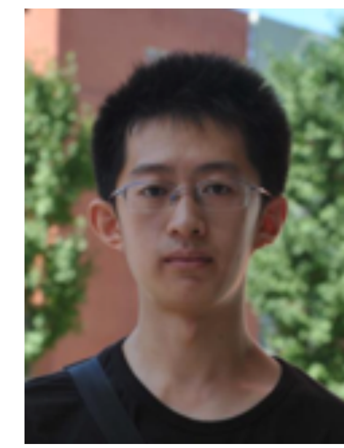
Kitaev materials, spin-1 pyrochlore antiferromagnet, and symmetry enriched topological orders

Gang Chen
Fudan University



李 非也 博士

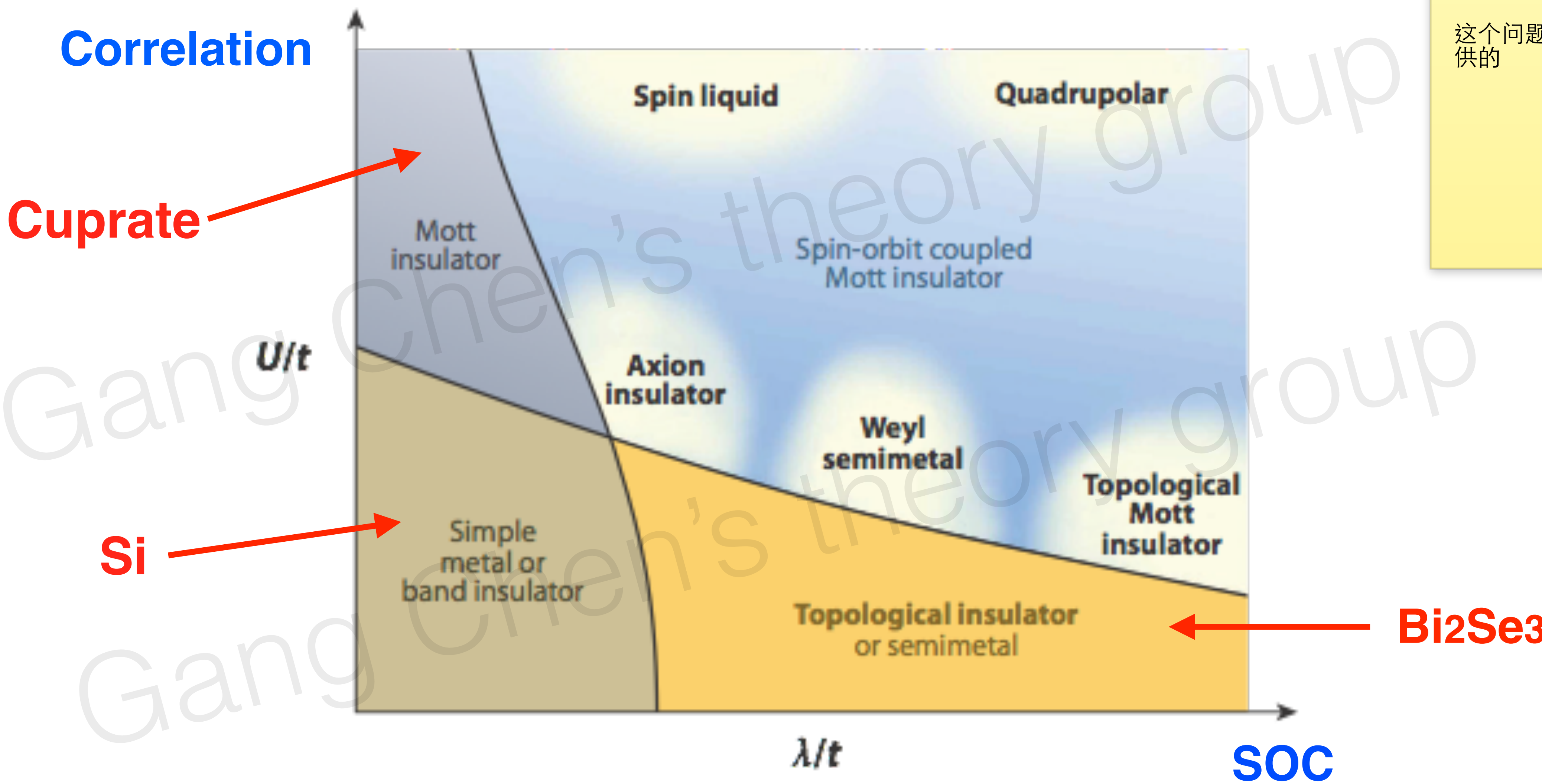
（复旦大学）

When correlation meets with spin-orbit coupling

$$H=\sum_{i,j;\alpha\beta} t_{ij,\alpha\beta}\, c^{\dagger}_{i\alpha} c_{j\beta} + \text{h.c.} + \lambda \sum_{i} \boldsymbol{L}_i \cdot \boldsymbol{S}_i + U \sum_{i,\alpha} n_{i\alpha}(n_{i\alpha}-1)\,,$$

当关联 遇到 SOC会有 很多理论上
新的现象和phase, 这是理论上提出
许多新的相。

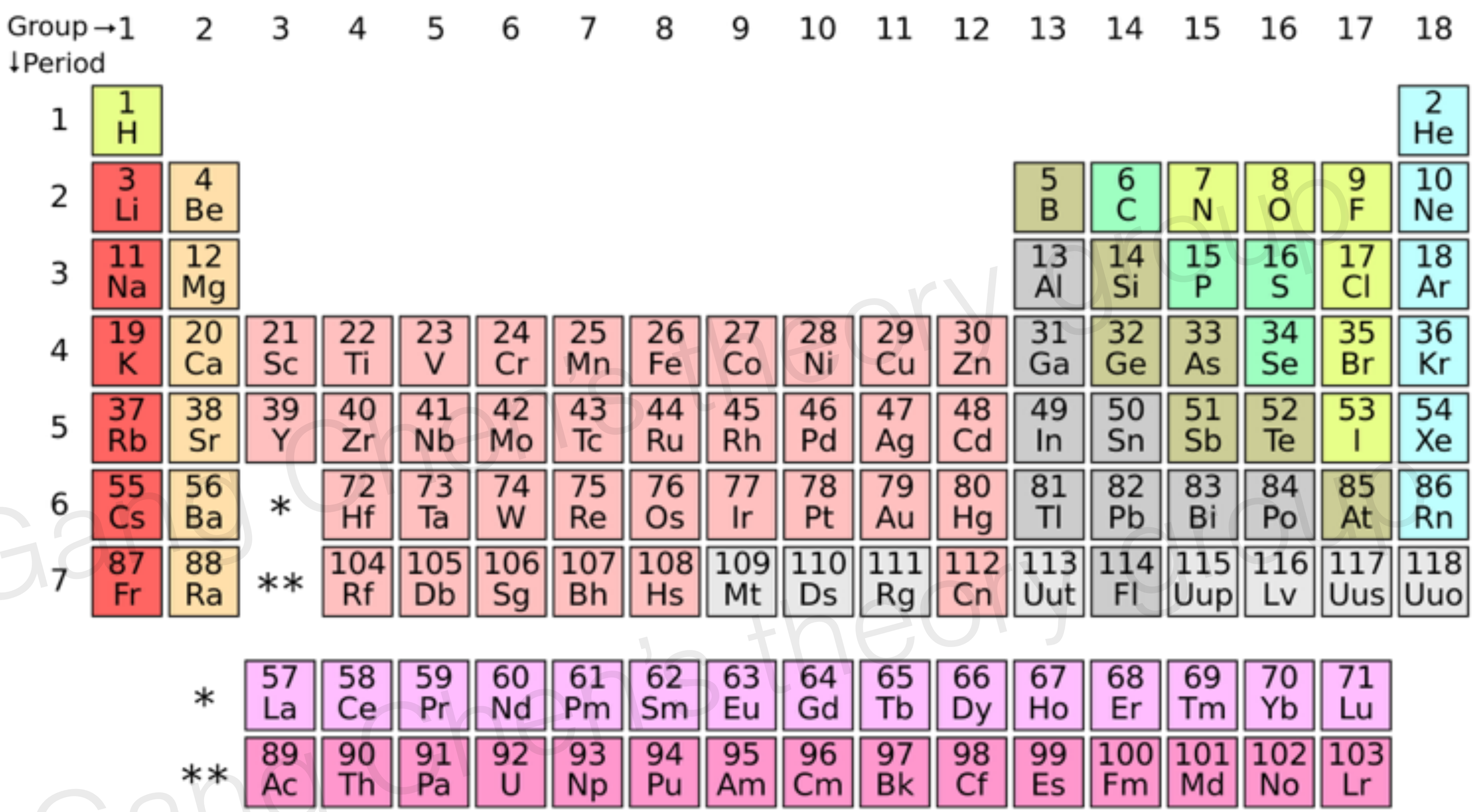
这个问题不仅仅是理论上的，也是
供的



"Spin-orbit coupled" Mott insulator is a relatively unexplored region.

