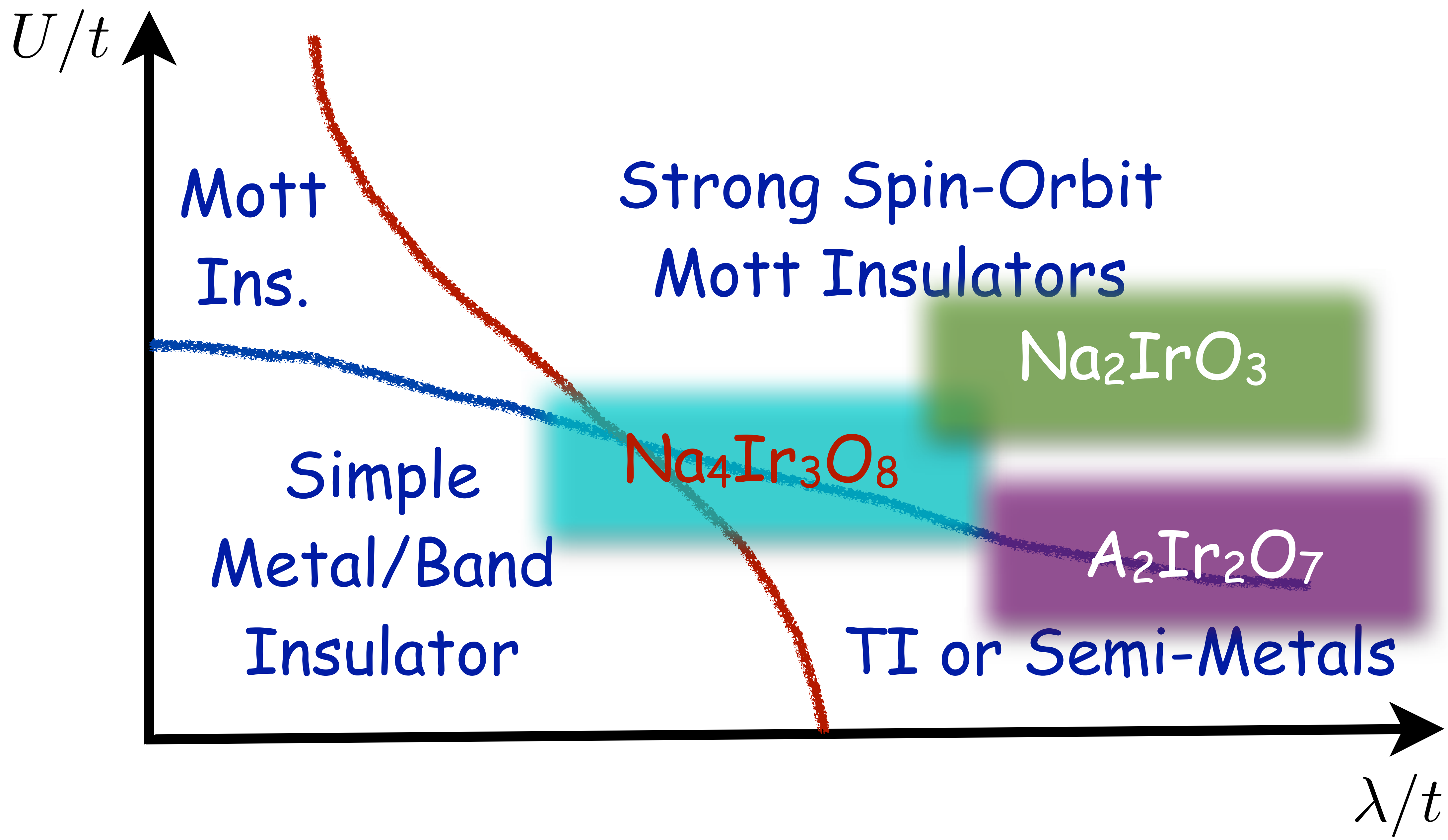
Non-trivial boundary states

Non-trivial topological invariant

Where can we find them ?
especially in
correlated materials

Interactions and Spin-Orbit Coupling

$$H = \sum_{ij,\alpha} t_{ij,\alpha\beta} c^\dagger_{i\alpha} c_{j\beta} - \lambda \sum_i \mathbf{L}_i \cdot \mathbf{S}_i + U \sum_i n_i(n_i - 1)$$



5d transition metal (Ir) oxides: New Playground

Energy(K)	3d TM (Fe,Co,Ni,Cu..)	4f Ln (Ce, Pr, Nd...)	5d TM (Re, Os, Ir, Pt...)
10^5	Coulomb U	Coulomb U	
10^4	Crystal field D	Spin-orbit coupling λ	Spin-orbit coupling λ, Coulomb U, Crystal field D
10^3			
10^2	Spin-orbit coupling λ	Crystal field D	
10^1			

5d: U ~ 0.5-1 eV

λ_{SO} ~ 0.5 eV

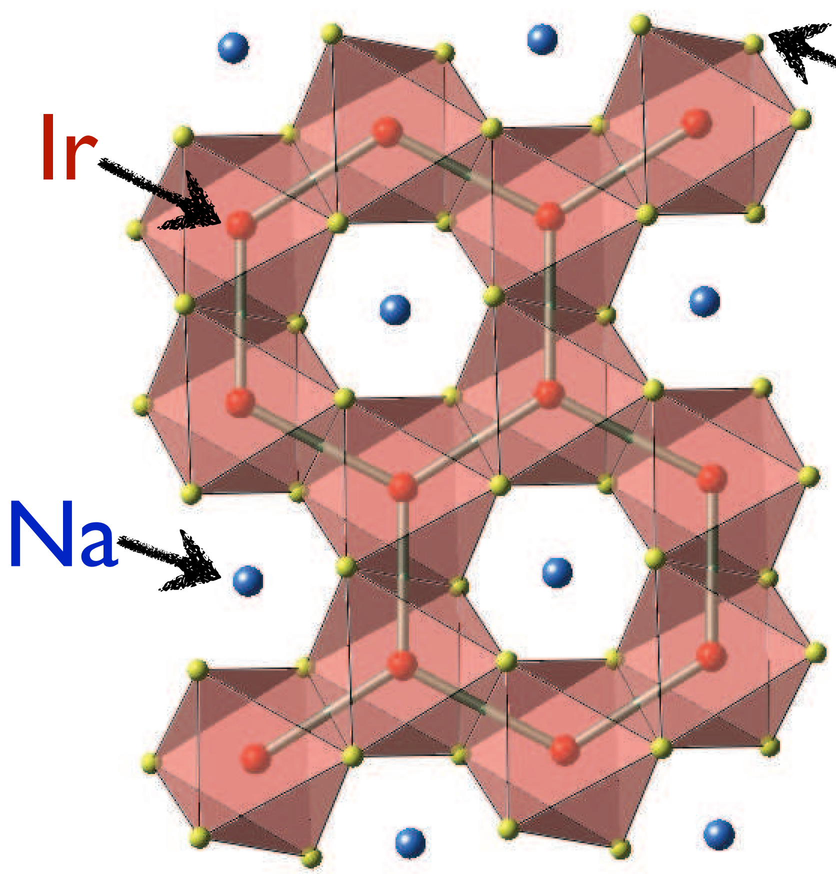
Traditional playground
for correlated electron physics

Honeycomb Iridates (A_2IrO_3)

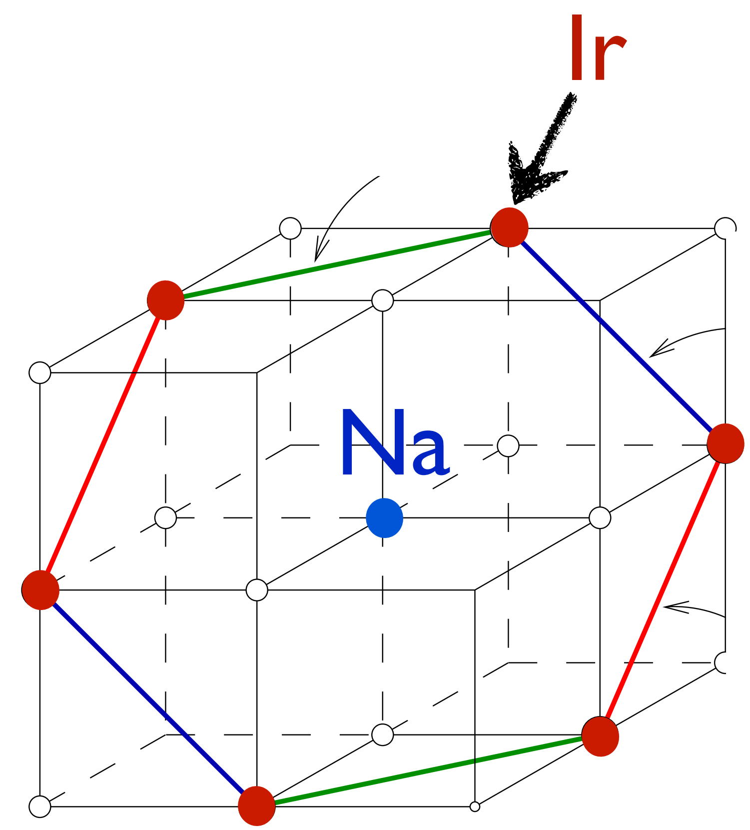
Type-I Topological Phases ?

Honeycomb Lattice of Ir^{4+}

Na_2IrO_3 5*d* transition metal oxides



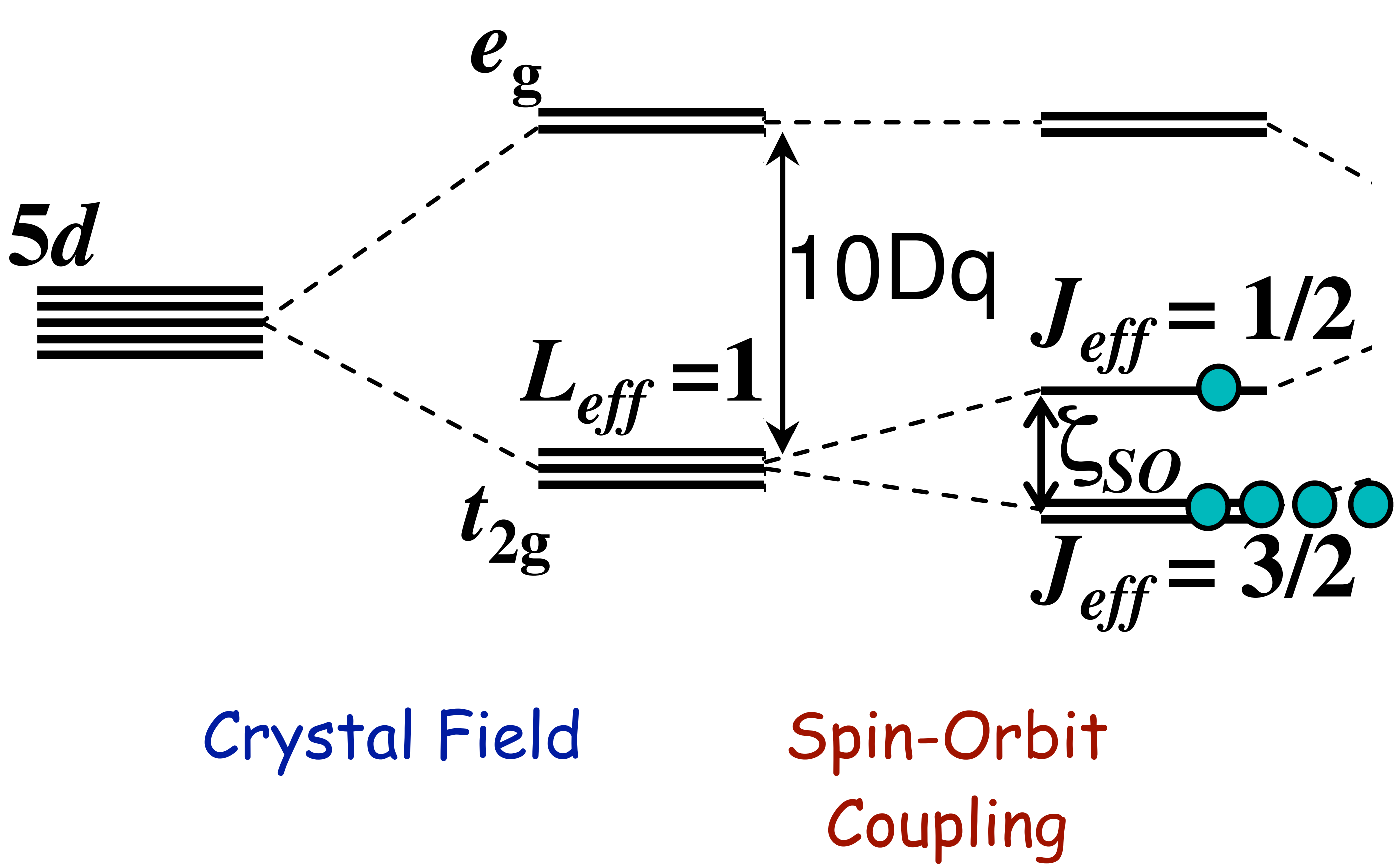
Edge-Sharing Oxygen Octahedra



Plane perpendicular to the [111] direction

5d orbitals of Ir^{4+}: large spin-orbit coupling

Ir^{4+} = [Xe] $4f^{14}\ 5d^5$



B.J.Kim, C. Kim, J.H.Park, T.W.Noh, G.Cao et al., PRL 101, 076402 (2008)

B.J.Kim, H.Takagi, et al, Science 323, 1329 (2009)

$$|\uparrow_j\rangle = \frac{1}{\sqrt{3}}(i|xz,\downarrow_s\rangle + |yz,\downarrow_s\rangle + |xy,\uparrow_s\rangle)$$

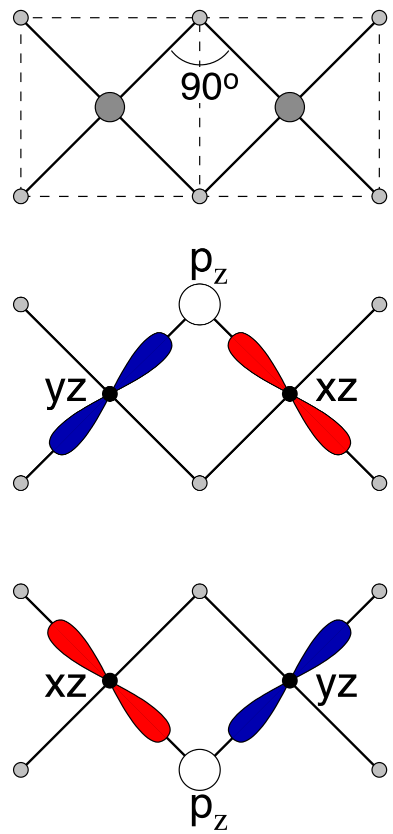
$$|\downarrow_j\rangle = -\frac{1}{\sqrt{3}}(i|xz,\uparrow_s\rangle - |yz,\uparrow_s\rangle + |xy,\downarrow_s\rangle)$$

$$\mathcal{P}_{t2g}\mathbf{L}_{\ell=2}\mathcal{P}_{t2g} = -\mathbf{L}^{\mathrm{eff}}_{\ell=1}$$

Strong Coupling Limit the Kitaev Model ?

