

Title: TBA

Date: Apr 25, 2014 11:00 AM

URL: <http://pirsa.org/14040142>

Abstract:

Condensed matter systems

Condensed matter systems

: systems with many ($\sim 10^{23}$) electrons and ions with Coulomb interaction

Weakly correlated systems

Many \approx sum of individuals

$$H_{tot}^e \sim \sum_{i=1}^N h_{eff}(i) \left(= \sum_{i=1}^N \frac{p_i^2}{2m^*} + v_{eff}(x_i) \right) \quad \begin{array}{l} \text{Free electron,} \\ \text{Kohn-Sham equation,} \\ \dots \end{array}$$

If a Hamiltonian is separable, it is essentially a one-body problem.

$$\hat{h}_{eff}(i)|\psi_i\rangle = \epsilon_i|\psi_i\rangle \quad \Longrightarrow \quad |\Psi\rangle \sim \prod_i^N |\psi_i\rangle \quad E_{tot} \sim \sum_{i=1}^N \epsilon_i$$

Weakly correlated systems

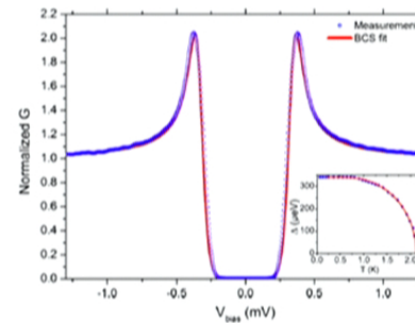
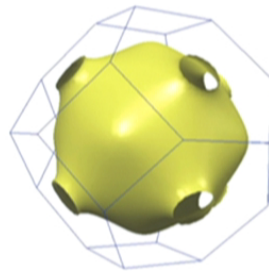
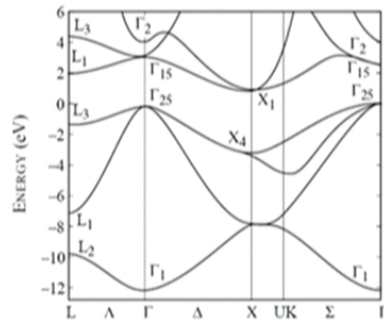
Many \approx sum of individuals

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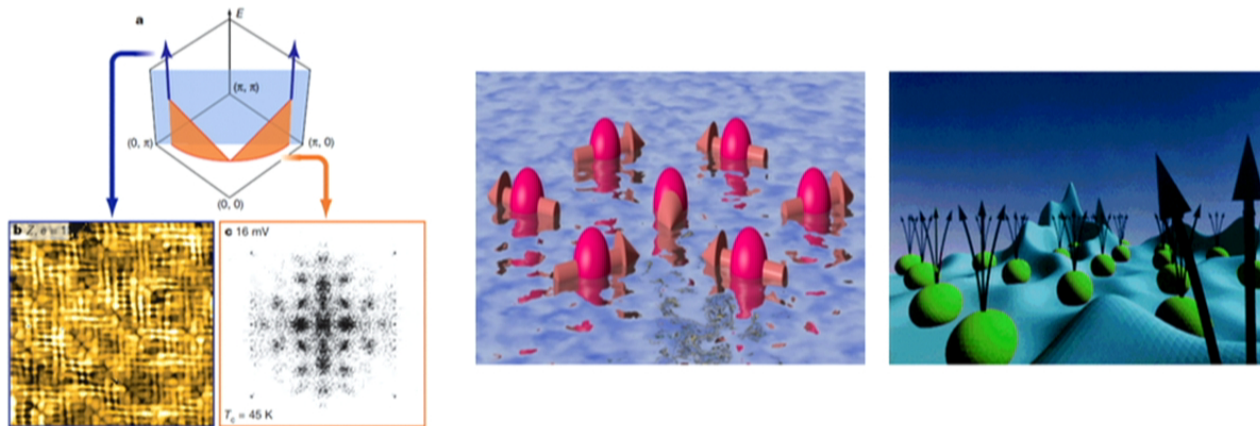
Triumph in 20th century physics (mostly from DFT)



Strongly correlated systems

Many \neq sum of individuals (*More is different*)

If a Hamiltonian is **not** separable, novel phenomena might happen!

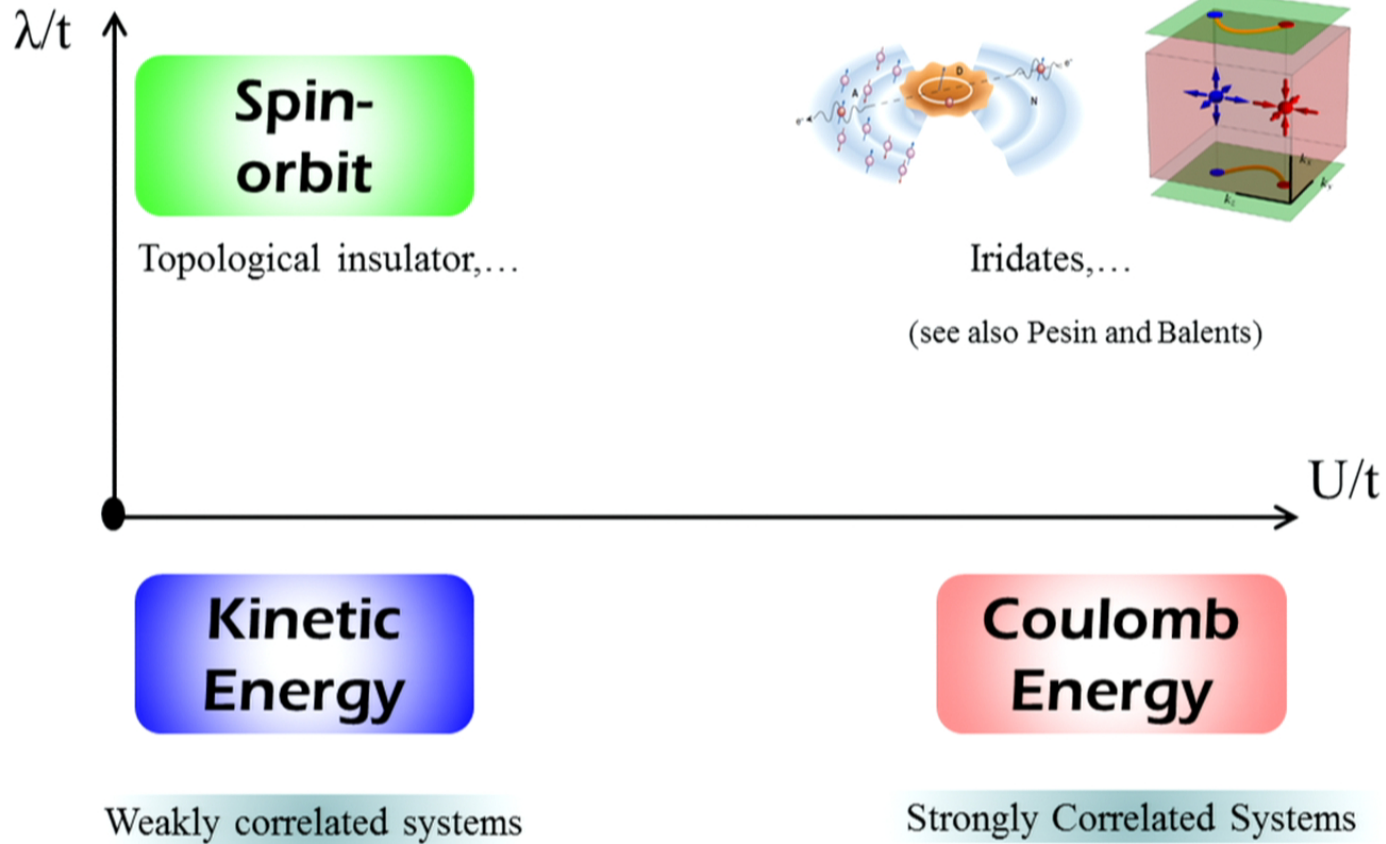


Coulomb interaction is important.

