Monopole condensation transition out of quantum spin ice

and

a quantum spin liquid with strong spin-orbit coupling

Gang Chen

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Job opening

- **Center for Theoretical Physics** of Fudan University is recruiting new members in all fields of theoretical physics.

- **Department of Physics** of Fudan University is recruiting new members.

- Finally **postdocs and visiting professors** are generously funded.

For questions, contact our department chair, Jian Shen <shenj5494@fudan.edu.cn>

OUTLINE

1. Monopole condensation transition out of quantum spin ice.

- I propose the Pr subsystem of the disordered **$Pr_2Ir_2O_7$** sample might be a quantum spin ice.

GC, in preparation.

2. Rare-earth triangular lattice quantum spin liquid: **$YbMgGaO_4$**

- To our best knowledge, this is the **first strong spin-orbit coupled** quantum spin liquid candidate with odd number of electrons per unit cell and effective spin-1/2 moment.

ArXiv **1509.06766**, accepted by **PhysRevLett.**

2. A rare-earth triangular lattice quantum spin liquid: $YbMgGaO_4$

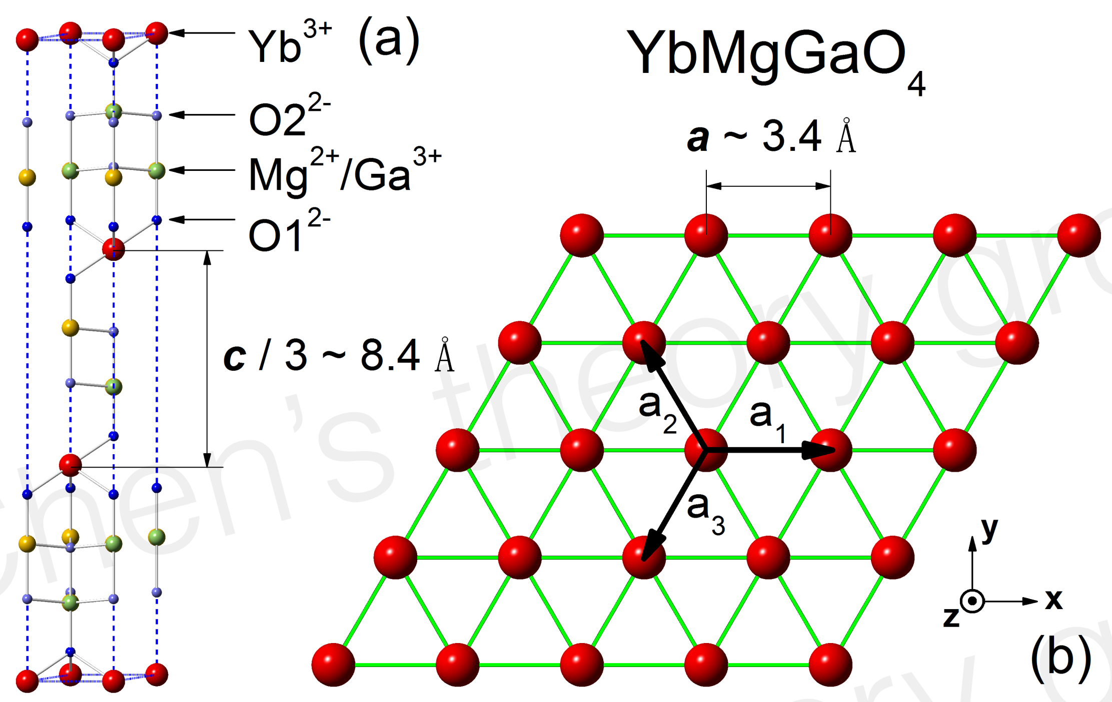
Dr. Yuesheng Li
from Renmin Univ of China

This part is in collaboration with experimentalists

Dr. Yuesheng Li (Renmin Univ, Beijing)
Prof. Qingming Zhang (Renmin Univ, Beijing)
Wei Tong (High Magnetic field Lab, Hefei)
Pi Li (High Magnetic field Lab, Hefei)
Juanjuan Liu (Renmin Univ, Beijing)
Zhaorong Yang (Institute of Solid-State Physics, Hefei)
Xiaoqun Wang (Renmin, Shanghai Jiaotong)