Considering only
Super-exchange processes

(b)



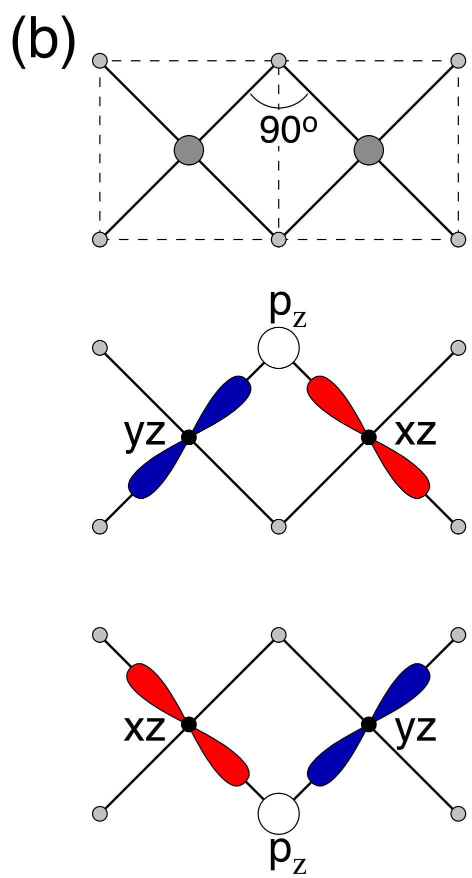
Edge-Sharing
Oxygen Octahedra

Isotropic Heisenberg
Exchange suppressed

Strong Coupling Limit the Kitaev Model ?

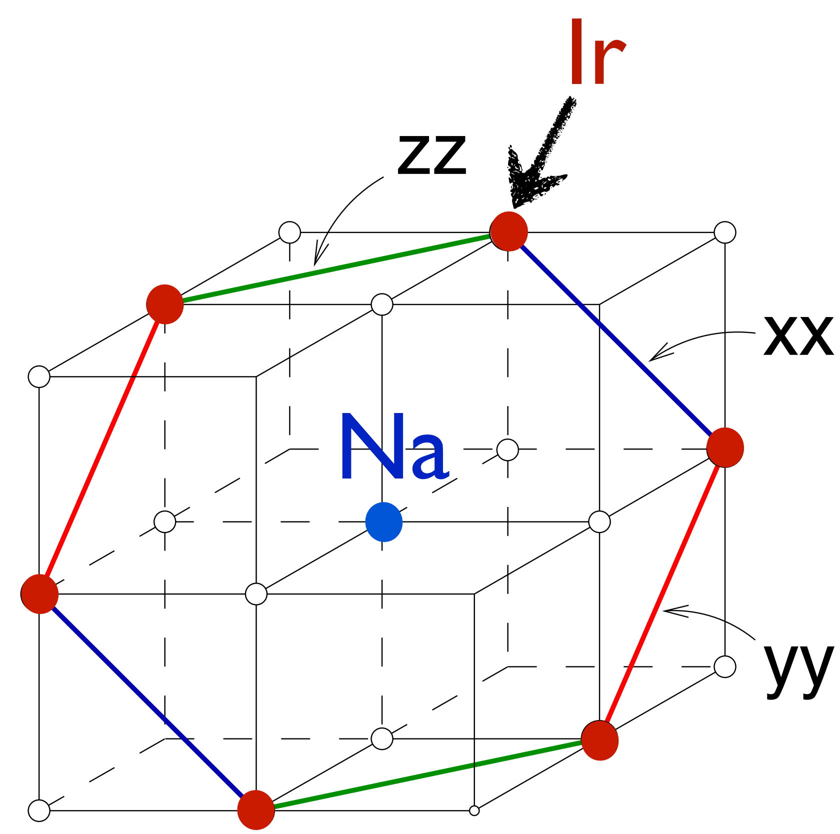
Including Hund's coupling and projecting to J_{eff}=1/2 manifold

$$\mathcal{H}_{ij}^{(\gamma)} = -JS_i^\gamma S_j^\gamma \qquad \gamma = x, y, z$$



Edge-Sharing Oxygen Octahedra

Isotropic Heisenberg Exchange suppressed



G. Jackeli and G. Khaliullin, PRL 102, 256403 (2009)

Strong Coupling Limit the Kitaev Model ?

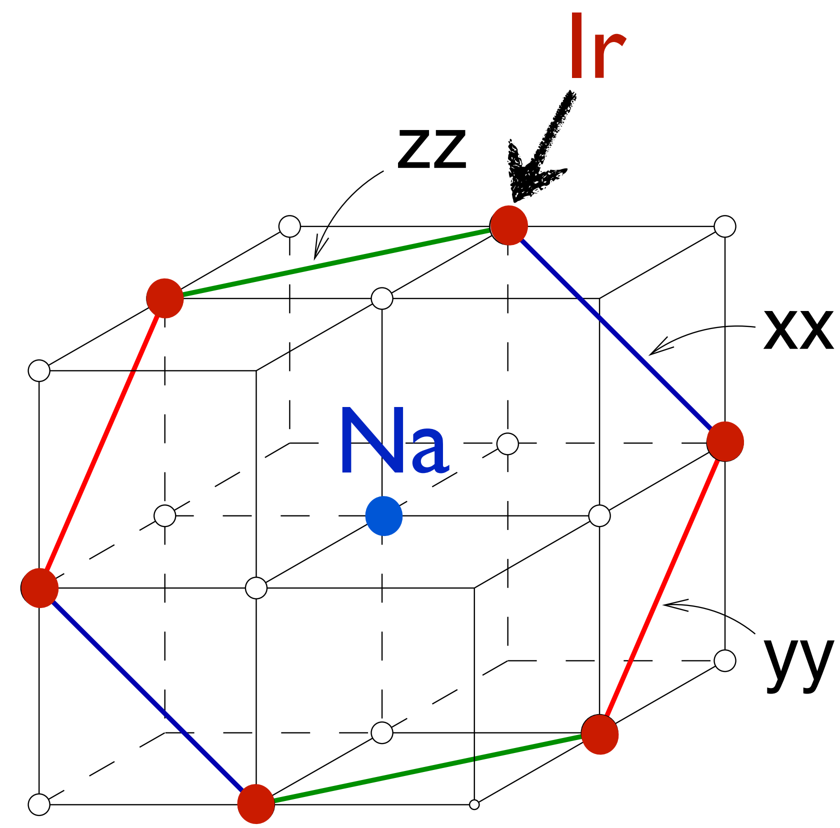
Including Hund's coupling and projecting to J_{eff}=1/2 manifold

$$\mathcal{H}_{ij}^{(\gamma)} = -J S_i^\gamma S_j^\gamma \qquad \gamma = x, y, z$$

Exactly Solvable

Quantum Spin Liquid Ground State

Spin-1/2 Spinons are Majorana Fermions (anti-particles to themselves)



G. Jackeli and G. Khaliullin, PRL 102, 256403 (2009)

Strong Coupling Limit
the Kitaev Model ?

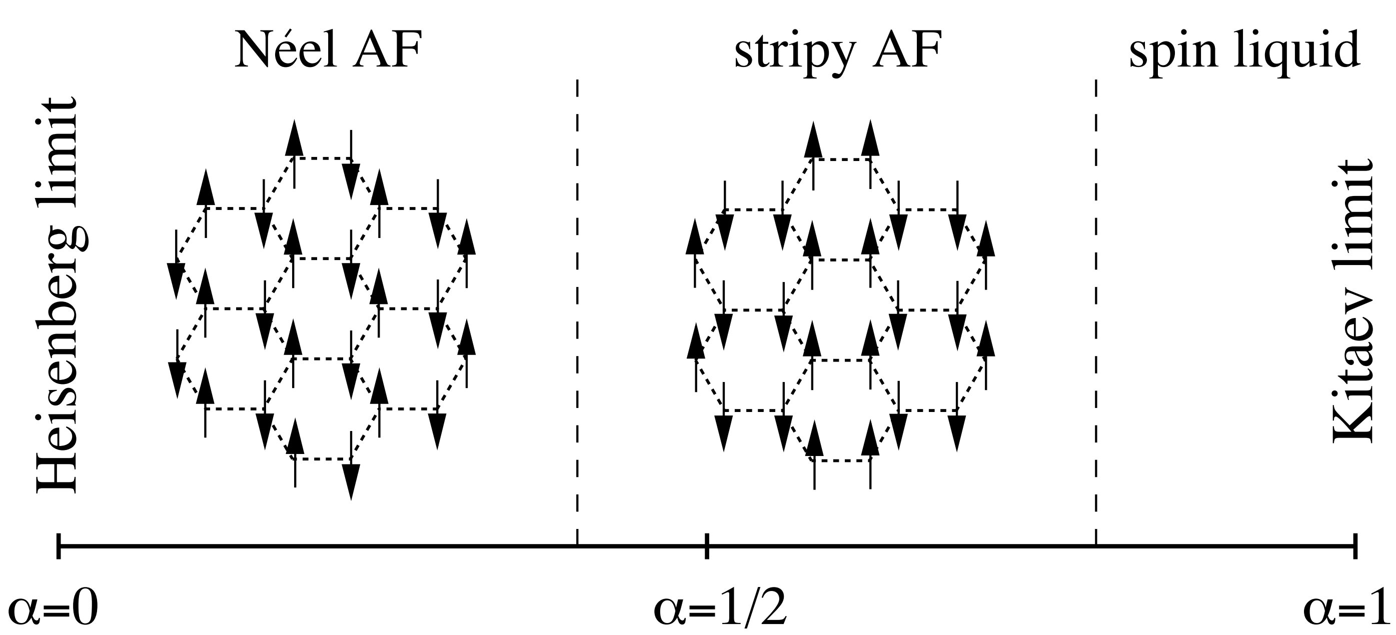
Including Hund's coupling
direct exchange,
spin-orbit

$$\mathcal{H}_{ij}^{(\gamma)} = -J_1\, S_i^\gamma S_j^\gamma + J_2\, \boldsymbol{S}_i \cdot \boldsymbol{S}_j \qquad \gamma = x, y, z$$

Heisenberg-Kitaev Model

J. Chaloupka, G. Jackeli and G. Khaliullin, PRL 105, 027204 (2010)

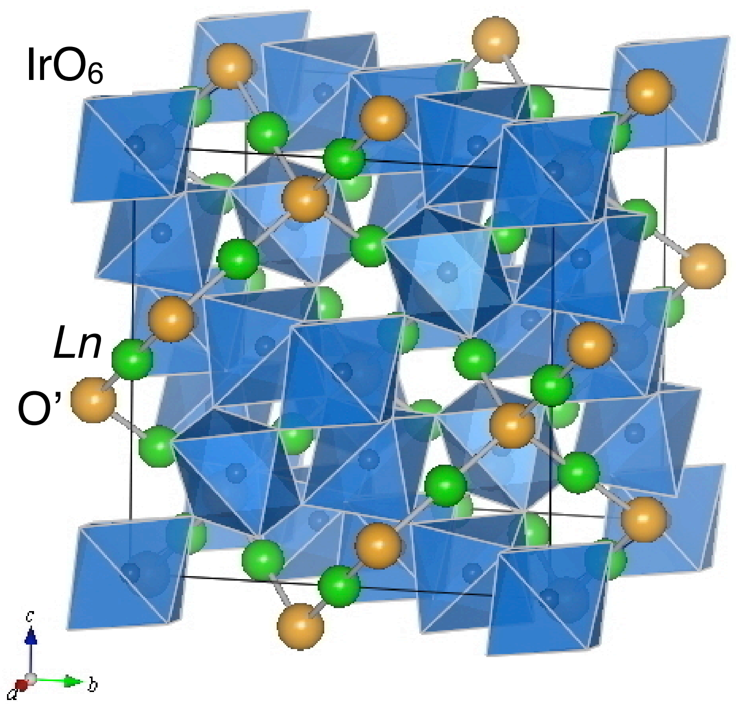
$$H_{\mathrm{HK}} = (1-\alpha)\sum_{\langle i,j\rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j - 2\alpha \sum_{\gamma-\mathrm{links}} \sigma_i^\gamma \sigma_j^\gamma$$

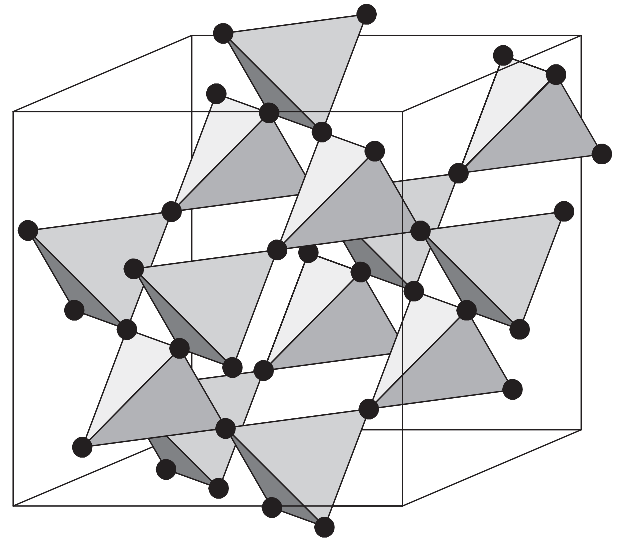


Pyrochlore Iridates ($A_2Ir_2O_7$)

Type-II Topological Phases ?