Two regimes

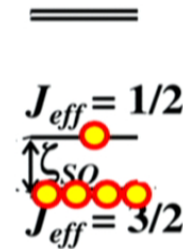
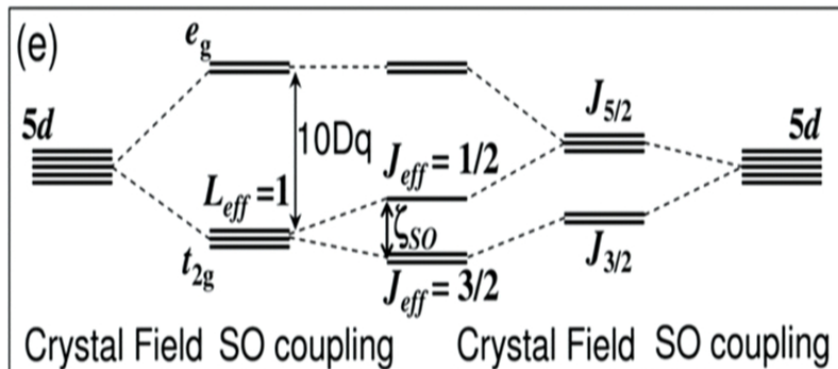


New regimes



Iridates

- $\text{Ir}^{4+} = 5d^5$
- Strong spin-orbit and coulomb interaction

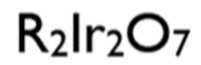
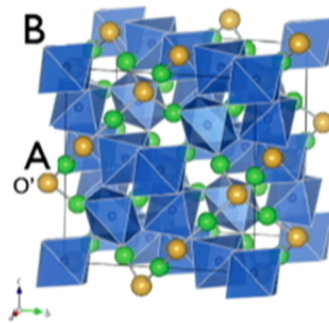
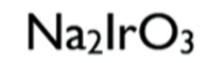
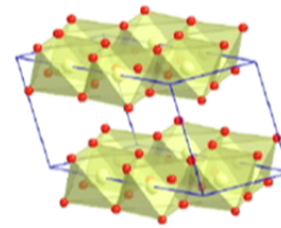
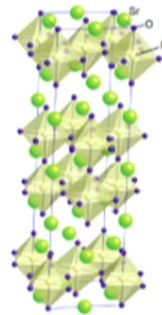
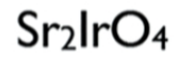
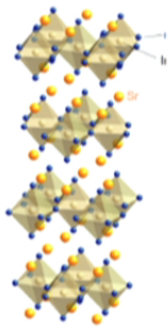


B.J. Kim. et.al. 2008

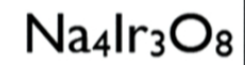
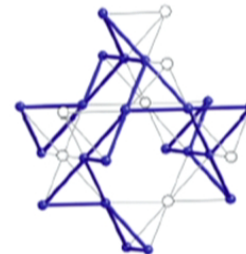
Local states : $J_{eff} = 1/2$ states (half-filling)

Iridates

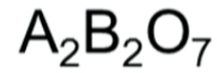
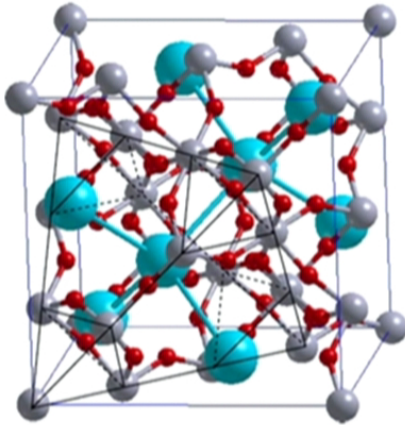
Structures



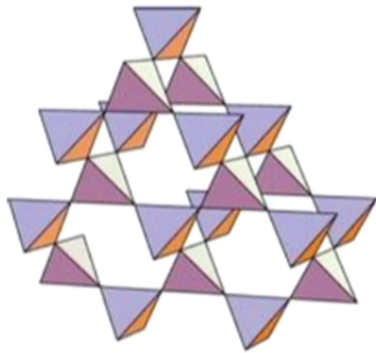
pyrochlores



Pyrochlore structure



A : rare earth B : Ir⁴⁺



Hydrogen 1 1.00794																	Helium 2 4.002602	
Lithium 3 6.941	Beryllium 4 9.012182											Boron 5 10.811	Carbon 6 12.011	Nitrogen 7 14.007	Oxygen 8 15.999	Fluorine 9 18.998	Neon 10 20.180	
Sodium 11 22.990	Magnesium 12 24.305											Aluminum 13 26.982	Silicon 14 28.086	Phosphorus 15 30.974	Sulfur 16 32.06	Chlorine 17 35.453	Argon 18 39.948	
Potassium 19 39.098	Calcium 20 40.078	Scandium 21 44.956	Titanium 22 47.887	Vanadium 23 50.942	Chromium 24 51.996	Manganese 25 54.938	Iron 26 55.845	Cobalt 27 58.933	Nickel 28 58.693	Copper 29 63.546	Zinc 30 65.38	Gallium 31 69.723	Germanium 32 72.63	Arsenic 33 74.922	Selenium 34 78.96	Bromine 35 79.904	Krypton 36 83.80	
Rubidium 37 85.468	Strontium 38 87.62	Yttrium 39 88.906	Zirconium 40 91.224	Niobium 41 92.906	Molybdenum 42 95.94	Technetium 43 98.906	Ruthenium 44 101.07	Rhodium 45 102.91	Palladium 46 106.42	Silver 47 107.87	Cadmium 48 112.41	Indium 49 114.82	Tin 50 118.71	Antimony 51 121.76	Tellurium 52 127.60	Iodine 53 126.905	Xenon 54 131.29	
Cesium 55 132.91	Barium 56 137.33	* 57-70	Lanthanum 57 138.91	Hafnium 72 178.49	Tantalum 73 180.95	Tungsten 74 183.85	Rhenium 75 186.21	Osmium 76 190.23	Iridium 77 192.22	Platinum 78 195.08	Gold 79 196.97	Mercury 80 200.59	Thallium 81 204.38	Lead 82 207.2	Bismuth 83 208.98	Polonium 84	Astatine 85	Rn 86
Francium 87 223	Radium 88 226	** 89-102	Lr 103	Rf 104	Db 105	Sg 106	Bh 107	Hs 108	Mt 109	Uun 110	Uuu 111	Uub 112						

* Lanthanide series

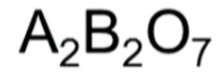
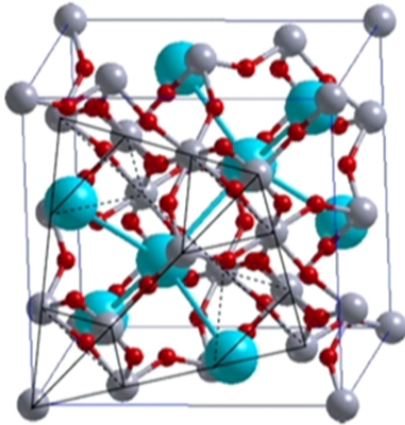
La 57 138.91	Ce 58 140.12	Pr 59 140.91	Nd 60 144.24	Pm 61	Sm 62 150.36	Eu 63 151.96	Gd 64 157.25	Tb 65 158.93	Dy 66 162.50	Ho 67 164.93	Er 68 167.26	Tm 69 168.93	Yb 70 173.05
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** Actinide series

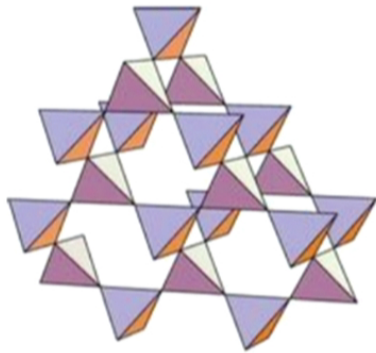
Ac 89 227	Th 90 232.04	Pa 91 231.04	U 92 238.03	Np 93	Pu 94 239	Am 95 243	Cm 96	Bk 97	Cf 98	Es 99	Fm 100	Md 101	No 102
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A (B) sublattice

Pyrochlore structure



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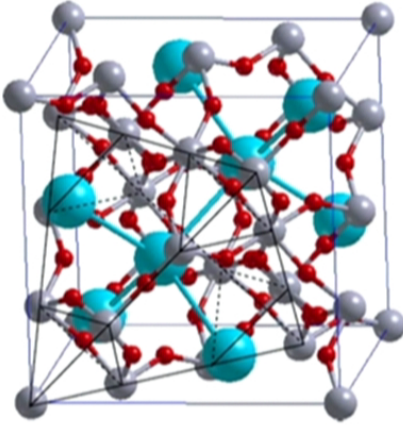
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A (B) sublattice

Pyrochlore iridates



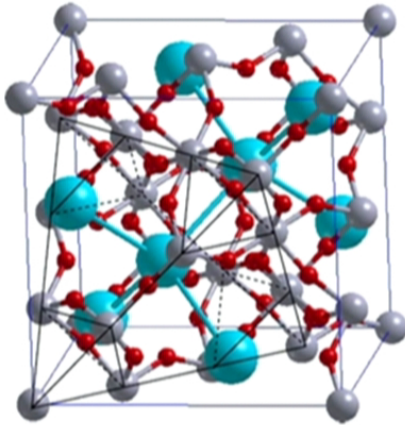
- Cubic symmetry
- Time reversal symmetry (paramagnetic phase)
- Strong spin-orbit
- Half-filling with sub-lattice structure

Representation of quantum states

O	E	\mathcal{R}	$3C_4^2 + 3\bar{\mathcal{R}}C_4^2$	$6C_4$	$6\mathcal{R}C_4$	$6C_2 + 6\bar{\mathcal{R}}C_2$	$8C_3$	$8\mathcal{R}C_3$
Γ_1	1	1	1	1	1	1	1	1
Γ_2	1	1	1	-1	-1	-1	1	1
Γ_{12}	2	2	2	0	0	0	-1	-1
$\Gamma_{15'}$	3	3	-1	1	1	-1	0	0
$\Gamma_{25'}$	3	3	-1	-1	-1	1	0	0
Γ_6	2	-2	0	$\sqrt{2}$	$-\sqrt{2}$	0	1	-1
Γ_7	2	-2	0	$-\sqrt{2}$	$\sqrt{2}$	0	1	-1
Γ_8	4	-4	0	0	0	0	-1	1

Tinkham, group theory

Pyrochlore iridates



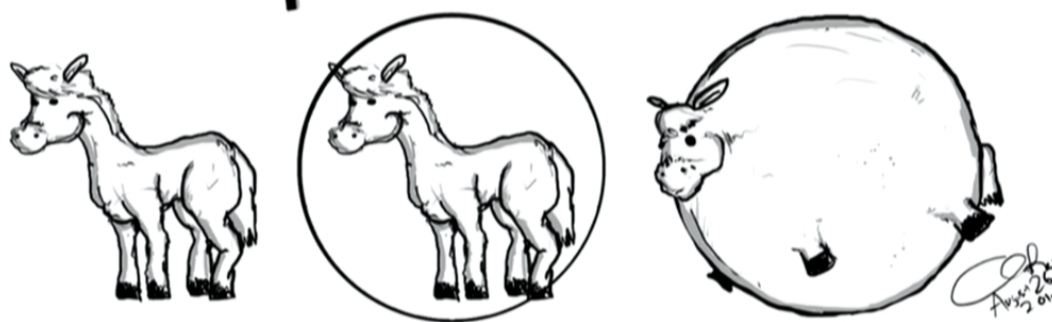
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- Time reversal symmetry
(paramagnetic phase)
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Phases in pyrochlore iridates ?