Witczak-Krempa, Gang Chen, YB Kim, Balents (Annu. Rev. CMP 2014)

Why do we care about this? **First it is real !**

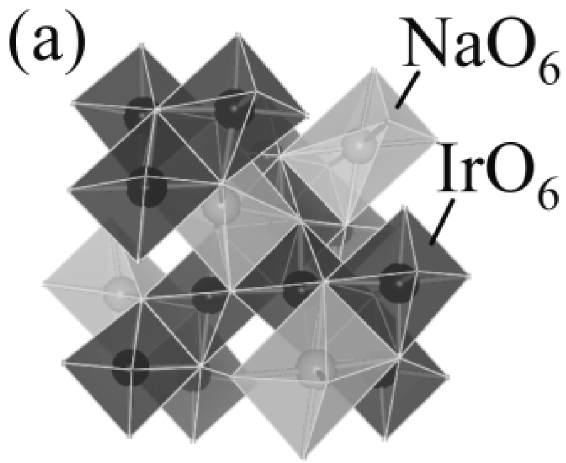


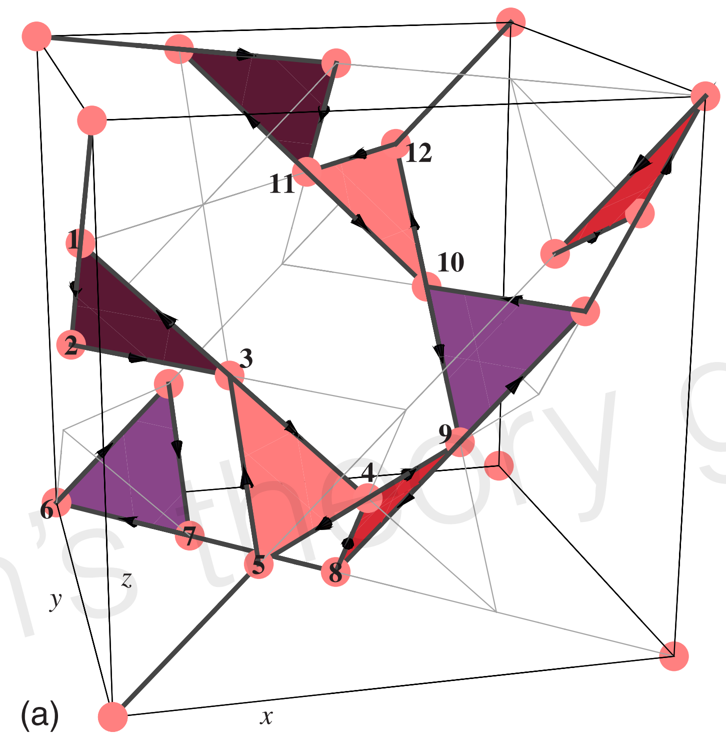
当 元素 变重以后，自
。。。

Heavy elements have stronger spin-orbit couplings.
For 4d, 5d, 4f, 5f electrons, even for 3d electrons (when the orbitals are degenerate), SOC needs to be seriously considered.

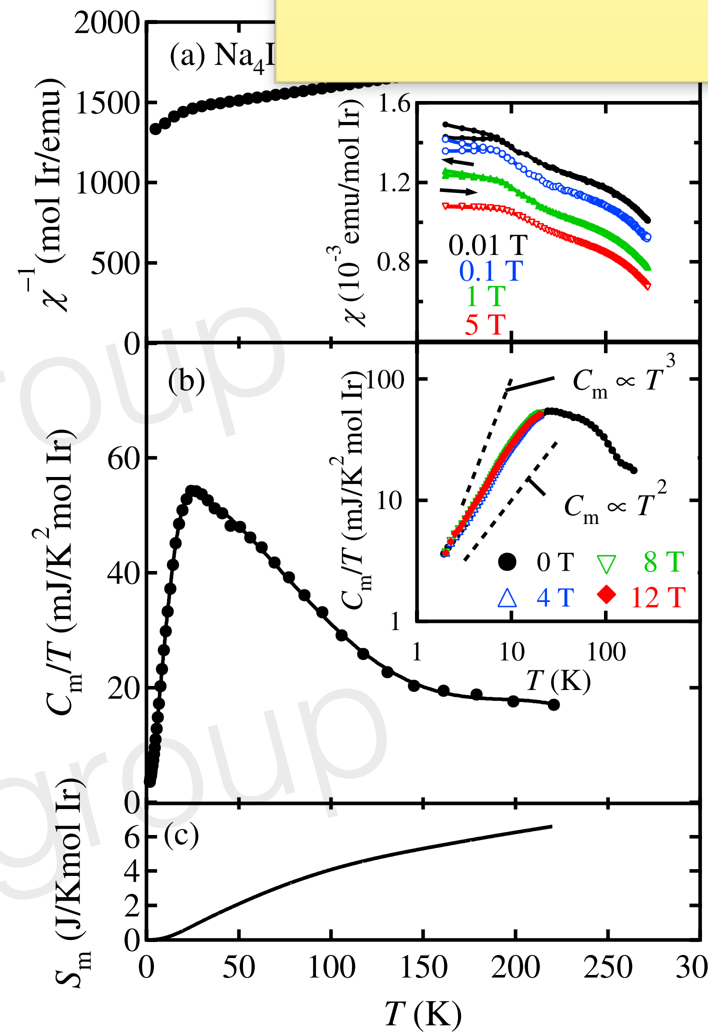
$Na_4Ir_3O_8$: hyperkagome quantum spin liq

我们原初的一个motivation 来源于 hyperkagome





hyperkagome lattice



Takagi,etc, PRL, **2007**

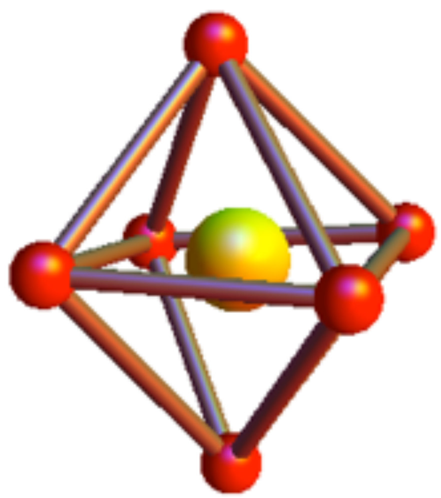
$\chi \sim \text{constant}, \quad C_v/T \sim \text{constant}$

Why Ir ion behaves as a spin-1/2 ?

Gang Chen, Leon Balents, PRB 2008

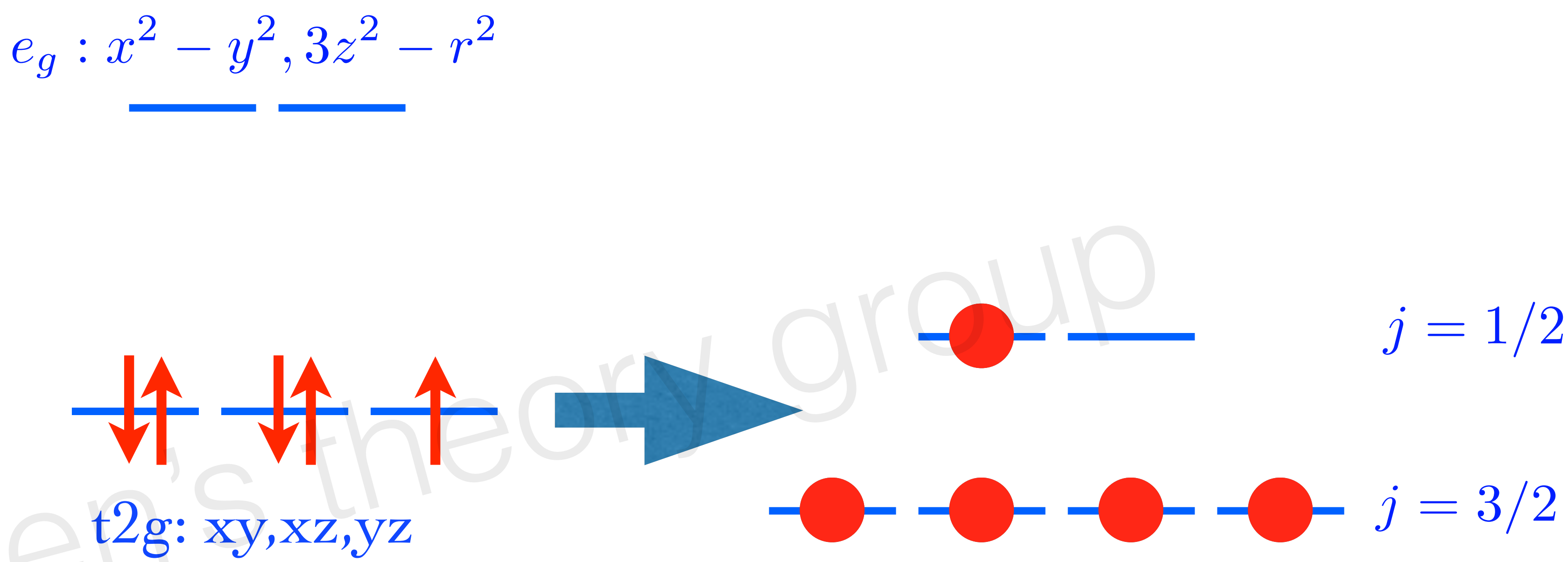
Yi Zhou (周毅), Fuchun Zhang (张富春), PA Lee, PRL 2008

t_{2g} orbitals in octahedral crystal field: **J=1/2**



IrO6 octahedron

$Ir^{4+} : 5d^5$



Crystal electric field

Spin-orbit coupling

$$\langle \{t_{2g}\} | \mathbf{L} | \{t_{2g}\} \rangle = -\mathbf{l}, \quad H_{soc} = -\lambda \mathbf{l} \cdot \mathbf{S}, \quad \mathbf{j} = \mathbf{l} + \mathbf{S}$$

It is interesting to look at how the magnetic moment M = L+2S = -l+2S varies.