Pyrochlore Iridates $A_2Ir_2O_7$





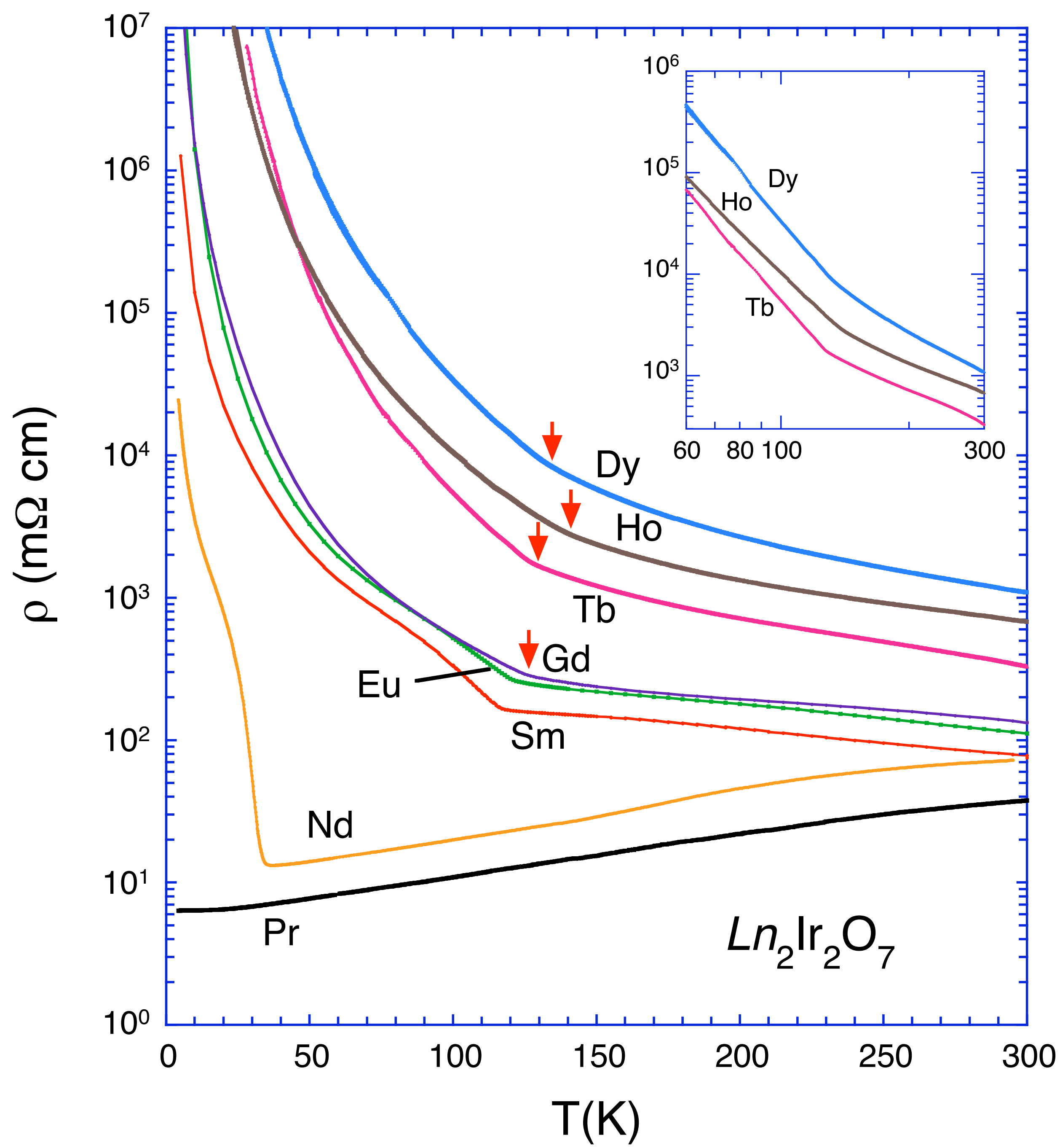
A= Y, Ho, Dy, Tb, Gd, Eu, Sm, Nd, Pr

A=Y, Ln and Ir reside on the inter-penetrating two pyrochlore lattices (cubic, FCC Bravais lattice)

D. Yanagishima and Y. Maeno, JPSJ 70, 2880 (2001)

K. Matsuhira et al JPSJ 76, 043706 (2007)

$A_2Ir_2O_7$ Metal to Insulator Transition ?



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Also Earlier Data from
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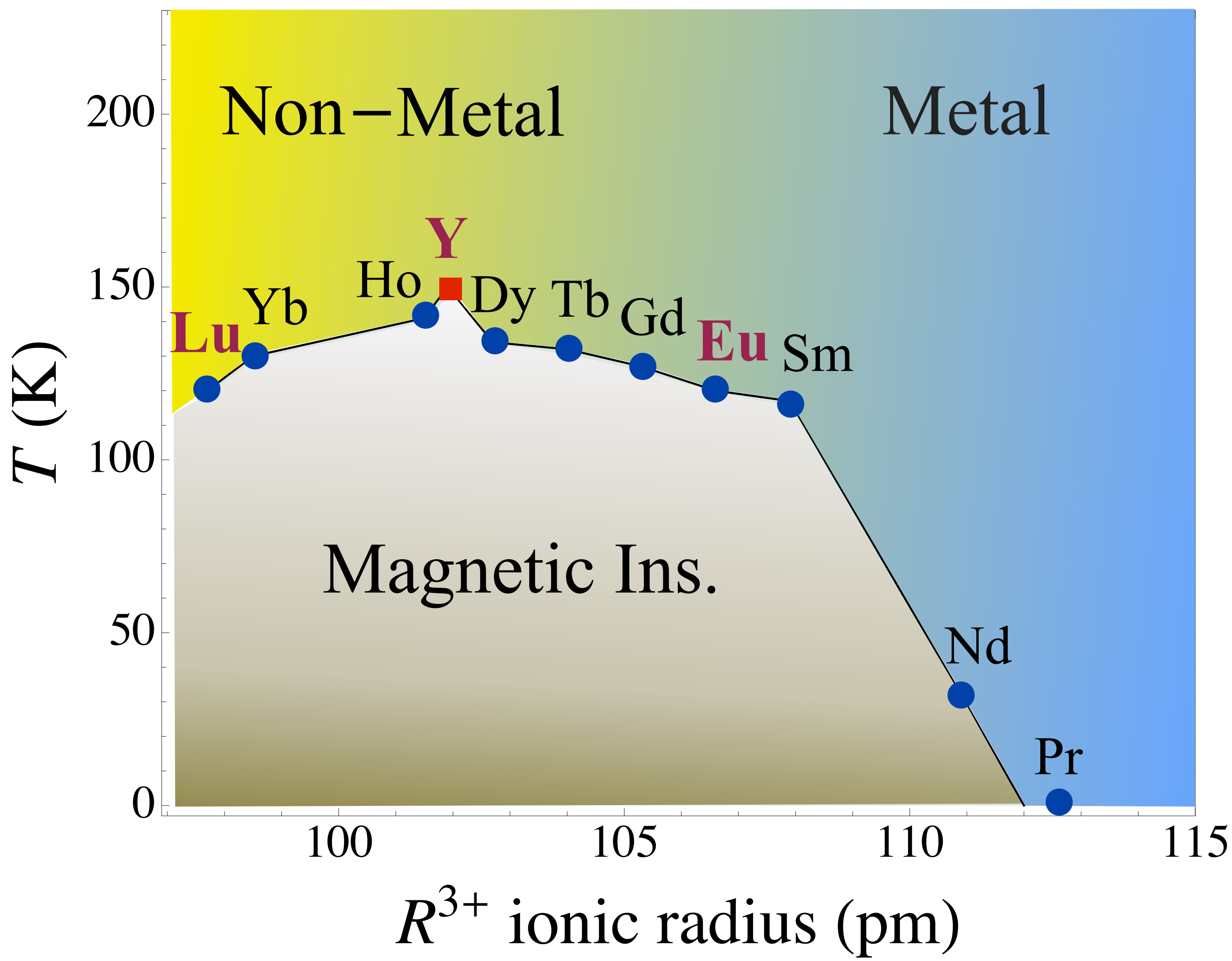

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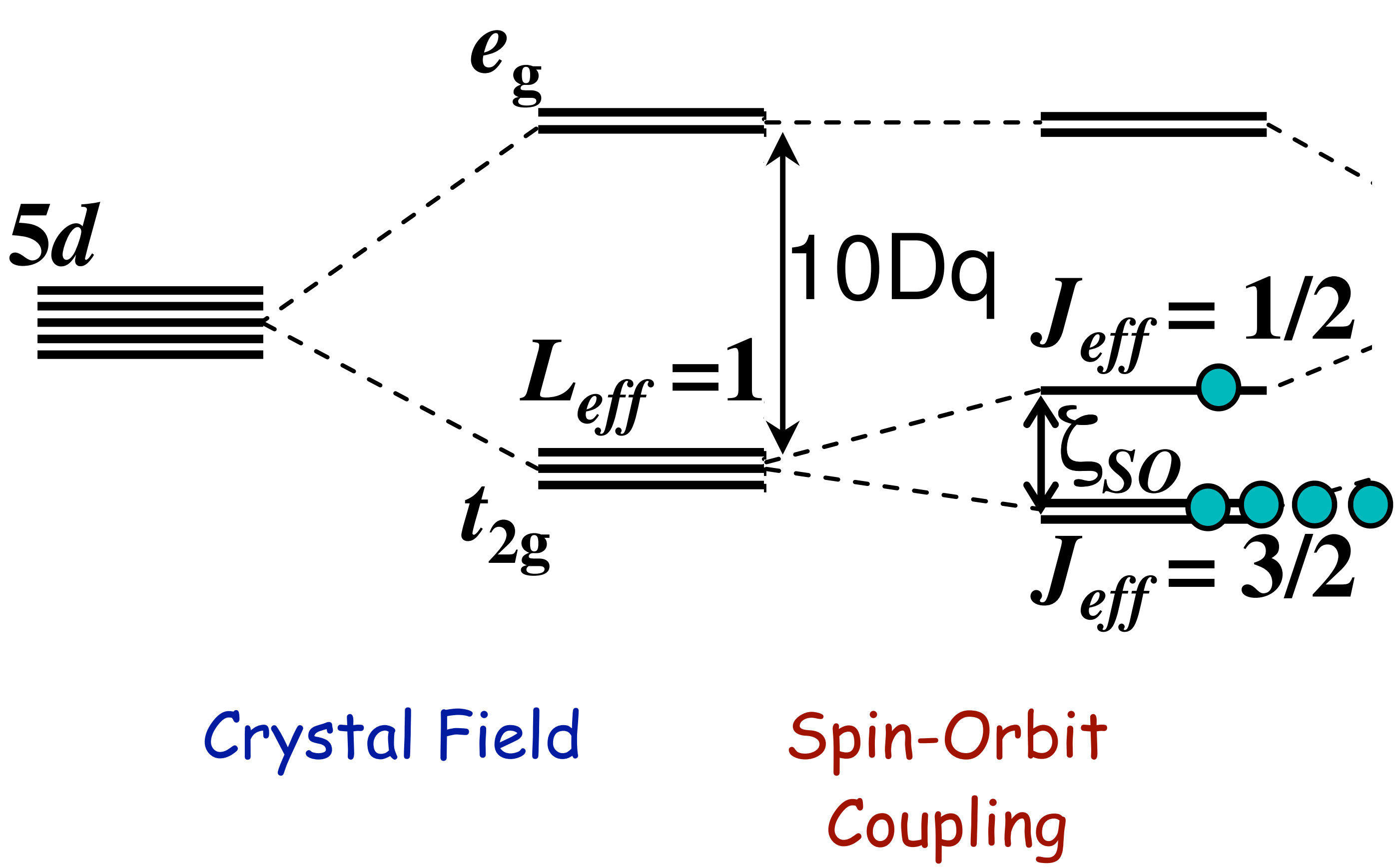

Construct tight binding model for J_{eff}=1/2

+

Hubbard U

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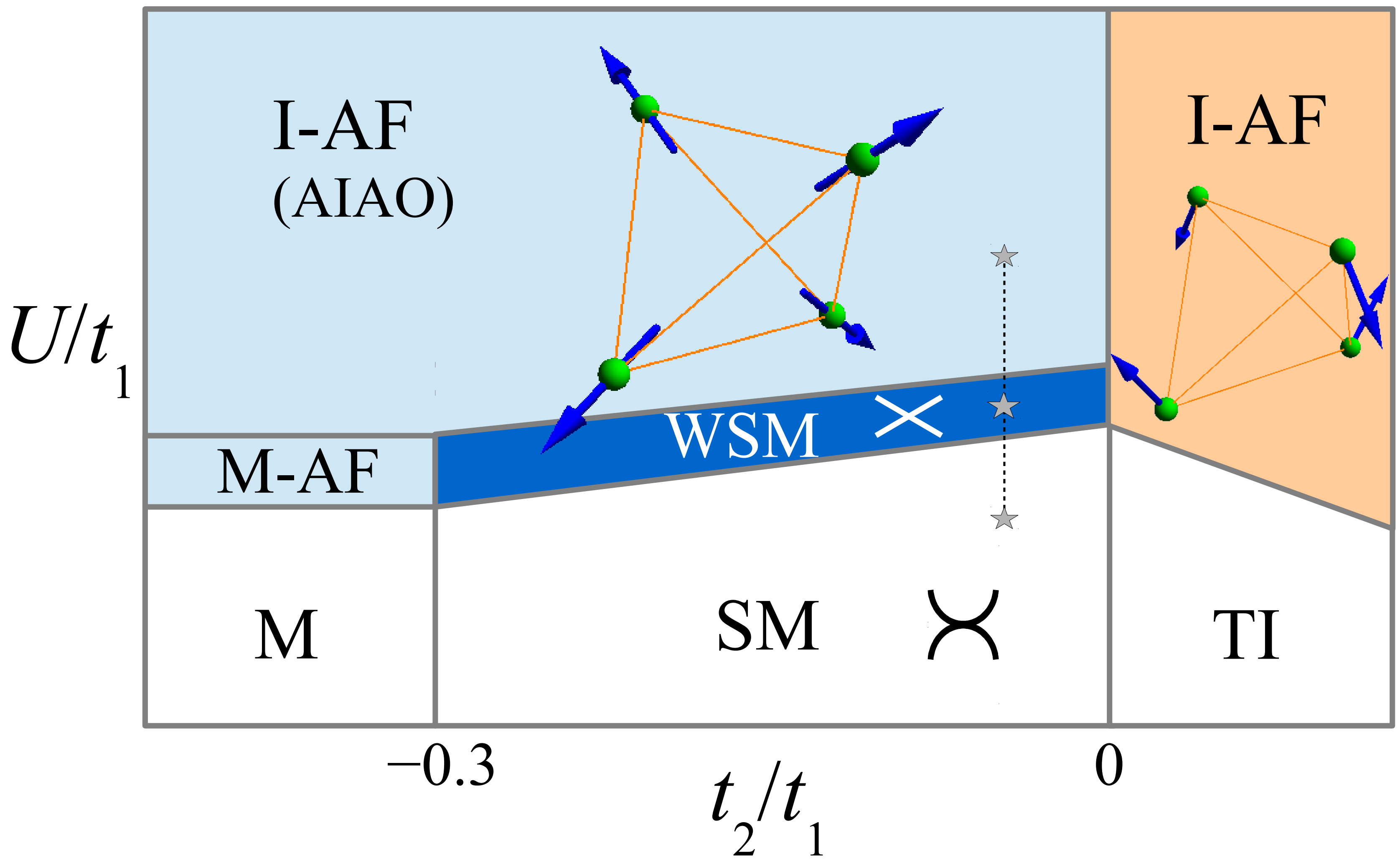
$$\mathcal{P}_{t2g}\mathbf{L}_{\ell=2}\mathcal{P}_{t2g} = -\mathbf{L}^{\text{eff}}_{\ell=1}$$