How to look at the world

Spherical horse in a vacuum

PHYSICS

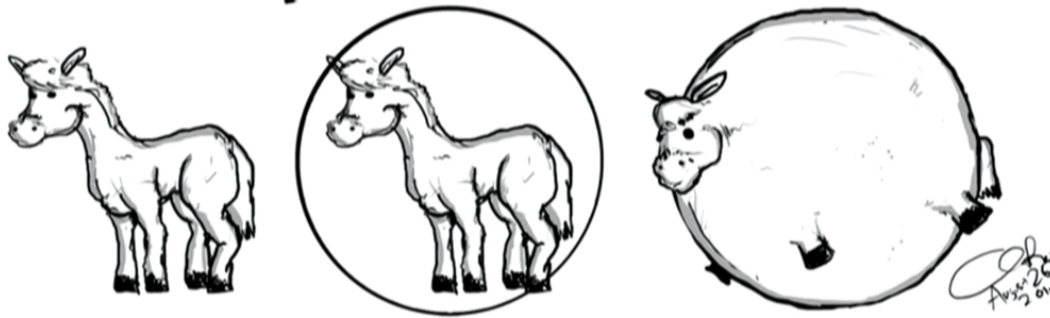


Phases in pyrochlore iridates ?

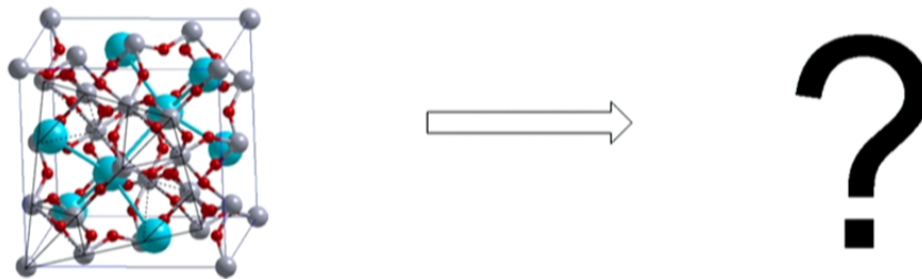
How to look at the world

Spherical horse in a vacuum

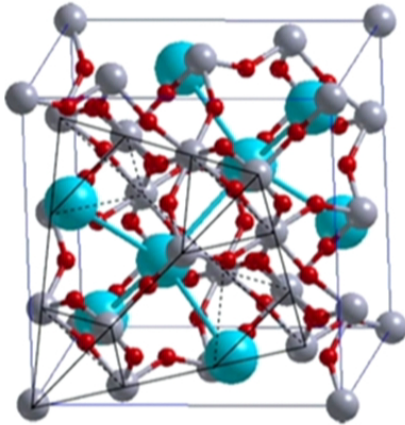
PHYSICS



Phases in pyrochlore iridates ?



Pyrochlore iridates



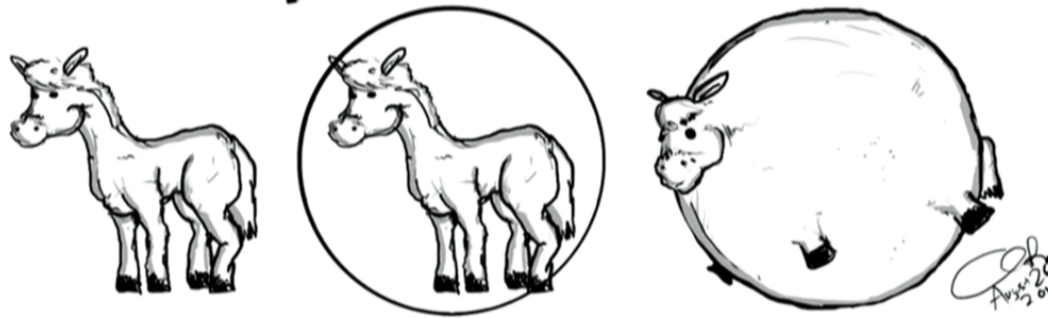
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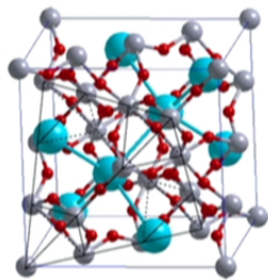
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PHYSICS



Phases in pyrochlore iridates ?



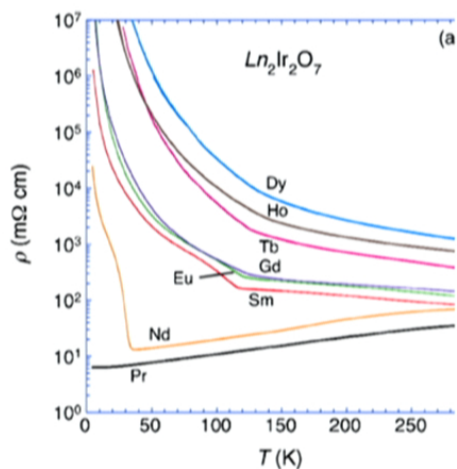
Band Insulator, Metal,

⋮

Non-Fermi liquid,

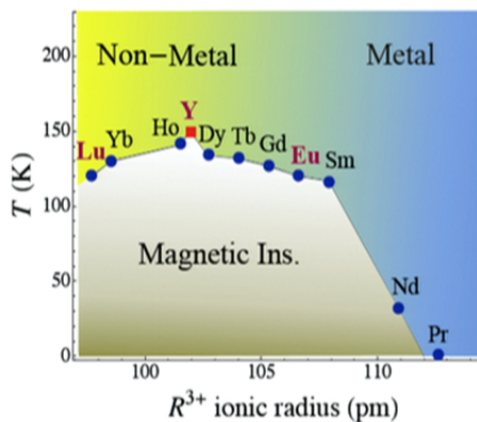
Topological insulator, Weyl SM....

Experiments



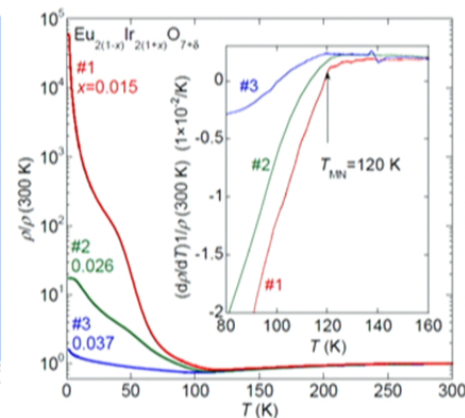
Matsuhira. et.al. 2011

2nd order metal-insulator transition (~magnetism)



Witzak-Krempa, et. al., 2013

Ionic radius dependence



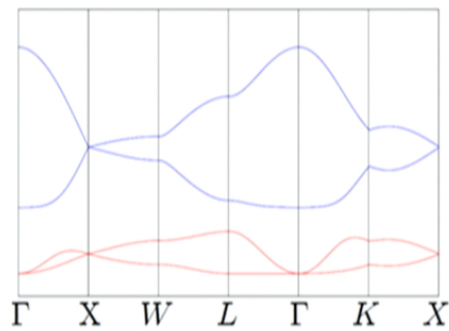
Ishikawa. et.al. 2012

Sensitive doping dependence

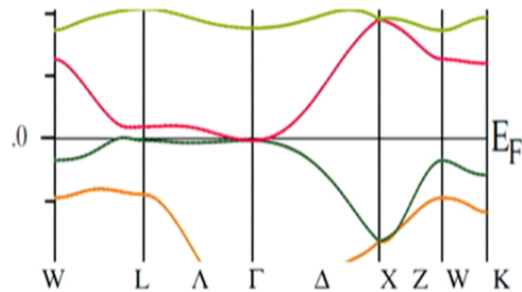
Neither good metal nor good insulator

Conventional phases (theory)

