Topology and Correlation in Quantum Materials with Strong Spin-Orbit Coupling I

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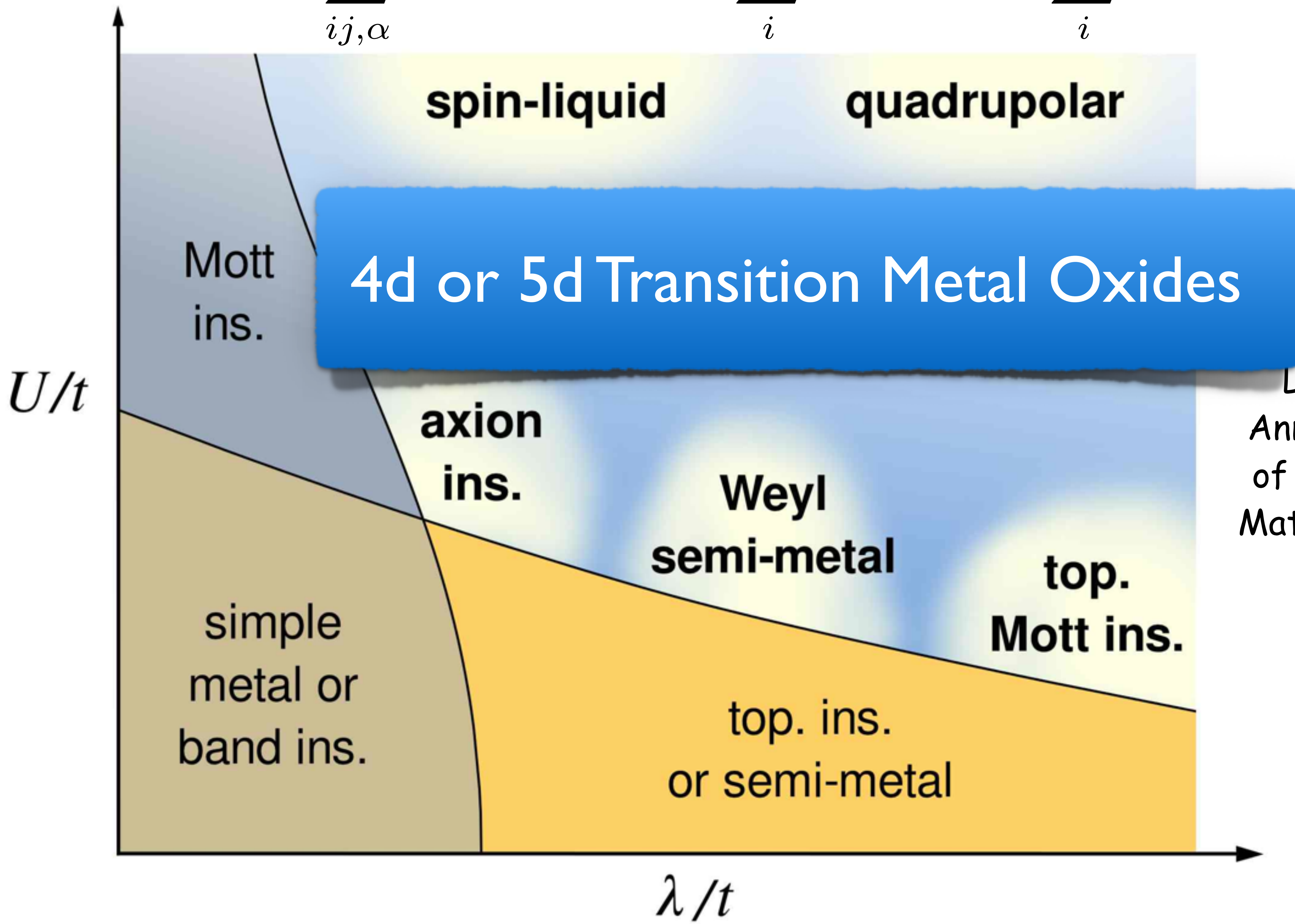
TPI Summer School, University of Minnesota
June 15, 2016

Correlations and Spin-Orbit Coupling

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



tczak-Krempa,
G. Chen,
Y.B.Kim,
L. Balents
Annual Review of Condensed Matter Physics (2014)

5d Transition Metal Oxides: Strong Spin-Orbit Coupling

Large-U

3d: U ~ 2-10 eV

Weak Spin-Orbit coupling

Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn
Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd
Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg

small-U

5d: U ~ 0.5 eV

λ_{SO} ~ 0.5 eV

Strong Spin-Orbit coupling

Interplay of U and λ_{SO}

5d transition metal (Ir) oxides

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	$\boxed{\text{Spin-orbit coupling } \lambda \quad \text{Coulomb U} \quad \text{Crystal field D}}$
10^3			5d: U ~ 0.5-1 eV
10^2	Spin-orbit coupling λ	Crystal field D	λ_{SO} ~ 0.5 eV
10^1			

Traditional playground
for correlated electron physics

Outline

General Intro: Iridates

Brief Introduction:
Topological Phases

Hyper-Honeycomb Iridates
β-Li_2IrO_3 γ-Li_2IrO_3

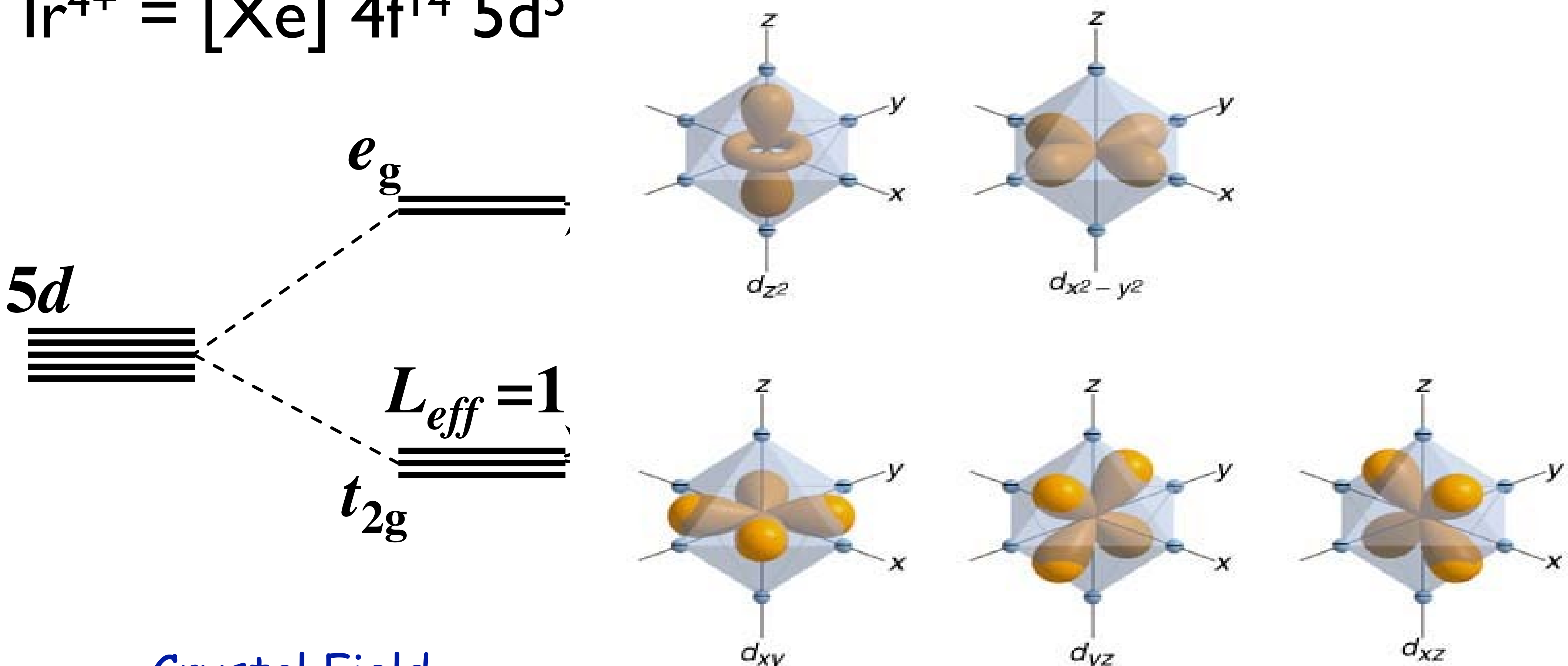
Pyrochlore Iridates (bulk and film)
$R_2Ir_2O_7$

Hyper-kagome Iridate:
$Na_4Ir_3O_8$

Iridates:
New Platforms for Discovery

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

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



Crystal Field

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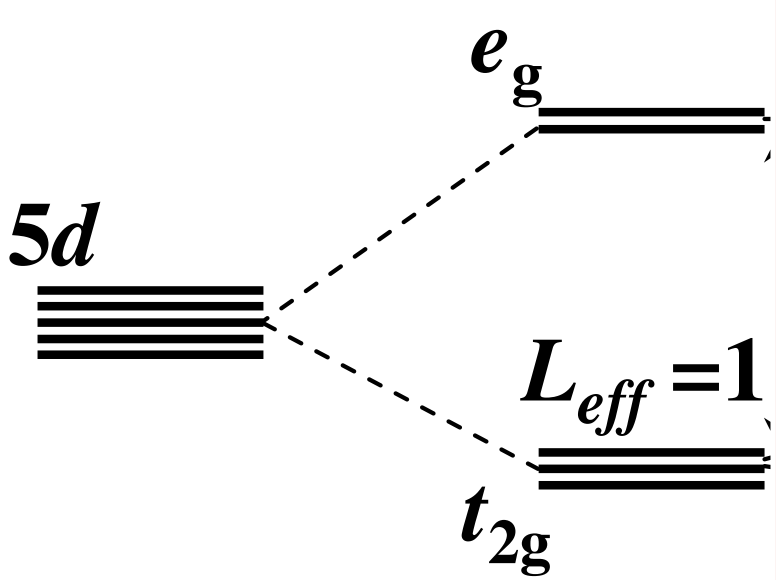

Crystal Field

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

$$\begin{array}{cc} & \begin{array}{ccccc} d_{yz} & d_{zx} & d_{xy} & d_{z^2} & d_{x^2-y^2} \end{array} \\ l_x = & \begin{bmatrix} 0 & 0 & 0 & -\sqrt{3}i & -i \\ 0 & 0 & i & 0 & 0 \\ 0 & -i & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

$$l_y = \begin{bmatrix} 0 & 0 & -i & 0 & 0 \\ 0 & 0 & 0 & \sqrt{3}i & -i \\ i & 0 & 0 & 0 & 0 \\ 0 & -\sqrt{3}i & 0 & 0 & 0 \\ 0 & i & 0 & 0 & 0 \end{bmatrix}$$

$$l_z = \begin{bmatrix} 0 & i & 0 & 0 & 0 \\ -i & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2i \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2i & 0 & 0 \end{bmatrix}$$

$$\Longleftrightarrow$$

$$\begin{array}{cc} & \begin{array}{ccc} p_x & p_y & p_z \end{array} \\ l_x = & \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix} \end{array}$$

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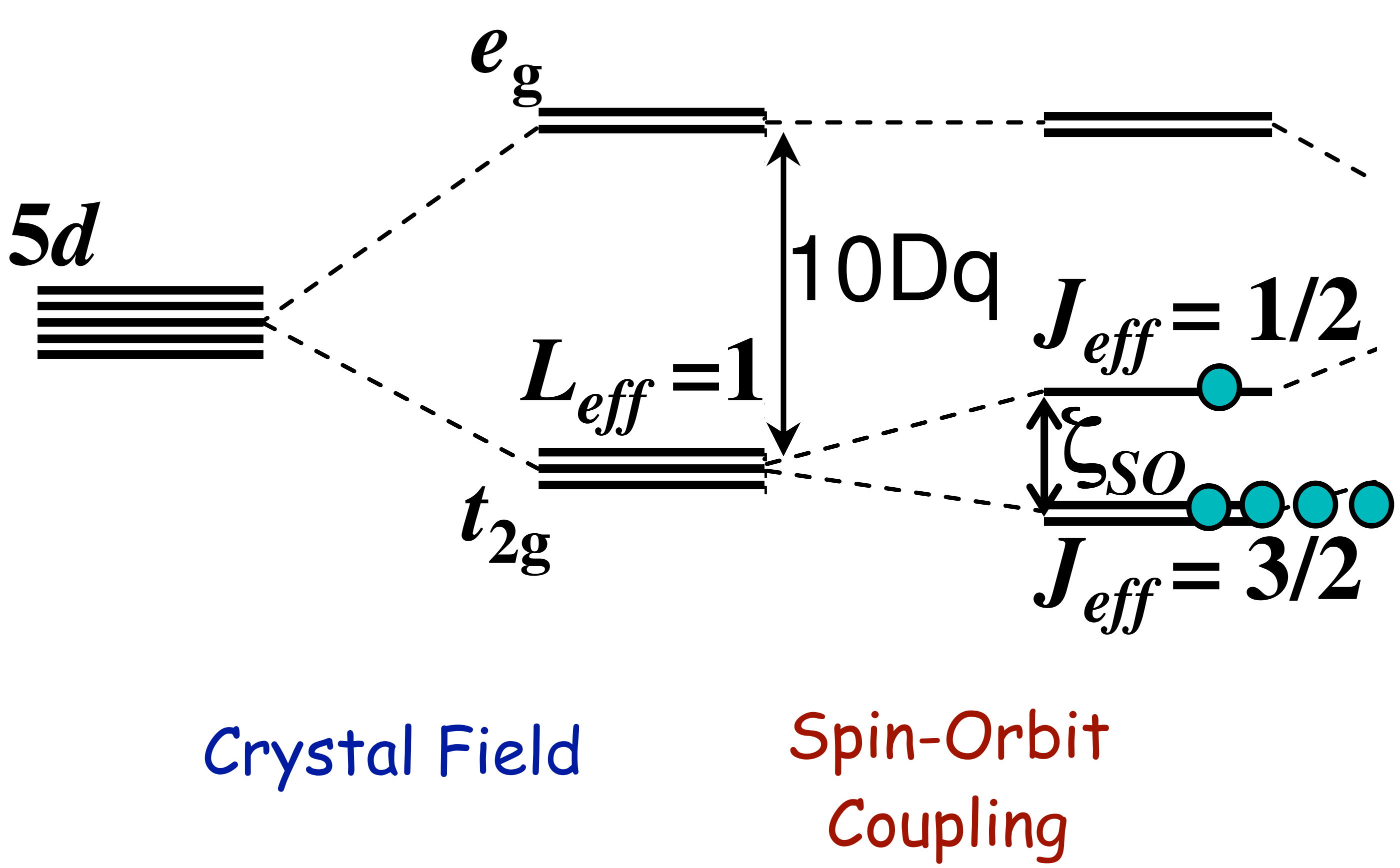