ArXiv **1509.06766**,
accepted by **PhysRevLett**

A rare-earth triangular lattice quantum spin liquid: **$YbMgGaO_4$**



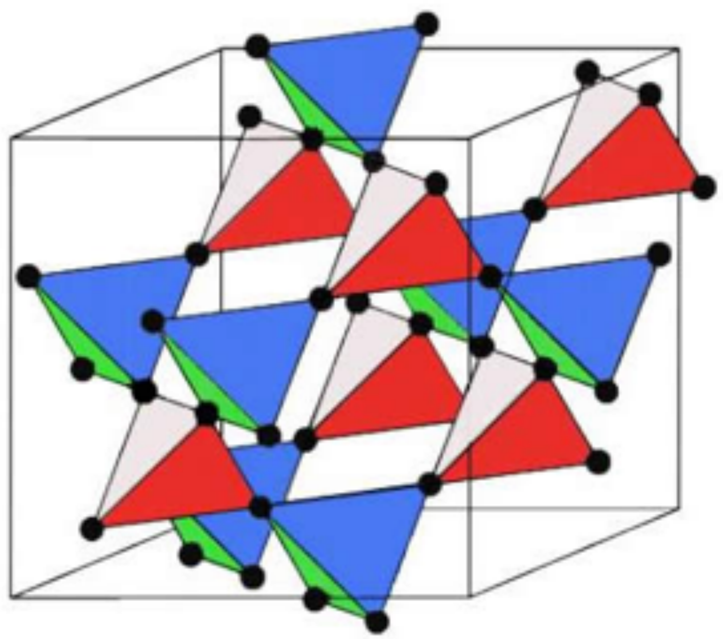
- Hastings-Oshikawa-Lieb-Shultz-Mattis theorem.
- Recent extension to spin-orbit coupled insulators (Watanabe, Po, Vishwanath, Zaletel, Arxiv1505).
- This is the **first** strong spin-orbit coupled QSL with odd number of electrons and effective spin-1/2.
- It is the **first** clear observation of $T^{2/3}$ heat capacity.
- We understand the microscopic Hamiltonian and the physical mechanism.

1. Monopole condensation transition out of quantum spin ice.

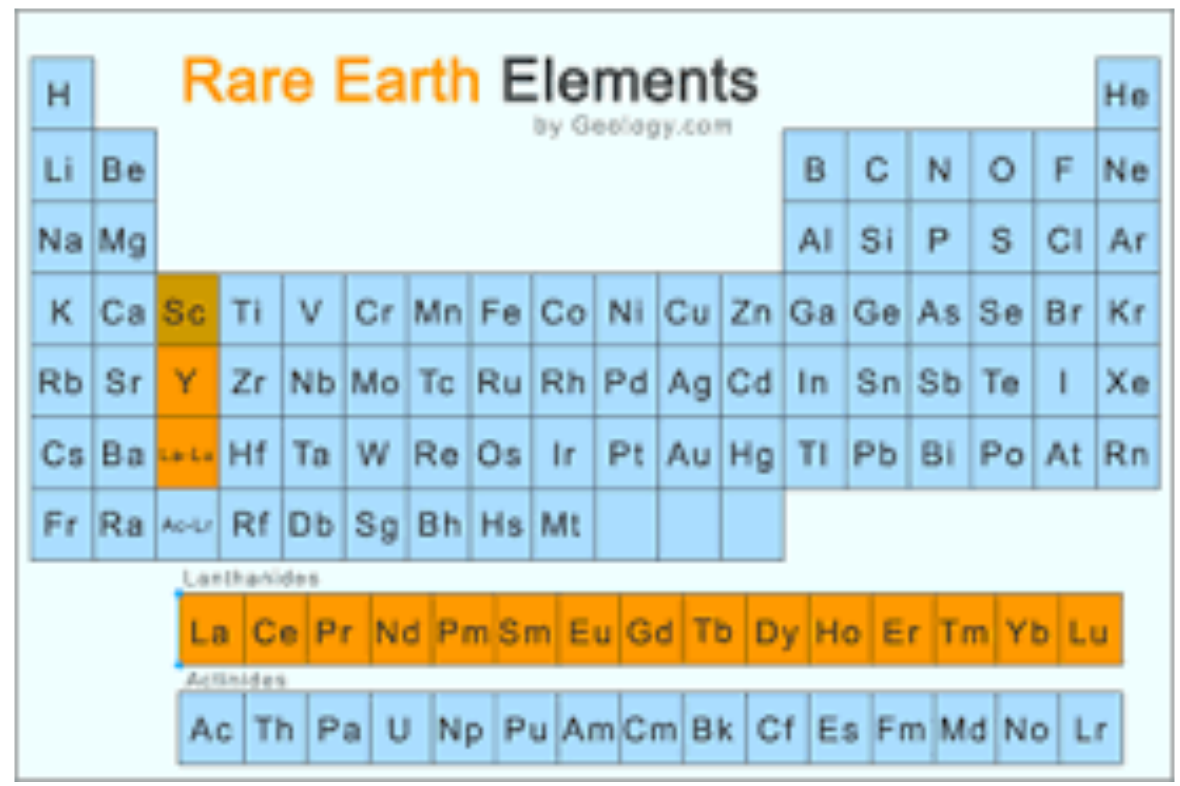
1. Monopole condensation out of quantum spin ice

- Introduction: does quantum spin ice exist in nature?
- Magnetic transition of quantum spin ice is confinement transition of compact QED
- Monopole condensation and proximate phases