Generic Phase Diagram



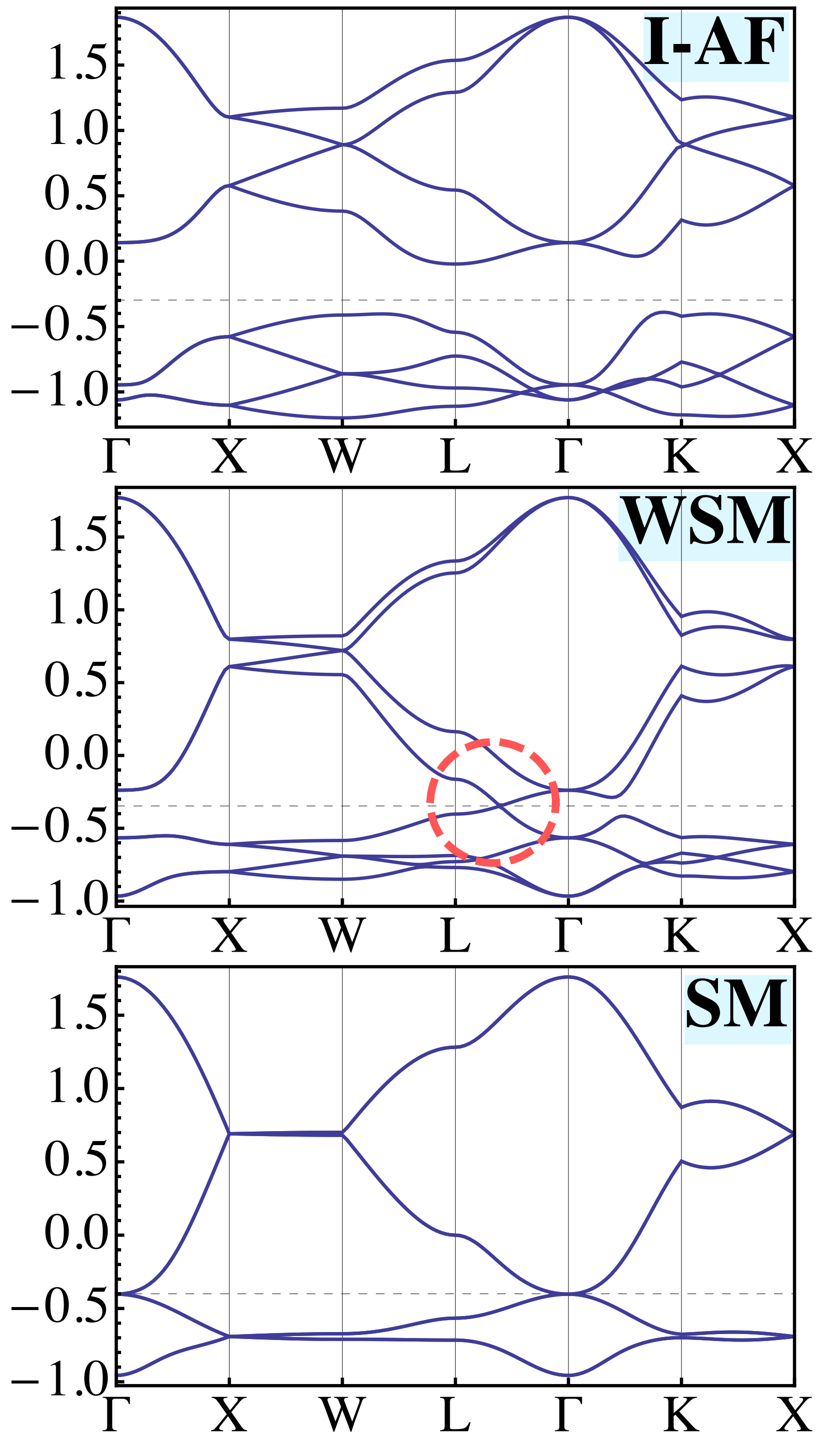
W. Witczak-Krempa,
Y. B. Kim
(2012)

WSM = Weyl Semi-Metal

Semi-metal with 3D Dirac points in the bulk

c.f. X. Wan, A. Turner, A. Vishwanath, S. Savrasov, PRB 83, 205101 (2011)

Effect of Interaction: Hartree-Fock



Magnetic Insulator

Weyl Semi-Metal

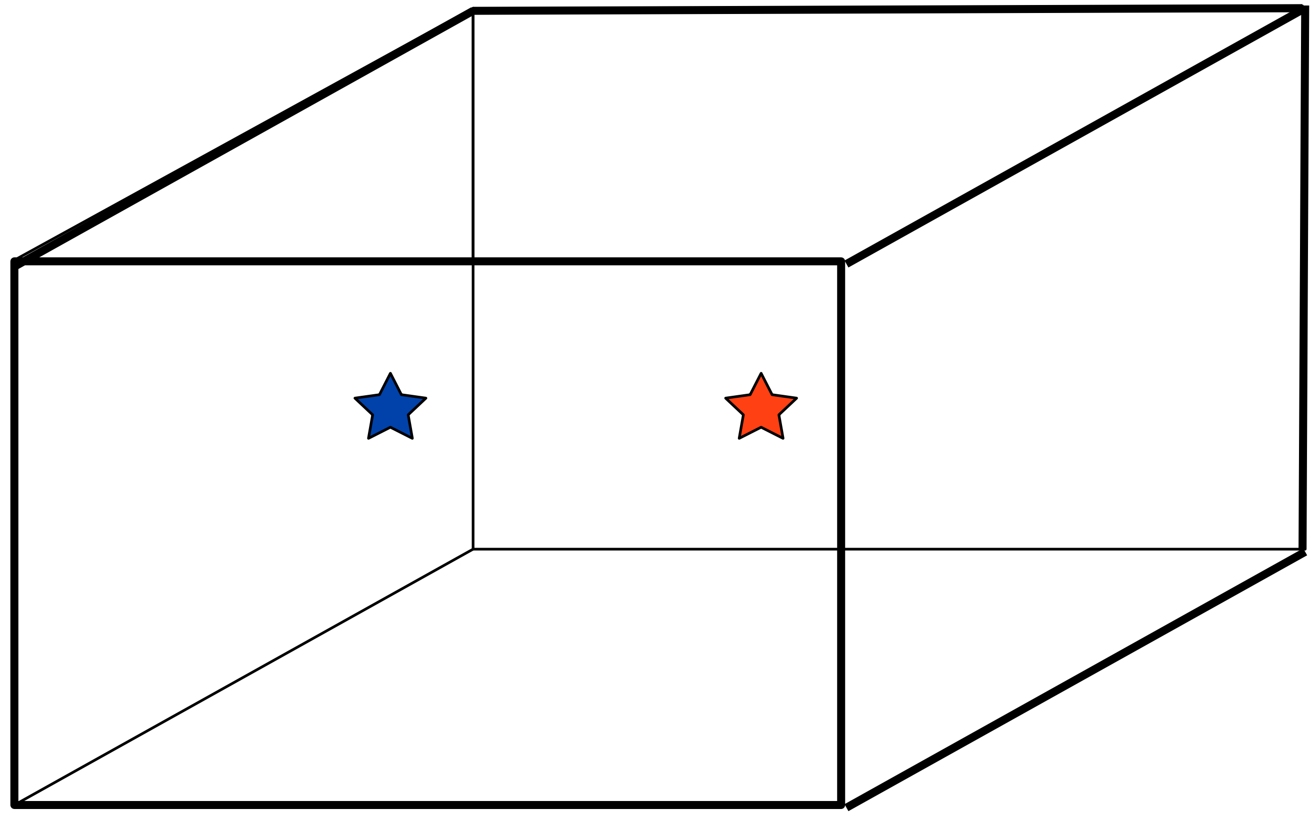
Semi-Metal

W. Witczak-Krempa, Y. B. Kim, PRB 85, 045124 (2012)

Weyl Semi-Metal

A pair of Weyl fermion points related by inversion; carry opposite chirality

$$\mathcal{H} = \sum_{i=1}^{3} \mathbf{v}_i \cdot \mathbf{k}\ \sigma_i \qquad c = \mathrm{sign}(\mathbf{v}_1 \cdot \mathbf{v}_2 \times \mathbf{v}_3) = \pm 1$$



Surface State: Fermi arcs at the surface BZ

X. Wan, A. Turner, A. Vishwanath, S. Y. Savrasov, PRB 83, 205101 (2011)

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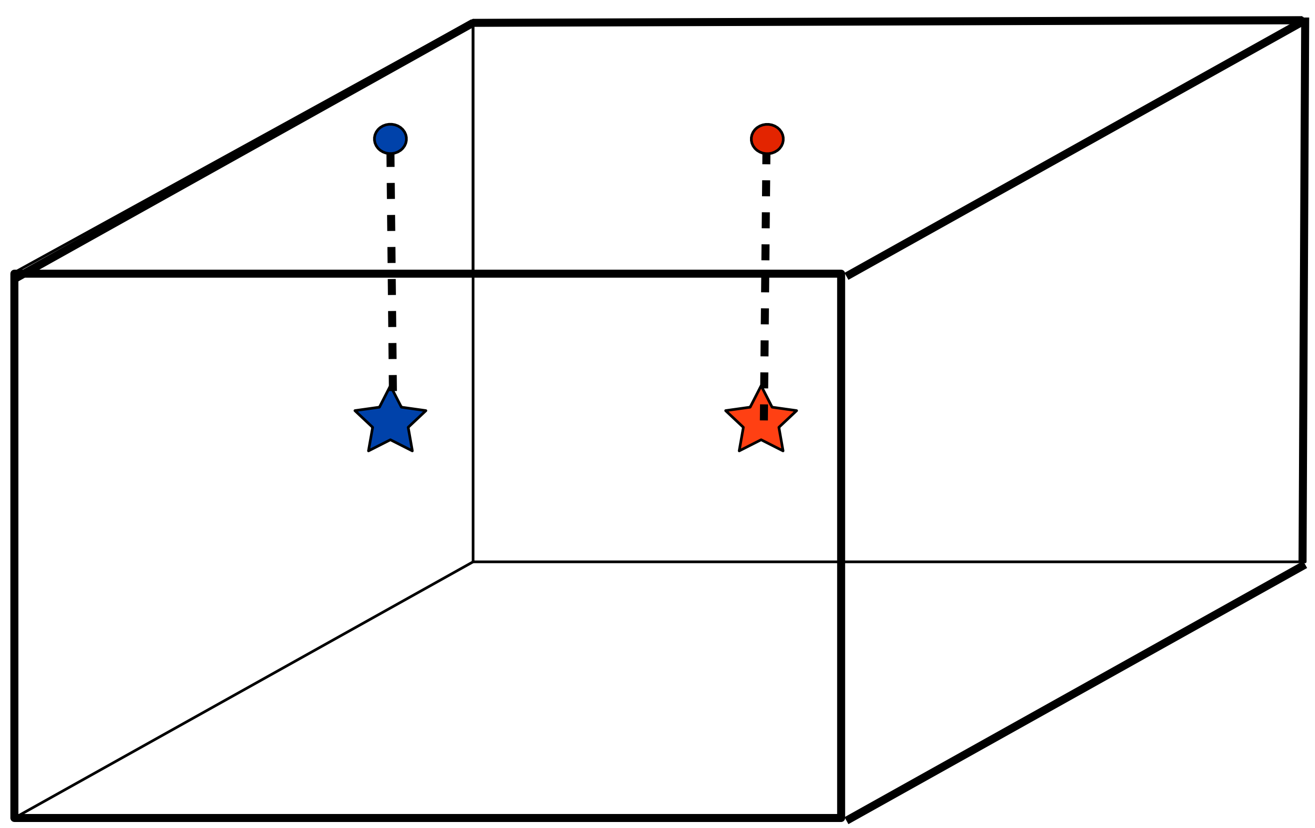

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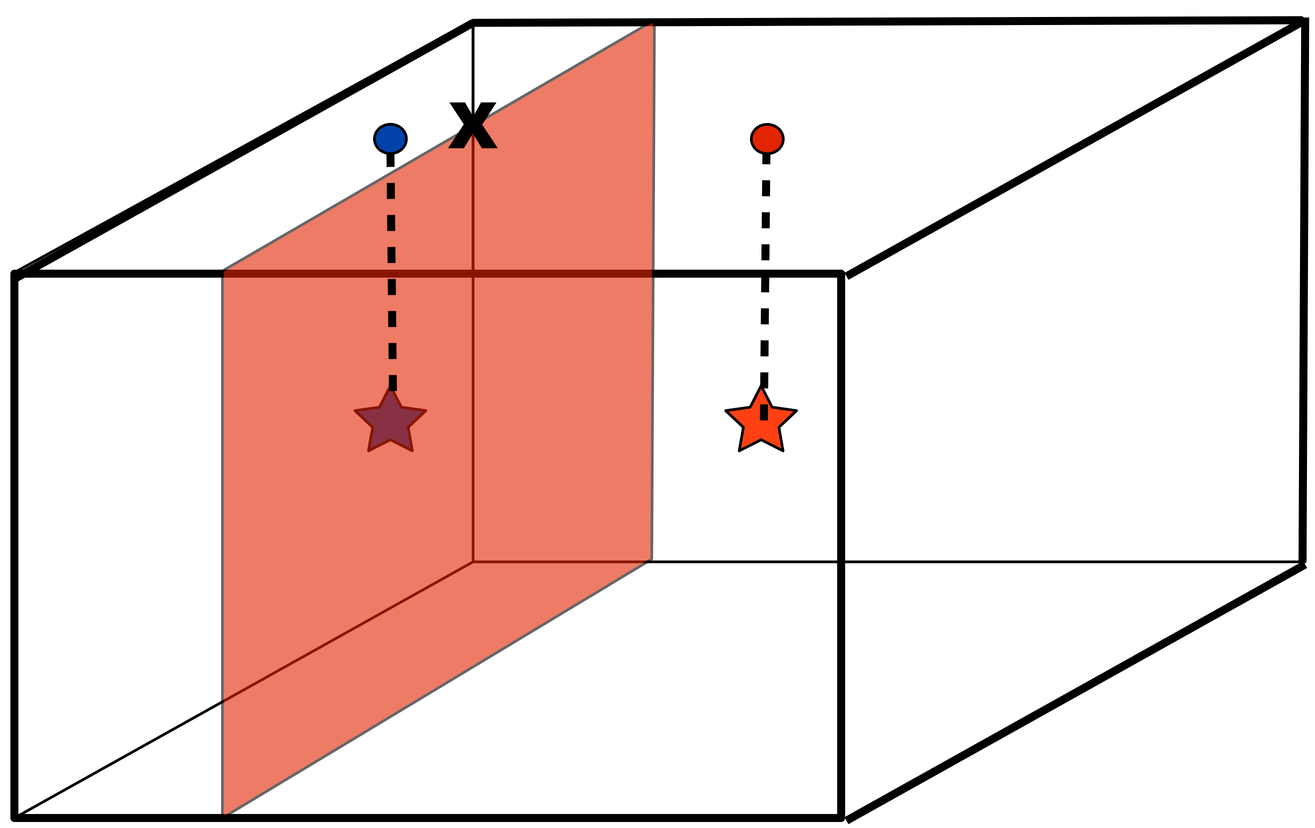