B.J.Kim, T.W.Noh, G.Cao et al. PRL (2008)

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

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

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

Strong Spin-Orbit Coupling leads to Spin-Orbit entangled pseudo-spin basis (Kramers Doublet)

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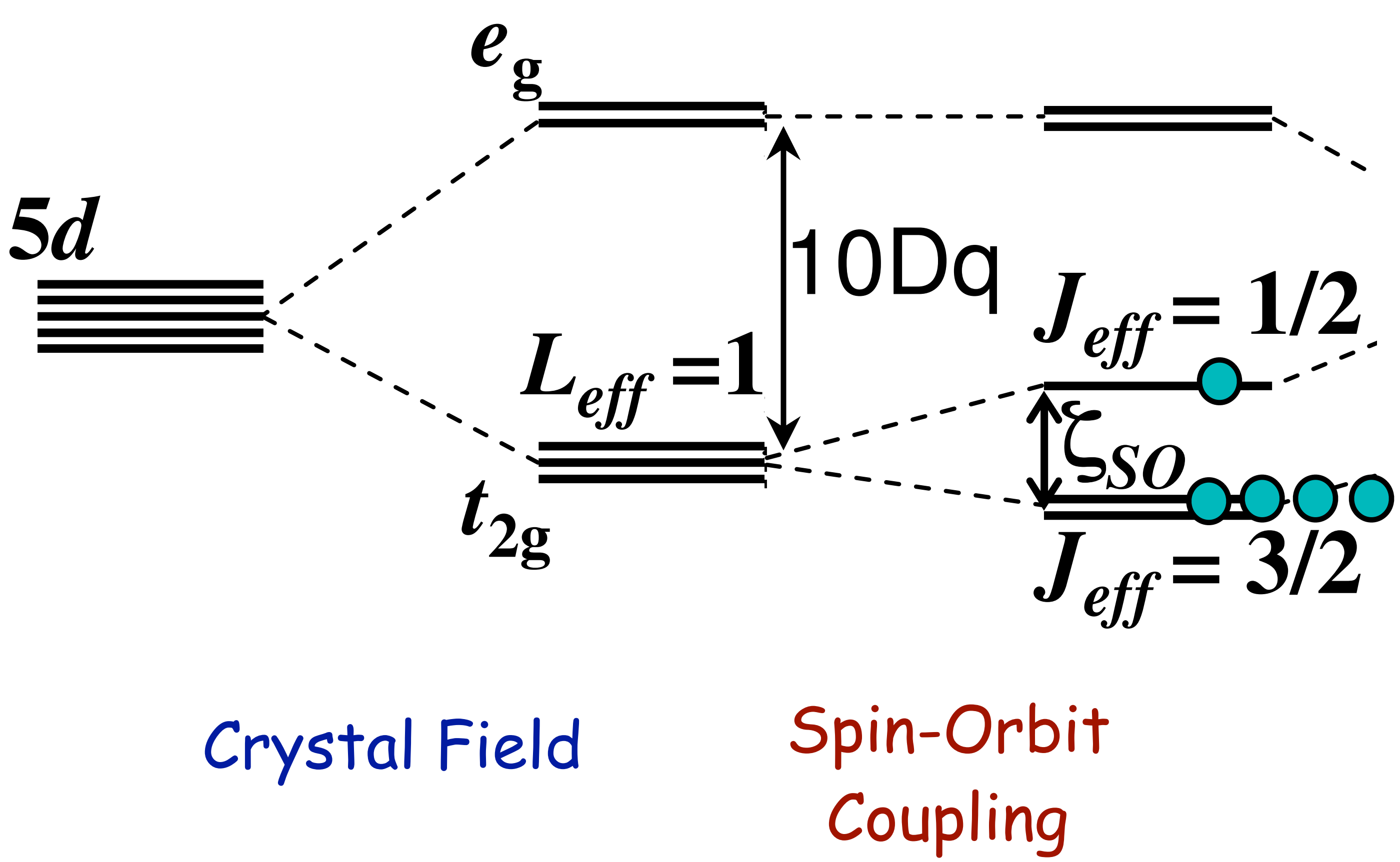

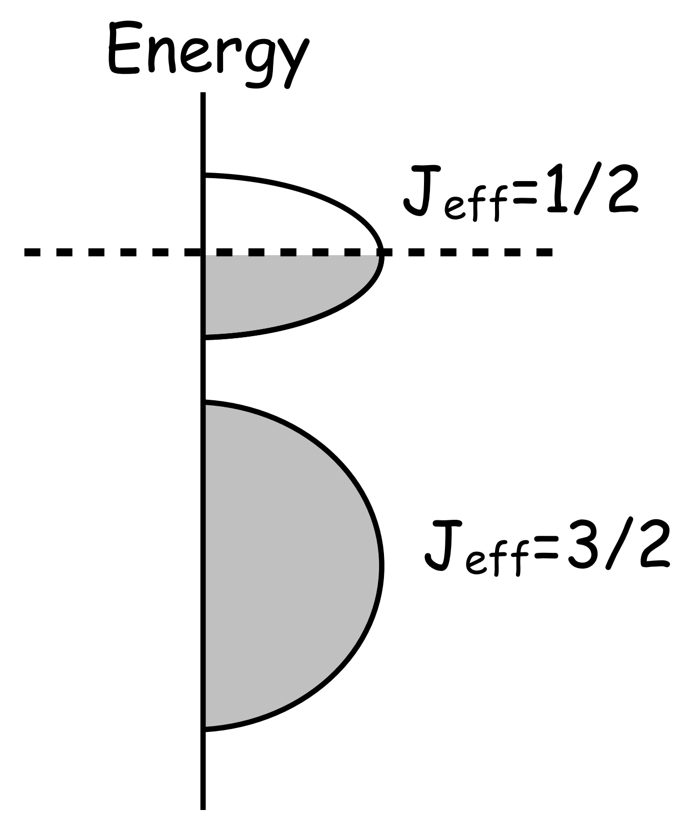

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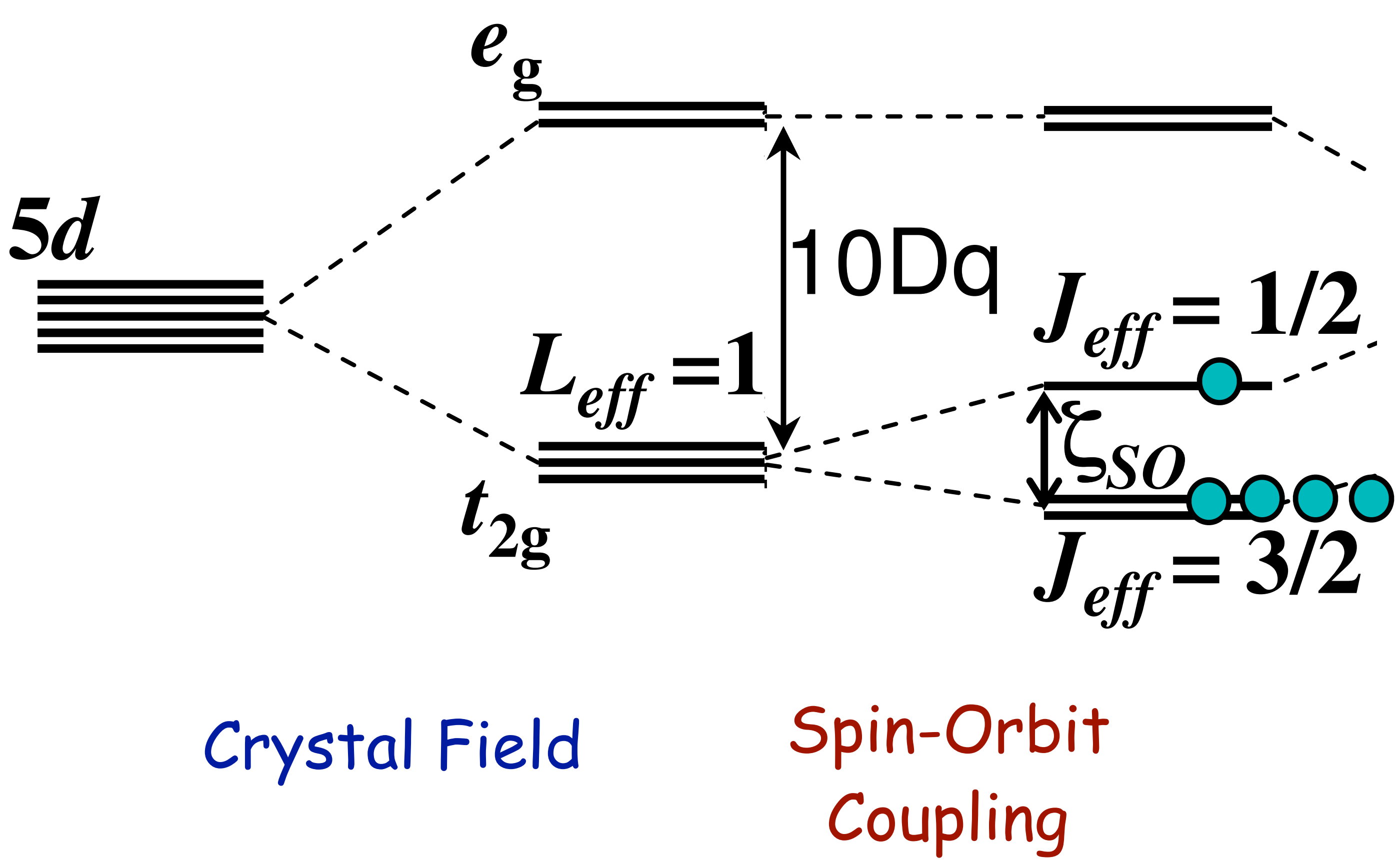

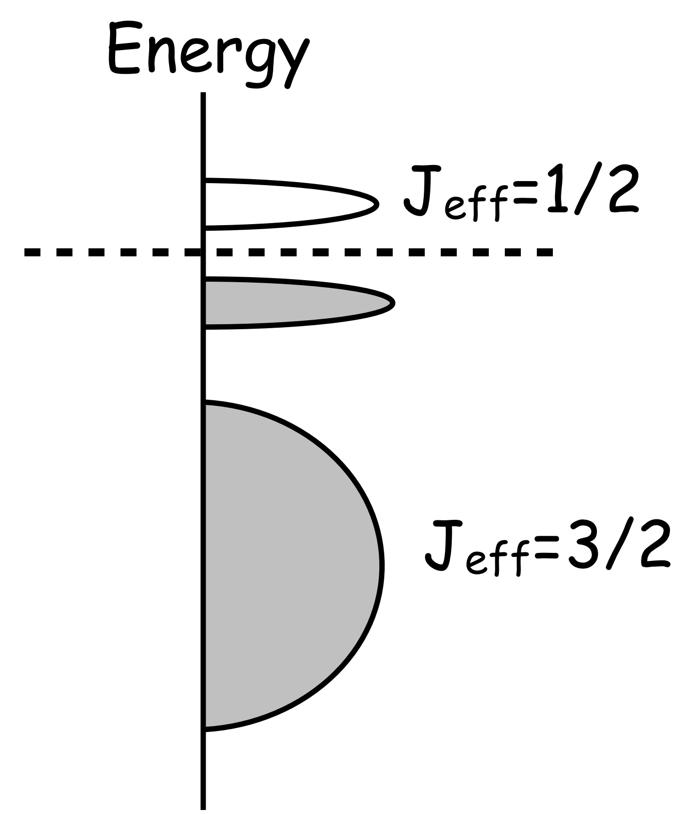

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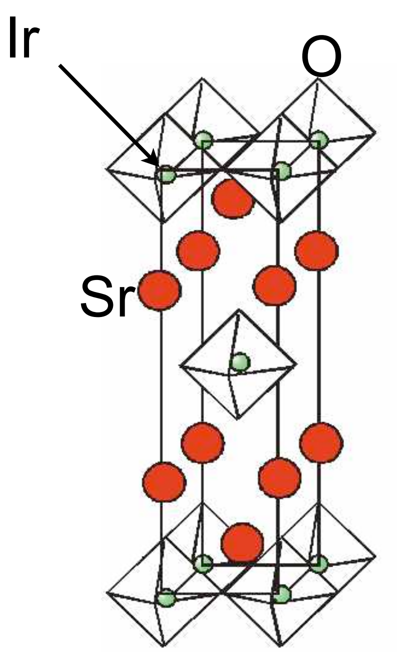
Sr_2IrO_4 is a Spin-Orbit Mott Insulator

5d transition metal (Ir) oxides

- ❑ Moderate strength of U → Mott Insulator
- ❑ Strong Spin-Orbit Coupling → Clever way to lift the orbital degeneracy !