Spin ice in rare-earth pyrochlores



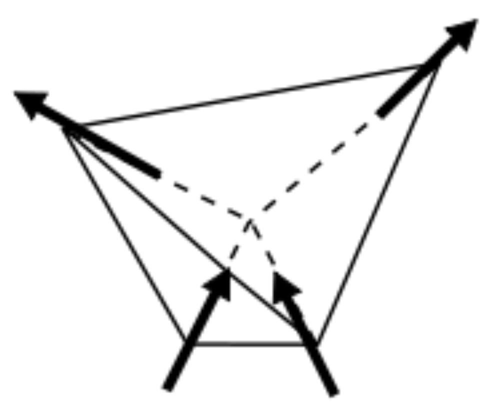
$RE_2M_2O_7$



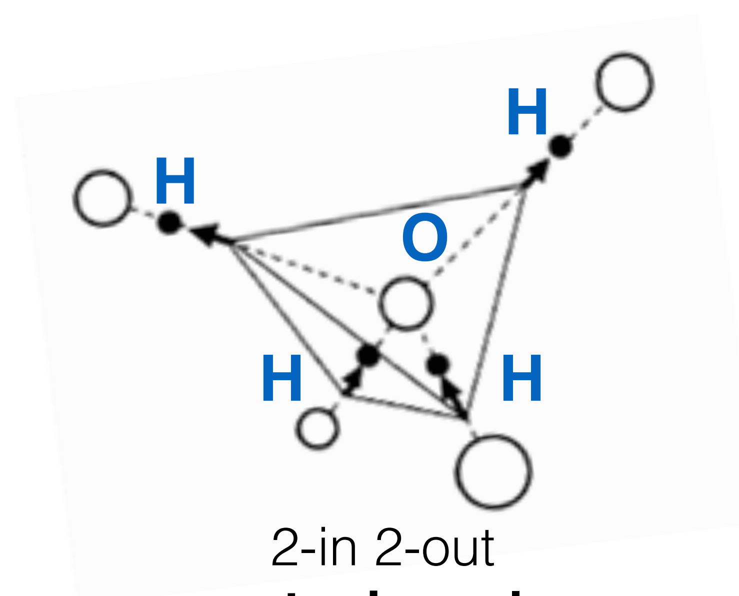
Spin ice in rare-earth pyrochlores

$$H = J_{zz} \sum_{\langle i,j \rangle} S_i^z S_j^z + \text{dipolar}$$

Castelnovo, Gingras, Moessner, Sondhi, Schiffer, Penc, …….

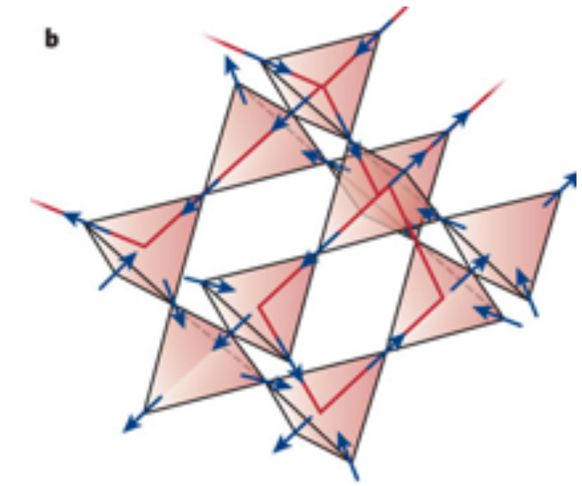


2-in 2-out
spin ice rule



2-in 2-out
water ice rule

from wiki



Classical spin ice

- The "2-in 2-out" states are extensively degenerate.
- At T < Jzz, the system **thermally** fluctuates within the ice manifold, leading to classical spin ice and interesting experimental discoveries.

Pinch points in spin correlation

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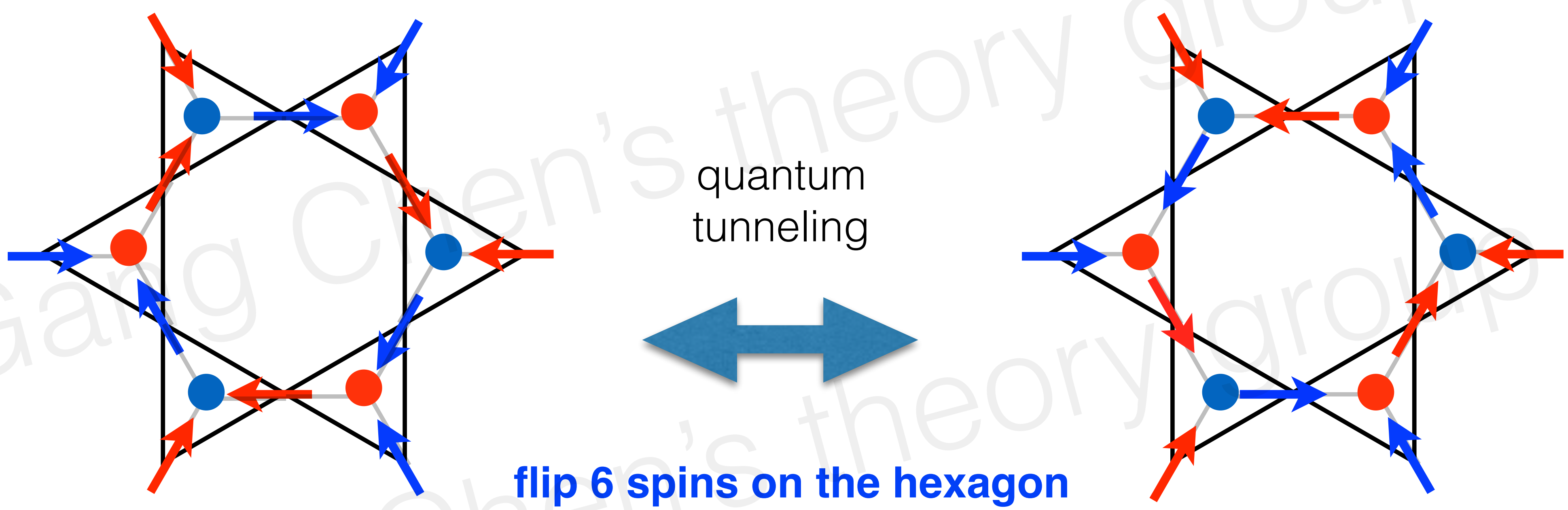
Quantum fluctuation can leads to U(1) QSL