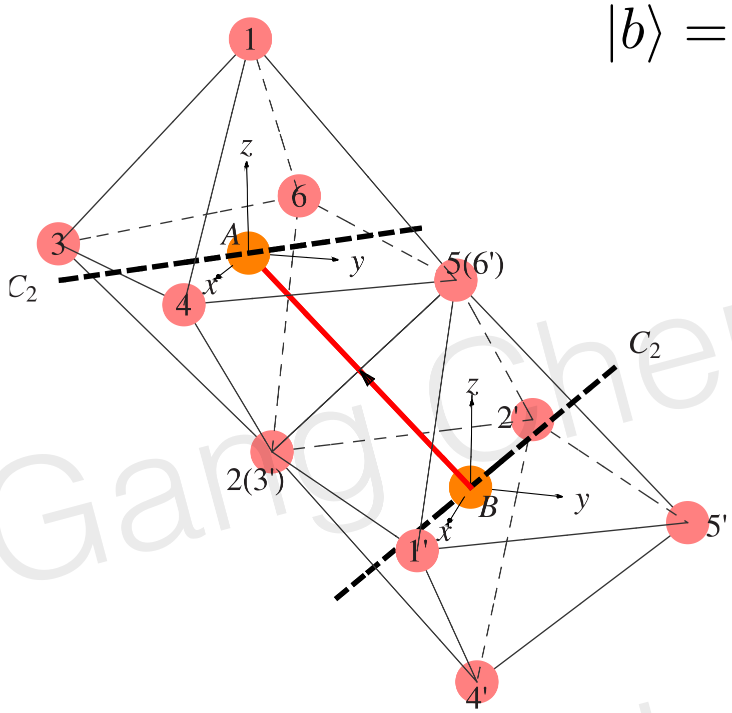
BTW, SOC is quenched for eg orbitals.

Gang Chen, Balents PRB 2008,
B.J. Kim etc, Science 2008,
G. Jackeli, G. Khaliullin PRL 2009.

Exchange interaction: direct

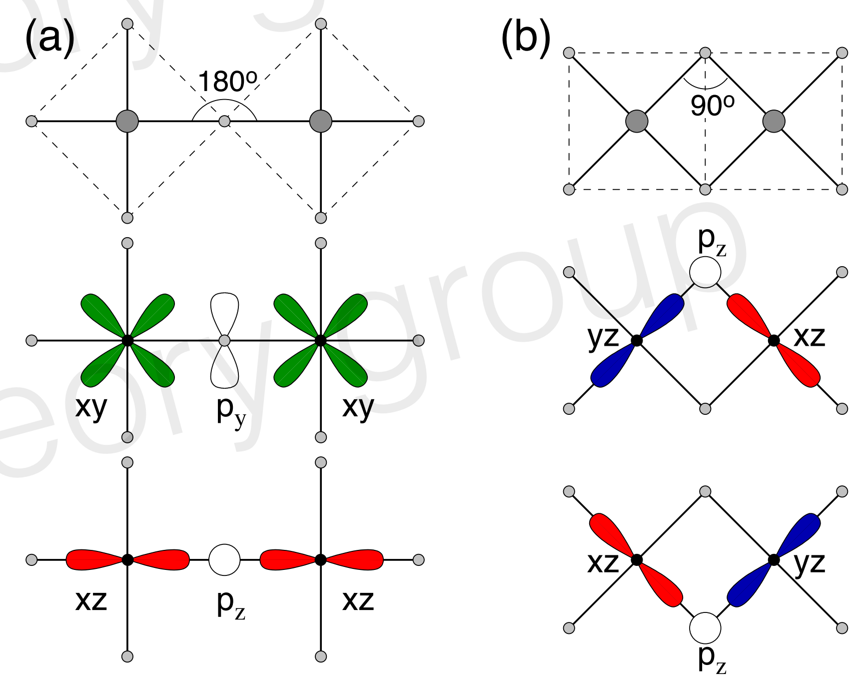
Spin-orbit entangled j=1/2 doublet

$$|a\rangle = \frac{1}{\sqrt{3}}(|d_{xy,\uparrow}\rangle + |d_{yz,\downarrow}\rangle + i|d_{zx,\downarrow}\rangle),$$
$$|b\rangle = \frac{1}{\sqrt{3}}(|d_{xy,\downarrow}\rangle - |d_{yz,\uparrow}\rangle + i|d_{zx,\uparrow}\rangle),$$



two neighboring IrO_6 octahedra:
they share 2 oxygens.

Gang Chen, Balents PRB 2008



Na2IrO3: Jackeli, Khaliullin PRL 2009

Surprisingly, direct hopping gives us a Heisenberg model !
This is very special especially since orbitals have orientations.

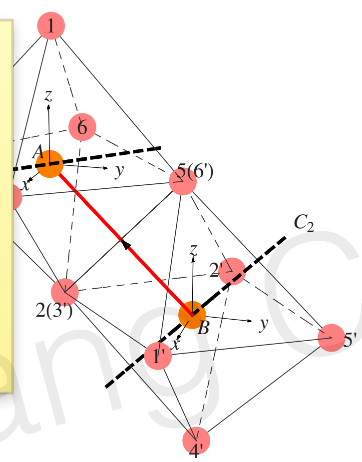
Gang Chen's theory group

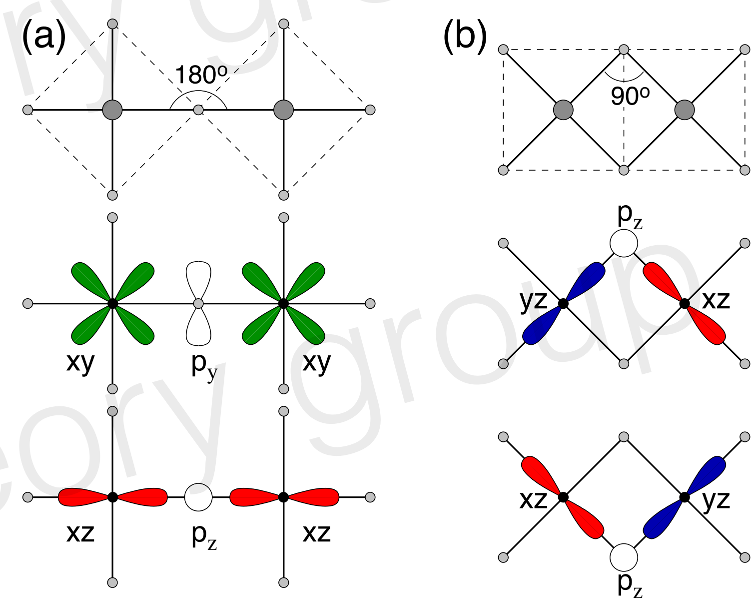
Exchange interaction: indirect, iridate as Kitaev material

Remark: almost all iridates have the same local structure,
- IrO6 form an octahedron,
- Neighboring IrO6 octahedra share 2 oxygens,
- Ir-O-Ir bond angle is close to be 90 degrees.
- The microscopic analysis may apply to many other iridate families.

G Jackeli

有了rucl3, 4d/5d 的kiteav
l,
onyecomb, harmonic honeycomb





$$\mathcal{H}_{AB} = -JS_A^x S_B^x + JS_A^y S_B^y + JS_A^z S_B^z$$

$$= -2JS_A^x S_B^x + J\mathbf{S}_A \cdot \mathbf{S}_B$$

anisotropic term for x bond after
including CEF splitting among t2g orbitals

Gang Chen, Balents PRB 2008

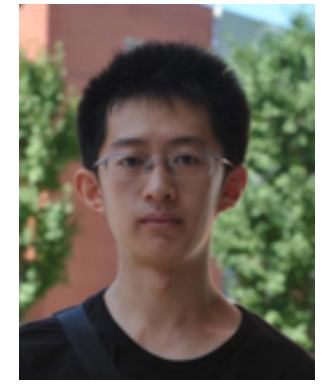
$$\mathcal{H}_{ij}^{(\gamma)} = -JS_i^\gamma S_j^\gamma$$

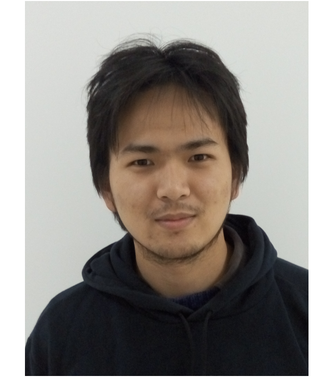
Kitaev term for gamma bond
after including Hund's coupling

Na2IrO3: Jackeli, Khaliullin PRL 2009

after Jackeli, Khaliullin's proposal, 后来才有了hyperhoneycomb, harmonic-honeycomb,
RuCl3 (**Shiyan Li, Weiqiang Yu, Jinsheng Wen, Liling Sun, Jianxin Li**)