  Avoid Kugel-Khomski
  + Large quantum fluctuations → Quantum Spin Liquid ?
  for $J_{eff}=1/2$ moment
- ❑ Doping half-filled $J_{eff}=1/2$ band → High T_c Superconductor ?
- ❑ Small Charge Gap Weak Mott Insulator
  Often close to a Metal-Insulator Transition
- ❑ Strong Spin-Orbit Coupling → Often semi-metal or could be a Topological Insulator
- ❑ Sensitive to Strain/Lattice → sensitive electronic properties

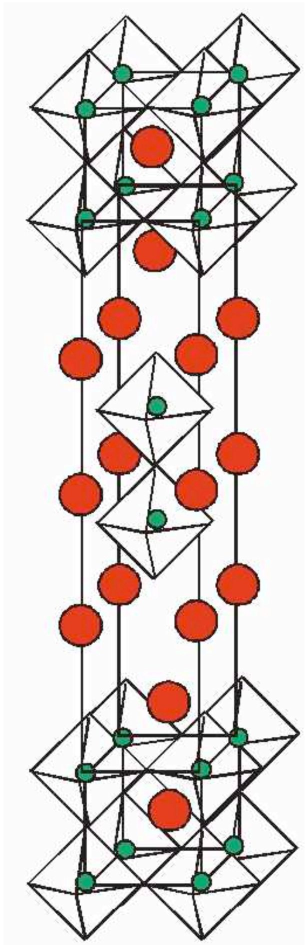
Bulk materials: layered perovskites
The Ruddlesden-Popper Series: $Sr_{1+n}Ir_nO_{1+3n}$



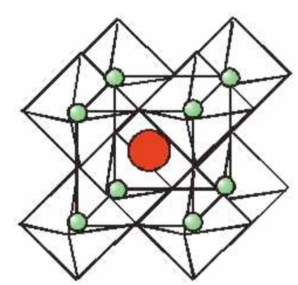
n=1

Sr2IrO4

Iso-structural
to Cuprates



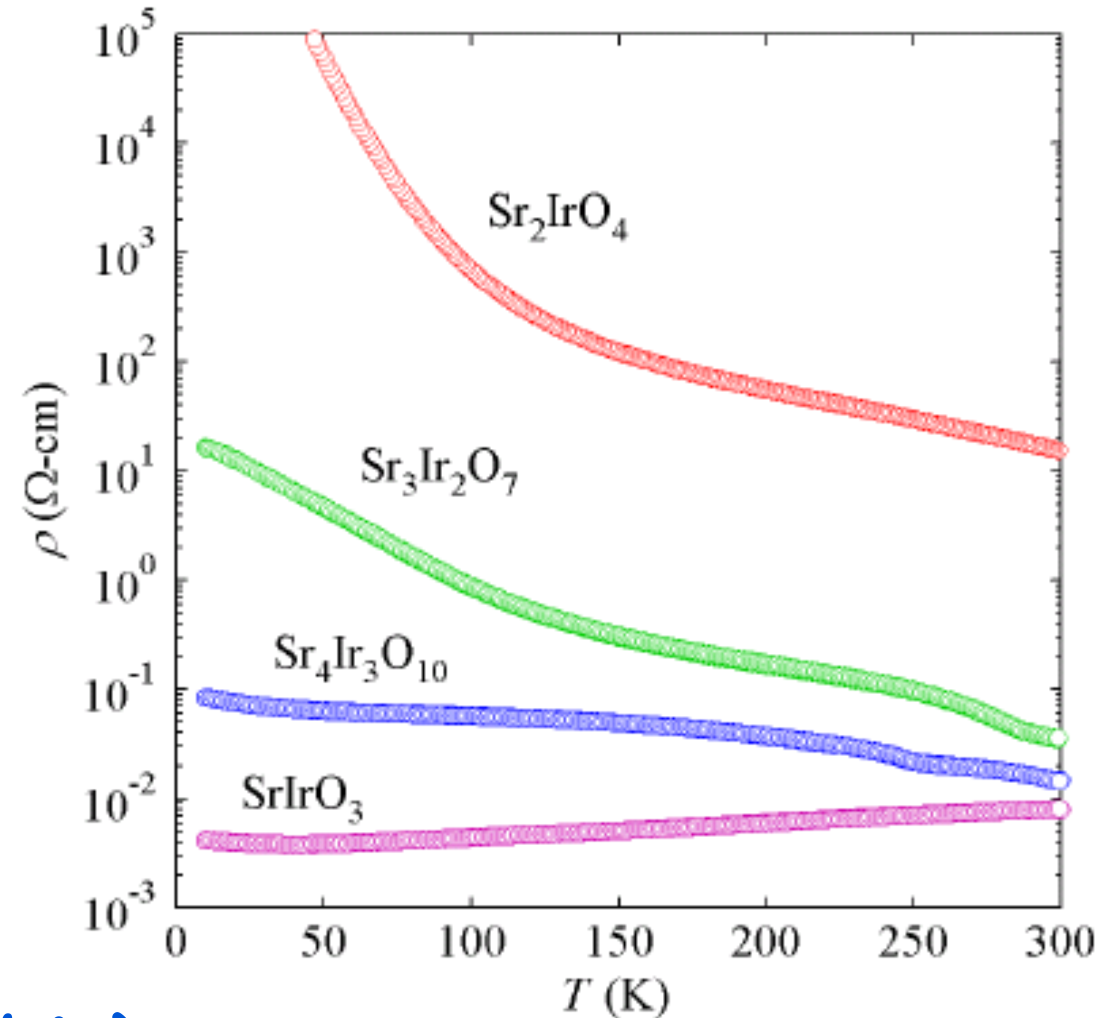
n=2
Sr3Ir2O7



n=∞

SrIrO3

Topological semi-metal (orthorhombic)



H. Takagi

Canted AF

magnetic, weaker insulator

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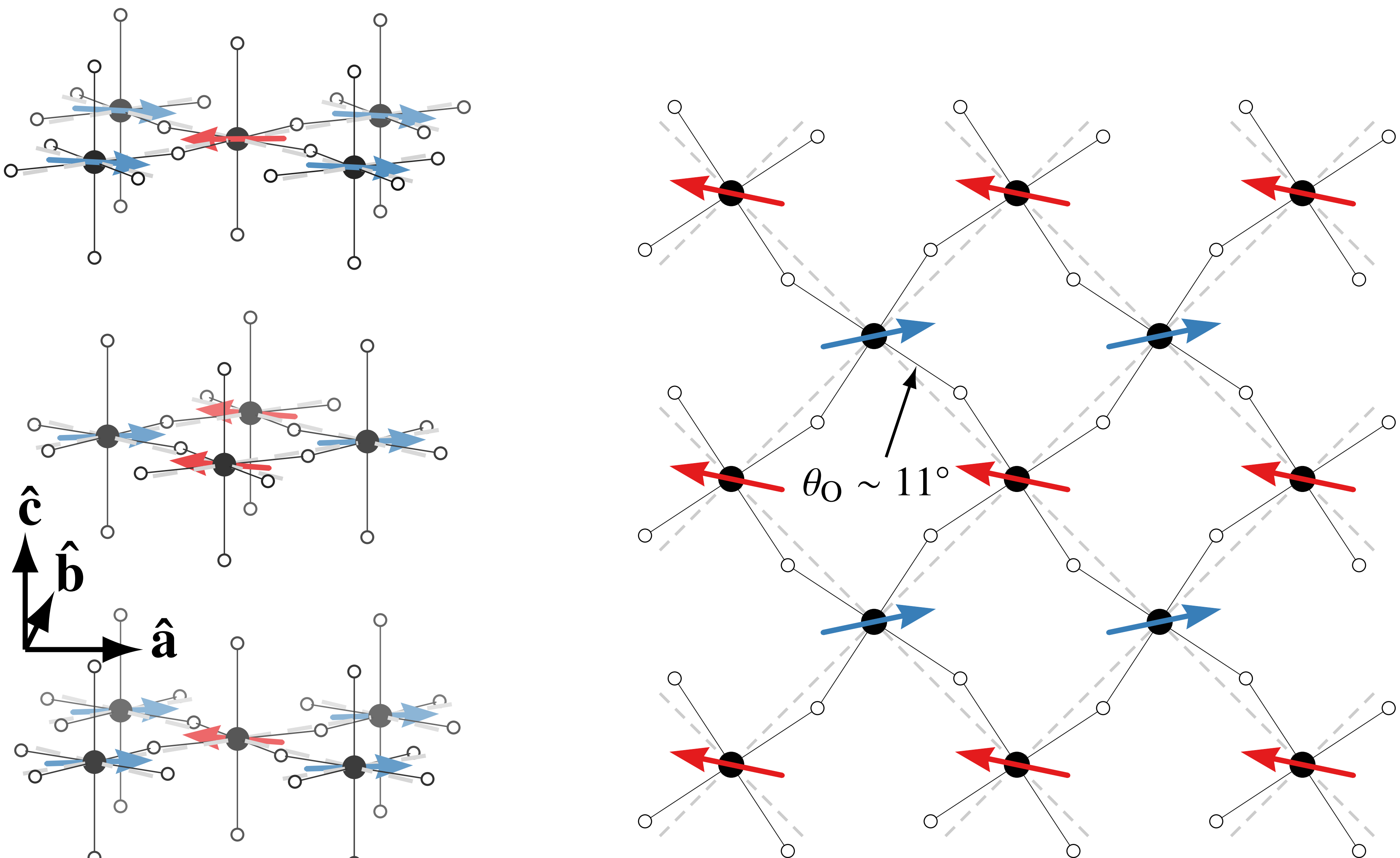

Sr_2IrO_4

Bulk materials: layered perovskites
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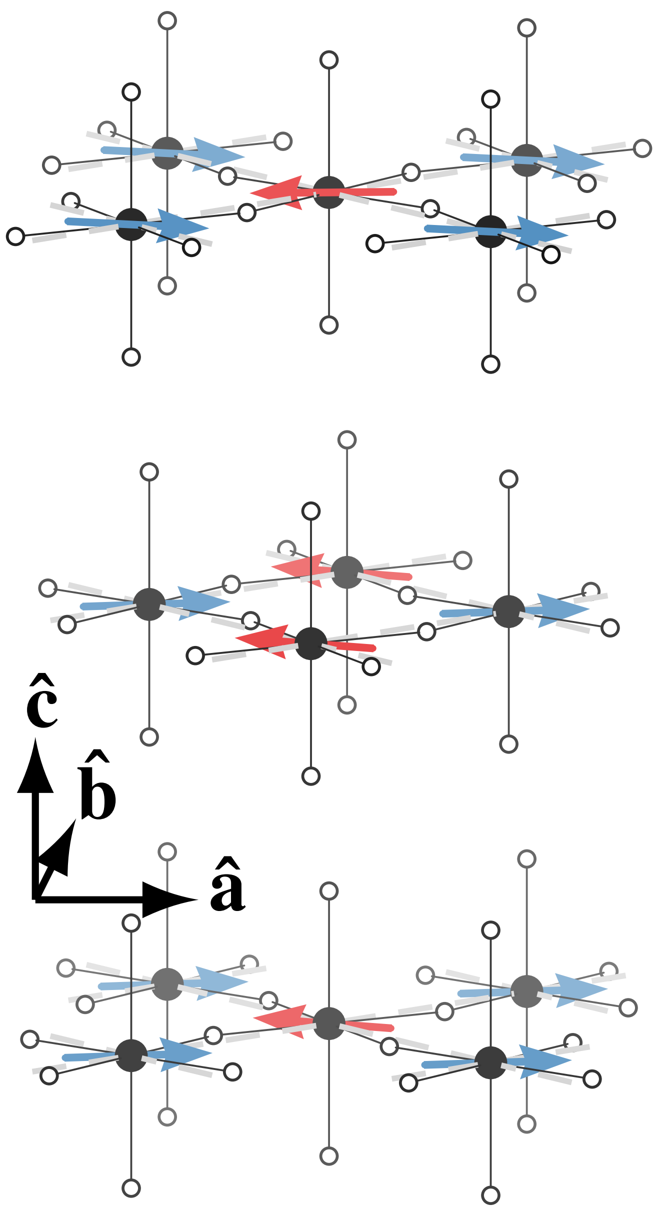
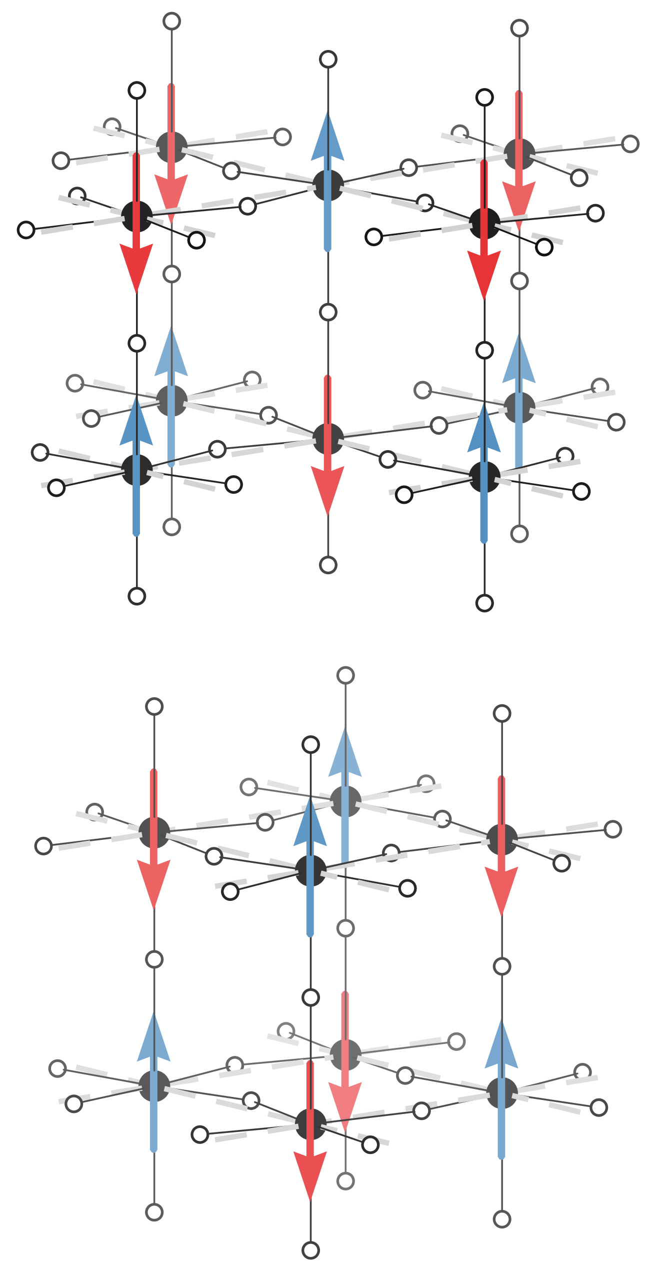