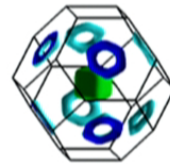
Examples of band structure calculation



(trivial) band Insulator



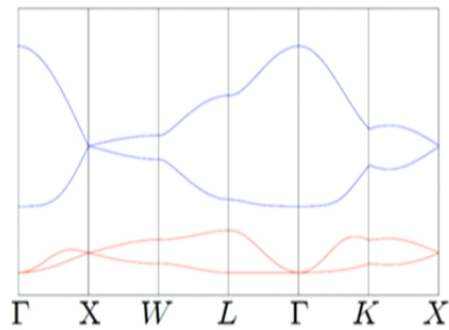
Metal



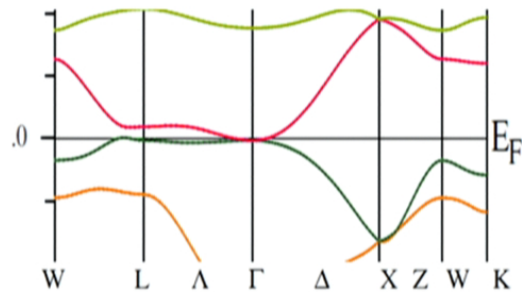
$$\int_{U_{2-2x}}^{I_{2+2x}} \circlearrowright + \delta$$

Conventional phases (theory)

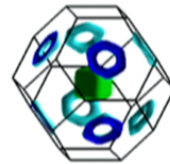
Examples of band structure calculation



(trivial) band Insulator



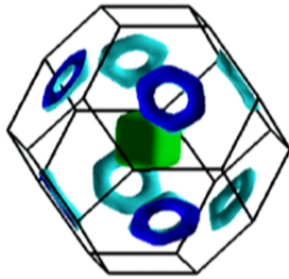
Metal



Conventional phases (theory)

Examples of band structure calculation

Metal



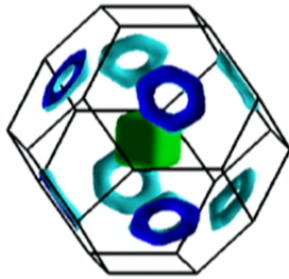
Coulomb interaction is rather weak.
(Thomas-Fermi screening)

$$E_F \gg E_{Coulomb} \sim \frac{1}{r} \quad (r \rightarrow \infty)$$

Zero Fermi Energy

Examples of band structure calculation

Metal



Coulomb interaction is rather weak.
(Thomas-Fermi screening)

$$E_F \gg E_{Coulomb} \sim \frac{1}{r} \quad (r \rightarrow \infty)$$

What happen if E_F is tiny or even zero?

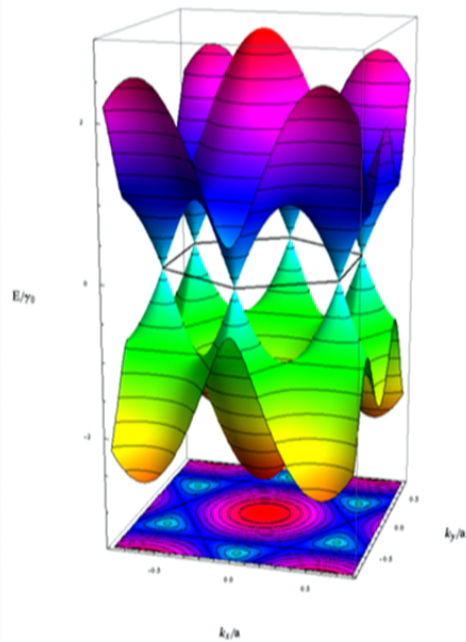
$$E_F = 0 \ll E_{Coulomb} \sim \frac{1}{r} \quad (r \rightarrow \infty)$$

Coulomb interaction is dominant! Exotic phase?

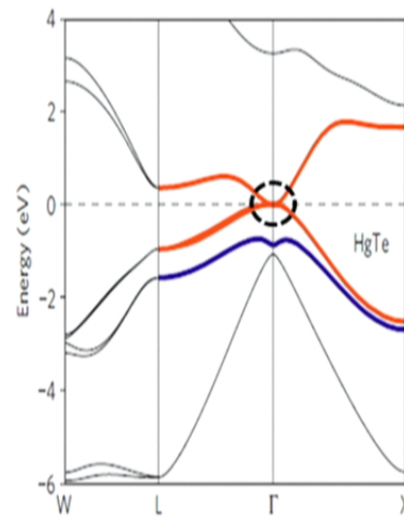
Zero Fermi Energy

Examples of zero E_F states

Graphene

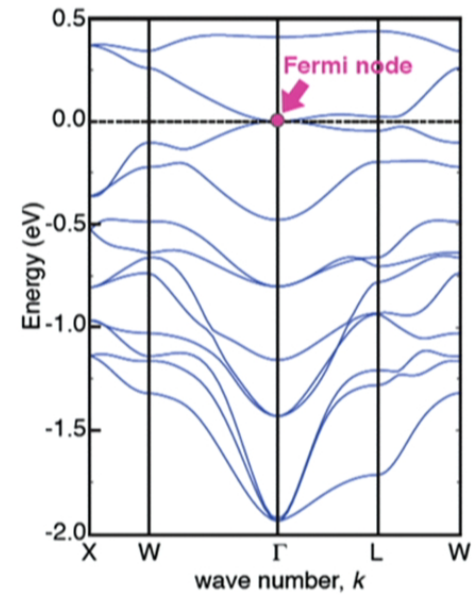


HgTe



Chadov et. al., (2010)

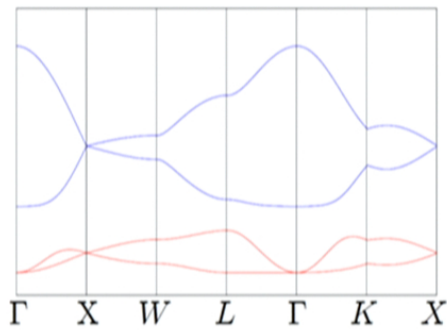
$\text{Pr}_2\text{Ir}_2\text{O}_7$ (LDA + mBJ)



T. Kondo, et. al. (to appear)

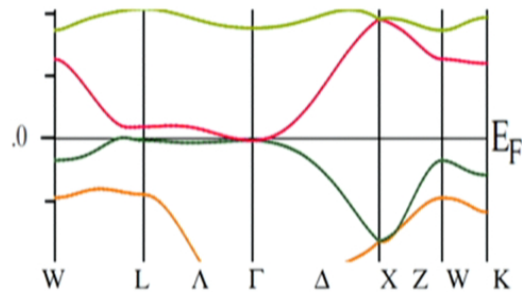
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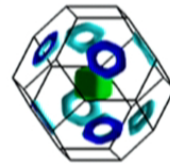


(trivial) band Insulator

the most well understood phase
(Kittel, Ashcroft-Mermin)



Metal

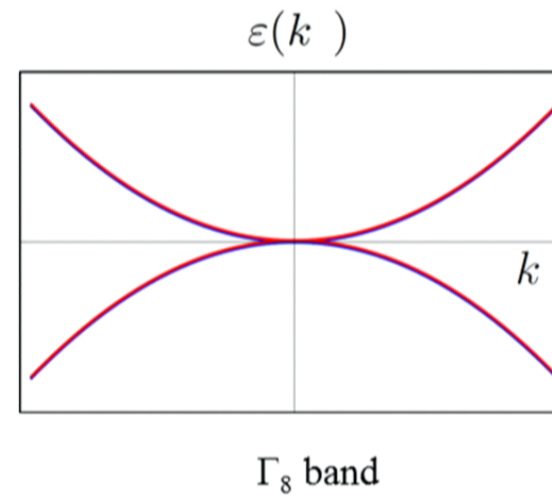
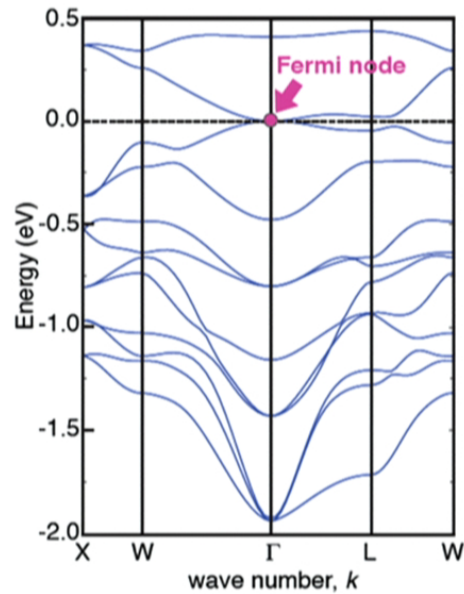
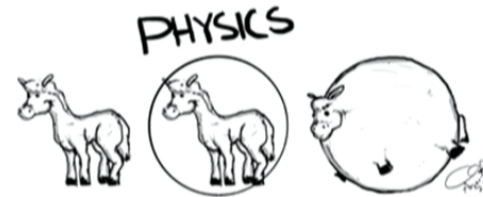


Gapless excitations from Fermi surfaces

Band structure and minimal model

■ Minimal model

- Four degenerate states, quadratic band touching
- Similar to the Luttinger model in semi-conductors