Integer Quantum Hall state: C=1

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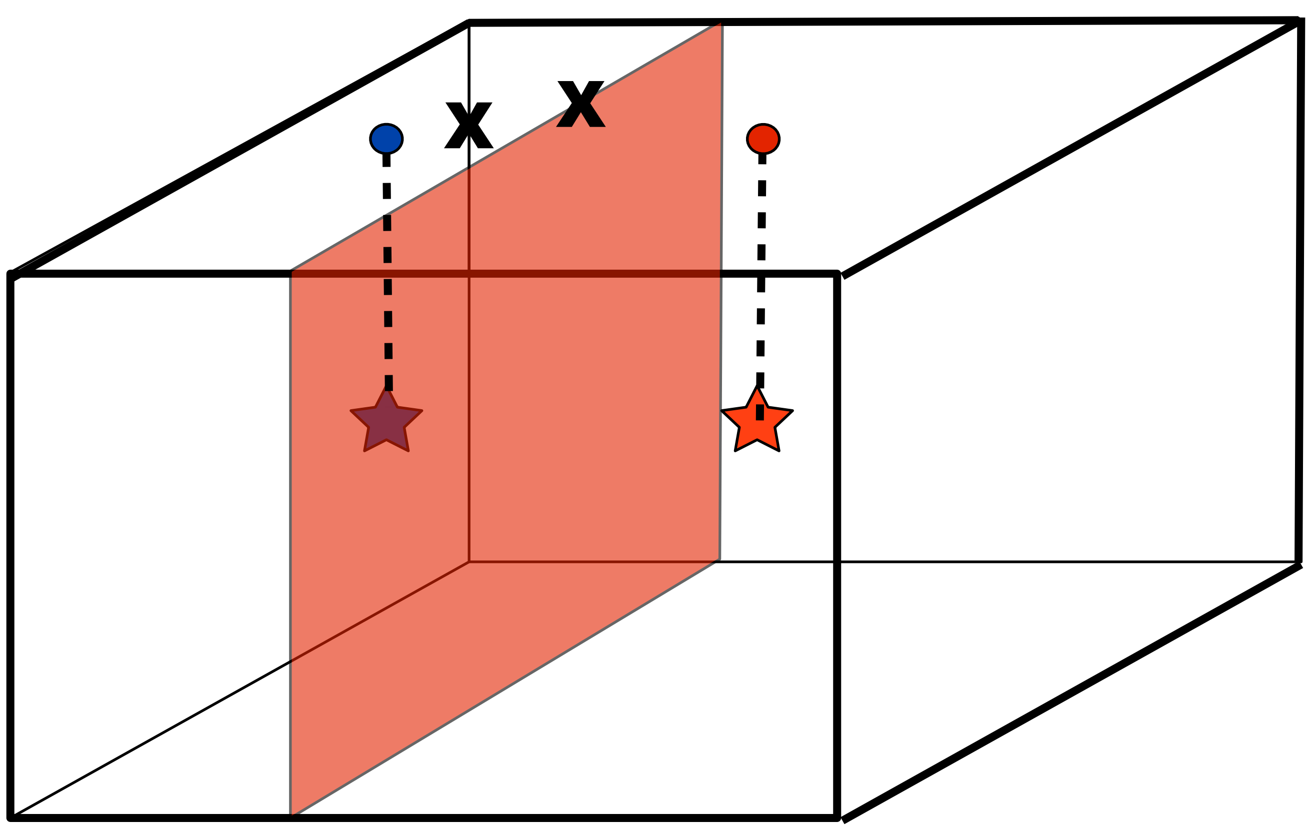

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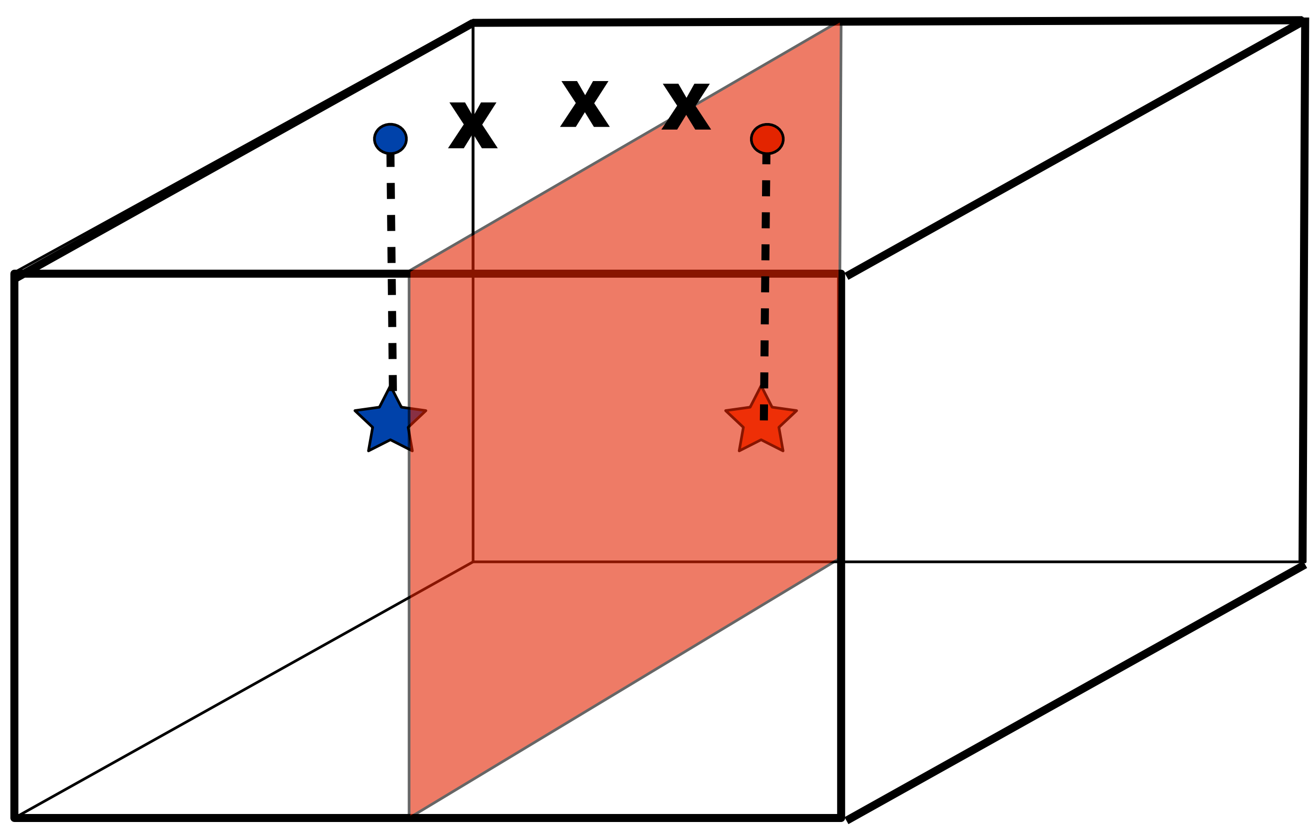

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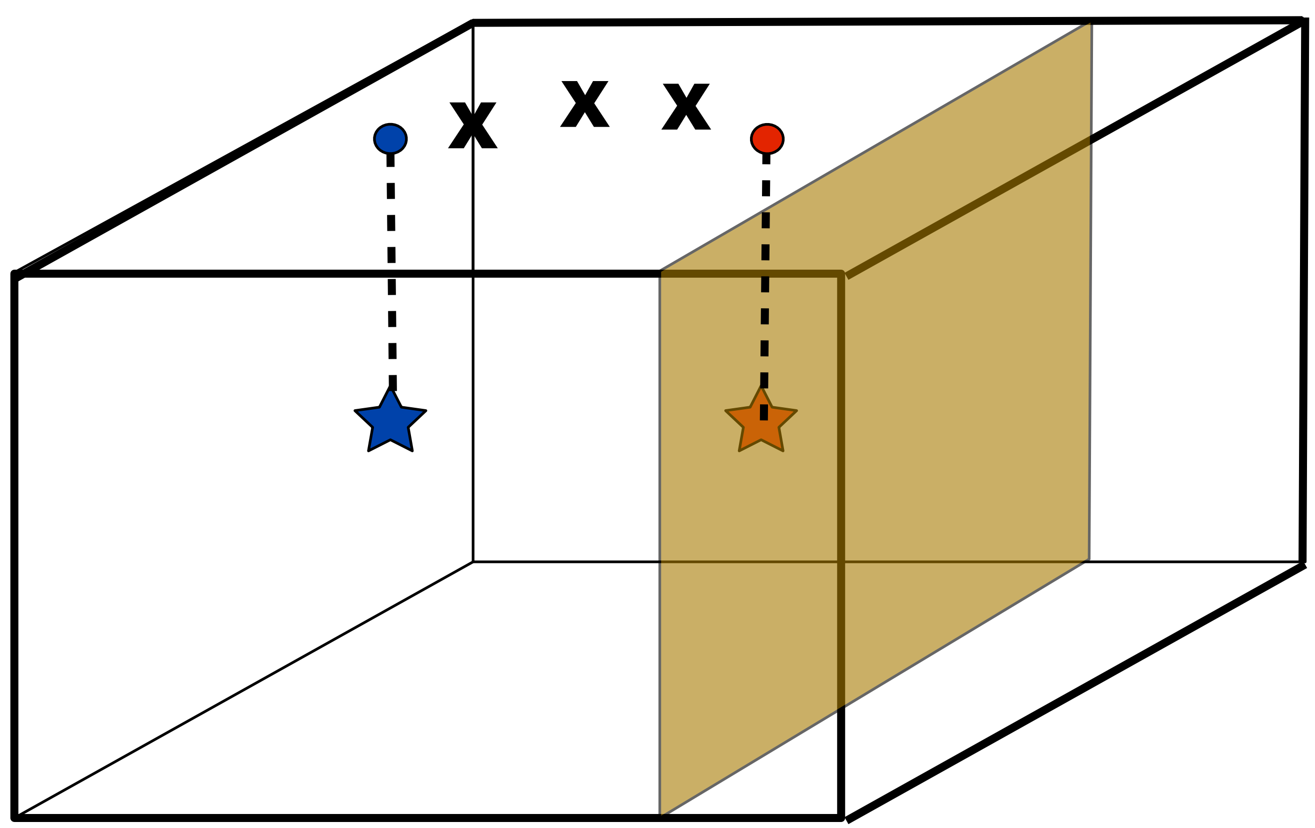

Trivial state: C=0

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X. Wan, A. Turner, A. Vishwanath, S. Y. Savrasov, PRB 83, 205101 (2011)

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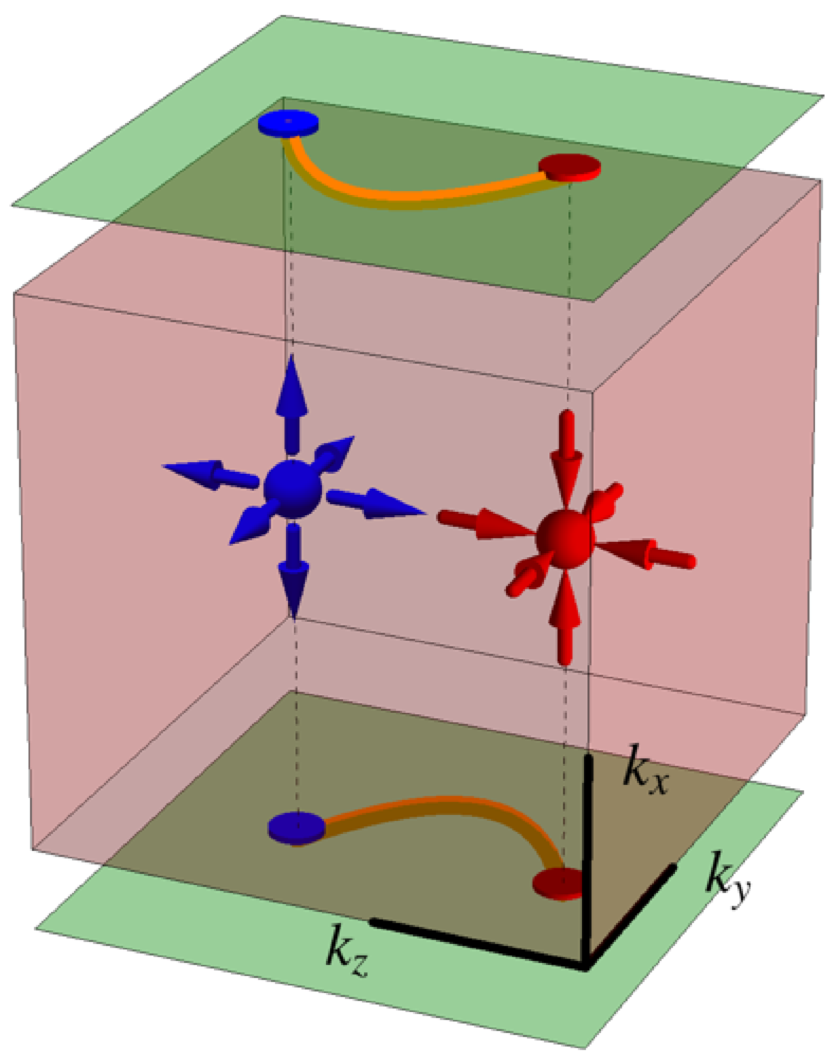