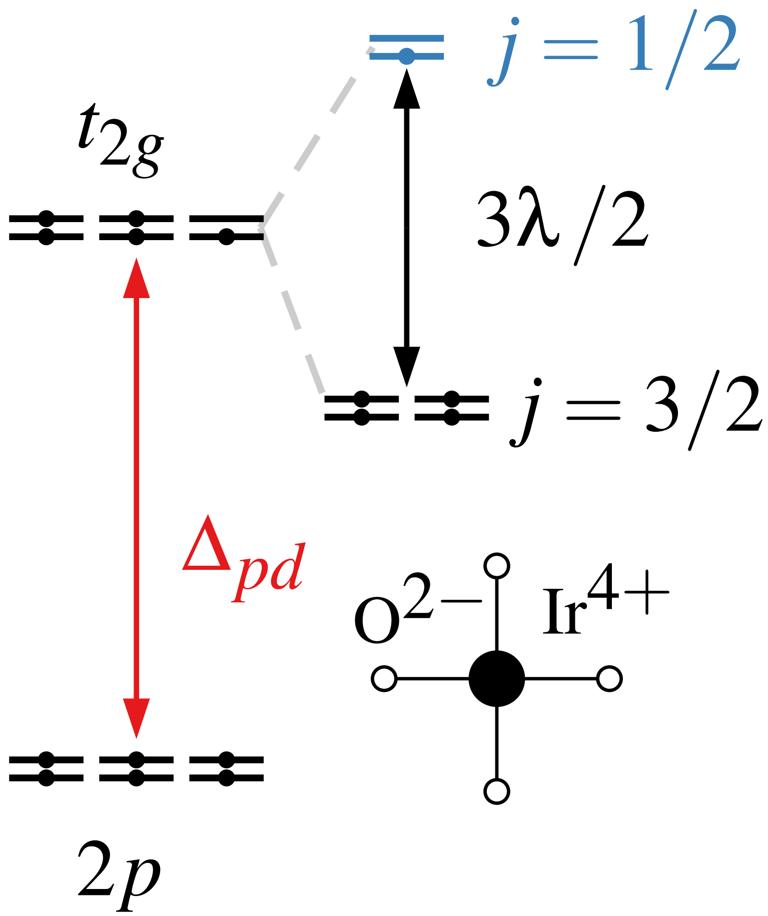
Sr_2IrO_4

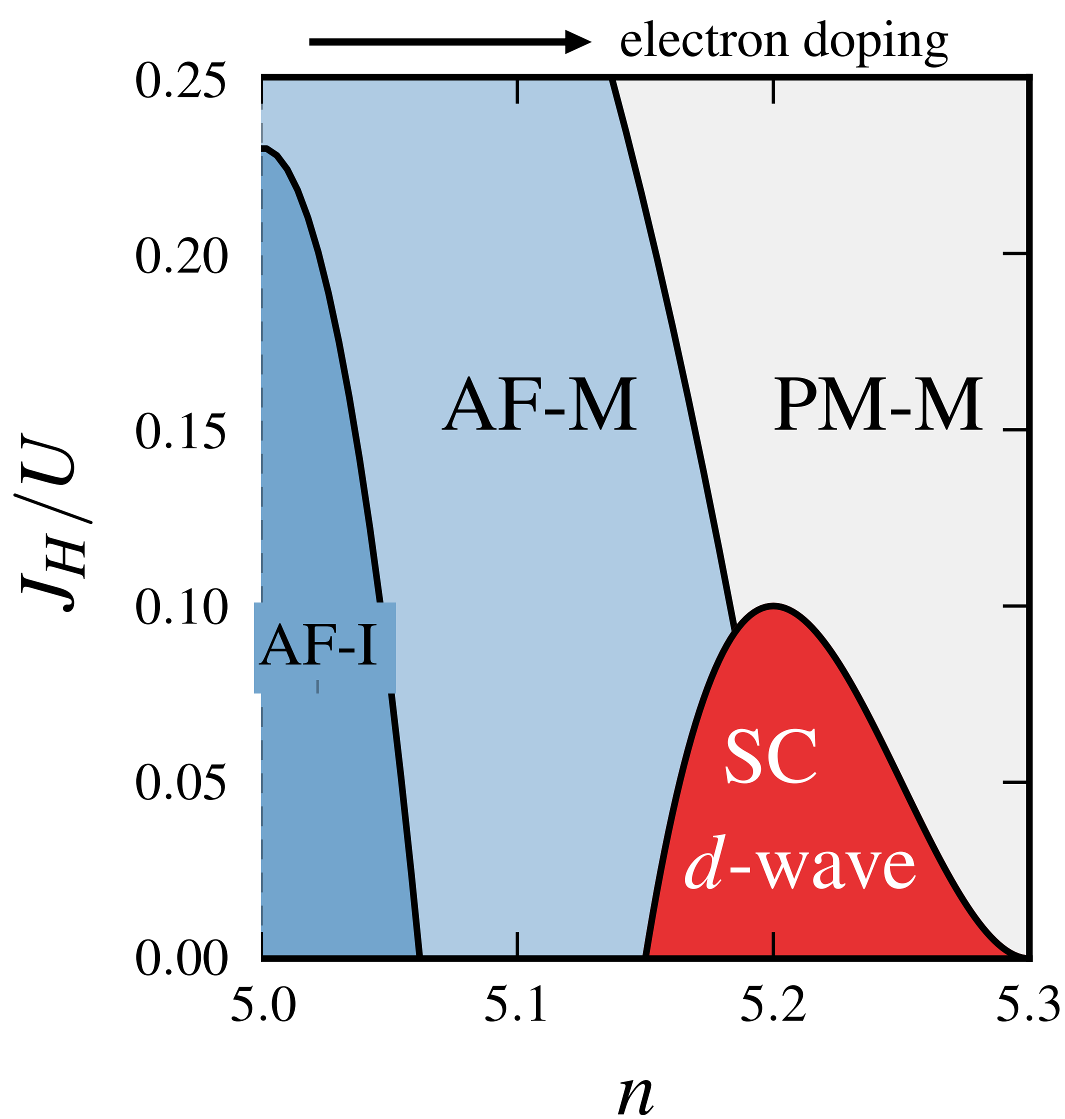


$Sr_3Ir_2O_7$

Superconductivity in doped Sr_2IrO_4 ?

Multi-orbital interaction may be important !





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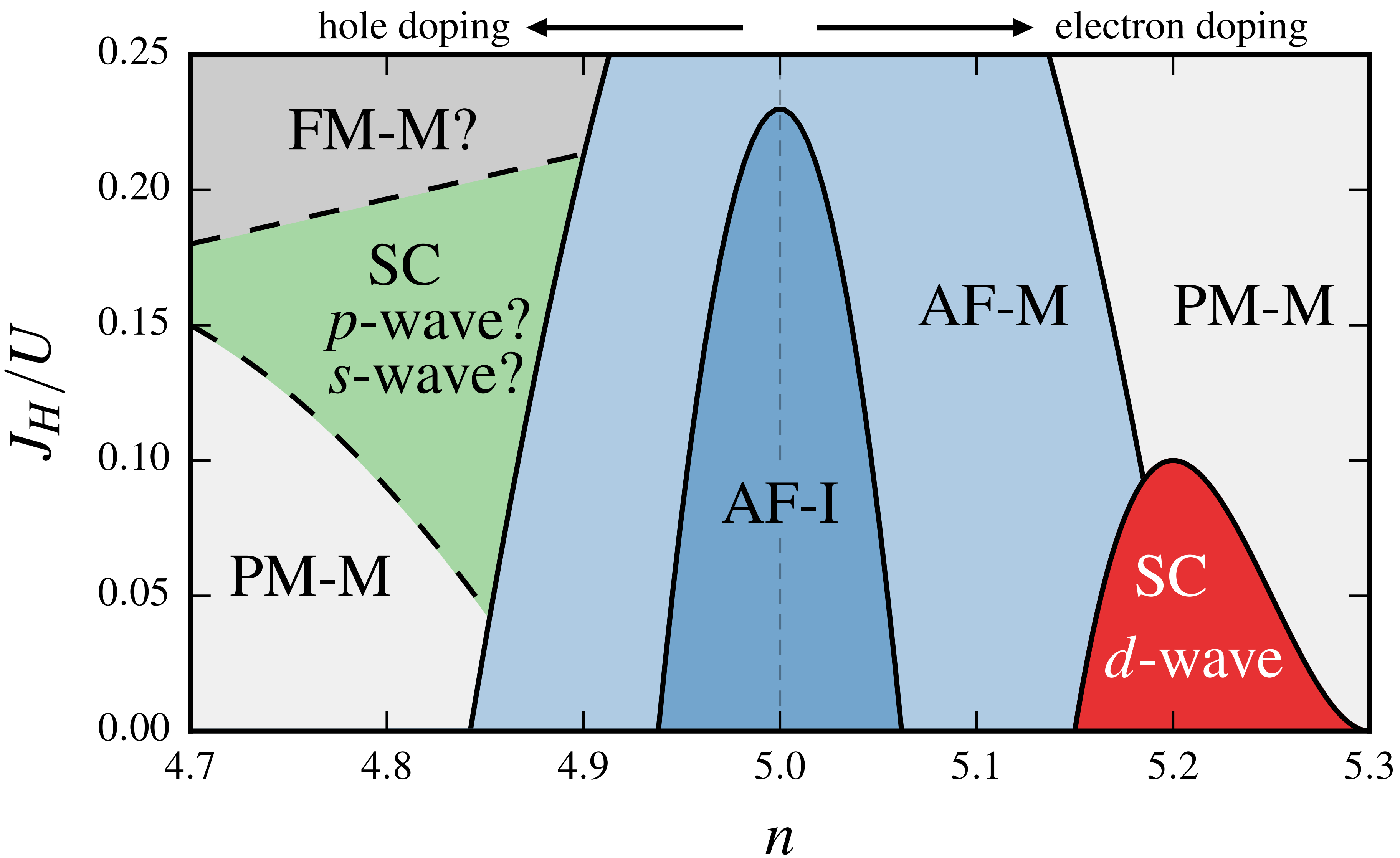

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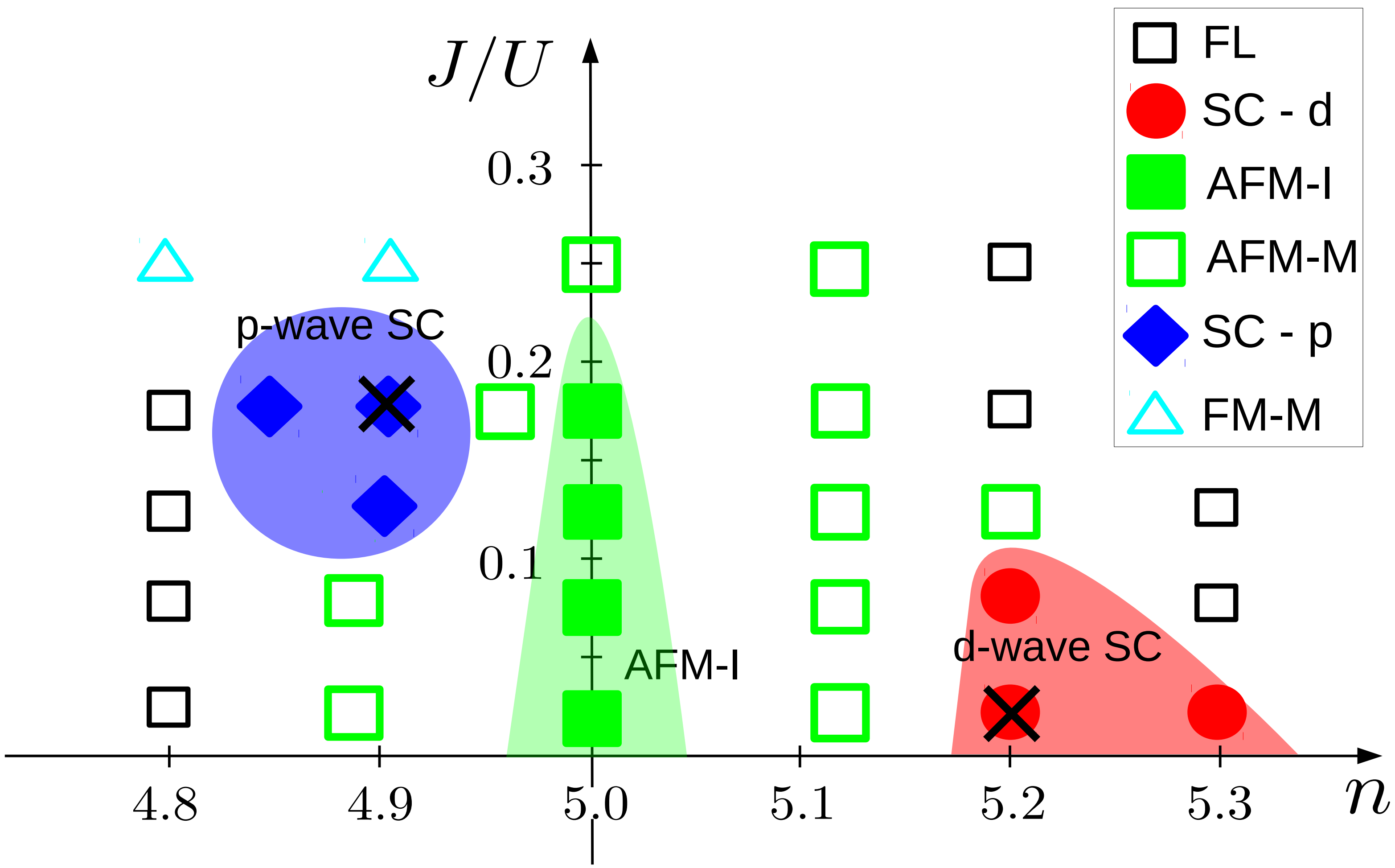
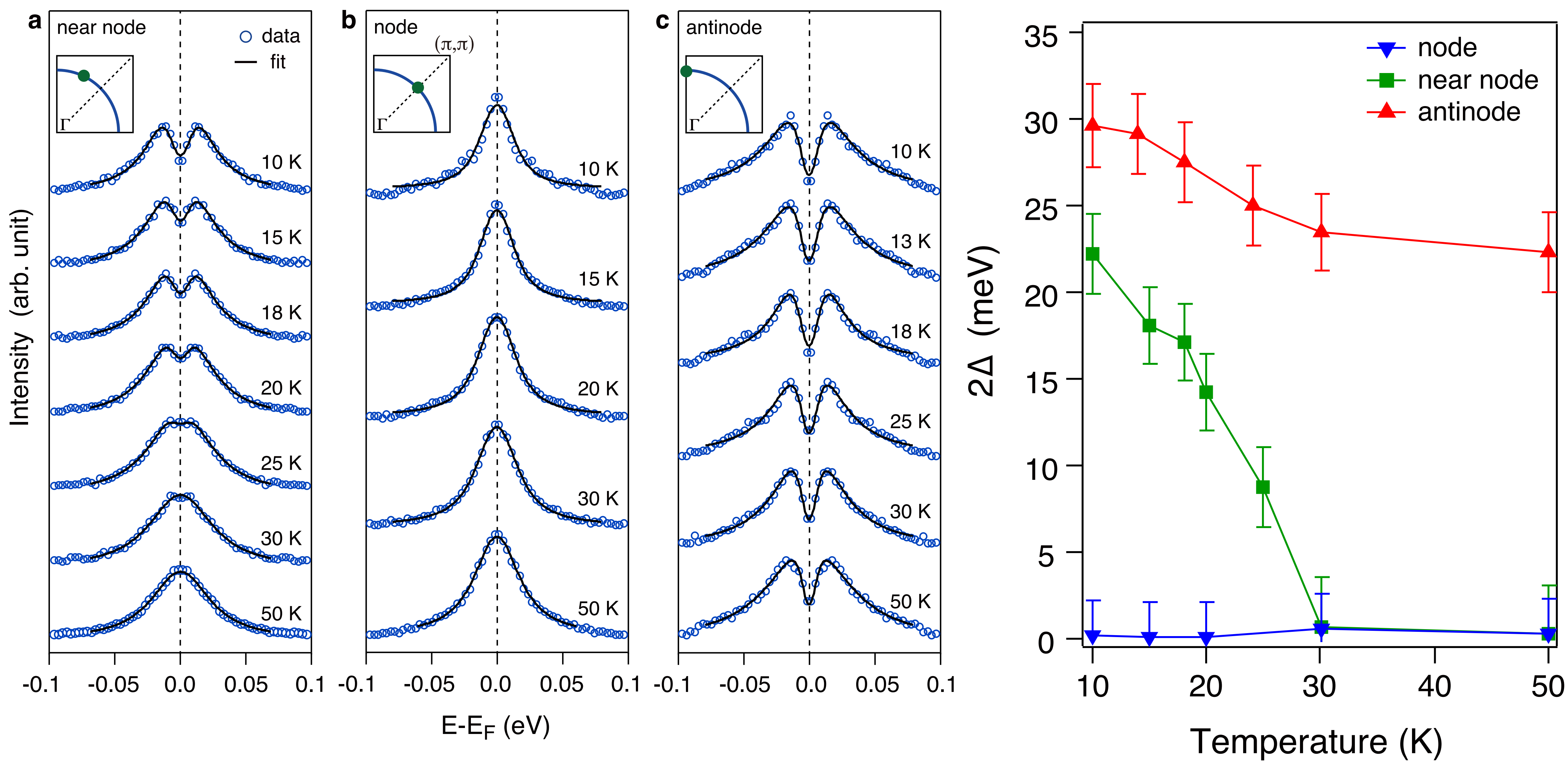