Kitaev materials beyond iridates/ruthenates





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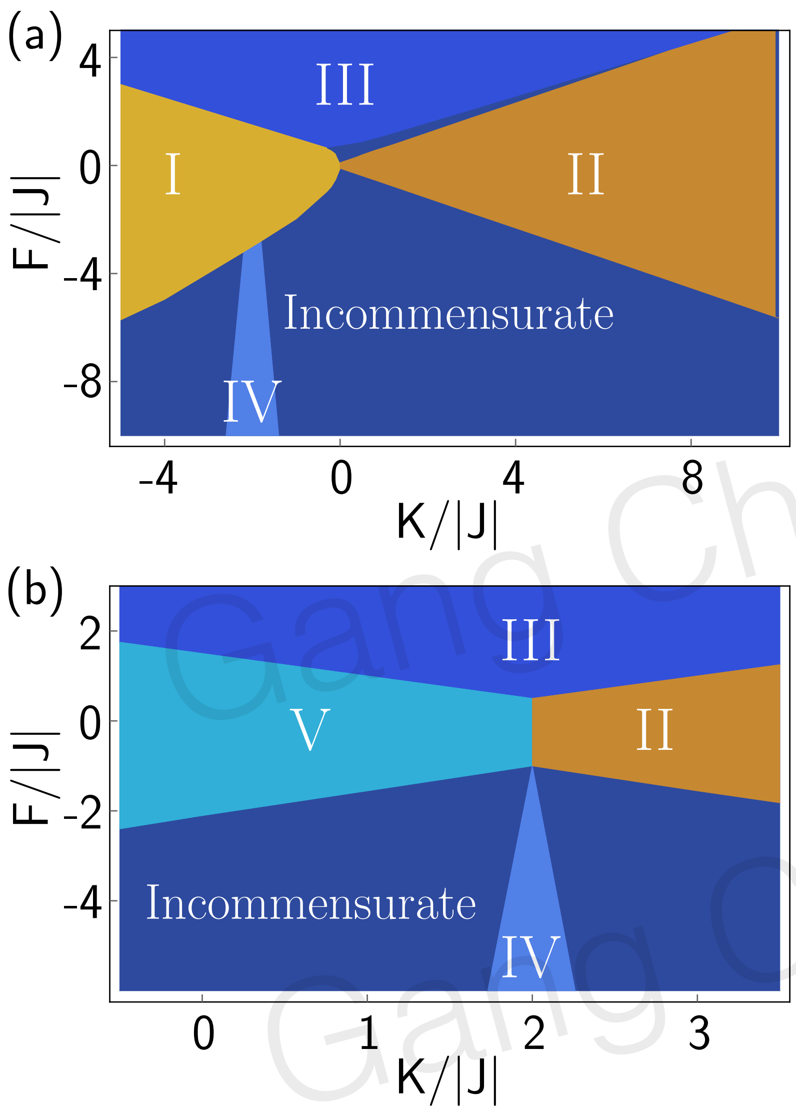

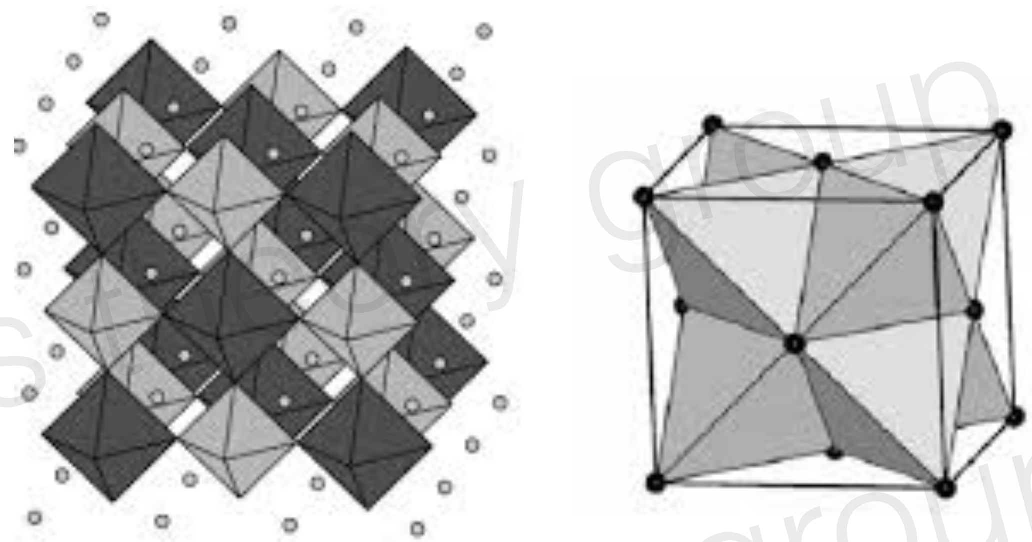

Ordered double perovskites
with rare-earth moments

$$H = \sum_{\langle ij \rangle_{\gamma\pm}} [J\, \mathbf{S}_i \cdot \mathbf{S}_j + K S_i^{\gamma} S_j^{\gamma} \pm F(S_i^{\alpha} S_j$$

其实从物理的角度，真正给予我
相互作用的不是 ir, ru, 这些元素

而是自选轨道耦合 以及 特定的
构，。。。 所以我们可以视野开
些，

从这个角度，稀土磁体会是更好
材料，更short range，更强的sc
没有中子吸收的问题。。。。

按照这个思想，我们提出了。。

指出可以在稀土材料里头实现ki
physics

我们指出Kitaev 材料应该远远超过目前的铱氧化物，我们讨论稀土材料里头的Kitaev 相互作用以及得到物理行为。 **所以要寻找honeycomb lattice稀土磁体。**

FY Li, YD Li, **……**, **Gang Chen***, Phys. Rev. B, 2017

Spin-1 Pyrochlore Antiferromagnet

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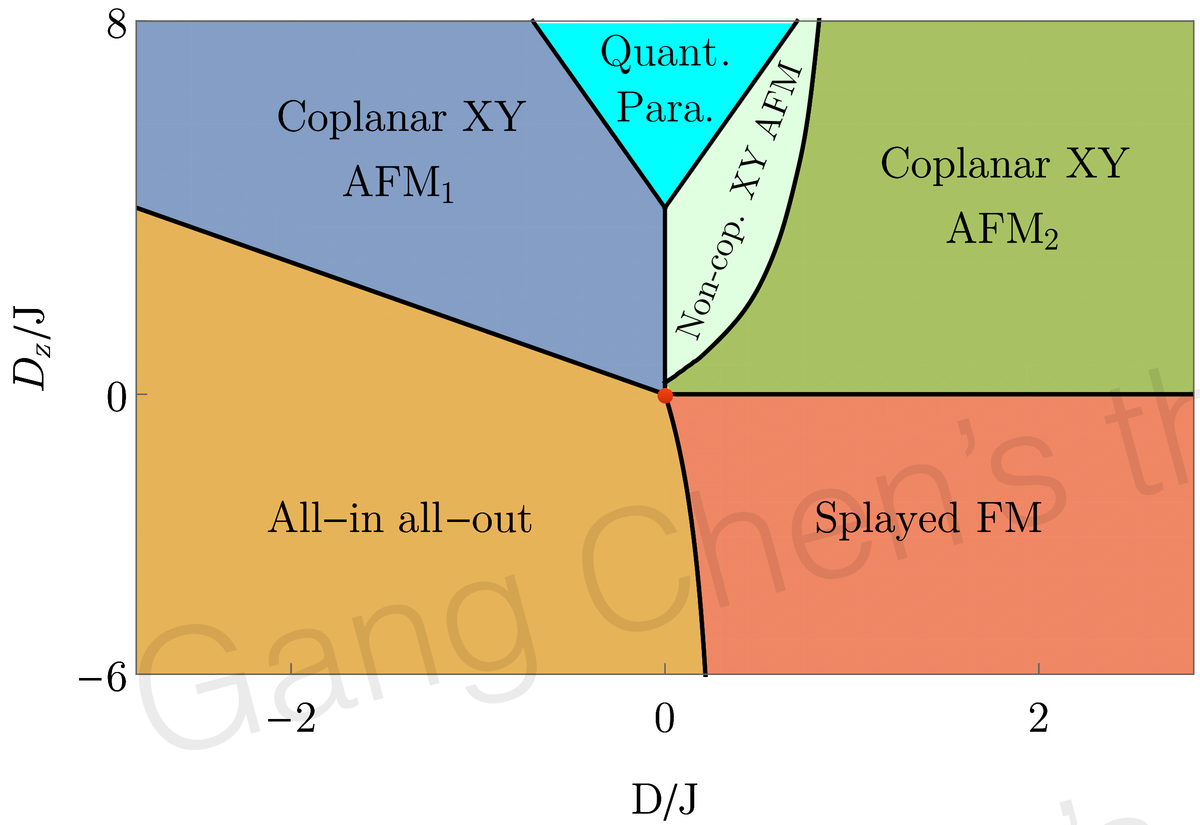
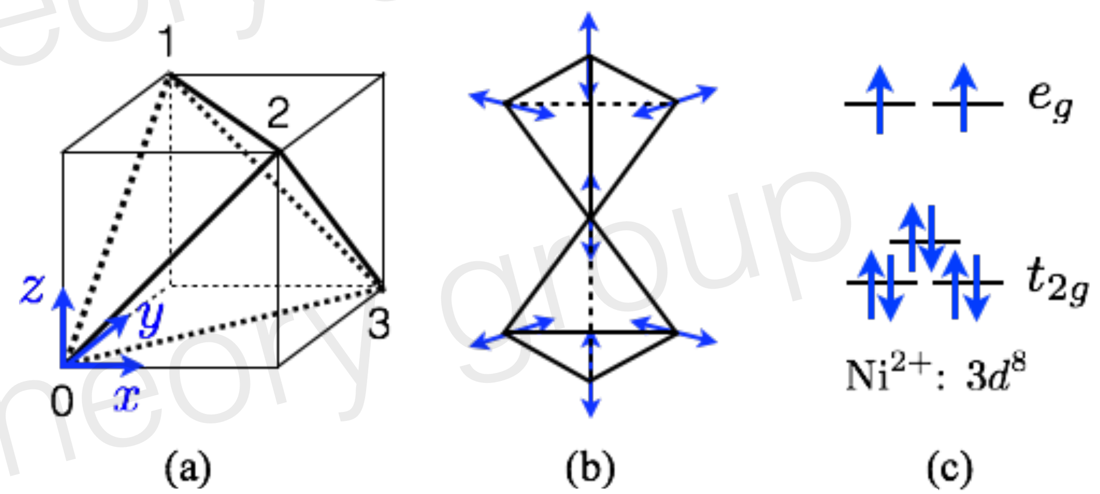
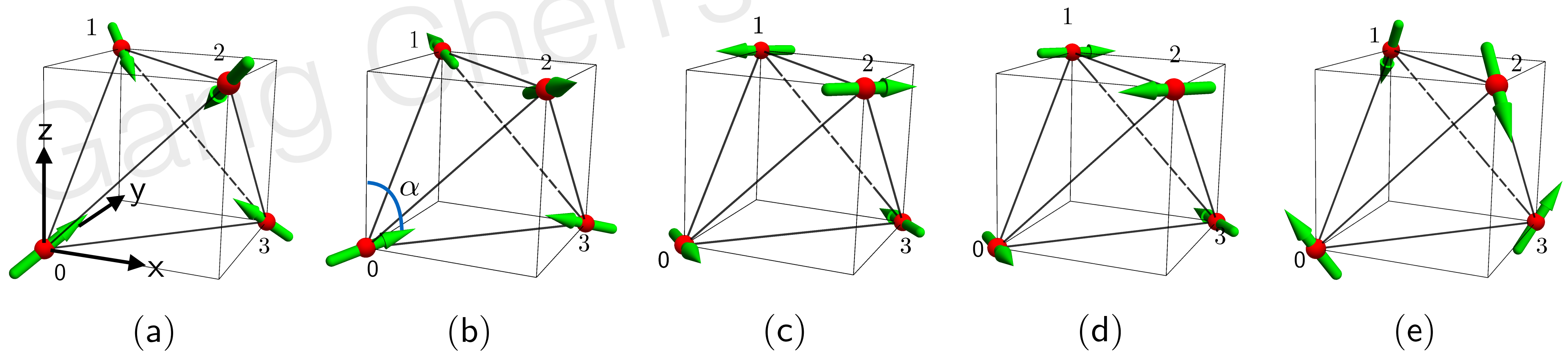