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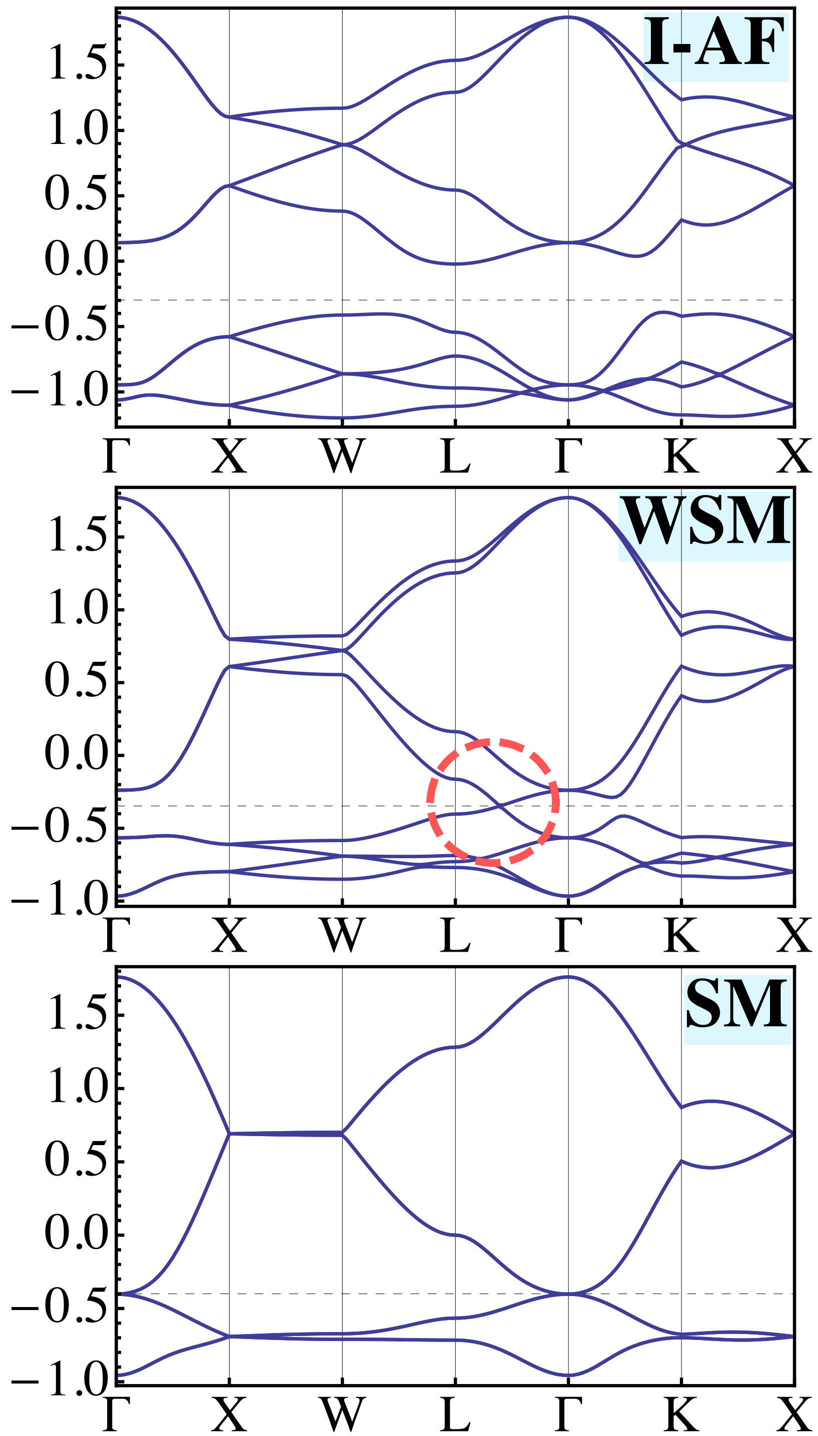


Magnetic Insulator

Weyl Semi-Metal

Semi-Metal

W. Witczak-Krempa, Y. B. Kim, PRB 85, 045124 (2012)

Minimal Hamiltonian: Luttinger Model

$\vec{k} \cdot \vec{p}$ expansion near Γ

$$\mathcal{H}_0(k) = \alpha_1 k^2 + \alpha_2 (\vec{k} \cdot \vec{J})^2 + \alpha_3 (k_x^2 J_x^2 + k_y^2 J_y^2 + k_z^2 J_z^2)$$

$$= \frac{k^2}{2\tilde{M}_0} + \frac{(\frac{5}{4}k^2 - \vec{k} \cdot \vec{J})^2}{2m} - \frac{(k_x^2 J_x^2 + k_y^2 J_y^2 + k_z^2 J_z^2)}{2M_c}$$

$\vec{J} = (J_x, J_y, J_z)$ are J=3/2, 4 x 4 matrices

Quadratic band touching of two doubly-degenerate bands

B. J. Yang, Y. B. Kim (2010)

Time-Reversal Symmetry Breaking

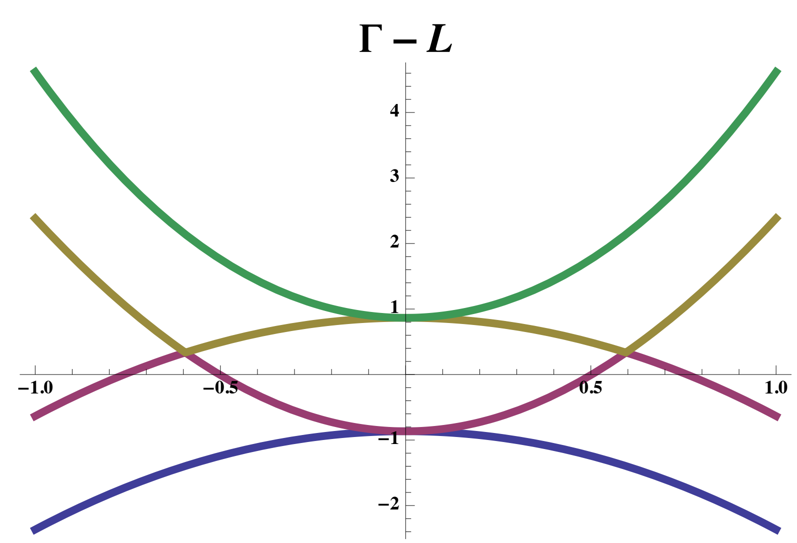
$$H_{\text{field}} = C_1(H_xJ_x + H_yJ_y + H_zJ_z) + C_2(H_xJ_x^3 + H_yJ_y^3 + H_zJ_z^3)$$

$$H_{\text{mag order}} = D_1(\{k_x, k_y\}V_z + \{k_y, k_z\}V_y + \{k_z, k_x\}V_y) + D_2(J_xJ_yJ_z + J_zJ_yJ_x)$$

$$V_x \equiv \{(J_y^2 - J_z^2)J_x\}, V_y \equiv \{(J_z^2 - J_x^2)J_y\}, V_z \equiv \{(J_x^2 - J_y^2)J_z\}$$

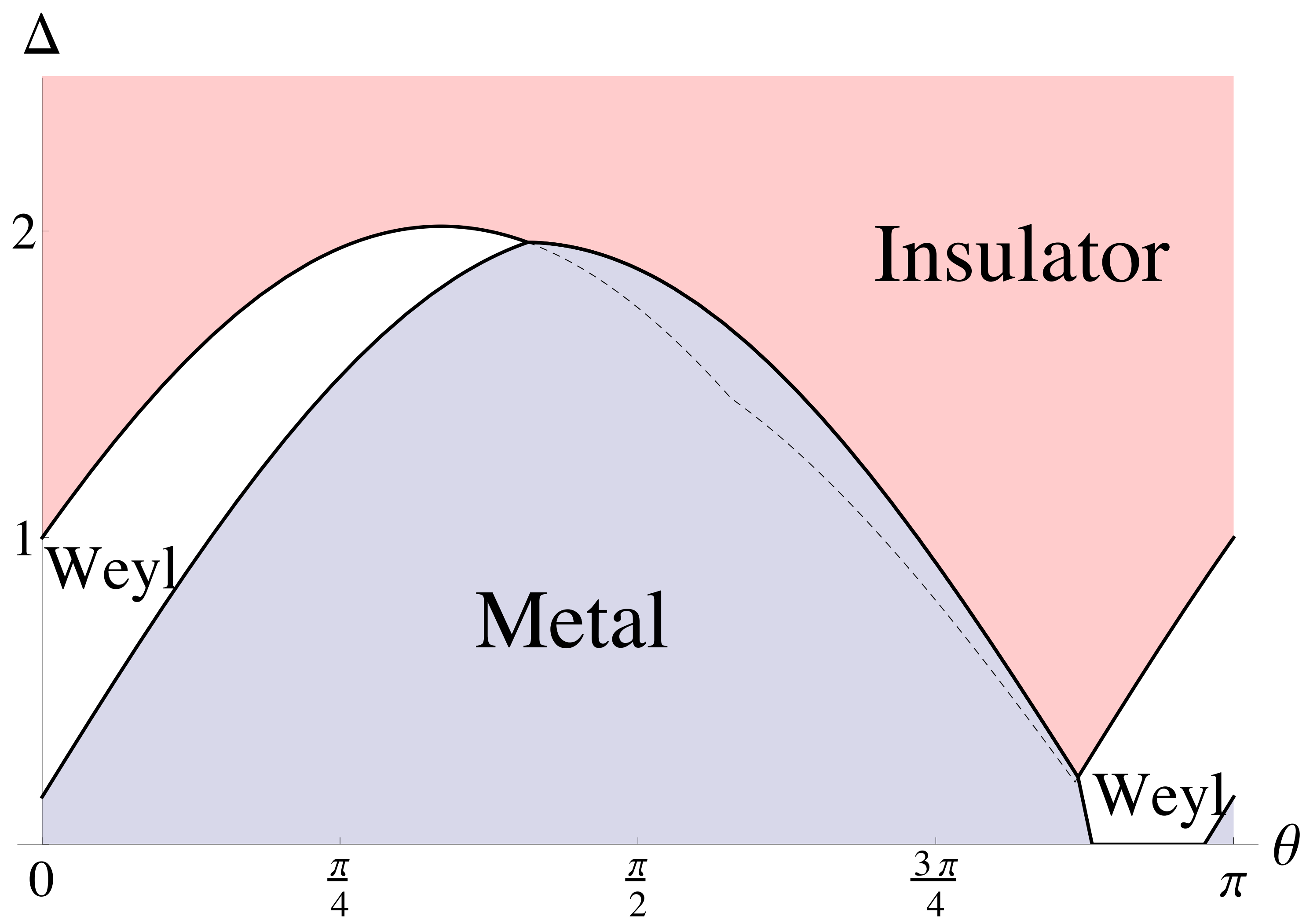
T. Hsieh, L. Fu (2012) E. G. Moon, C. Xu, Y. B. Kim, L. Balents (2012)

Both types of perturbations can generate Weyl fermions



Time-Reversal Symmetry Breaking and Strain

$$\mathcal{H}' = -\delta(J_z^2 - \frac{5}{4}) - H(\cos(\theta)J_z + \sin(\theta)J_z^3),$$



E. G. Moon, C. Xu, Y. B. Kim, L. Balents, arXiv:1212.1168

Long-range Coulomb interaction

Relevant in RG sense near the non-interacting limit

$\varepsilon = 4 - d$ expansion leads to non-trivial interacting (isotropic) fixed point

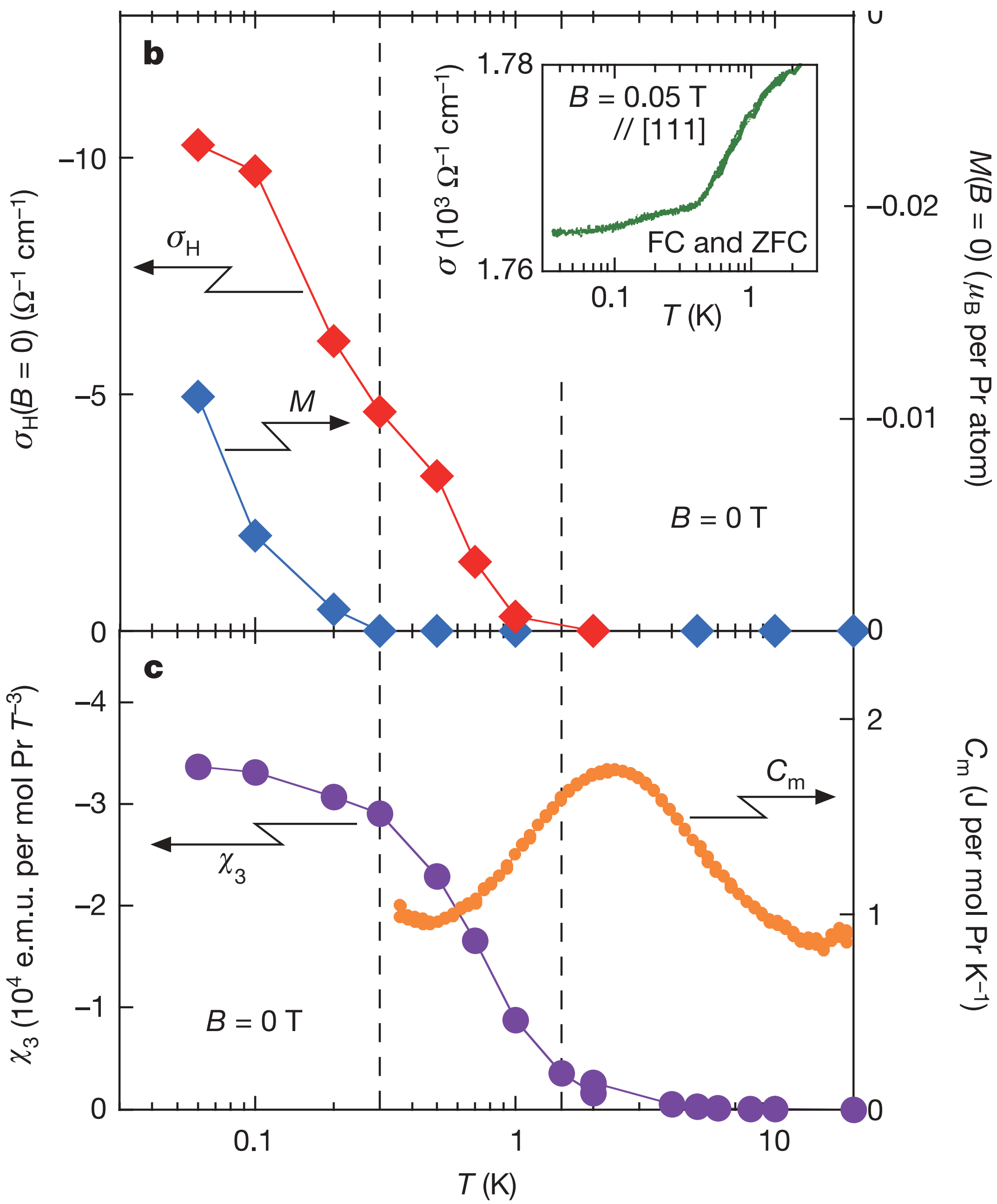
Non-Fermi Liquid scaling in physical quantities

$$z \approx 1.8 \qquad C_v \sim T^{d/z} \approx T^{1.7} \qquad \chi \sim a + bT^{0.5}$$

$$\chi_3 = \left.\frac{\partial^3 M}{\partial H^3}\right|_{H=0} \sim T^{-1.7} \qquad \sigma(\omega, T) \sim T^{1/z}\mathcal{F}(\omega/T) \qquad \sigma_{xy} \sim M^{0.51}$$