DMFT (CTQMC)
+ Parquet Equations
Z.Meng,
H.-Y.Kee,
Y.B.Kim,
PRL 2014

hole doping electron doping

Electron doping on the surface: Sr_2IrO_4



B.J.Kim et al (2015)

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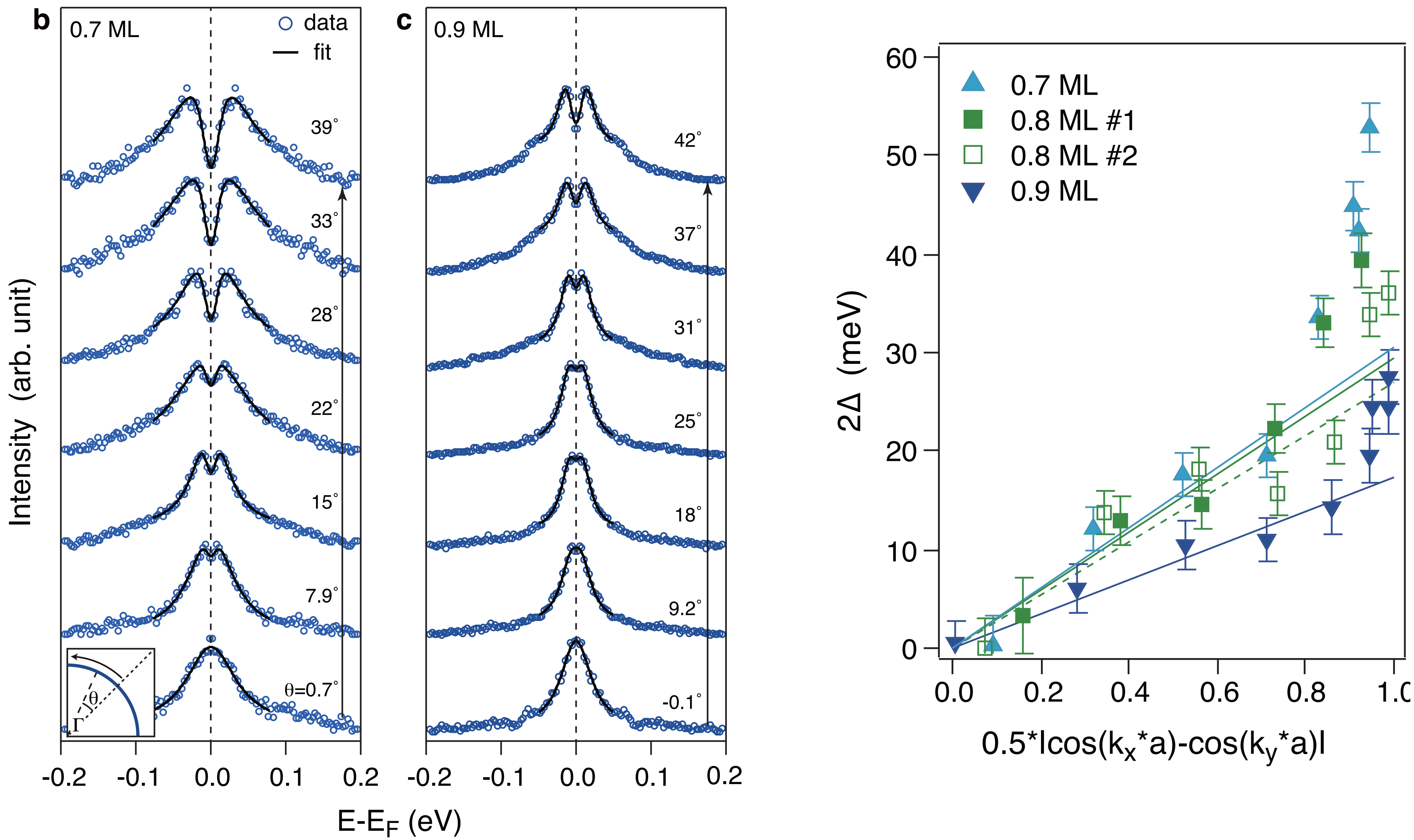

B.J.Kim et al (2015)

nature COMMUNICATIONS

ARTICLE

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OPEN

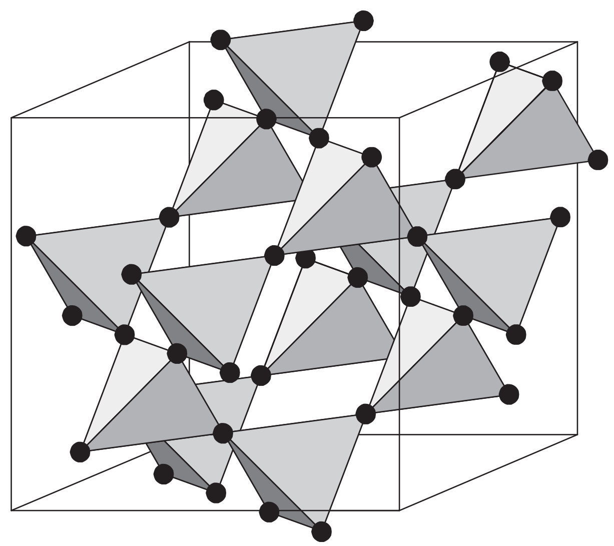
Hallmarks of the Mott-metal crossover in the hole-doped pseudospin-1/2 Mott insulator Sr_2IrO_4

Yue Cao[1,†], Qiang Wang[1,†], Justin A. Waugh[1], Theodore J. Reber[1,†], Haoxiang Li[1], Xiaoqing Zhou[1], Stephen Parham[1], S.-R. Park[1,2], Nicholas C. Plumb[3], Eli Rotenberg[4], Aaron Bostwick[4], Jonathan D. Denlinger[4], Tongfei Qi[5], Michael A. Hermele[1], Gang Cao[5] & Daniel S. Dessau[1]

Here we investigate the evolution of electronic structure and dynamics of the hole-doped pseudospin-1/2 Mott insulator Sr_2IrO_4. The effective hole doping is achieved by replacing Ir with Rh atoms, with the chemical potential immediately jumping to or near the top of the lower Hubbard band. The doped iridates exhibit multiple iconic low-energy features previously observed in doped cuprates—pseudogaps, Fermi arcs and marginal-Fermi-liquid-like electronic scattering rates.

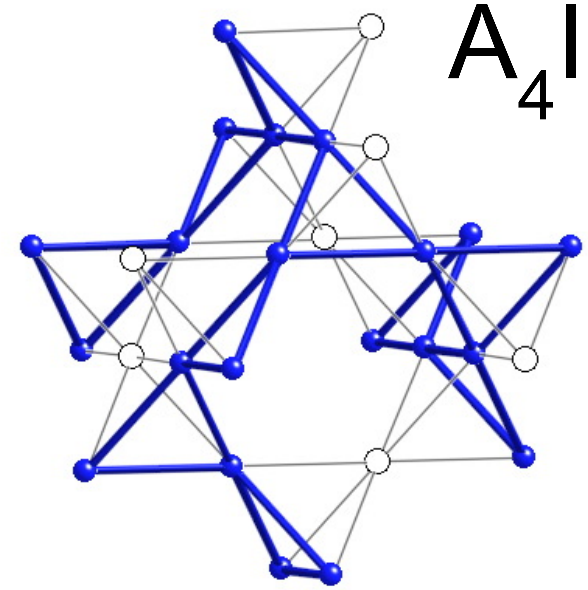
Pyrochlore

$A_2Ir_2O_7$



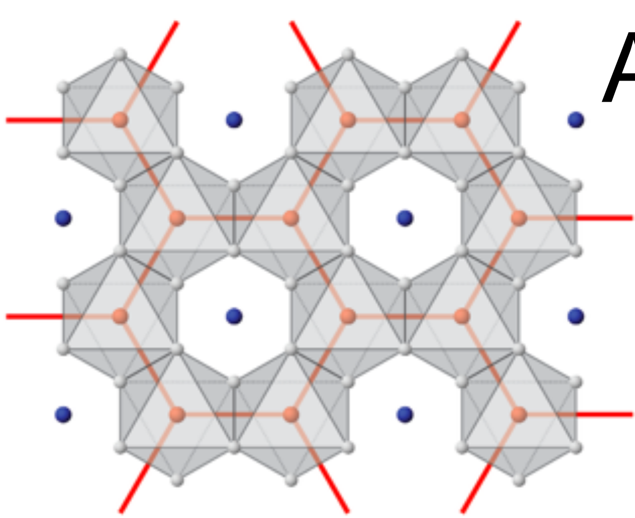
Hyperkagome

$A_4Ir_3O_8$



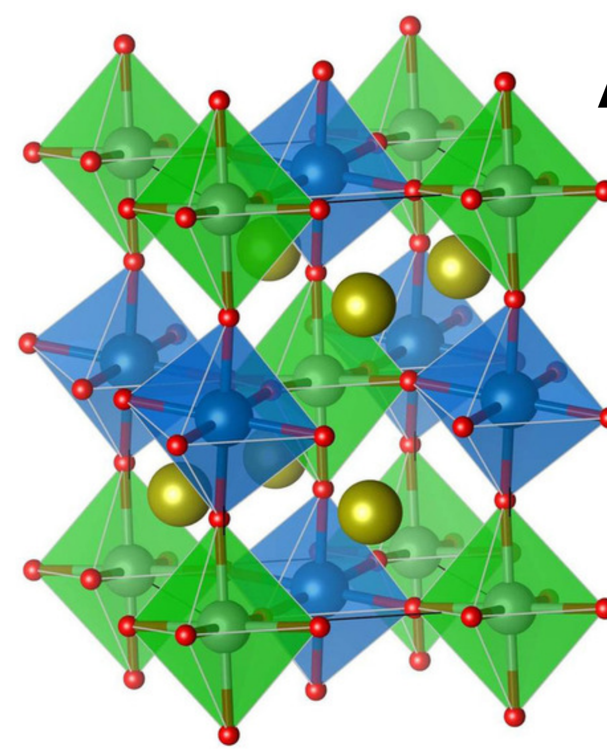
Honeycomb

A_2IrO_3



Double Perovskite

A_2BIrO_6



Pyrochlore

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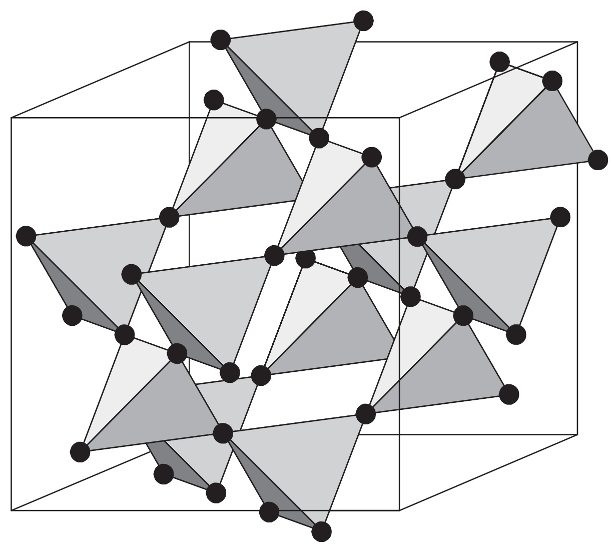