Band structure and minimal model

- Minimal model

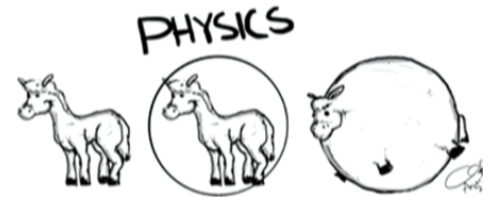
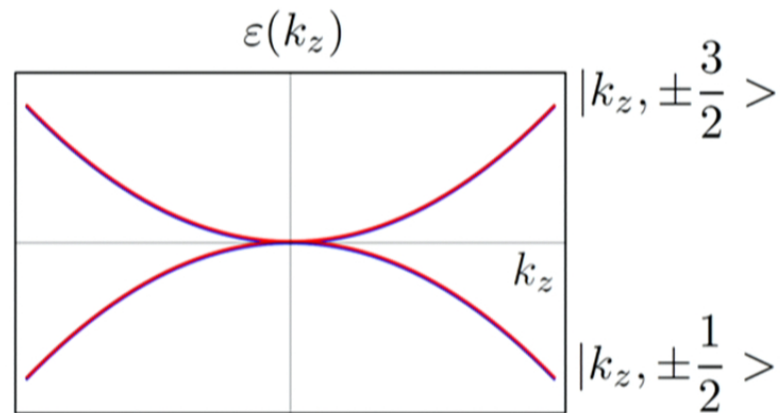
- Four degenerate states, quadratic band touching
- Similar to the Luttinger model in semi-conductors

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

$J_{x,y,z}$: 4x4 angular momentum matrices

$$\mathcal{H}(k_z \hat{z}) = \frac{k_z^2}{2m} (J_z^2 - \frac{5}{4})$$

$$J_z = \begin{pmatrix} +\frac{3}{2} & 0 & 0 & 0 \\ 0 & +\frac{1}{2} & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & -\frac{3}{2} \end{pmatrix}$$



Band structure and minimal model

- Minimal model

- Four degenerate states, quadratic band touching
- Similar to the Luttinger model in semi-conductors

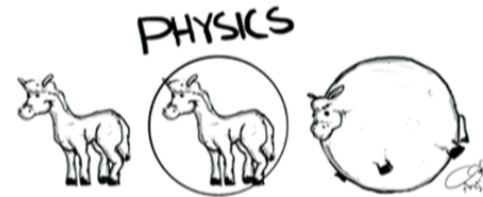
$$\mathcal{H}_0(k) = \alpha_1 k^2 + \alpha_2 (\vec{k} \cdot \vec{J})^2 + \alpha_3 (k_x^2 J_x^2 + k_y^2 J_y^2 + k_z^2 J_z^2)$$

$J_{x,y,z}$: 4x4 angular momentum matrices

- Coulomb interaction effect

$$H_{eff} = \int d^3x \overset{\text{"kinetic" term}}{\psi^\dagger \mathcal{H}_0(-i\nabla) \psi} + \overset{\text{Coulomb}}{\frac{e^2}{2} \int \frac{n(x)n(y)}{|x-y|} d^3x d^3y}$$

$$\{\psi^\dagger(\vec{k})|\text{vac}\rangle\} = \{|\vec{k}, J_z = \pm \frac{3}{2}\rangle, |\vec{k}, J_z = \pm \frac{1}{2}\rangle\}$$



Outline

1. Introduction : *bird's eye-view of correlated electron systems*
2. Band structure and minimal model : *theoretical starting point*
3. Strong Coulomb interaction : *correlation, correlation, and correlation*
4. Symmetry breaking and topological phases
5. Conclusion

Strong Coulomb interaction

- Estimation of Coulomb interaction

- Coulomb interaction : $E_C \sim \frac{e^2}{r}$ - kinetic energy: $E_{kin}(k) \sim k^2$

- Heisenberg uncertainty relation : $E_{kin} \sim \frac{1}{mr^2}$, $E_C \sim \frac{e^2}{r}$

$$E_{kin} \ll E_C \quad r \rightarrow \infty$$

Strong Coulomb interaction

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Coulomb interaction is dominant!
Exotic phases?

Strong Coulomb interaction

- Estimation of Coulomb interaction

- Coulomb interaction : $E_C \sim \frac{e^2}{r}$
- kinetic energy: $E_{kin}(k) \sim k^2$
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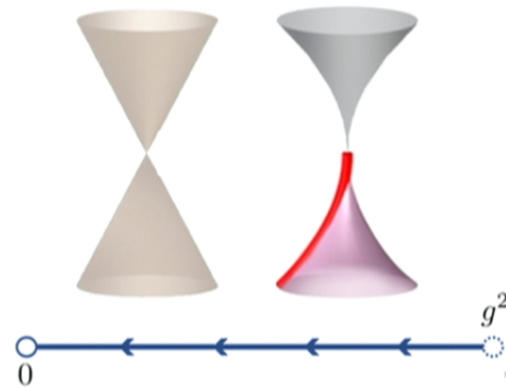
$$E_{kin} \ll E_C \quad r \rightarrow \infty$$

cf) graphene at zero doping

- kinetic energy : $E_{kin}(k) \sim k$
- Coulomb interaction : $E_C \sim \frac{e^2}{r}$

$$E_{kin} \sim E_C$$

marginal Coulomb interaction
 → velocity renormalization



$$g^2 = \frac{e^2}{2\pi}$$

$$\int_{U^2-2x}^{I} \frac{1}{2+2x} dx$$



Strong Coulomb interaction

- Renormalization group

$$\mathcal{H}_0(k) = \alpha_1 k^2 + \alpha_2 (\vec{k} \cdot \vec{J})^2 + \alpha_3 (k_x^2 J_x^2 + k_y^2 J_y^2 + k_z^2 J_z^2) \quad J_{x,y,z} : 4 \times 4 \text{ matrices}$$

$$S_L = \int d\tau d^d x \left\{ \psi^\dagger \left[\partial_\tau - ie\varphi + \mathcal{H}_0 \right] \psi + \frac{c_0}{2} (\partial_i \varphi)^2 \right\}$$

Scaling analysis ($z=2, d=3$):

$$\begin{aligned} x &\rightarrow x e^{-l} & [\psi^\dagger \psi] &= d & [\varphi^2] &= d \\ \tau &\rightarrow \tau e^{-z l} \end{aligned}$$

$$[e^2] = 1 \quad \text{relevant!}$$

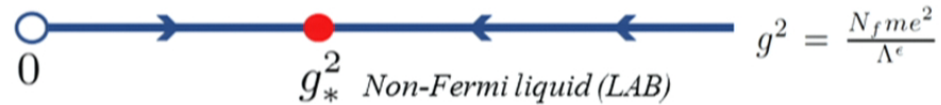
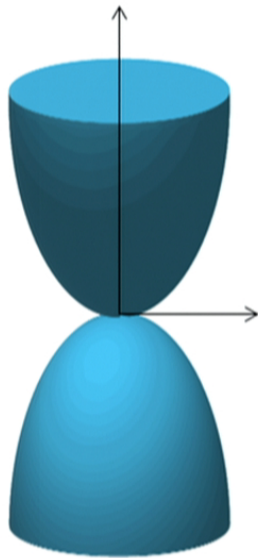
Two methods : $\varepsilon (=4-d)$ expansion, Large N_f expansion ($d=3$)

Strong Coulomb interaction

- Renormalization group

1. $\epsilon(=4-d)$:

$$\frac{d\tilde{g}}{dl} = \epsilon\tilde{g} - N_f\tilde{g}^2 \quad \eta_b = \epsilon + O\left(\frac{\epsilon^2}{N_f}\right)$$



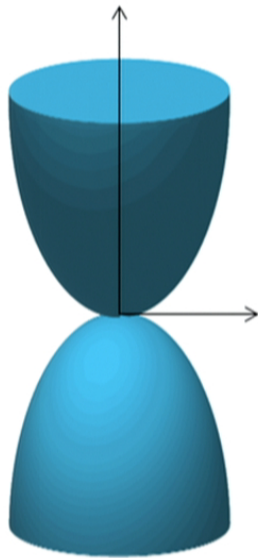
Strongly interacting **quantum critical phase** in $d=3$!