$$H = \sum_{\langle ij \rangle} [J \boldsymbol{S}_i \cdot \boldsymbol{S}_j + \boldsymbol{D}_{ij} \cdot (\boldsymbol{S}_i \times \boldsymbol{S}_j)] + \sum_i D_z (\boldsymbol{S}_i \cdot \hat{z}_i)^2,$$





FY Li, Gang Chen, 2017

(Topological) Flavor wave theory

张富春教授

BER 16 PHYSICAL REVIEW LETTERS

SU(4) Theory for Spin Systems with Orbital Degeneracy

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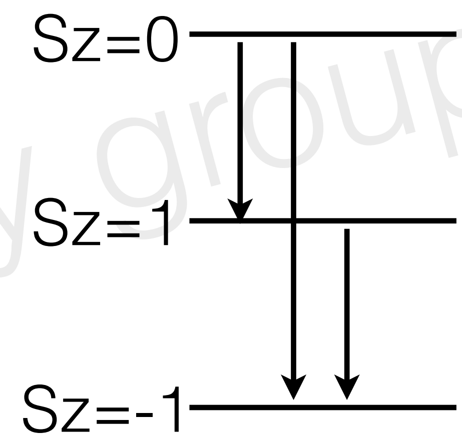
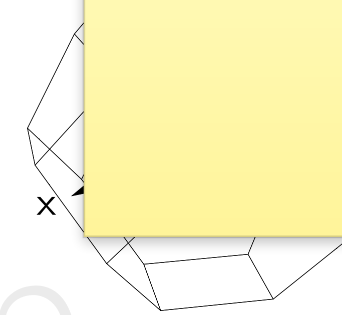
(Received 15 April 1998)

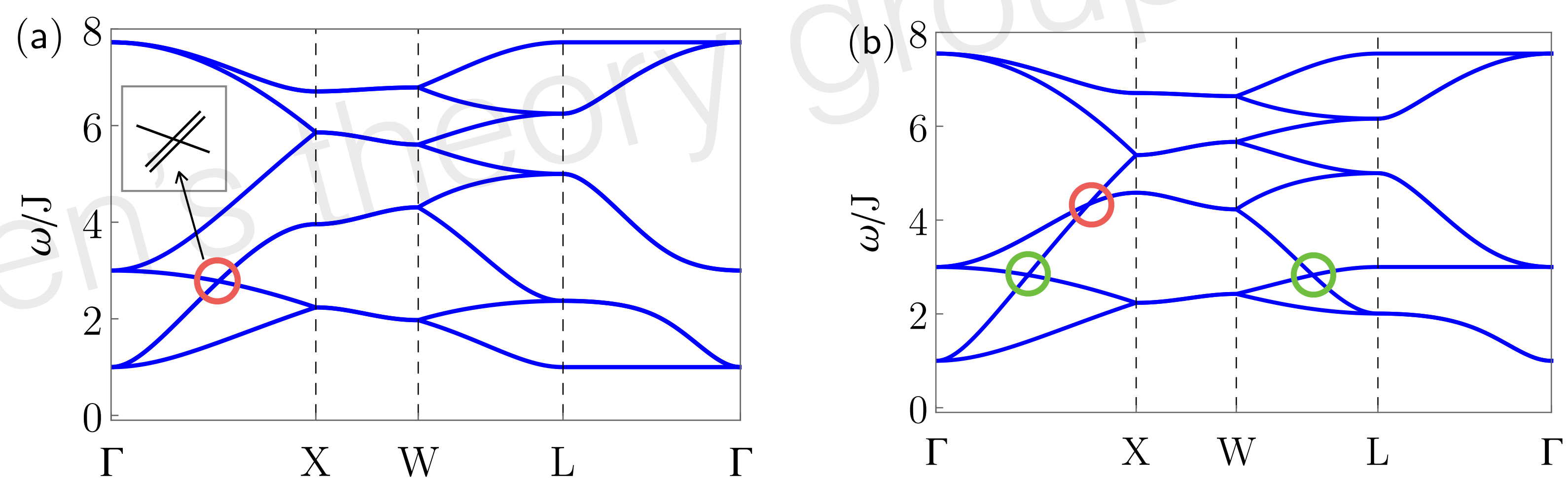
$$H = \sum_{\langle i,j \rangle} (2\vec{s}_i \cdot \vec{s}_j + 1/2)(2\vec{\tau}_i \cdot \vec{\tau}_j + 1/2),$$





这是超越模型的物理

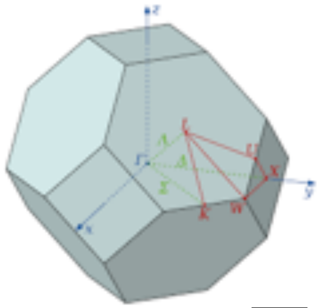
$$S_0^0(i) = 1 - a_1^\dagger(i)a_1(i) - a_{\bar{1}}^\dagger(i)a_{\bar{1}}(i),$$
$$S_1^0(i) = a_1^\dagger(i)[1 - a_1^\dagger(i)a_1(i) - a_{\bar{1}}^\dagger(i)a_{\bar{1}}(i)]^{\frac{1}{2}},$$
$$S_{\bar{1}}^0(i) = a_{\bar{1}}^\dagger(i)[1 - a_1^\dagger(i)a_1(i) - a_{\bar{1}}^\dagger(i)a_{\bar{1}}(i)]^{\frac{1}{2}},$$
$$S_{\bar{1}}^1(i) = a_{\bar{1}}^\dagger(i)a_1(i),$$
$$S_1^1(i) = a_1^\dagger(i)a_1(i),$$
$$S_{\bar{1}}^{\bar{1}}(i) = a_{\bar{1}}^\dagger(i)a_{\bar{1}}(i),$$



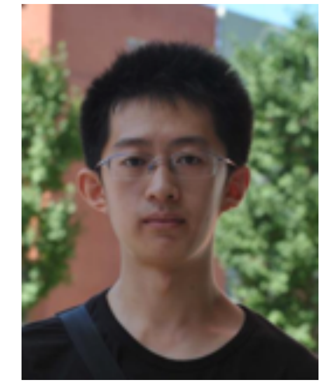
topological flavor wave

triply degenerate band touching:
"new fermion"

Type-II Weyl



Topological (Weyl) magnons



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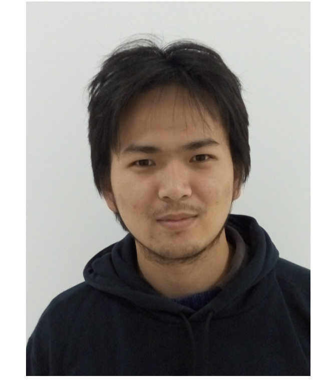
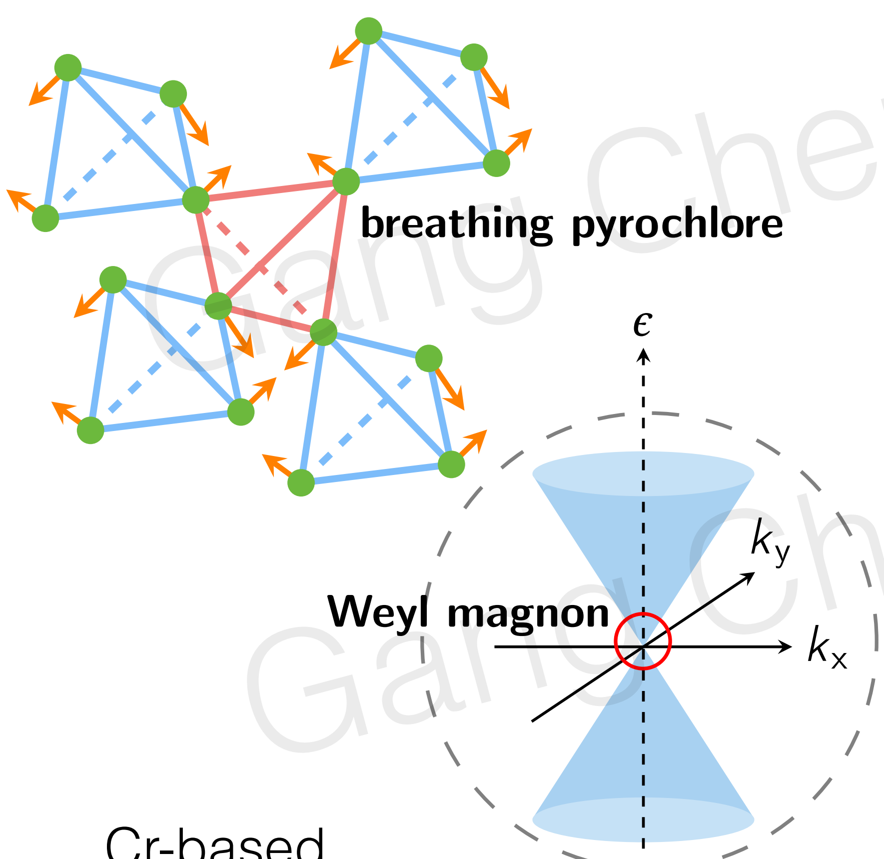
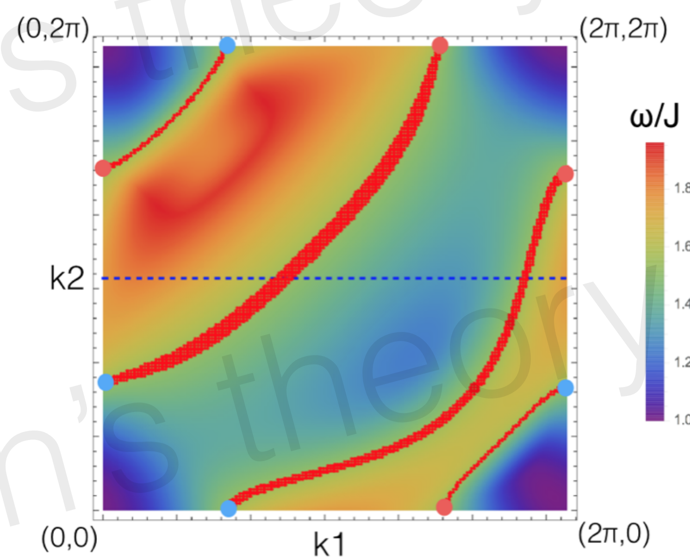