TI

Weyl semi-metal

Non-Fermi liquid

Hyperkagome

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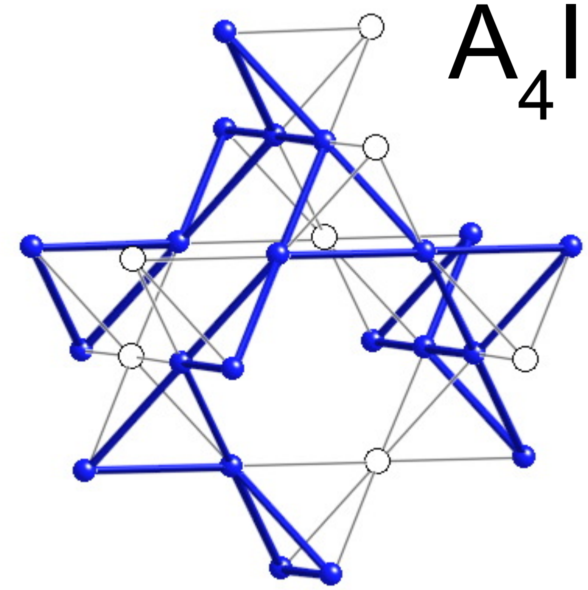
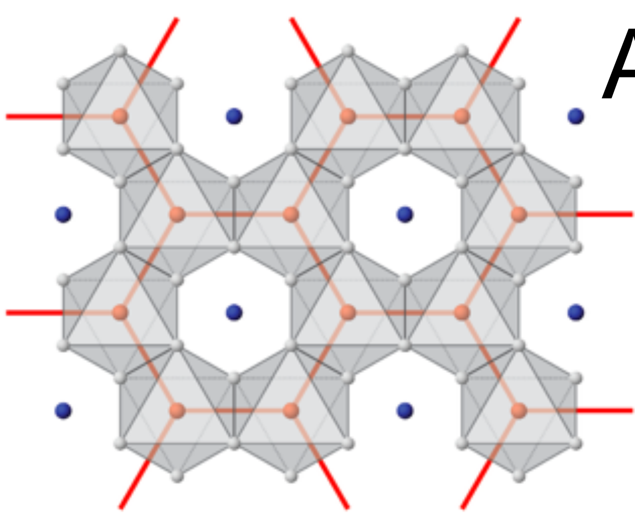


quantum spin liquid ?

Honeycomb

A_2IrO_3



quantum spin liquid ?

Double Perovskite

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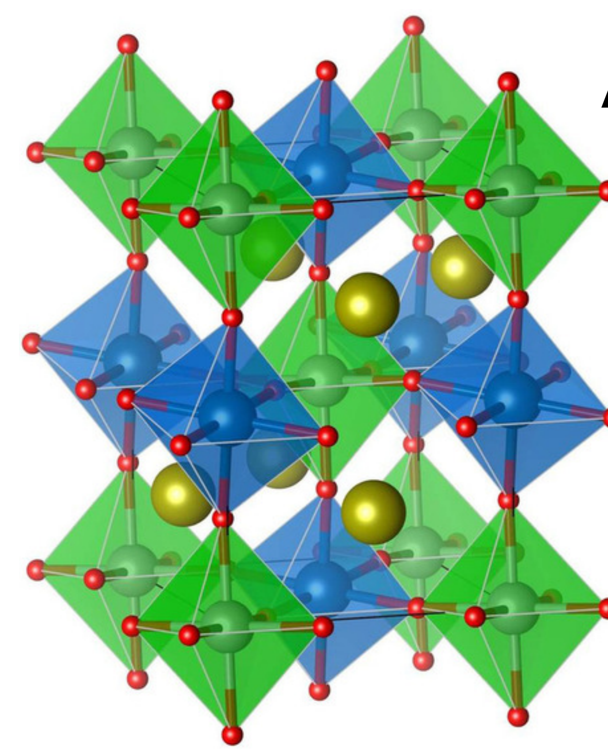
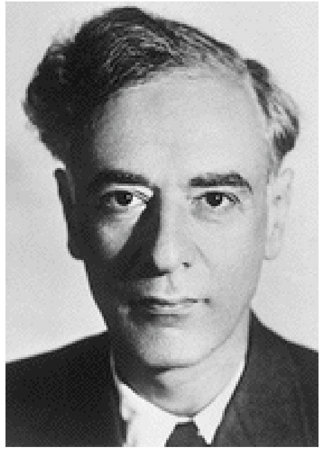


Multipolar Order ?

Brief Introduction: Topological Phases

Broken-Symmetry Phases

"Measure" Order Parameter experimentally to determine the broken symmetry



Lev Landau

X-ray: Crystal Structure, Charge Density Modulation

Neutron: Magnetic Structure, Spin Density Modulation

Landau Order Parameter allows the classification of different broken-symmetry phases

e.g. Crystal Structure

Magnetic Order

Superconductivity

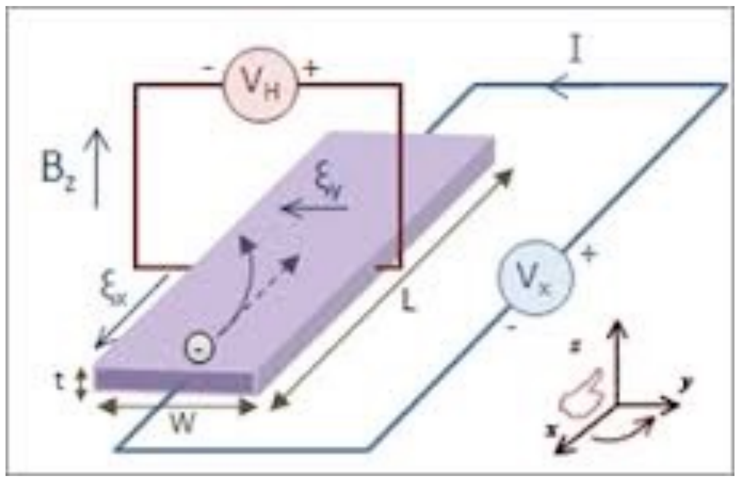
Order is boring ?   from Matthew P. A. Fisher

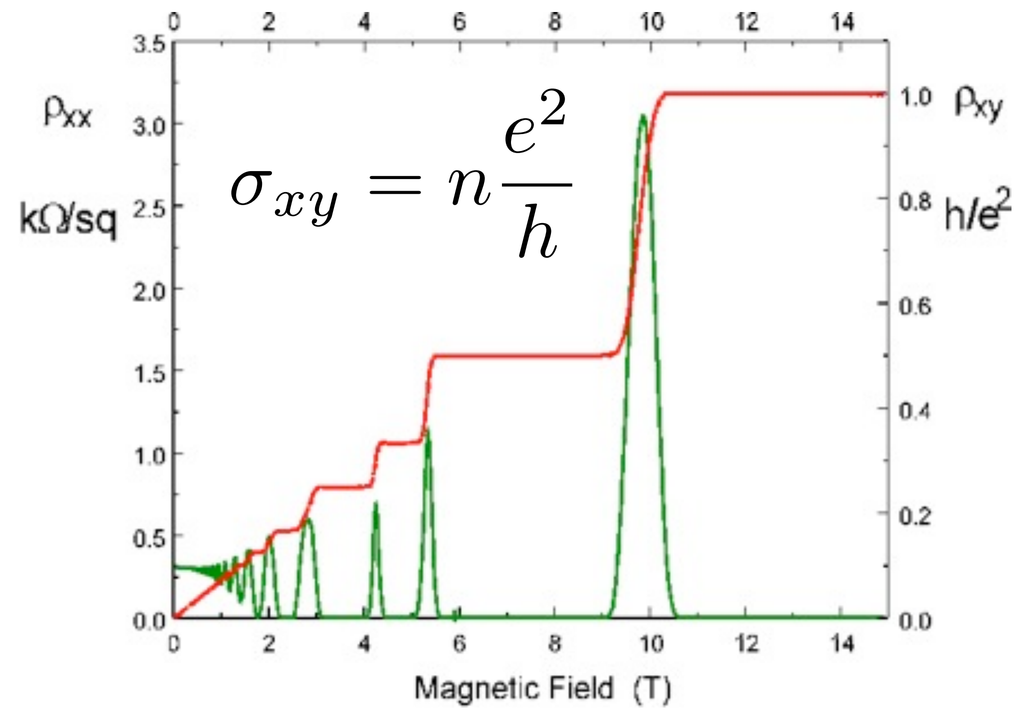
Beyond Landau Paradigm ?