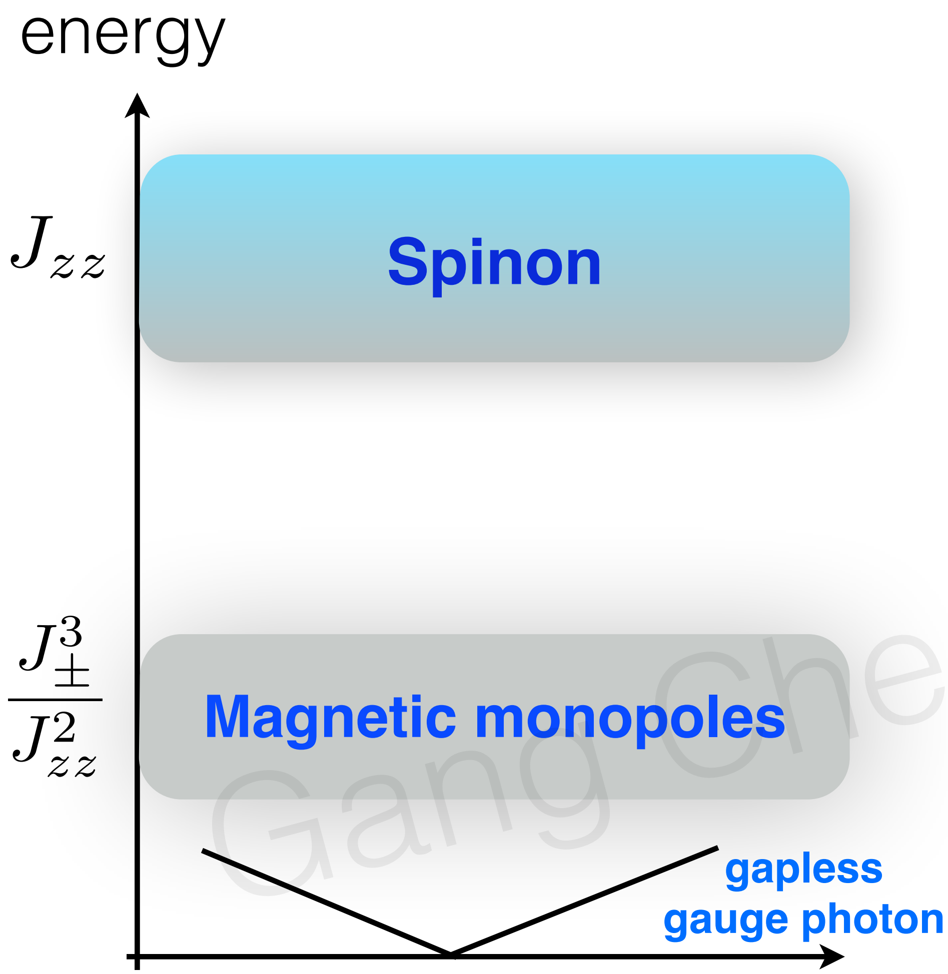
$$H = J_{zz} \sum_{\langle i,j \rangle} S_i^z S_j^z - J_{\pm} \sum_{\langle i,j \rangle} (S_i^+ S_j^- + S_i^- S_j^+) + \cdots\cdots$$