李耀东
(复旦-> Santa Barbara)

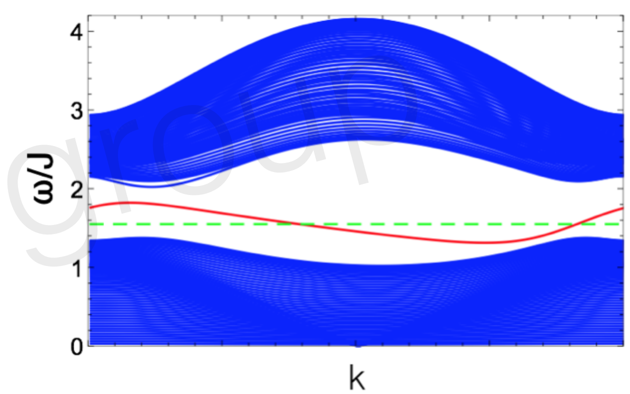
有序态一般可能是平庸的，但是基态的平庸并不代表激发态也是平庸的.磁有序态的元激发可以拥有非平庸的拓扑能带结构。



Cr-based spinel



(a)



(b)

拓扑保护的表面弧

三维威尔磁子 (Weyl Magnon)

F-Y Li, Y-D Li, ….., **Gang Chen***,

Nature Communications, 7, 12691, (2016)

Candidate spin-1 pyrochlore

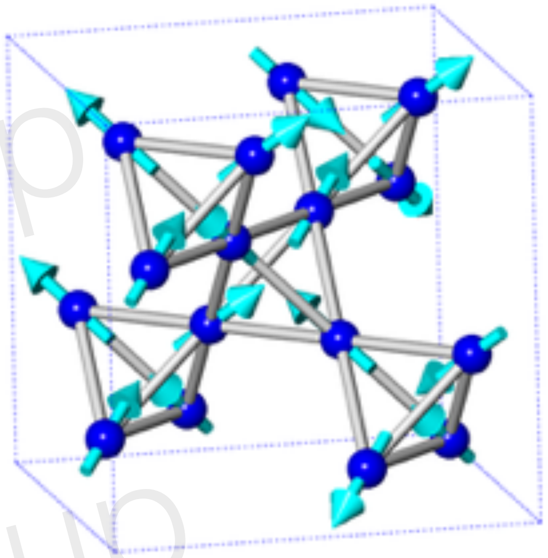
materials	magnetic ions	Θ_{CW}	magnetic transitions	magnetic structure	refs
$NaCaNi_2F_7$	$Ni^{2+}(3d^8)$	-129K	glassy transition at 3.6K	spin glass	66
$Y_2Ru_2O_7$	$Ru^{4+}(4d^4)$	-1250K	AFM transition at 76K	canted AFM $\boldsymbol{Q} = \mathbf{0}$	78
$Tl_2Ru_2O_7$	$Ru^{4+}(4d^4)$	-956K	structure transition at 120K	gapped paramagnet	79
$Eu_2Ru_2O_7$	$Ru^{4+}(4d^4)$	-	Ru order at 118K	Ru order	80
$Pr_2Ru_2O_7$	$Ru^{4+}(4d^4)$, $Pr^{3+}(4f^2)$	-224K	Ru AFM order at 162K	Ru AFM order	81 and 82
$Nd_2Ru_2O_7$	$Ru^{4+}(4d^4)$, $Nd^{3+}(4f^3)$	-168K	Ru AFM order at 143K	Ru AFM order	83
$Gd_2Ru_2O_7$	$Ru^{4+}(4d^4)$, $Gd^{3+}(4f^7)$	-10K	Ru AFM order at 114K	Ru AFM order $\boldsymbol{Q} = \mathbf{0}$	84
$Tb_2Ru_2O_7$	$Ru^{4+}(4d^4)$, $Tb^{3+}(4f^8)$	-16K	Ru AFM order at 110K	Ru AFM order $\boldsymbol{Q} = \mathbf{0}$	85
$Dy_2Ru_2O_7$	$Ru^{4+}(4d^4)$, $Dy^{3+}(4f^9)$	-10K	Ru AFM order at 100K	Ru AFM order	86
$Ho_2Ru_2O_7$	$Ru^{4+}(4d^4)$, $Ho^{3+}(4f^{10})$	-4K	Ru AFM order at 95K	Ru FM order $\boldsymbol{Q} = \mathbf{0}$	87 and 88
$Er_2Ru_2O_7$	$Ru^{4+}(4d^4)$, $Er^{3+}(4f^{11})$	-16K	Ru AFM order at 92K	Ru AFM order $\boldsymbol{Q} = \mathbf{0}$	89 and 90
$Yb_2Ru_2O_7$	$Ru^{4+}(4d^4)$, $Yb^{3+}(4f^{13})$	-	Ru AFM order at 83K	Ru AFM order	88
$Y_2Mo_2O_7$	$Mo^{4+}(4d^2)$	-200K	Mo spin glass at 22K	Mo spin glass	91–94
$Lu_2Mo_2O_7$	$Mo^{4+}(4d^2)$	-160K	Mo spin glass at 16K	Mo spin glass	95
$Tb_2Mo_2O_7$	$Mo^{4+}(4d^2)$, $Tb^{3+}(4f^8)$	20K	spin glass at 25K	spin glass	96–98

TABLE I. A list of candidate spin-one pyrochlore materials. The null entry means that the data is not available.

这些系统并没有被仔细研究，这里我们把它们搜罗归纳整理出来

FY Li, Gang Chen, 2017

Symmetry Enriched U(1) Topological orders / spin liquids



Gang Chen*, Phys. Rev. B 96, 085136, 2017
Gang Chen*, Phys. Rev. B 96, 195127, 2017

The field is not only about **finding** spin liquid,
is more about **confirming** spin liquid!

Pyrochlore ice U(1) spin liquid

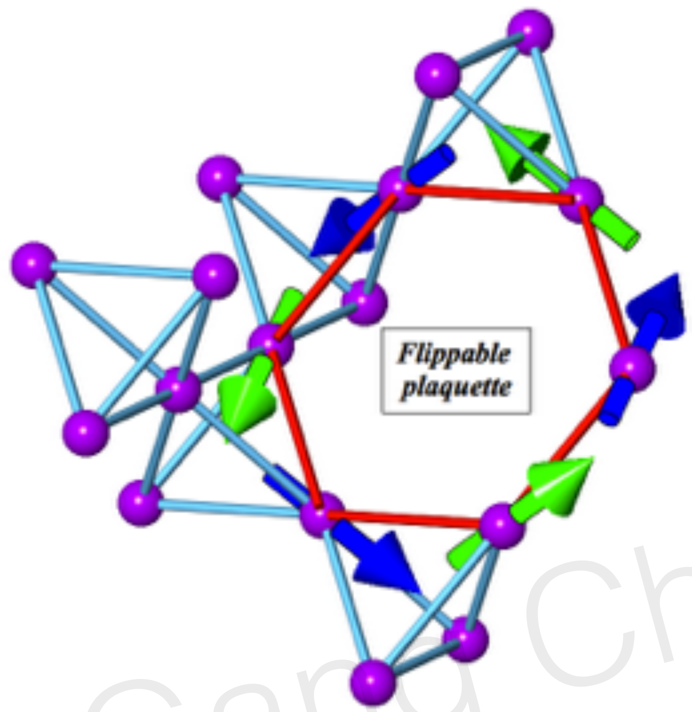


Figure from Michel Gingras

$$\mathcal{H}_{\text{XXZ}} = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z - J_{\perp}(S_i^+ S_j^- + S_i^- S_j^+),$$