Strong Coulomb interaction

- Renormalization group

1. $\epsilon(=4-d)$:

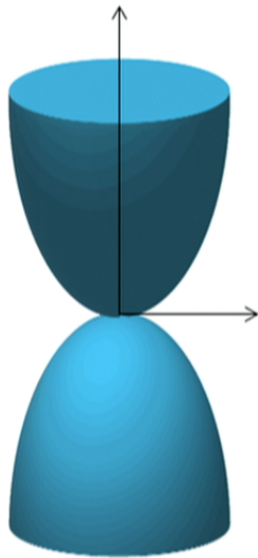
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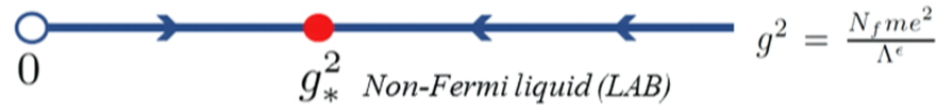
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Strong Coulomb interaction

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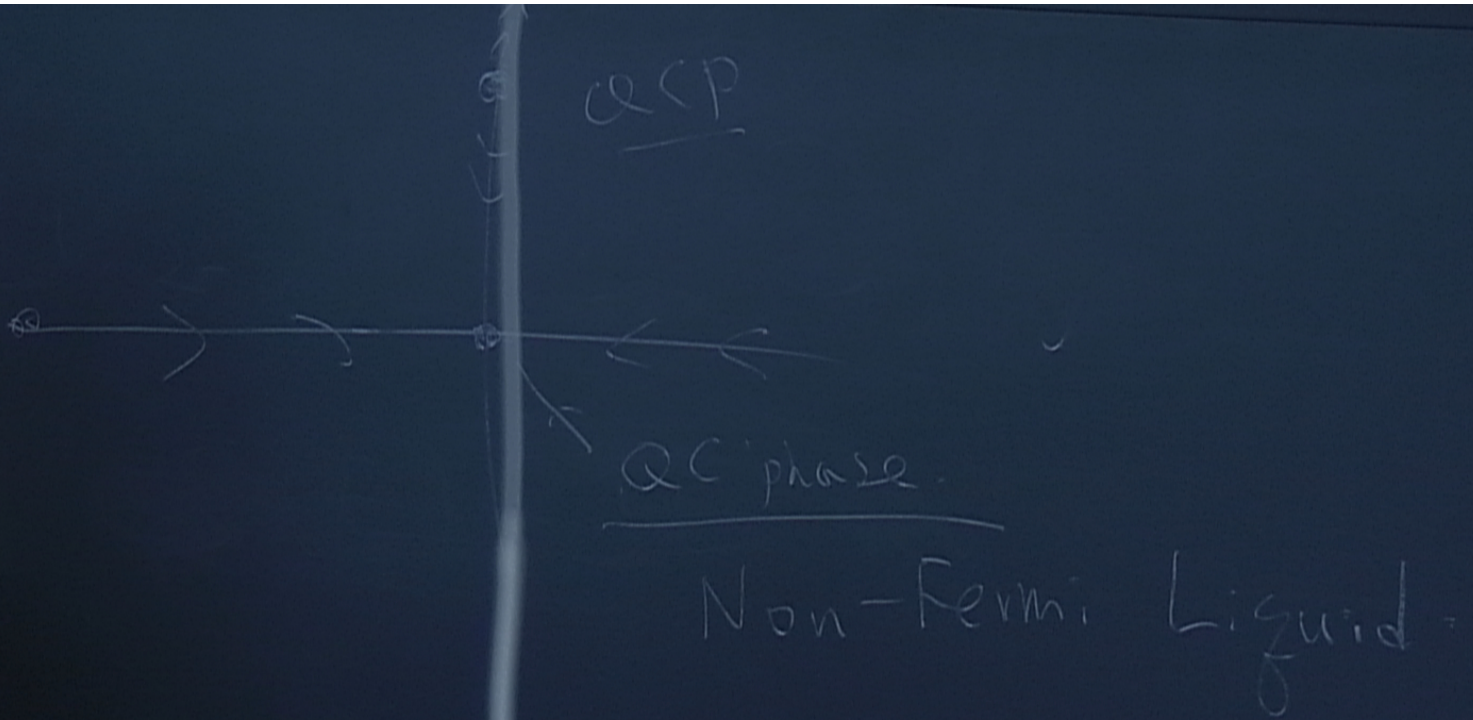
$$1. \varepsilon(=4-d) : \quad \frac{d\tilde{g}}{dl} = \varepsilon\tilde{g} - N_f\tilde{g}^2 \quad \eta_b = \varepsilon + O\left(\frac{\varepsilon^2}{N_f}\right)$$



$$2. \text{Large } N_f : \quad \eta_b = 1 \quad \eta_f = \frac{0.17}{N_f} \quad z = 2 - \frac{0.069}{N_f}$$

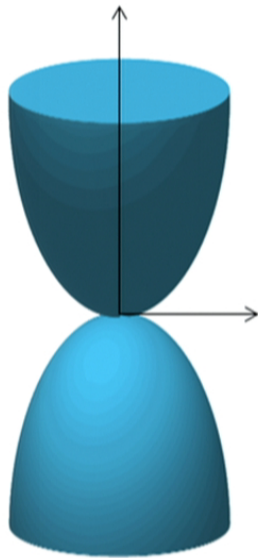
Two methods are consistent! $V_c(q) \sim \frac{1}{q^2} \rightarrow \frac{1}{q^{2-\eta_b}}$

Strongly interacting **quantum critical phase** in $d=3$!

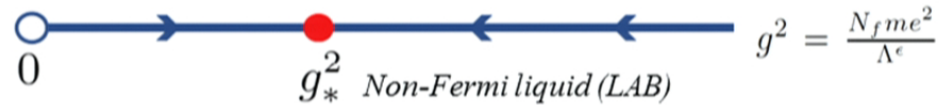


Strong Coulomb interaction

- Renormalization group



$$1. \varepsilon(=4-d) : \quad \frac{d\tilde{g}}{dl} = \varepsilon\tilde{g} - N_f\tilde{g}^2 \quad \eta_b = \varepsilon + O\left(\frac{\varepsilon^2}{N_f}\right)$$



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Strongly interacting **quantum critical phase** in d=3!

Implication

$$S_L = \int d\tau d^d x \left\{ \psi^\dagger \left[\partial_\tau - ie\varphi + \mathcal{H}_0 \right] \psi + \frac{c_0}{2} (\partial_i \varphi)^2 \right\}$$

Symmetry broken states

$$E_{1,2} = \pm \sqrt{k_x^2 + k_y^4}$$

$$E_{1,1,2} = \pm \sqrt{k_x^2 + k_y^2 + k_z^4}$$

$$E_{2,2,1} = \pm \sqrt{(k_x^2 + k_y^2)^2 + k_z^2}$$

Physical realization?

Coulomb interaction effect?

Non Fermi liquid

- LAB (Luttinger-Abrikosov-Beneslaevski) phase
 - **Anomalous dimensions** in physical quantities
 - Symmetry protection (cubic+ time reversal)
 - Emergent symmetries (particle-hole and full rotation)

Dispersion relation : $\omega \sim k^z \approx k^{1.7}$

Specific Heat : $c_v \sim T^{\check{d}/z} \approx T^{1.7}$

Susceptibility : $\chi(T) \sim a + b T^{(d-z+2\eta_{12})/z} \approx a + b T^{0.5}$

Non linear susceptibility : $\chi_3 = \partial^3 M / \partial H^3 \Big|_{H=0} \approx T^{-1.7}$

Anomalous Hall : $\sigma_{xy} \sim H^{1/(z-\eta_{12})} \approx H^{0.51}$

Outline

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3. Strong Coulomb interaction : *Correlation, correlation, and correlation*
4. Symmetry breaking and topological phases : *World without symmetry*
5. Conclusion

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$$S_L = \int d\tau d^d x \left\{ \psi^\dagger \left[\partial_\tau - ie\varphi + \mathcal{H}_0 \right] \psi + \frac{c_0}{2} (\partial_i \varphi)^2 \right\}$$

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Physical realization?

Coulomb interaction effect?

Implication

$$S_L = \int d\tau d^d x \left\{ \psi^\dagger \left[\partial_\tau - ie\varphi + \mathcal{H}_0 \right] \psi + \frac{c_0}{2} (\partial_i \varphi)^2 \right\}$$

Mono-layer graphene

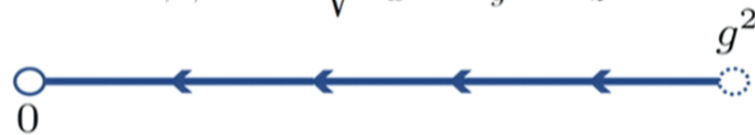
$$E_{1,1} = \pm \sqrt{k_x^2 + k_y^2}$$

Bi-layer graphene

$$E_{2,2} = \pm (k_x^2 + k_y^2)$$

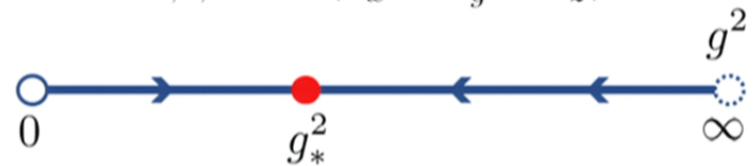
*Quantum electrodynamics
(linear Weyl semi-metal)*