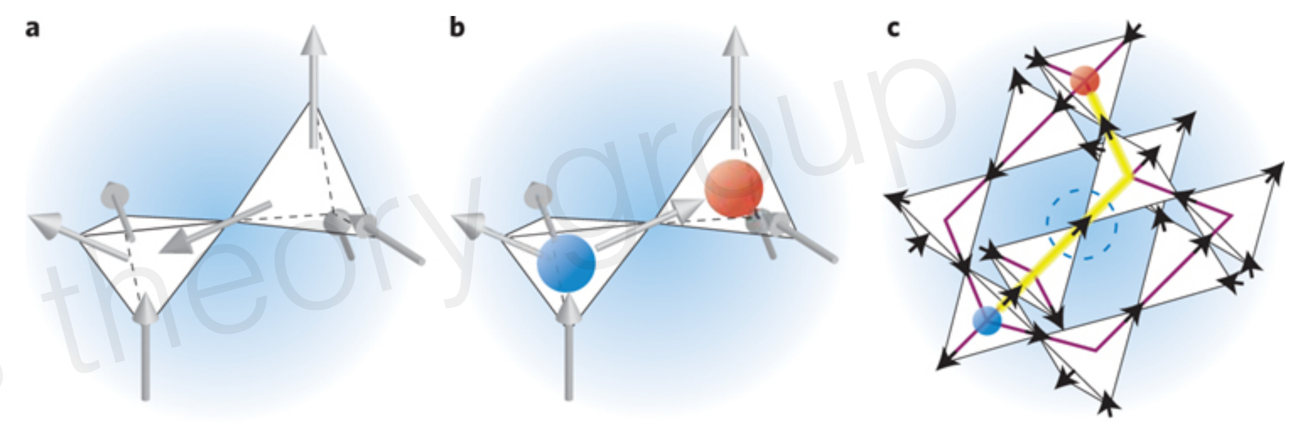
Hermele, Fisher, Balents, Moessner, Isakov, YB Kim….



- Pretty much one can add any term to create **quantum** tunneling, as long as it is not too large to induce magnetic order, the **ground state** is a quantum spin ice !

QSI is NOT a Landau symmetry breaking phase





Figs from Moessner&Schiffer,2009

Spinon deconfinement

- Unlike CSI, QSI is a **novel phase of matter**. No LRO, no symmetry breaking, **cannot** be understood in Landau's paradigm!
- The right description is in terms of fractionalization and emergent gauge structure.

Important question: does QSI exist in experiments?

Probably.

Realistic models

- Kramers' doublet

$$H = \sum_{\langle ij \rangle} \{ J_{zz} S_i^z S_j^z - J_{\pm}(S_i^+ S_j^- + S_i^- S_j^+) + J_{\pm\pm}(\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-) + J_{z\pm}[S_i^z(\zeta_{ij} S_j^+ + \zeta_{ij}^* S_j^-) + i \leftrightarrow j] \},$$

S. H. Curnoe, PRB (2008).

Savary, Balents, PRL 2012

- Non-Kramers' doublet

$$H = \sum_{\langle ij \rangle} \{ J_{zz} S_i^z S_j^z - J_{\pm}(S_i^+ S_j^- + S_i^- S_j^+) + J_{\pm\pm}(\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-) \}$$

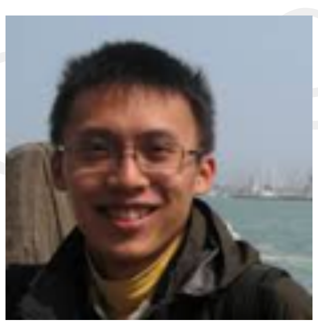
S. Onoda, etc, 2009

SB Lee, Onoda, Balents, 2012

- Dipole-octupole doublet

$$H = \sum_{\langle ij \rangle} J_x S_i^x S_j^x + J_y S_i^y S_j^y + J_z S_i^z S_j^z + J_{xz}(S_i^x S_j^z + S_i^z S_j^x).$$