3rd order degenerate perturbation
(Hermele, Fisher, Balents 2004)

$$\mathcal{H}_{\text{eff}} = -\frac{12 J_{\perp}^3}{J_{zz}^2} \sum_{\hexagon_{\text{p}}} (S_i^+ S_j^- S_k^+ S_l^- S_m^+ S_n^- + h.c.),$$

$$E_{\boldsymbol{r}\boldsymbol{r}'} \simeq S^z_{\boldsymbol{r}\boldsymbol{r}'}$$

$$e^{iA_{\boldsymbol{r}\boldsymbol{r}'}} \simeq S^{\pm}_{\boldsymbol{r}\boldsymbol{r}'}$$

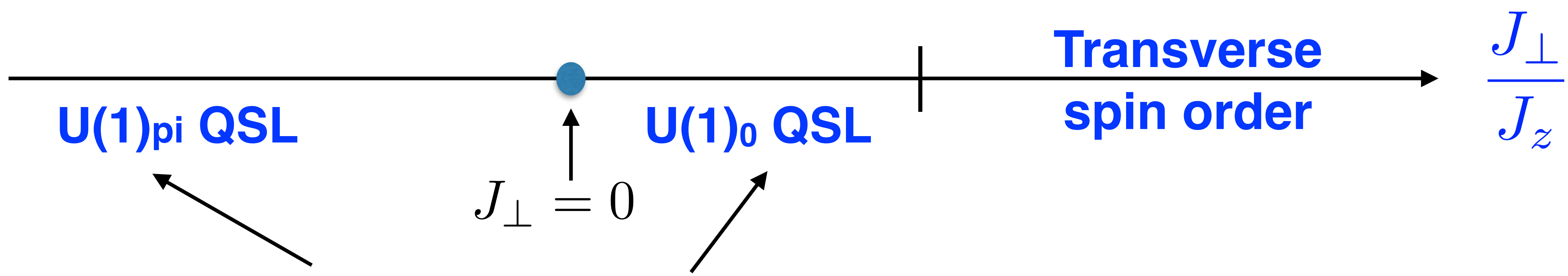
$$K = 24 J_{\perp}^3 / J_{zz}^2$$

Lattice gauge theory
on the diamond lattice

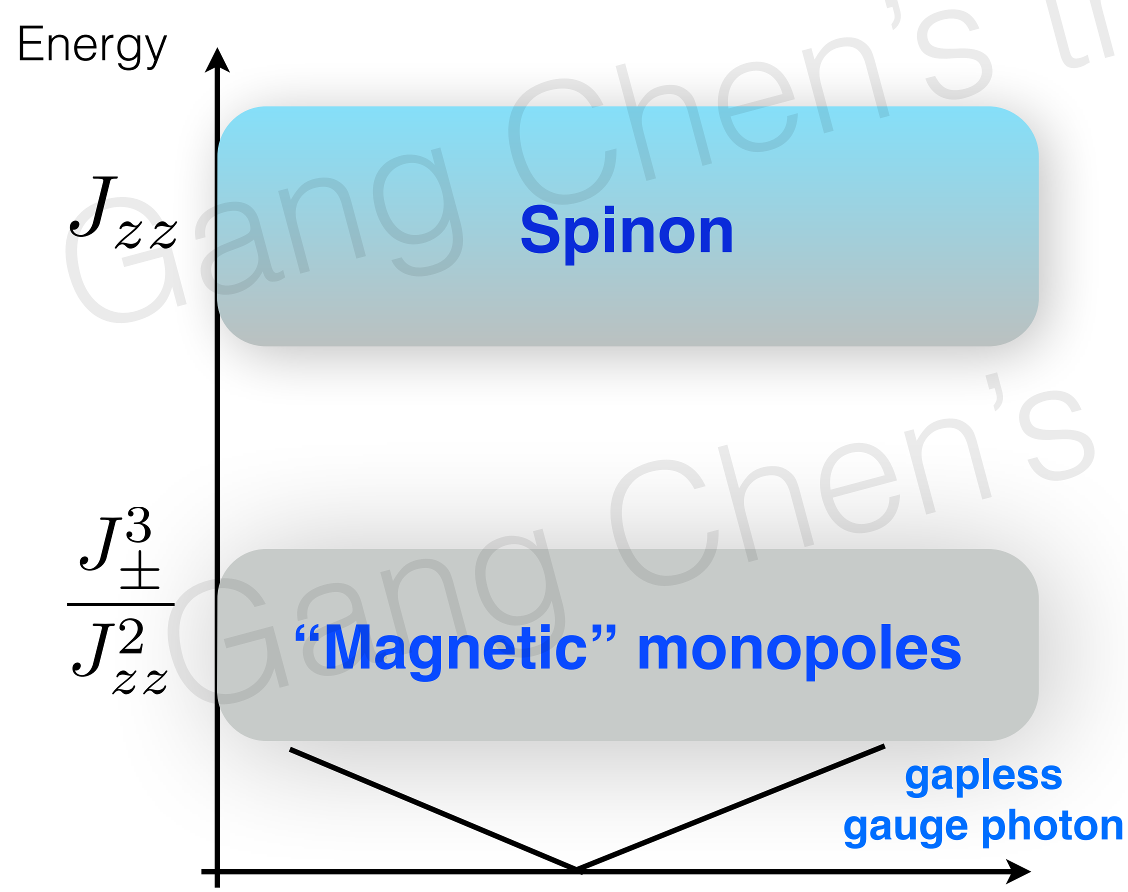
$$\mathcal{H}_{\text{LGT}} = -K \sum_{\hexagon_{\text{d}}} \cos(\text{curl}\, A) + U \sum_{\boldsymbol{r}\boldsymbol{r}'} (E_{\boldsymbol{r}\boldsymbol{r}'} - \frac{\eta_{\boldsymbol{r}}}{2})^2$$

inserting spinon matter (Savary Balents 2012)

$$H = \sum_{\mathbf{r} \in \text{I,II}} \frac{J_{zz}}{2} Q_{\mathbf{r}}^2 - J_{\pm} \left\{ \sum_{\mathbf{r} \in \text{I}} \sum_{\mu, \nu \neq \mu} \Phi^{\dagger}_{\mathbf{r}+\mathbf{e}_\mu} \Phi_{\mathbf{r}+\mathbf{e}_\nu} \mathsf{s}^-_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu} \mathsf{s}^+_{\mathbf{r},\mathbf{r}+\mathbf{e}_\nu} + \sum_{\mathbf{r} \in \text{II}} \sum_{\mu, \nu \neq \mu} \Phi^{\dagger}_{\mathbf{r}-\mathbf{e}_\mu} \Phi_{\mathbf{r}-\mathbf{e}_\nu} \mathsf{s}^+_{\mathbf{r},\mathbf{r}-\mathbf{e}_\mu} \mathsf{s}^-_{\mathbf{r},\mathbf{r}-\mathbf{e}_\nu} \right\}$$

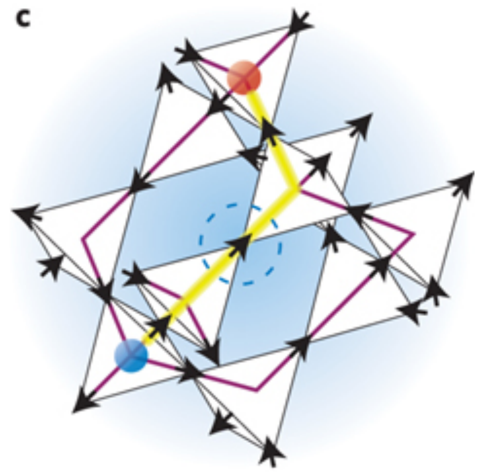


Related by unitary transformation (Hermele, Fisher, Balents PRB 2004)



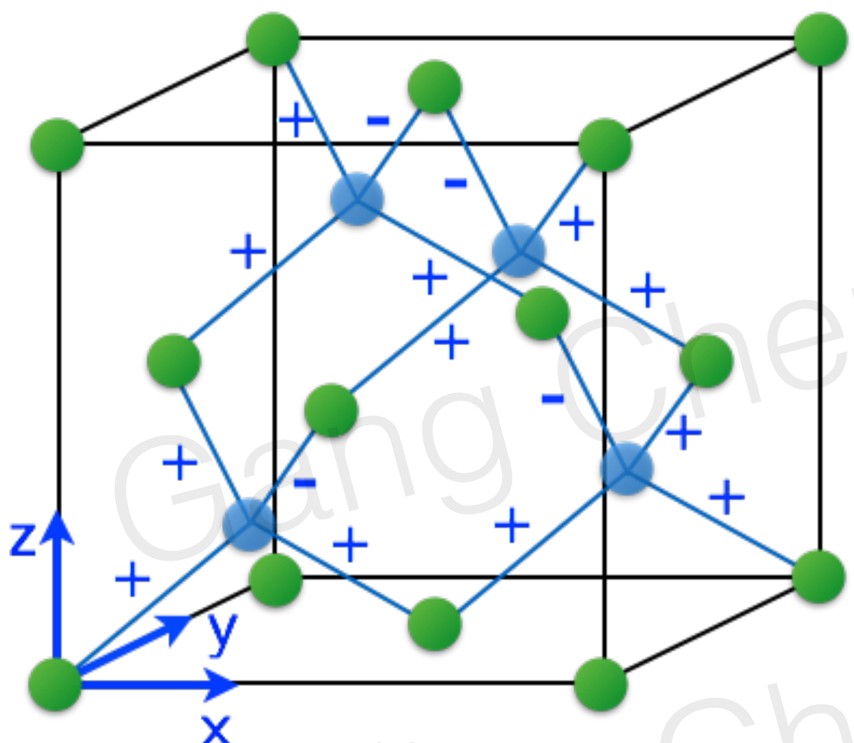
Besides the quantitative differences, are there sharp distinctions between U(1)pi QSL on the left and U(1)0 QSL on the right?