E. G. Moon, C. Xu, Y. B. Kim, L. Balents, arXiv:1212.1168

$Pr_2Ir_2O_7$



Y. Machida *et al*, 2010

Large anomalous Hall effect with "small" magnetization

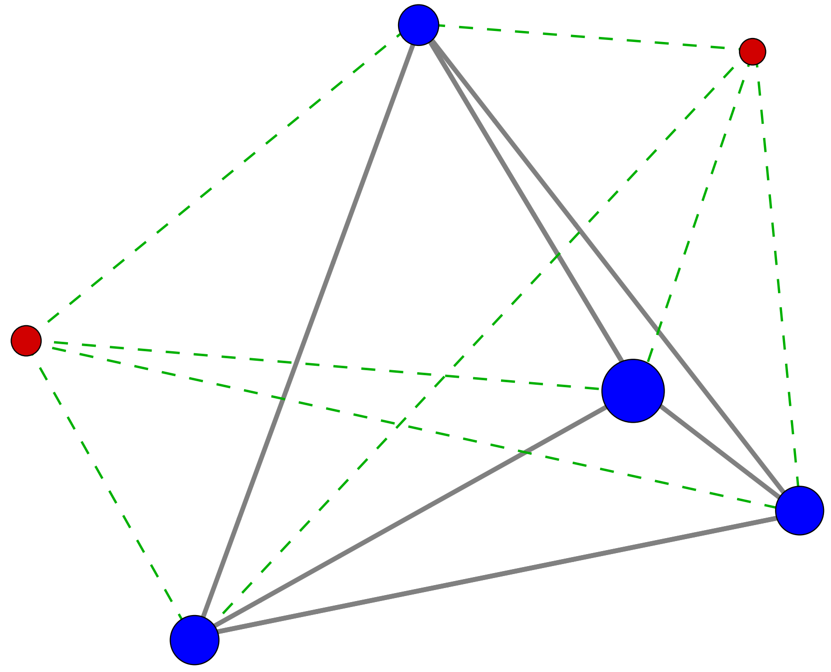
Large χ_3

Beyond Single-Particle Picture

Cluster Dynamical Mean-Field Theory (CDMFT)

Interaction Effect in CDMFT

$$H = \sum_{\langle \mathbf{R}i, \mathbf{R}'i' \rangle, \sigma\sigma'} ([T_o]^{ii'}_{\sigma\sigma'} + [T_d]^{ii'}_{\sigma\sigma'}) c^\dagger_{\mathbf{R}i\sigma} c_{\mathbf{R}'i'\sigma'} - \mu \sum_{\mathbf{R}i,\sigma} c^\dagger_{\mathbf{R}i\sigma} c_{\mathbf{R}i\sigma} + U \sum_{\mathbf{R}i} n_{\mathbf{R}i\uparrow} n_{\mathbf{R}i\downarrow}$$



- Cluster (Tetrahedron) with N_c=4
- Bath Sites with N_b=8

A. Go, W. Witczak-Krempa, G.S.Jeon, K. Park, Y.B.Kim, PRL (2012)

Green's function criteria for correlated topological phases — inversion symmetry

$$\hat{G}^{-1}(\omega, \mathbf{\Gamma}_i) \, |\alpha(\omega, \mathbf{\Gamma}_i)\rangle = \mu_\alpha(\omega, \mathbf{\Gamma}_i) \, |\alpha(\omega, \mathbf{\Gamma}_i)\rangle$$

$$\hat{P} \, |\alpha(\omega, \mathbf{\Gamma}_i)\rangle = \eta_\alpha \, |\alpha(\omega, \mathbf{\Gamma}_i)\rangle$$

$\mathbf{\Gamma}_i$: TRIM (time reversal invariant momentum)

$\eta_\alpha = \pm 1$ Parity Eigenvalue

$$\boxed{(-1)^\Delta = \prod_{\text{R-zero}} \eta_\alpha^{1/2}}$$

$$\text{R-zero} \Leftrightarrow \mu_\alpha(0, \mathbf{k}) > 0$$

$$\Delta = 0, 1$$

$\Delta = 1$: Correlated Topological Insulator

Z. Wang, X.-L.Qi, and S.-C. Zhang, arXiv: 1201.6431 (2012)

Green's function criteria for correlated topological phases inversion symmetry

$$\boxed{(-1)^{\Delta} = \prod_{\text{R-zero}} \eta_{\alpha}^{1/2}}$$

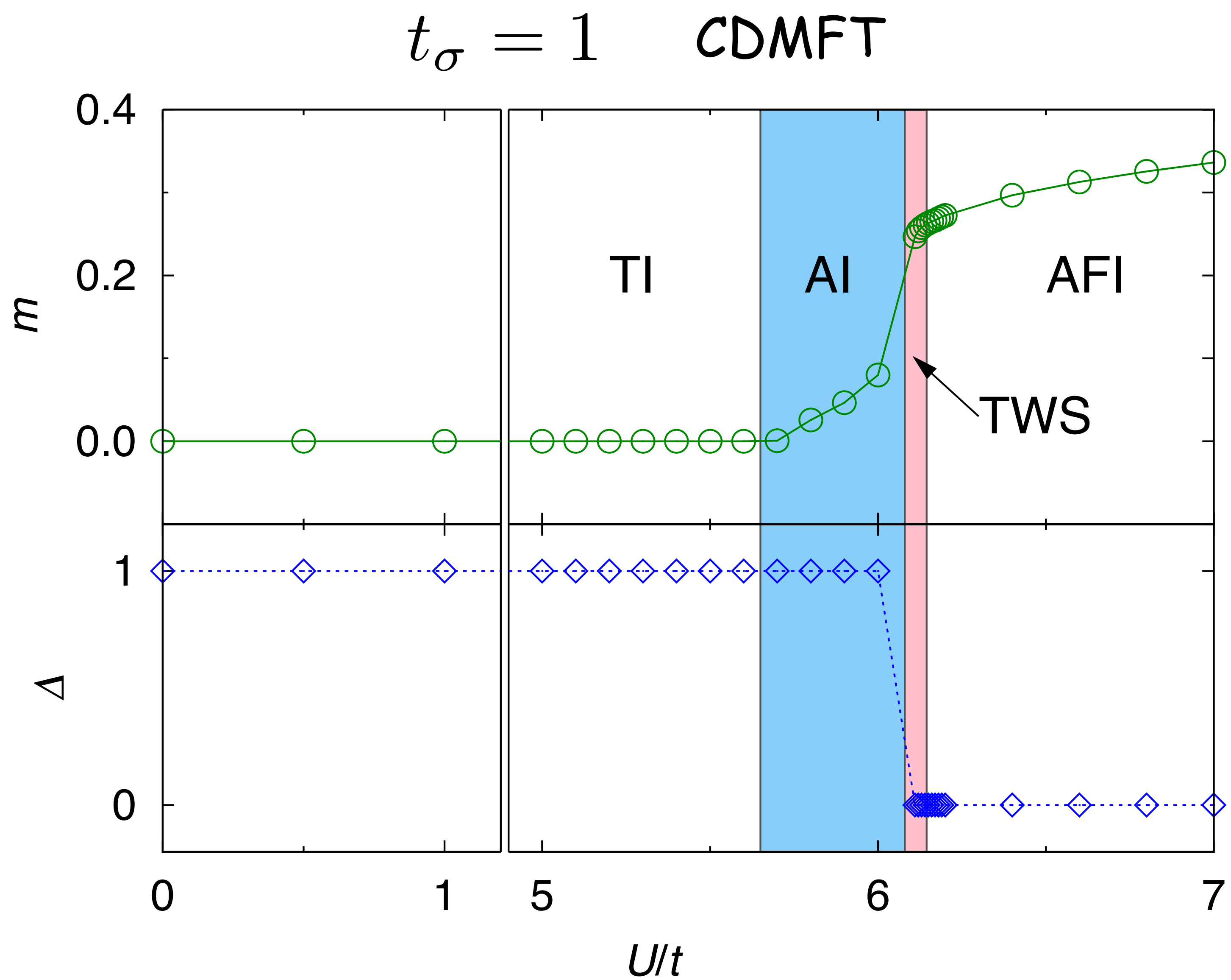
$$\text{R-zero} \Leftrightarrow \mu_{\alpha}(0,\mathbf{k}) > 0$$

Magneto-Electric effect

$$\mathbf{P} = \theta \frac{\alpha}{(2\pi)^2}\mathbf{B} \qquad \mathcal{L}_{\theta} = \theta \frac{\alpha}{(2\pi)^2}\mathbf{E}\cdot\mathbf{B}$$

For TI, $\Delta = 1 \qquad \theta = \pi$

Z. Wang, X.-L.Qi, and S.-C. Zhang, arXiv: 1201.6431 (2012)



A. Go,
W. Witczak-Krempa,
G.S.Jeon,
K. Park,
Y.B.Kim,
PRL 109, 066401 (2012)

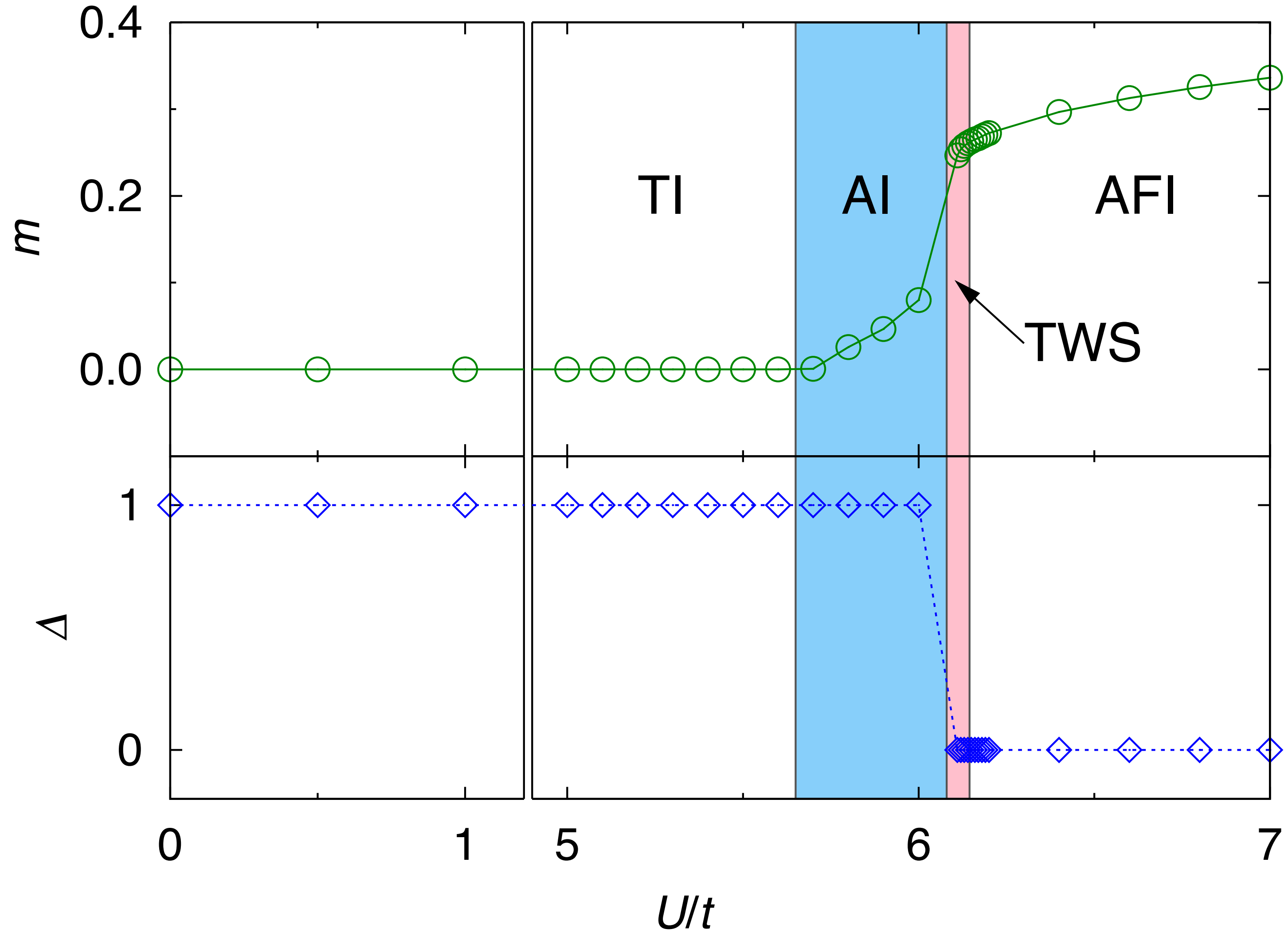
TWS: Topological Weyl Semimetal

AI: Axion Insulator $\Delta = 1$ $\theta = \pi$ Magnetic Order

$$\mathbf{P} = \theta \frac{\alpha}{(2\pi)^2} \mathbf{B} \qquad \mathcal{L}_\theta = \theta \frac{\alpha}{(2\pi)^2} \mathbf{E} \cdot \mathbf{B}$$

Inversion Symmetry

$t_\sigma = 1$ CDMFT



A. Go,
W. Witczak-Krempa,
G.S.Jeon,
K. Park,
Y.B.Kim,
PRL 109, 066401 (2012)

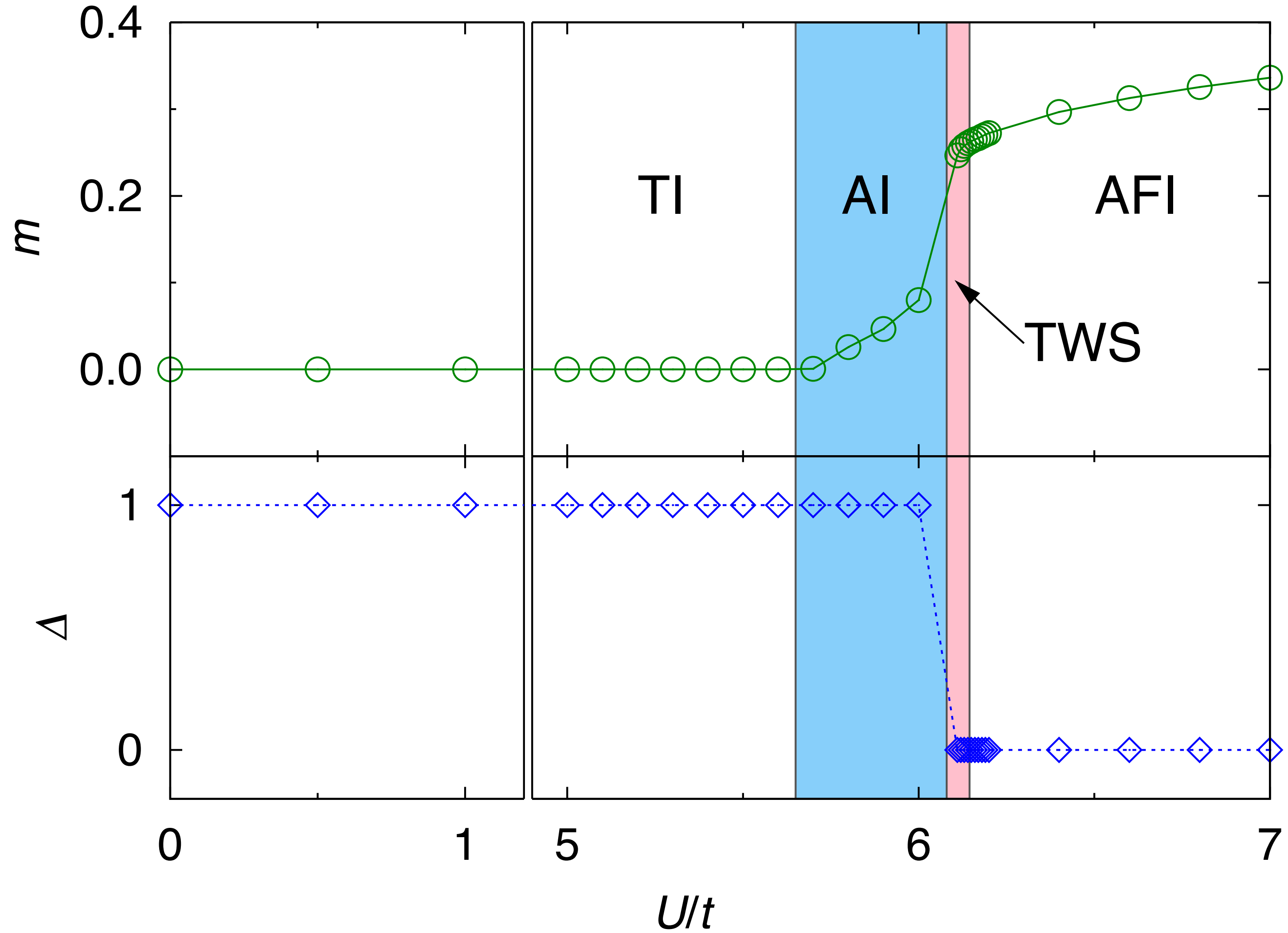
TWS: Topological Weyl Semimetal

AI: Axion Insulator $\Delta = 1$ $\theta = \pi$ Magnetic Order

Gapped surface state Magneto-Electric Effect

possibility discussed in X. Wan, et al, PRB 83, 205101 (2011)