$\Downarrow$

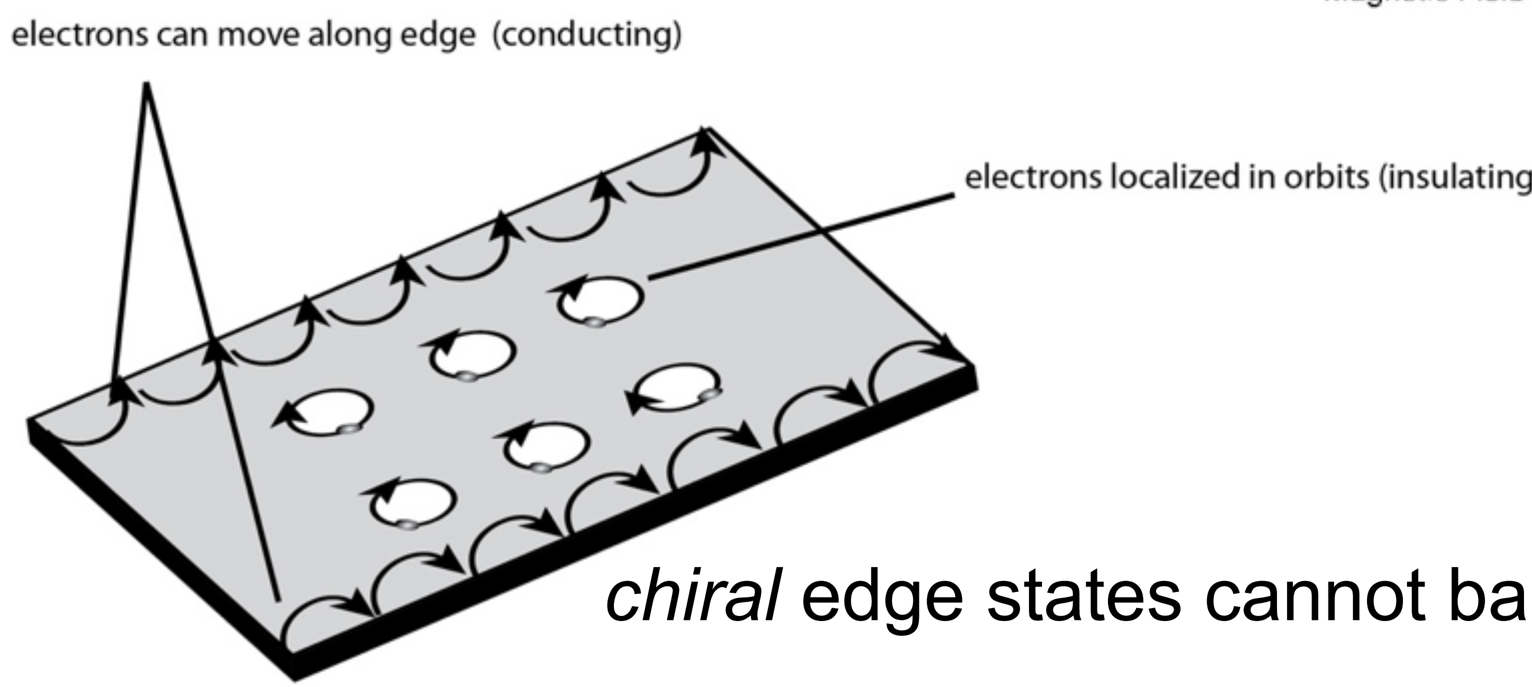
Topological Phases

The First "Topological Insulator/Phase": Integer Quantum Hall States



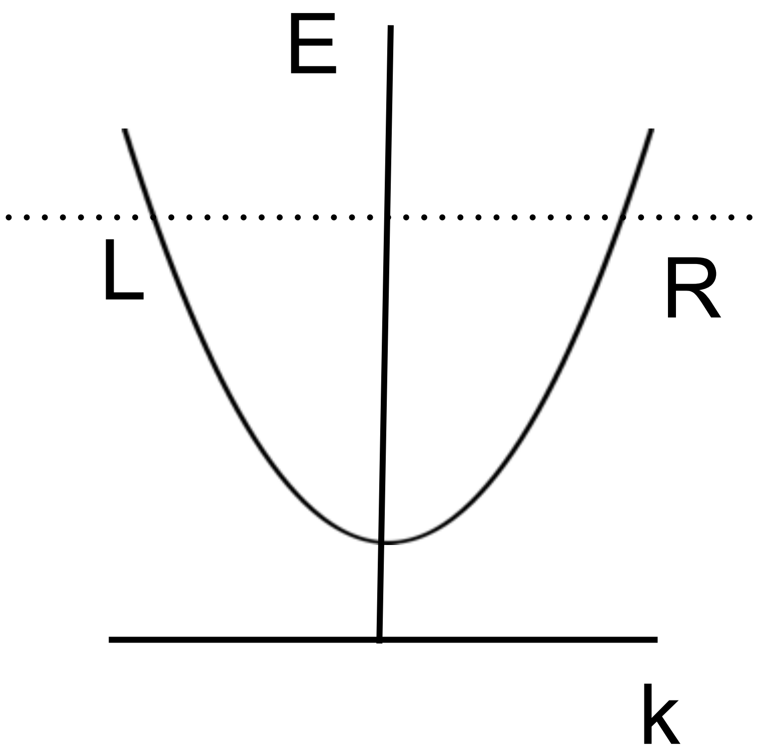


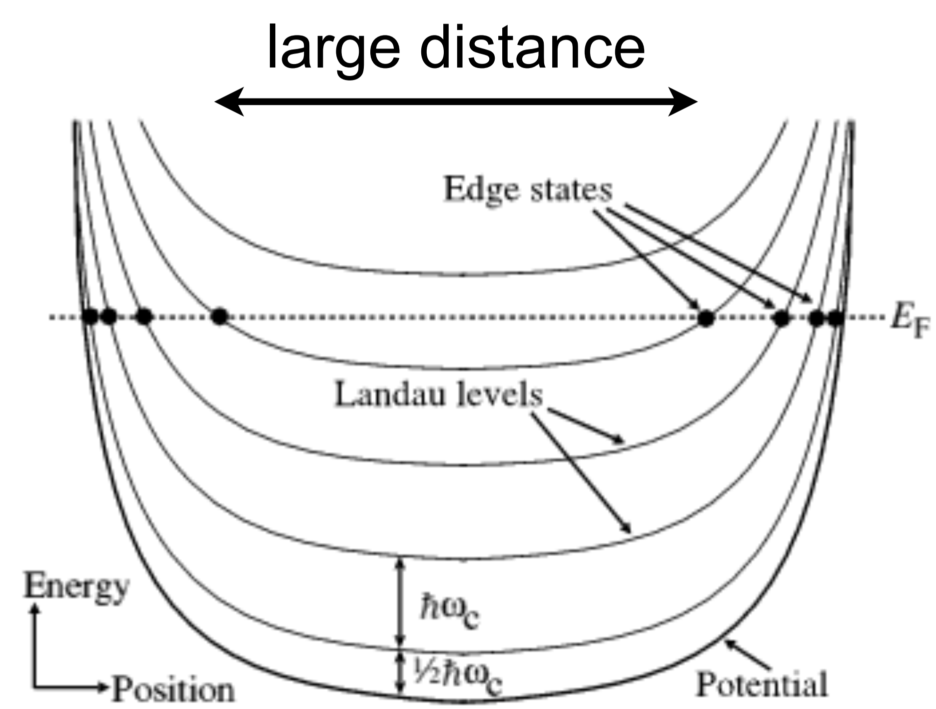
$$\sigma_{xy} = n\frac{e^2}{h}$$



chiral edge states cannot backscatter

Edge states are "half" of the low energy excitations in a 1D electron gas





B. I. Halperin 1982

The boundary chiral edge states cannot be realized in a stand-alone 1D electron system

Topological Invariant

Semiclassical Dynamics of electrons

$$\hbar\dot{\mathbf{k}} = -e\dot{\mathbf{r}} \times \mathbf{B}$$

$$\dot{\mathbf{r}} = \hbar^{-1}\nabla_{\mathbf{k}}\varepsilon_n(\mathbf{k}) - \dot{\mathbf{k}} \times \mathcal{B}_n(\mathbf{k})$$

Bloch states $\psi_n(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{n,\mathbf{k}}(\mathbf{r})$

Berry Gauge Field $\mathcal{A}_n = \langle u_{n,\mathbf{k}} | -i\nabla_{\mathbf{k}} | u_{n,\mathbf{k}} \rangle$ $\mathcal{B}_n = \nabla_{\mathbf{k}} \times \mathcal{A}_n$

Net Berry Flux is the Chern Number $C_n = \frac{1}{2\pi}\int d^2k \; B_n^z$

The total Chern number of occupied states is an integer topological invariant, and gives the Hall conductance

$$\sigma_{xy} = \frac{e^2}{h} \sum_{\varepsilon_n < \varepsilon_F} C_n$$

TKNN formula 1982

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"

Intrinsic 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)

Intrinsic 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:

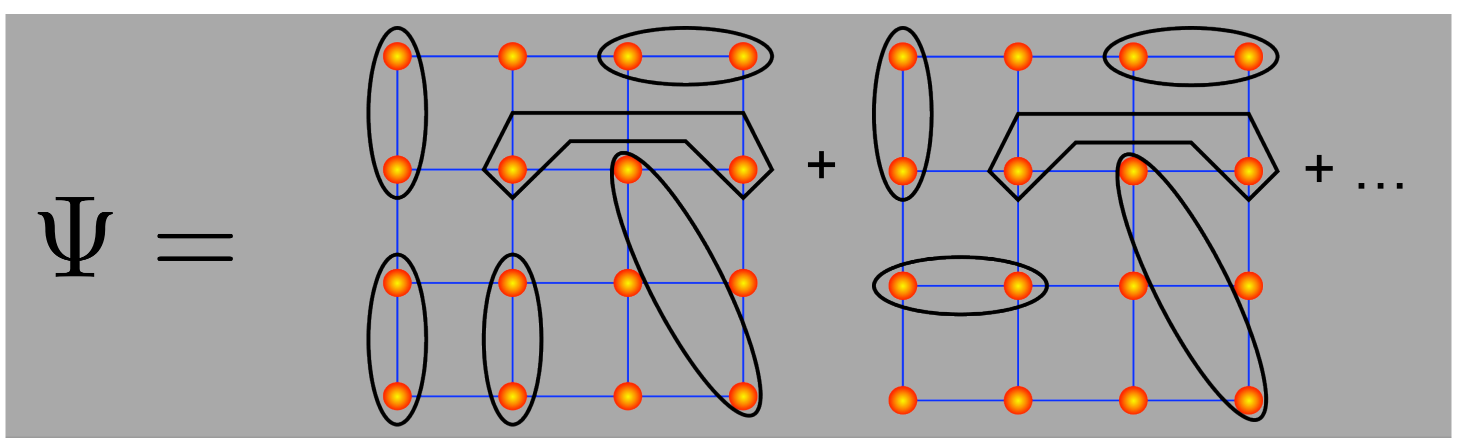
Fractionally charged e/3 Laughlin quasi-particles

Intrinsic Topological Phases (Gapped Phases)

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

Correlated insulator with no broken translational symmetry

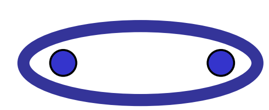
Resonating Valence Bond state (RVB);
Superposition of Valence Bond coverings



P.W.Anderson

Rokhsar-Kivelson

$$|RVB\rangle = \sum_{vb} A_{vb} |vb\rangle$$



$= \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$ 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 $|BCS\rangle \propto e^{\sum_{\mathbf{r},\mathbf{r}'} g(\mathbf{r}-\mathbf{r}') c^\dagger_{\mathbf{r}\uparrow} c^\dagger_{\mathbf{r}'\downarrow}} |0\rangle$

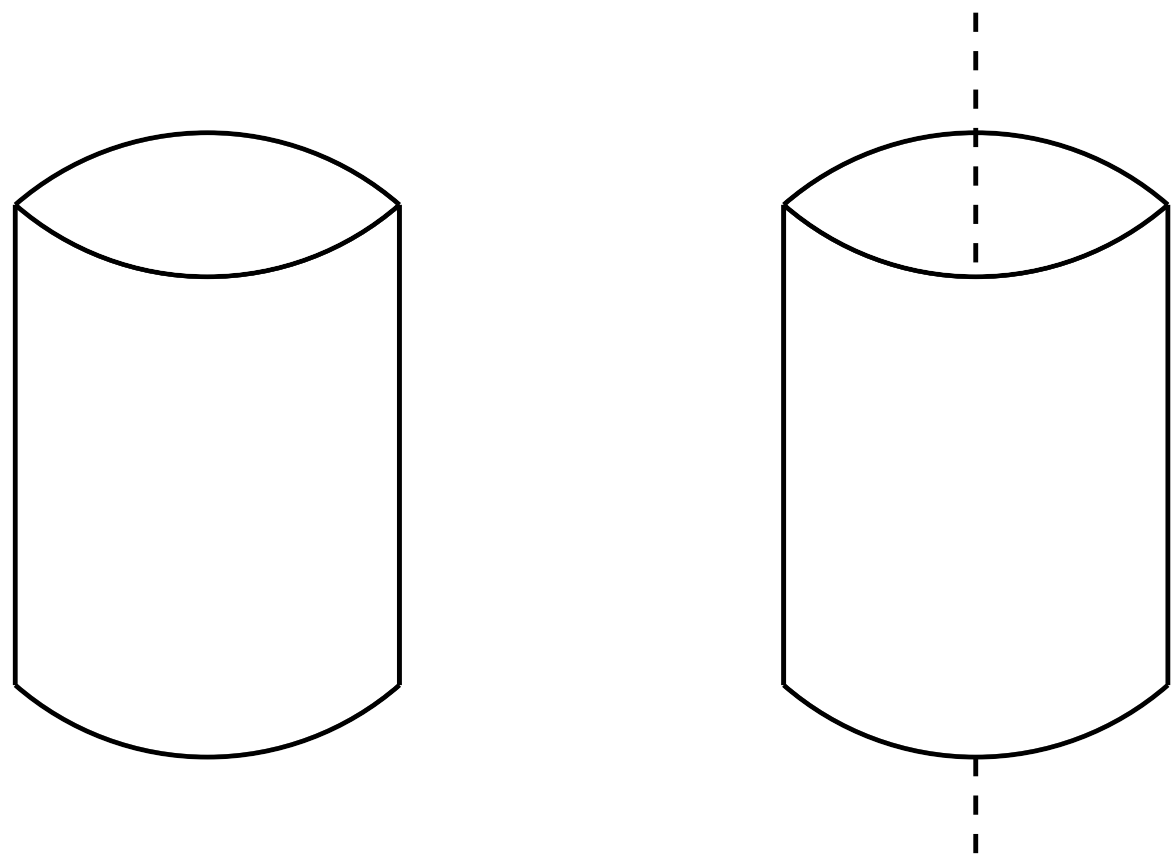
- RVB wave function $|RVB\rangle = P_G|BCS\rangle \propto \sum_{vb} A_{vb}|vb\rangle$

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



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

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

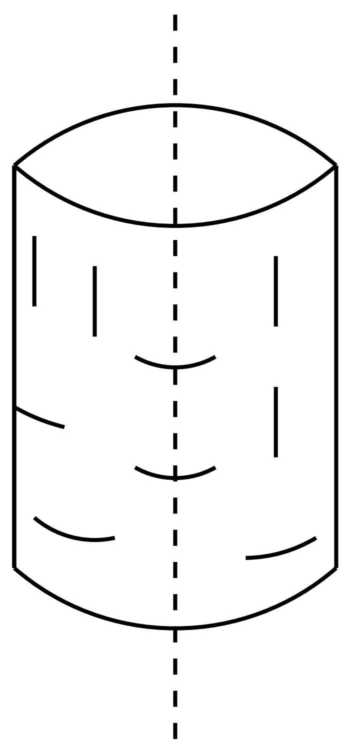
No local measurement can distinguish these phases

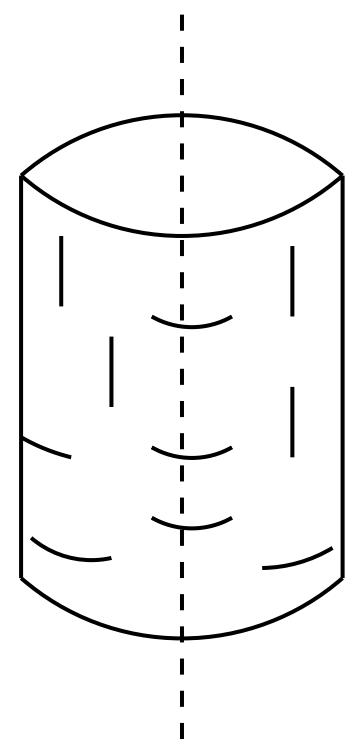
Short 'Coherence Length' Limit

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

TWO topologically distinct valence bond coverings

intersecting
even number
of dimers





intersecting
odd number
of dimers

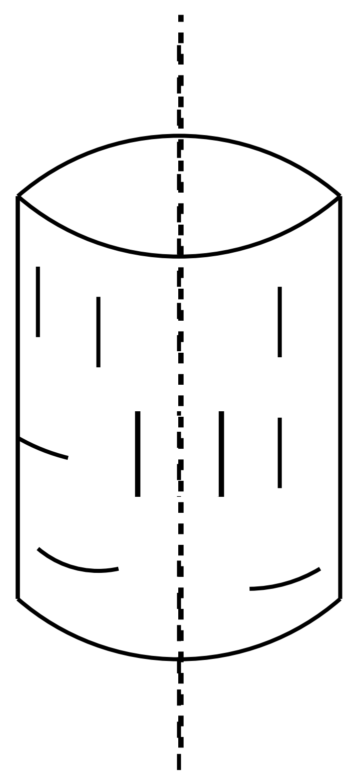
Non-trivial ground state degeneracy

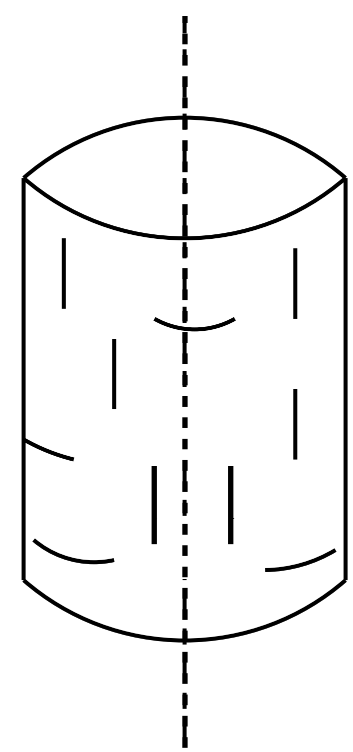
Short ‘Coherence Length’ Limit

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

TWO topologically distinct valence bond coverings

intersecting
even number
of dimers





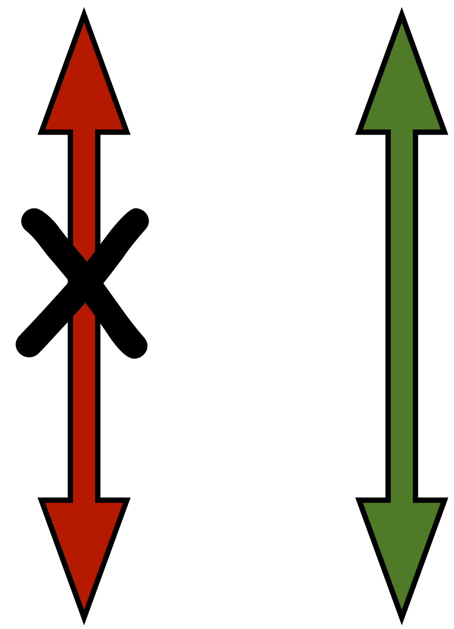
intersecting
odd number
of dimers

Non-trivial ground state degeneracy

“Symmetry-Protected” Topological Phases (Gapped Phases)