Y-P Huang, **Gang Chen**, M Hermele, PRL 2014



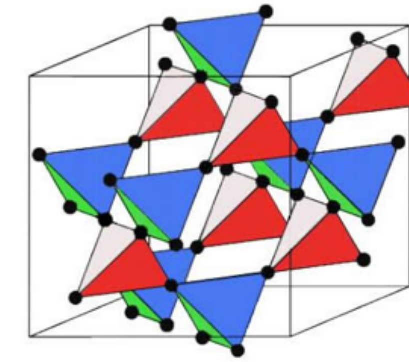
Yi-Ping Huang

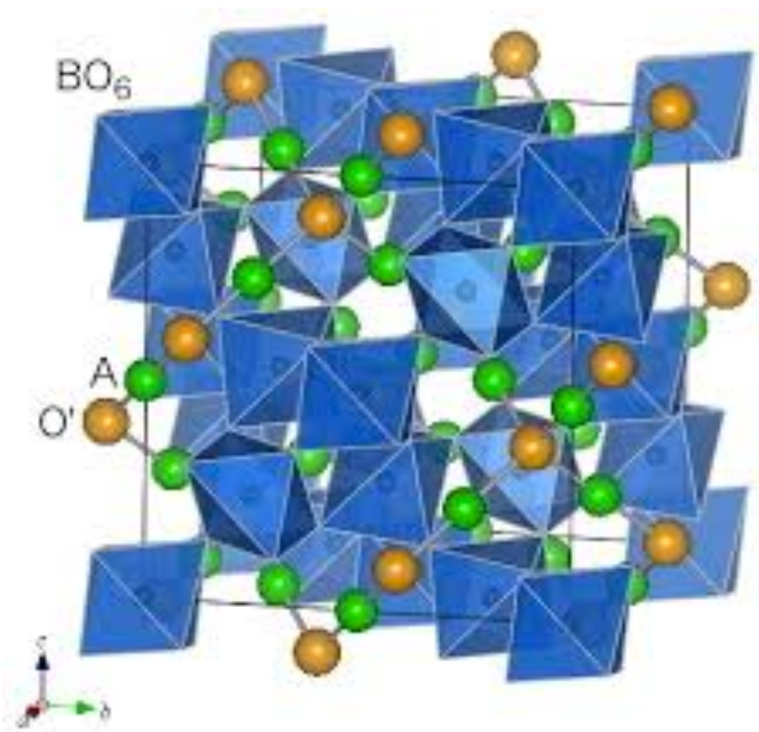
$Nd_2Ir_2O_7$, $Nd_2Sn_2O_7$, $Nd_2Zr_2O_7$, etc

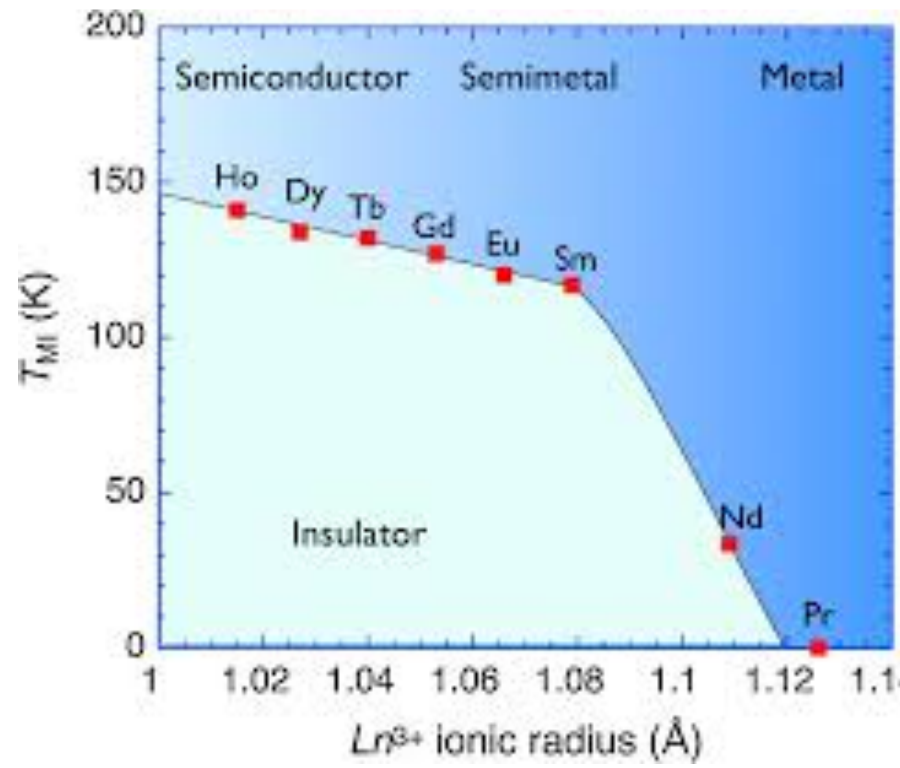
no sign problem for QMC on any lattice.