$$E_{1,1,1} = \pm \sqrt{k_x^2 + k_y^2 + k_z^2}$$



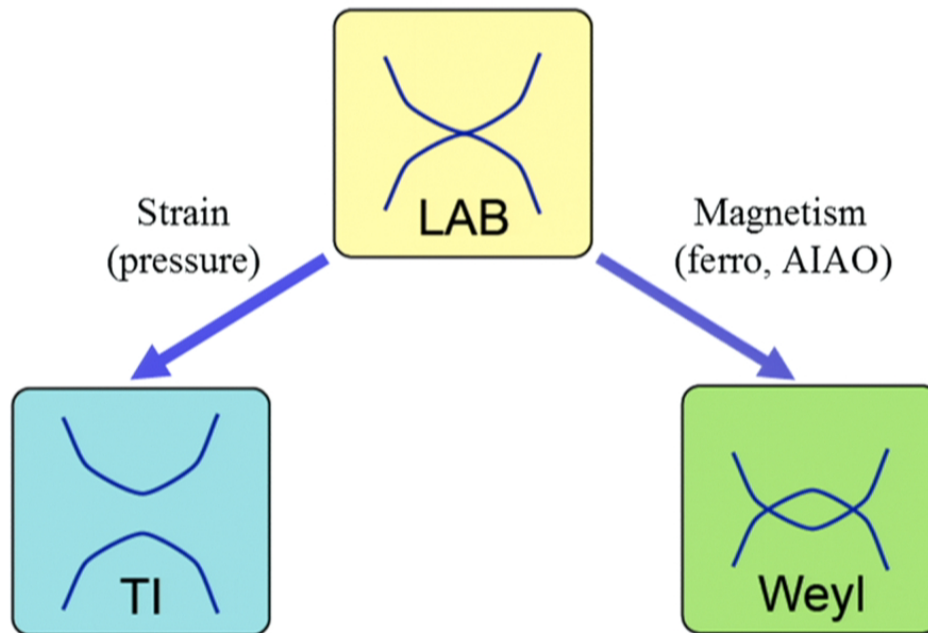
Pr₂Ir₂O₇

$$E_{2,2,2} = \pm (k_x^2 + k_y^2 + k_z^2)$$



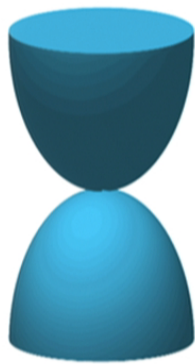
Symmetry breaking

- Topological phases around the NFL



Coulomb interaction in Weyl semimetals

Spin-orbit + cubic + time reversal : quadratic band touching (QBT)



Break some symmetry
: QBT becomes unstable.
ex) linear Weyl (LW) semimetal



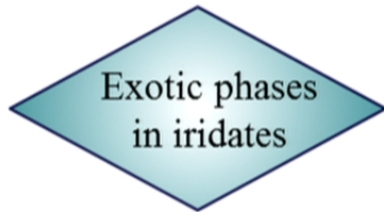
Coulomb interaction in LW
(~quantum electrodynamics)

$$\mathcal{H}_{LW} = k_x \sigma_x + k_y \sigma_y + k_z \sigma_z$$



Hosor et. al. , PRL 2012

Current Situation (Exp)



NFL

Maybe?

Nakatusji group, Nature 2010

Weyl SM

Maybe?

Tokura group, PRL 2012

TI

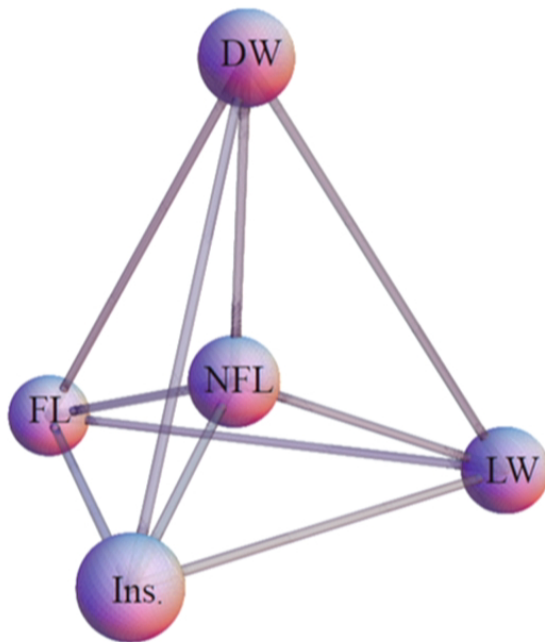
Not yet!

...

Clean sample,
bulk and thin film,
Charge probe (transport,
optical, ARPES, q-
oscillation,...),
Theory and Exp,...

Summary of phases

Phases and phase transitions in pyrochlore iridates



FL : Fermi liquids

DOS = Constant

$$C_v \sim T$$

Ins : Insulator (band, magnetism...)

DOS = zero

$$C_v \sim e^{-\frac{\Delta}{T}}$$

LW : Linear Weyl semi-metal

DOS(E) $\sim E^2$

$$C_v \sim T^3$$

DW : Double Weyl semi-metal

DOS(E) $\sim E$

$$C_v \sim T^2$$

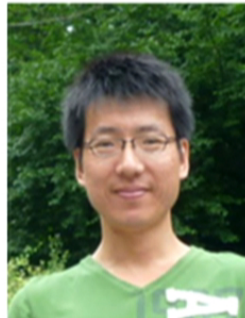
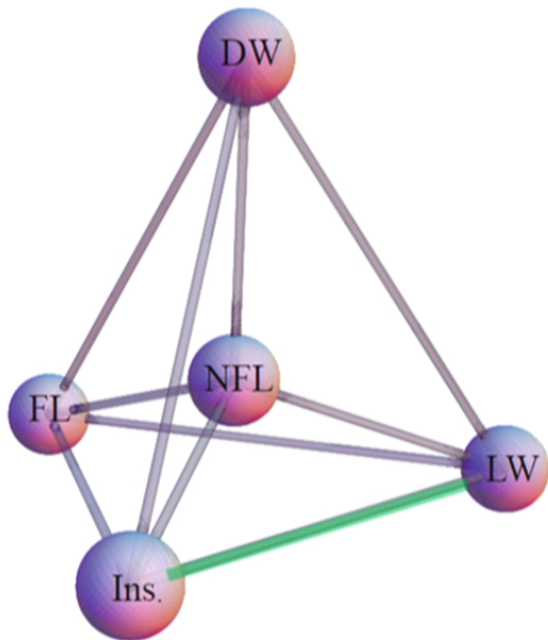
NFL : Non-Fermi liquids

(Luttinger-Abrikosov-Beneslavskii)

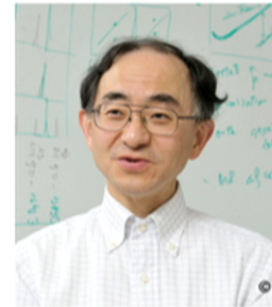
$$C_v \sim T^{1.5+\delta} \quad \delta \sim 0.2 + O(\epsilon^2)$$

Collaborators

Phases and phase transitions in pyrochlore iridates



B.J. Yang
Riken



N. Nagaosa,
Riken

Quantum criticality of topological phase transitions in 3d interacting electrons
Yang, *EGM*, *Isobe*, and *Nagaosa* (to appear)

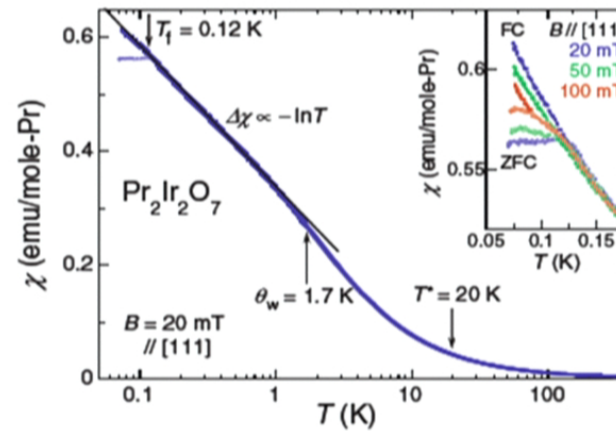
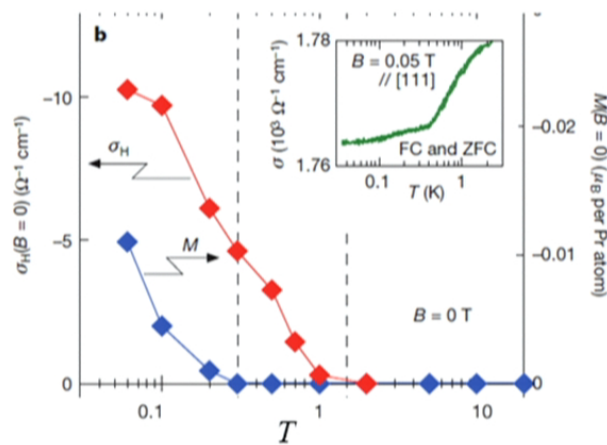
Thank you for your attention!

Symmetry breaking

- Observed non-Fermi liquid

Non Fermi liquid behavior in $\text{Pr}_2\text{Ir}_2\text{O}_7$

Anomalous Hall effect, large non-linear susceptibility, logarithmic susceptibility, etc.