Topological Phases

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



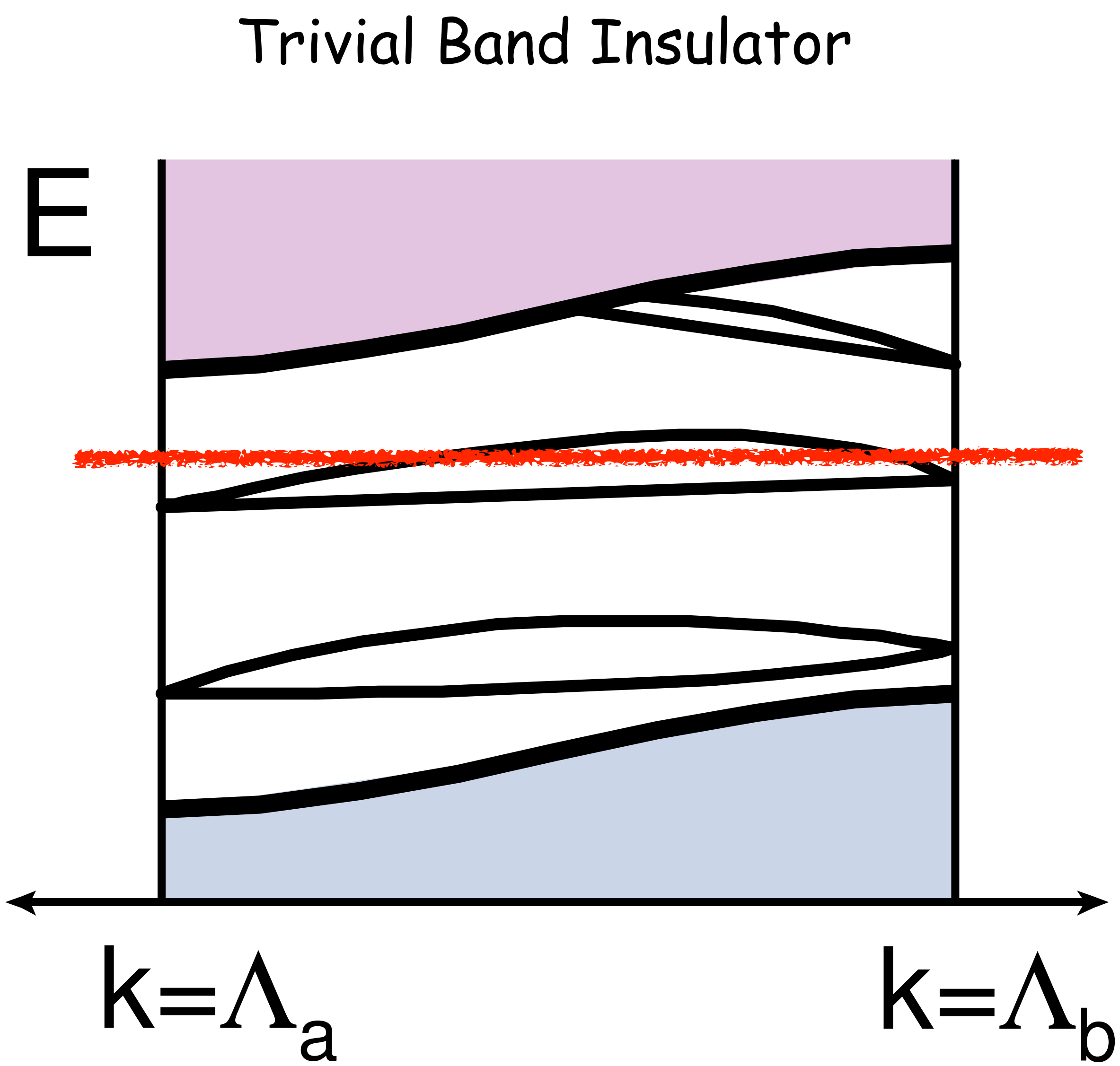
Symmetry-Breaking “Path” without closing the bulk gap

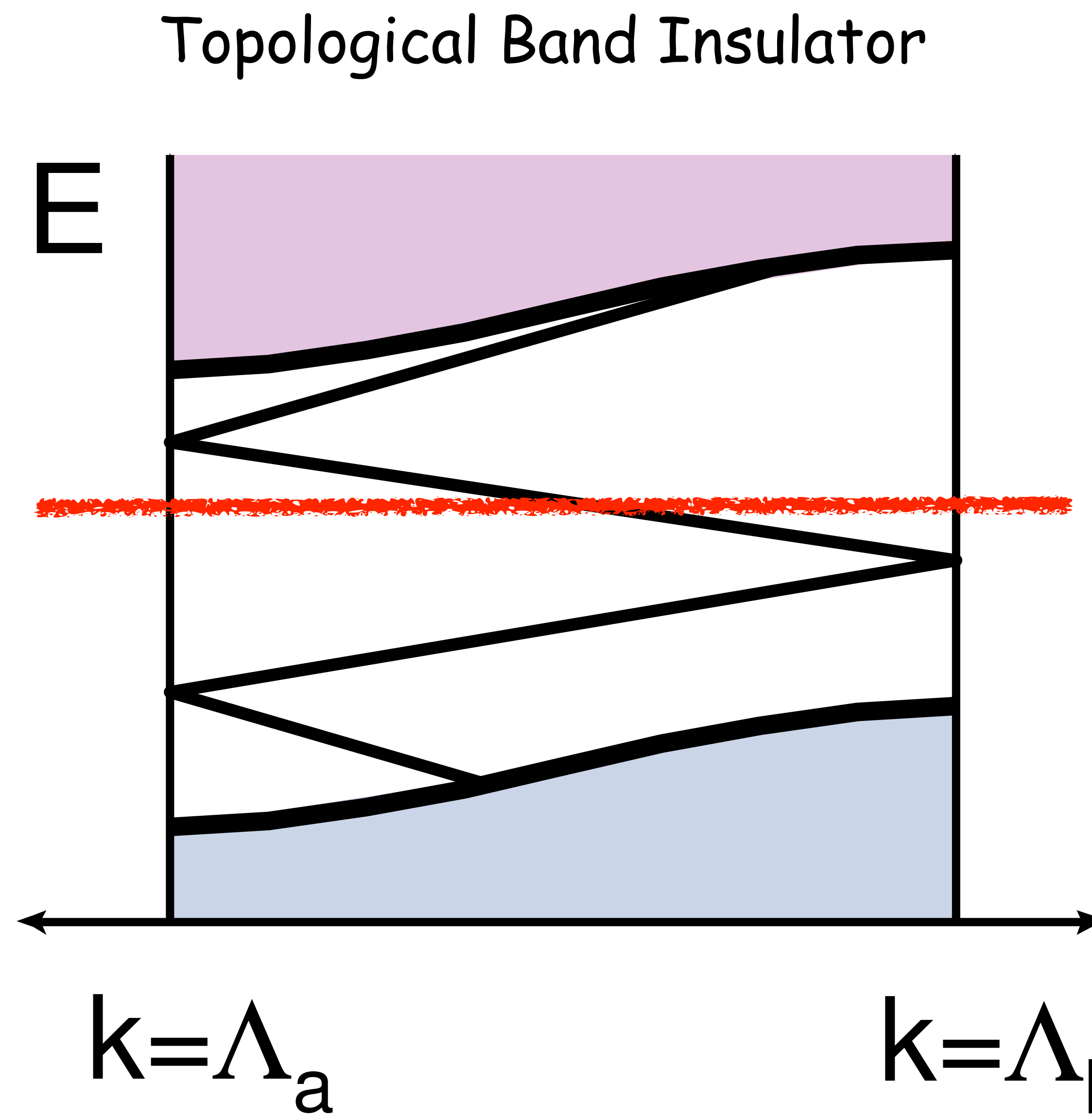
“simple phases”

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

Topological Band Insulator

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





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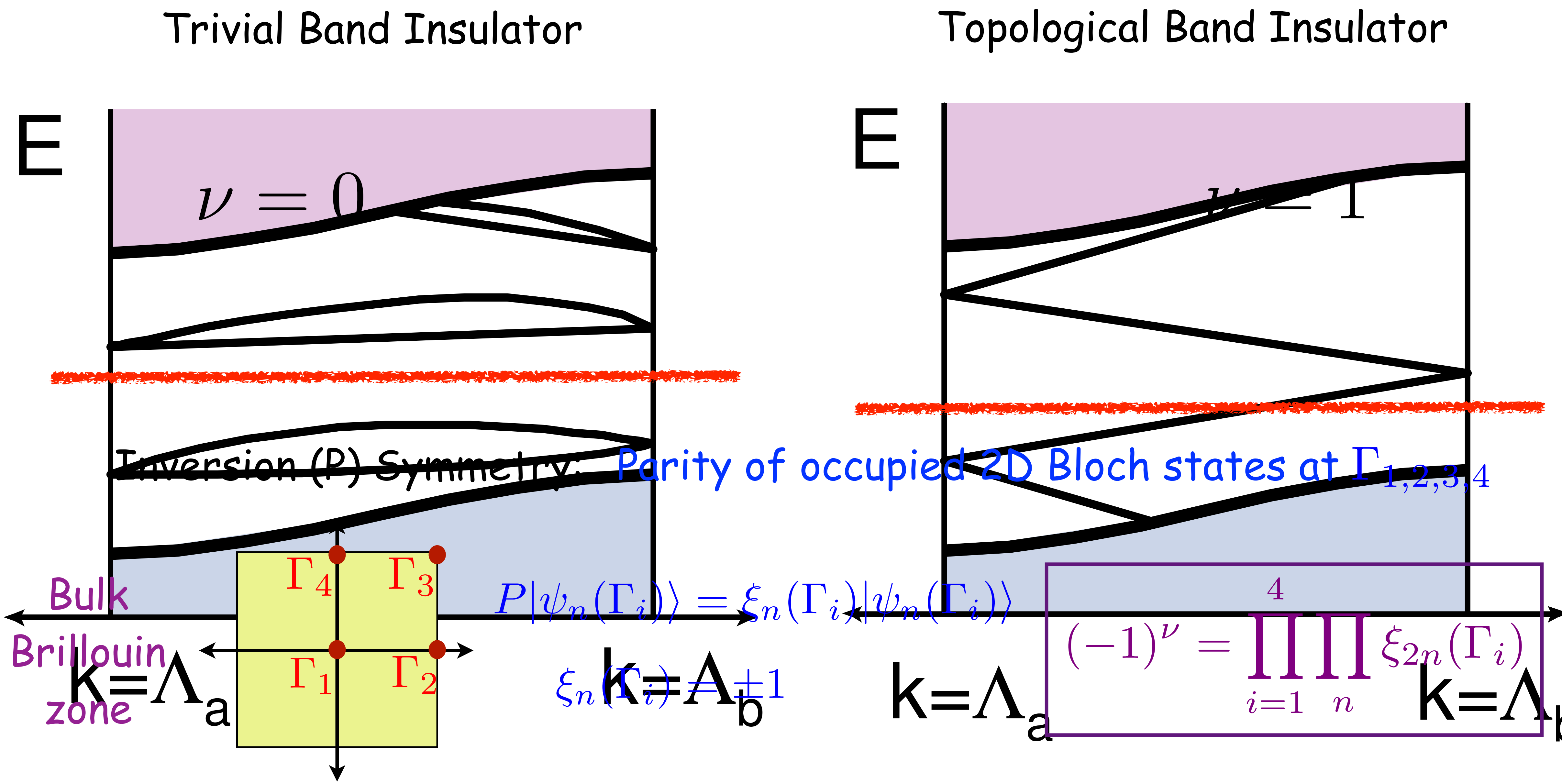
Topological Band Insulator

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



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

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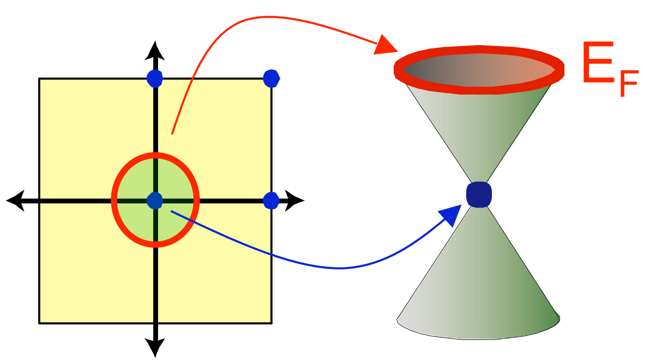
3D Topological Band Insulator

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

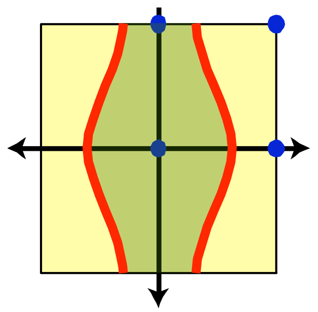
$\nu = 1$: Strong Topological Insulator

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

Symmetry-Protected Topological Phases with Interactions

Recent theoretical activities focus on "interacting" versions of Topological Insulators (not possible without interactions)

Requirement: No bulk topological order (bulk is gapped and trivial, just like non-interacting TI)

Surface States: Gapless, or break symmetries, or has intrinsic topological order (even though bulk is trivial)

D-1 dimensional surface states in D dimensional interacting TI cannot be realized in a stand-alone D-1 dimensional system !