It supports nontrivial phase like quantum spin ice

Pyrochlore Iridates: $Pr_2Ir_2O_7$



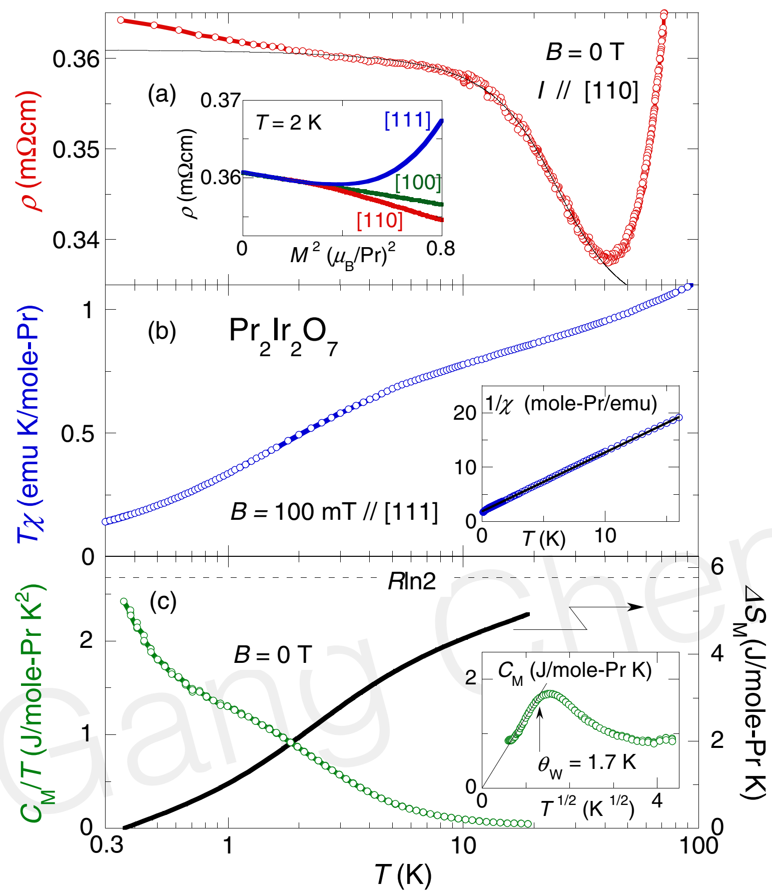




$R_2Ir_2O_7$

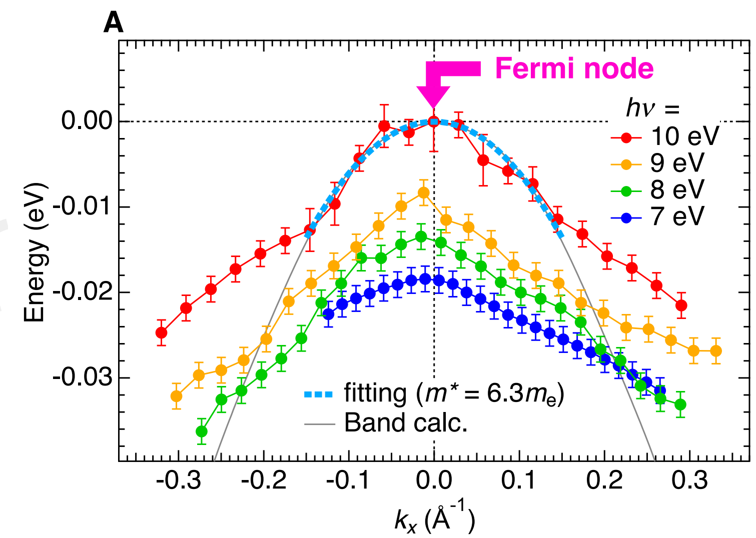
K Matsuhira, M Wakeshima, Y Hinatsu, S. Takagi
JPSJ, 2011

Experiments: a featureless state near an ordered state



Nakatsuji, etc PRL **96,** 087204 (2006)

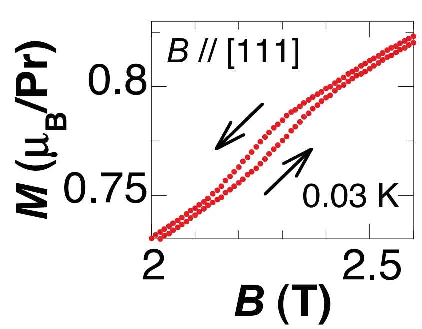
ARPES: quadratic band touching of Ir d electrons



Valence band approaches the Fermi energy at few meV resolution

T. Kondo, S Shin, etc 2014 (unpublished)

$Pr_2Ir_2O_7$



metamagnetic transition

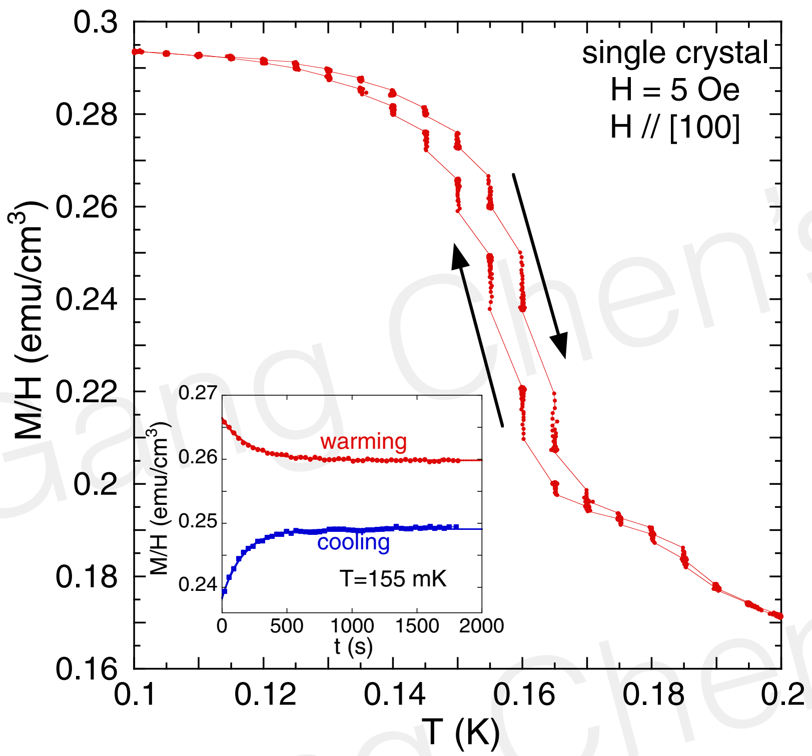
Expts are **sample dependent**, some samples are AFM ordered.