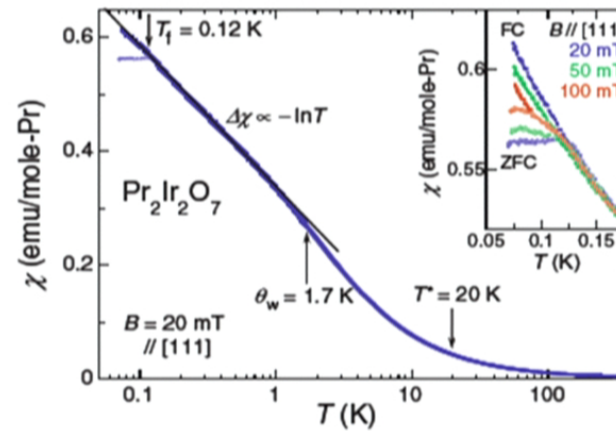
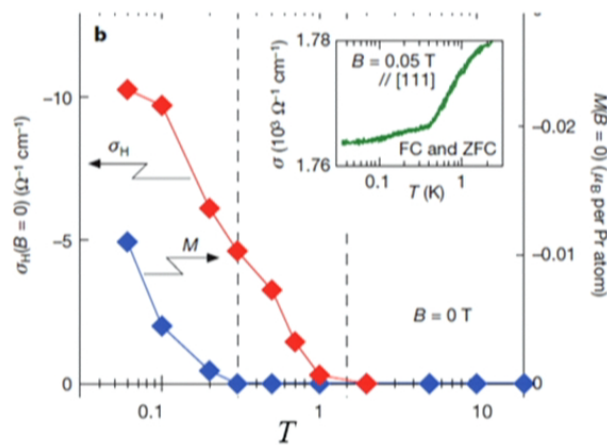
Machida. et.al. 2010

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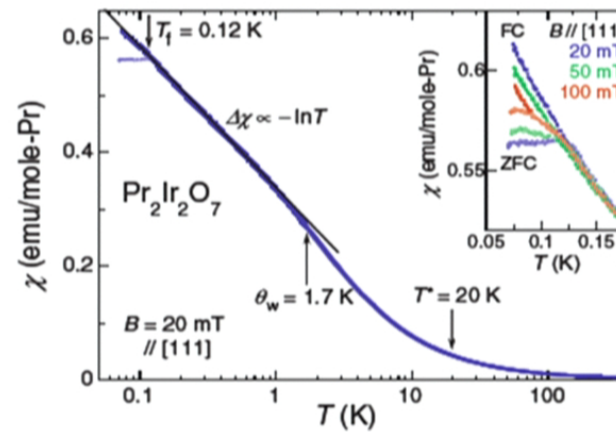
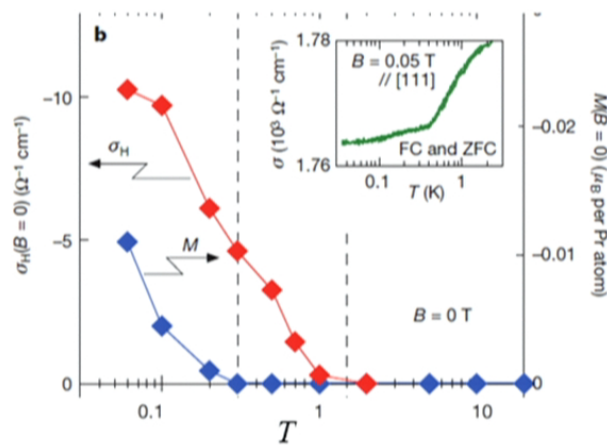
Machida. et.al. 2010

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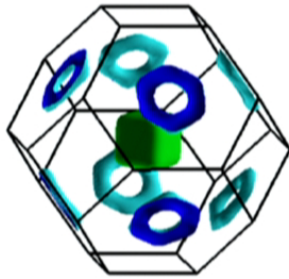


Machida. et.al. 2010

Conventional phases (theory)

Examples of band structure calculation

Metal



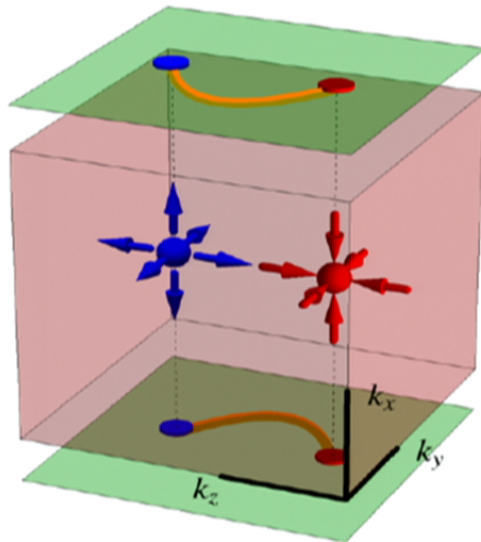
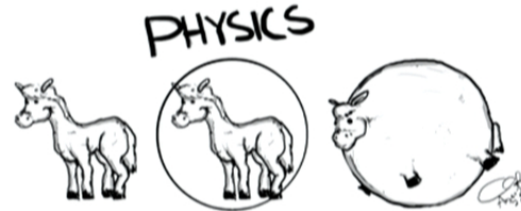
Coulomb interaction is rather weak.
(Thomas-Fermi screening)

$$E_F \gg E_{Coulomb} \sim \frac{1}{r} \quad (r \rightarrow \infty)$$

Symmetry breaking

- Weyl semi-metal

$$\mathcal{H}_2^\pm = \pm k_z \tau^z + \frac{\sqrt{3}}{2} (k_x^2 - k_y^2) \tau^x + \sqrt{3} k_x k_y \tau^y$$



Surface :
Fermi "arc"

Bulk :
Weyl points

Anomalous Hall effect (3d) :

$$\sigma_{\mu\nu}^H = \frac{e^2}{h} \epsilon_{\mu\nu\lambda} K_\lambda$$

Surface contribution

$$\frac{K_w^2}{2m} \sim \mu_B H \quad K_w \sim H^{0.5}$$

$$\sigma_H = \frac{e^2}{h} K_w \sim H^{0.5} \gg H$$

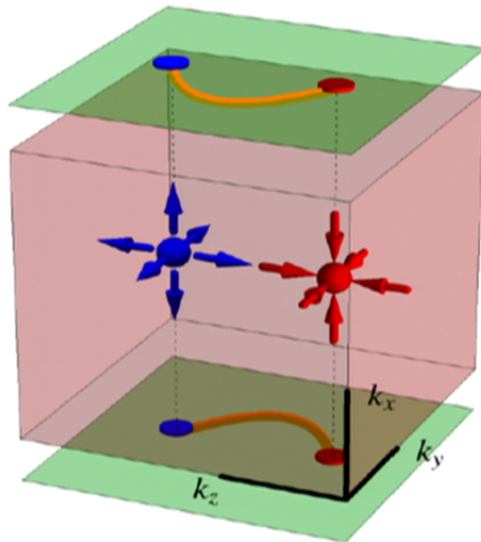
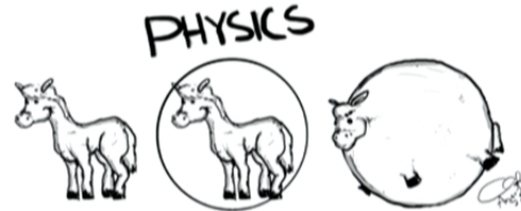
(for small H)

Witzak-Krempa, et. al., 2013

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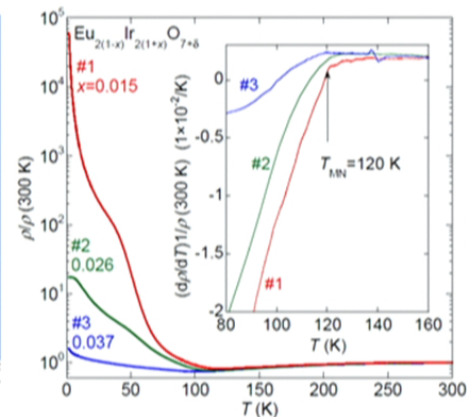
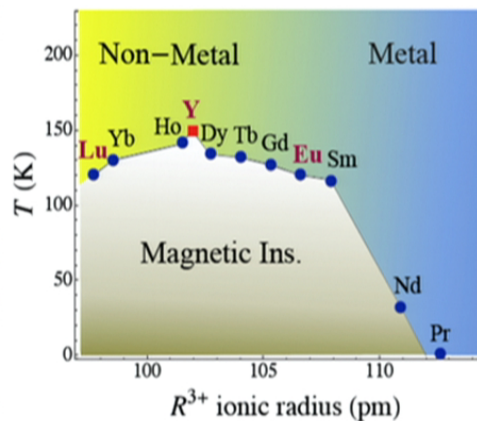
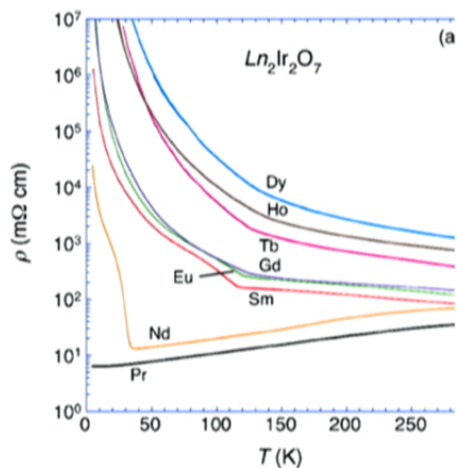
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(for small H)

Witzak-Krempa, et. al., 2013

Experiments



Matsuhira. et.al. 2011

2nd order metal-insulator transition (\sim magnetism)

Witzak-Krempa, et. al., 2013

Ionic radius dependence

Ishikawa. et.al. 2012

Sensitive doping dependence

Neither good metal nor good insulator