with modern understanding of topological phase,

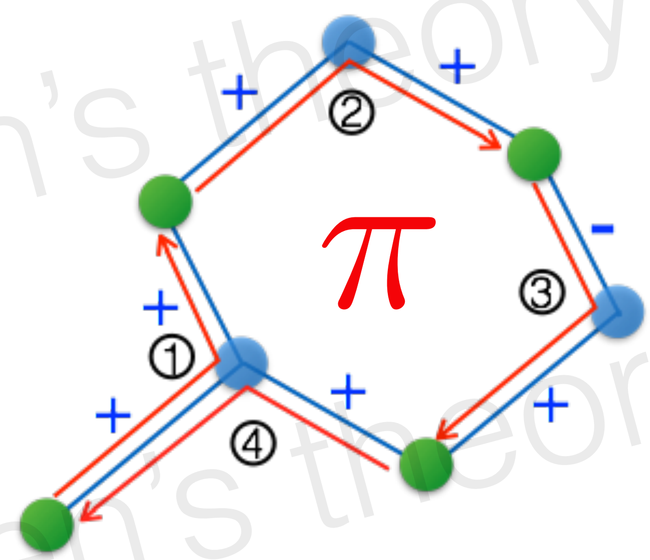


Pi flux and the spinon translation

$$\mathcal{H}_{\mathrm{LGT}} = -K \sum_{\hexagon_{\mathrm{d}}} \cos(\mathrm{curl}\, A) + U \sum_{\boldsymbol{rr'}} (E_{\boldsymbol{rr'}} - \frac{\eta_{\boldsymbol{r}}}{2})^2$$



(a)



(b)

If $K < 0, \ curl A = \pi$

If $K > 0, \ curl A = 0$

$$T^s_\mu T^s_\nu (T^s_\mu)^{-1} (T^s_\nu)^{-1} \ = \pm 1$$

$$H = \sum_{\mathbf{r} \in \mathrm{I,II}} \frac{J_{zz}}{2} Q^2_{\mathbf{r}} - J_{\pm} \left\{ \sum_{\mathbf{r} \in \mathrm{I}} \sum_{\mu, \nu \neq \mu} \Phi^\dagger_{\mathbf{r}+\mathbf{e}_\mu} \Phi_{\mathbf{r}+\mathbf{e}_\nu} \mathrm{s}^-_{\mathbf{r},\mathbf{r}+\mathbf{e}_\mu} \mathrm{s}^+_{\mathbf{r},\mathbf{r}+\mathbf{e}_\nu} + \sum_{\mathbf{r} \in \mathrm{II}} \sum_{\mu, \nu \neq \mu} \Phi^\dagger_{\mathbf{r}-\mathbf{e}_\mu} \Phi_{\mathbf{r}-\mathbf{e}_\nu} \mathrm{s}^+_{\mathbf{r},\mathbf{r}-\mathbf{e}_\mu} \mathrm{s}^-_{\mathbf{r},\mathbf{r}-\mathbf{e}_\nu} \right\}$$

Aharonov-Bohm flux experienced by spinon via the 4 translation
is identical to the flux in the hexagon.

Pi flux means crystal symmetry fractionalization

with definitive momentum
quantum number

It is like symmetry breaki

$$T^s_\mu T^s_\nu = -T^s_\nu T^s_\mu$$

2-spinon scattering state in an inelastic neutron scattering measurement

$$|a\rangle \equiv |\boldsymbol{q}_a; z_a\rangle,$$

construct another 3 equal-energy states by translating one spinon by 3 lattice vectors

$$|b\rangle = T^s_1(1)|a\rangle, \quad |c\rangle = T^s_2(1)|a\rangle, \quad |d\rangle = T^s_3(1)|a\rangle$$

$$T_1|b\rangle = T^s_1(1)T^s_1(2)T^s_1(1)|a\rangle = +T^s_1(1)[T_1|a\rangle],$$
$$T_2|b\rangle = T^s_2(1)T^s_2(2)T^s_1(1)|a\rangle = -T^s_1(1)[T_2|a\rangle],$$
$$T_3|b\rangle = T^s_3(1)T^s_3(2)T^s_1(1)|a\rangle = -T^s_1(1)[T_3|a\rangle],$$

$\Rightarrow$

$$\mathbf{q}_b - \mathbf{q}_a = 2\pi(100)$$

Xiao-Gang Wen, 2001, 2002, Essin, Hermele, 2014
Gang Chen, PRB 2017

Calculation to demonstrate the above prediction

$$\mathcal{H}_{\mathrm{XXZ}} = \sum_{\langle ij \rangle} J_{zz} S_i^z S_j^z - J_{\perp}(S_i^+ S_j^- + S_i^- S_j^+),$$

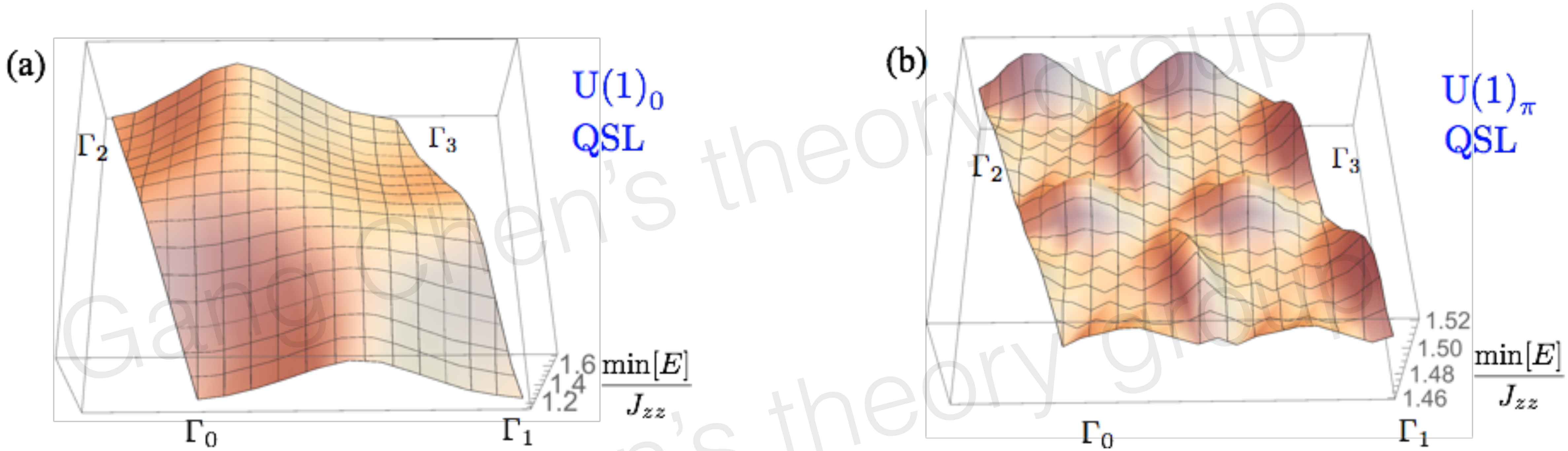
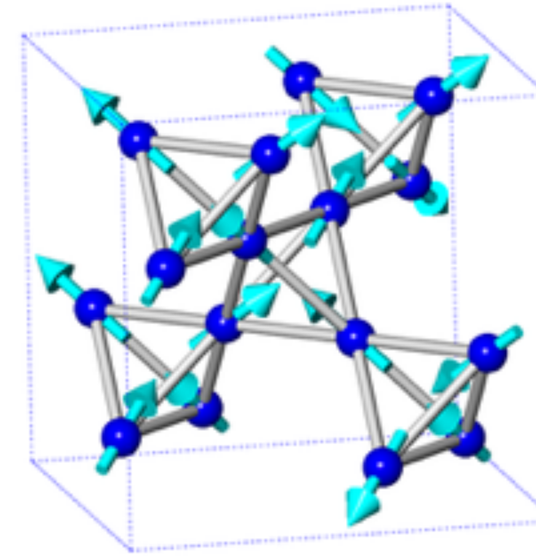


FIG. 3. (Color online.) The lower excitation edge of the spinon continuum in U(1)$_0$ and U(1)$_\pi$ QSLs. Here, $\Gamma_0\Gamma_1 = 2\pi(\bar{1}11), \Gamma_0\Gamma_2 = 2\pi(1\bar{1}1)$. We set $J_\perp = 0.12 J_{zz}$ for U(1)$_0$ QSL in (a) and $J_\perp = -J_{zz}/3$ for U(1)$_\pi$ QSL in (b).

绝大部分参数空间拥有
这个性质！

Lower excitation edge of spinon continuum



Lots of pyrochlore materials

1. rare-earth pyrochlores: $Ho_2Ti_2O_7$, $Dy_2Ti_2O_7$, $Ho_2Sn_2O_7$, $Dy_2Sn_2O_7$, Er_2Ti_2O7, $Yb_2Ti_2O_7$, $Tb_2Ti_2O_7$, $Er_2Sn_2O_7$, $Tb_2Sn_2O_7$, $Pr_2Sn_2O_7$, $Nd_2Sn_2O_7$, $Gd_2Sn_2O_7$, ……

2. rare-earth B-site spinel: $CdEr_2S_4$,$CdEr_2Se_4$, $CdYb_2S_4$, $CdYb_2Se_4$, $MgYb_2S_4$, $MgYb_2S_4$, $MnYb_2S_4$, $MnYb_2Se_4$, $FeYb_2S_4$, $CdTm_2S_4$ $CdHo_2S_4$, $FeLu_2S_4$, $MnLu_2S_4$, $MnLu_2Se_4$, ….

所以要在这些材料里头寻找**谱周期的增强效应**

总结

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复杂量子磁性材料 不仅是 spin liquid 物理的载体，
更是提供了实现其他有趣物理的可能性。

我们这里的几个工作指出了一系列体系、新的物理、
以及这些物理对应的观测量效应。