$t_\sigma = 1$ CDMFT



A. Go,
W. Witczak-Krempa,
G.S.Jeon,
K. Park,
Y.B.Kim,
PRL 109, 066401 (2012)

TWS: Topological Weyl Semimetal

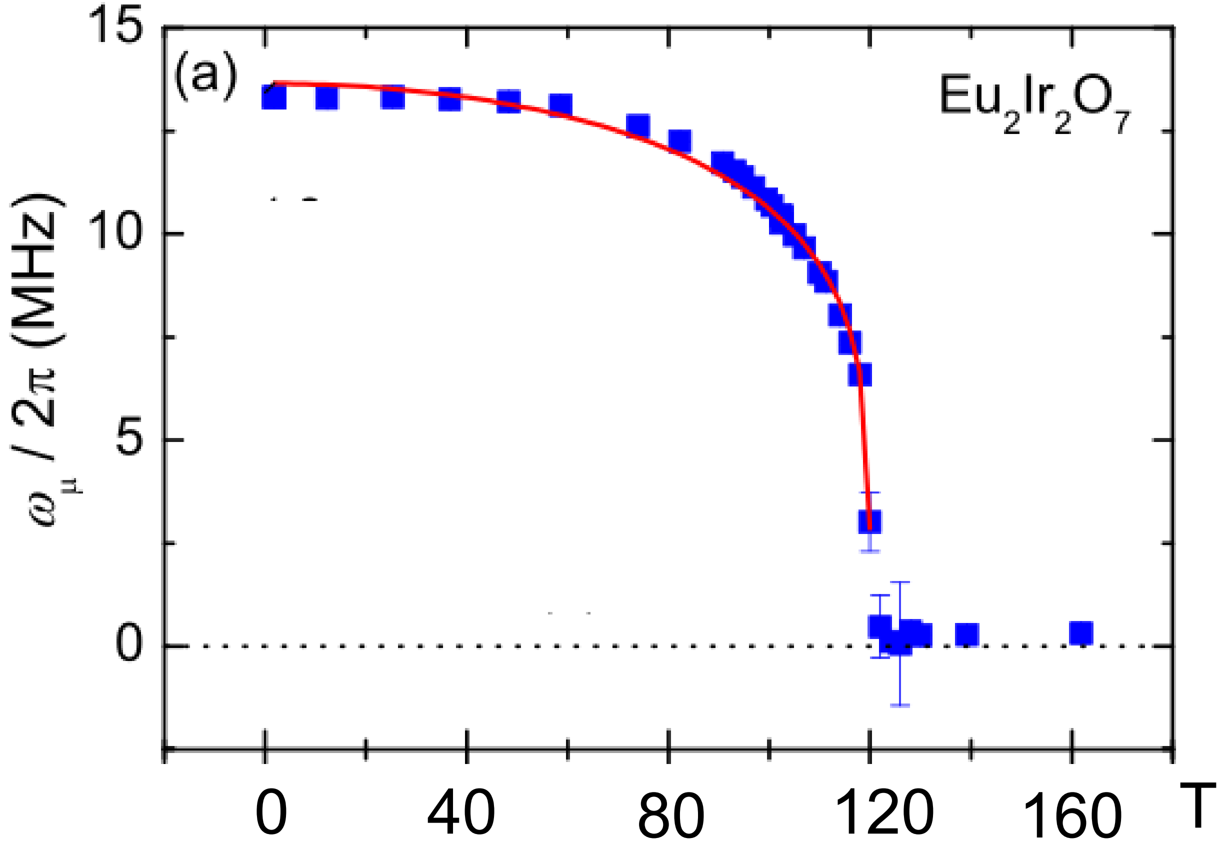
AI: Axion Insulator $\Delta = 1$ $\theta = \pi$ Magnetic Order

Correlation in the cluster important; non-existent in HF

possibility discussed in X. Wan, et al, PRB 83, 205101 (2011)

Connection to Experiments

muSR: Magnetic Order ?



S. Zhao, D. E. MacLaughlin, S. Nakatsuji et al, (2011)

$Eu_2Ir_2O_7$

Eu^{3+} is non-magnetic

Magnetic moments from Ir^{4+}

$$T_M = 120K$$

Non-magnetic A-site	muSR	Neutron (elastic/inelastic)
$Eu_2Ir_2O_7$ (single crystal)	Yes (< 120K) S. Zhao, D. MacLaughlin, Nakatsuji et al, (2011)	?
$Y_2Ir_2O_7$	Yes (< 150K) S. M. Disseler et al, (2012)	$< 0.5\mu_B$ M.C. Shapiro, I. R. Fisher et al, (2012) S. M. Disseler et al, (2012)
Magnetic A-site		
$Nd_2Ir_2O_7$ J=9/2	Damped (< 8K) S. M. Disseler et al, (2012)	Nd^{3+} ordered ? K. Tomiyasu, K. Yamada et al, (2011) Not detected S. M. Disseler et al, (2012)
$Yb_2Ir_2O_7$ J=7/2	Yes (< 130K) S. M. Disseler et al, (2012)	$< 0.5\mu_B$ S. M. Disseler et al, (2012)

Elastic Resonant X-ray Scattering

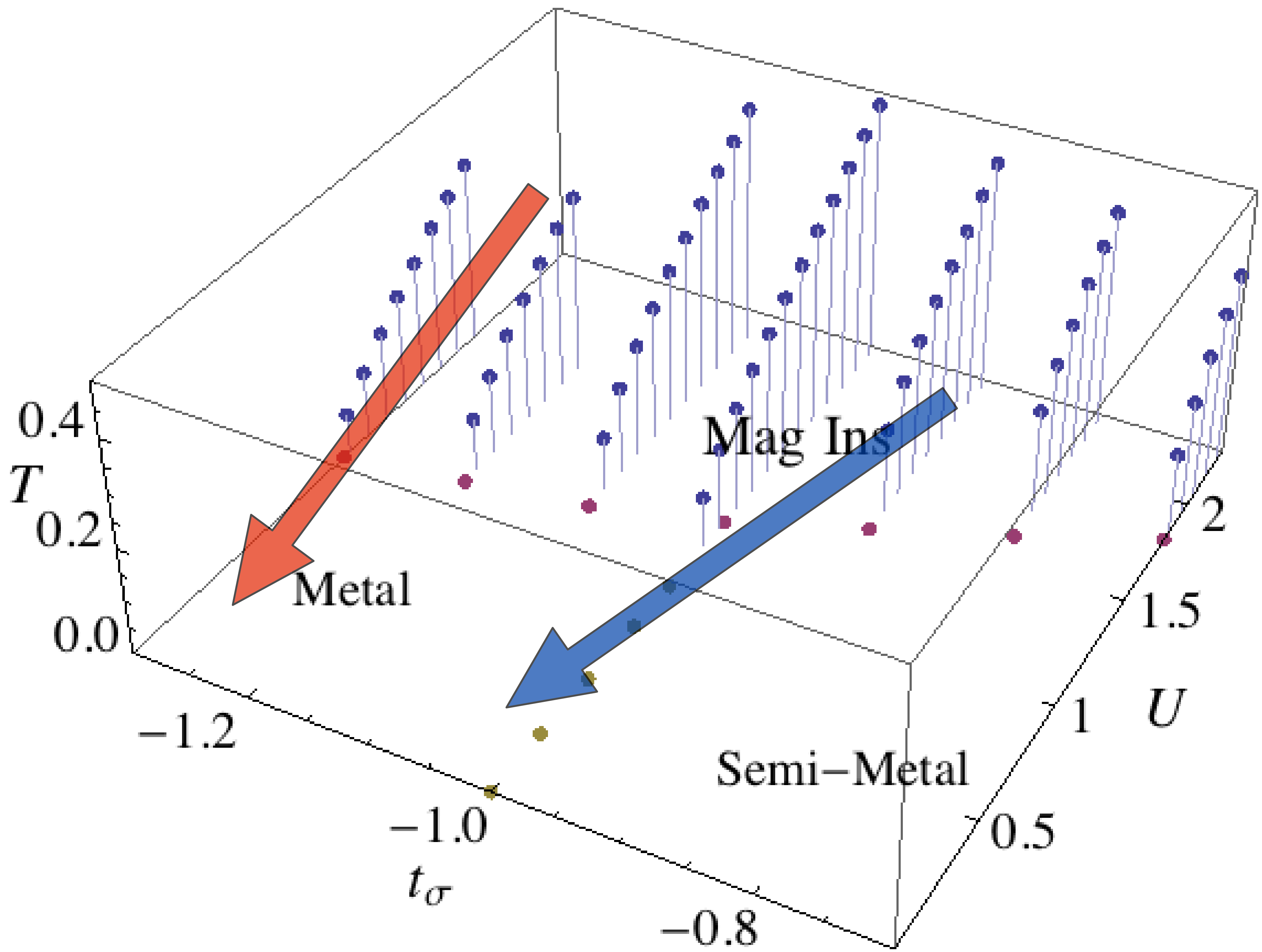
H. Sagayama, D. Uematsu, T. Arima, K. Sugimoto, J. J. Ishikawa, E. O'Farrell, S. Nakatsuji (2013)

$Eu_2Ir_2O_7$

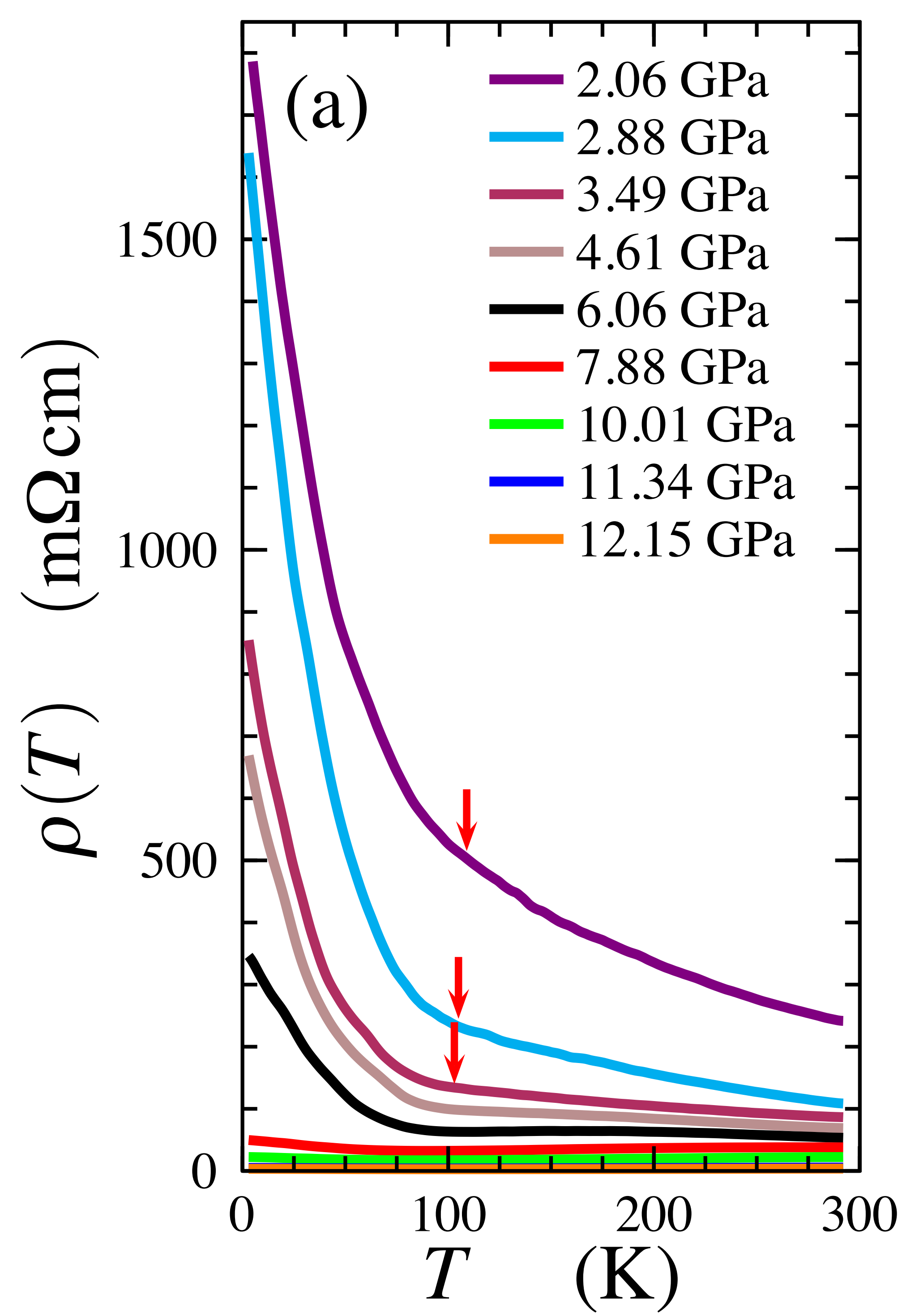
q=0 magnetic order confirmed

But need inelastic resonant X-ray scattering to directly prove the all-in/all-out order

Finite Temperature (Hartree-Fock)



High Pressure Experiment



$Eu_2Ir_2O_7$

F. F. Tafti,
J. J. Ishikawa,
A. McCollam,
S. Nakatsuji,
S. R. Julian,
2012

Spin-Orbit + Interactions + Frustration

Exotic Phases of Matter !

W. Witczak-Krempa, G. Chen, Y.-B.Kim, L. Balents
Review article arXiv:1305.2193