Experiments: a featureless state near an ordered state

PHYSICAL REVIEW B **89**, 224419 (2014)

First-order magnetic transition in $Yb_2Ti_2O_7$

E. Lhotel,[1,*] S. R. Giblin,[2] M. R. Lees,[3] G. Balakrishnan,[3] L. J. Chang,[4] and Y. Yasui[5]



Some samples have FM LRO with 1st transition. Some samples do not have order.

PHYSICAL REVIEW X **1**, 021002 (2011)

Quantum Excitations in Quantum Spin Ice

Kate A. Ross,[1] Lucile Savary,[2] Bruce D. Gaulin,[1,3,4] and Leon Balents[5,*]

waves [14]. Although one neutron study [15] supported ferromagnetic order in $Yb_2Ti_2O_7$, intriguingly, the majority of neutron scattering measurements have reported a lack of magnetic ordering and the absence of spin waves at low fields in this material [16–18]. In a recent study,

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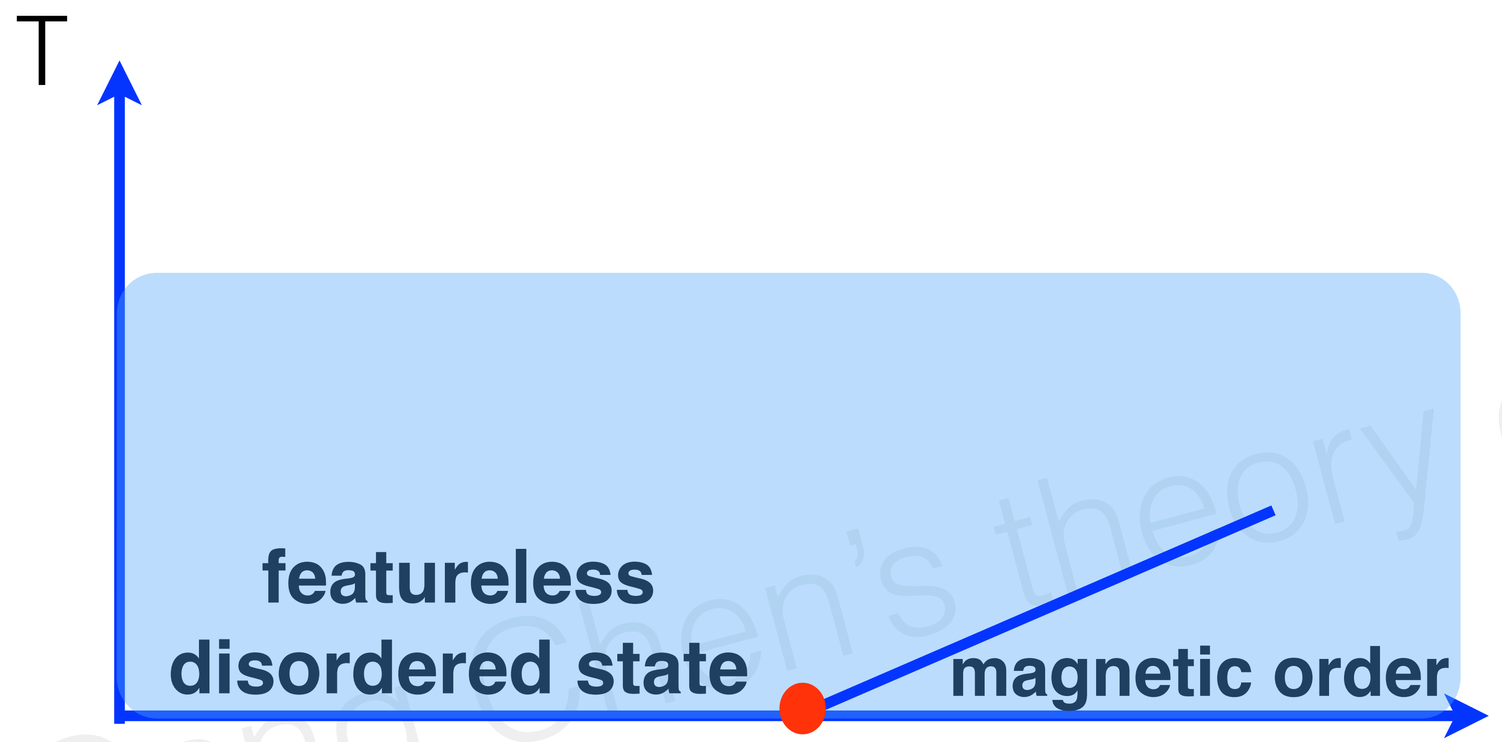
Summary of experimental results



- What is the structure of the magnetic order?
- What is the relationship between the featureless disordered state and various magnetic states?
- What is the nature of the featureless disordered states? Is it **QSI**?

Insight from high-Tc superconductors

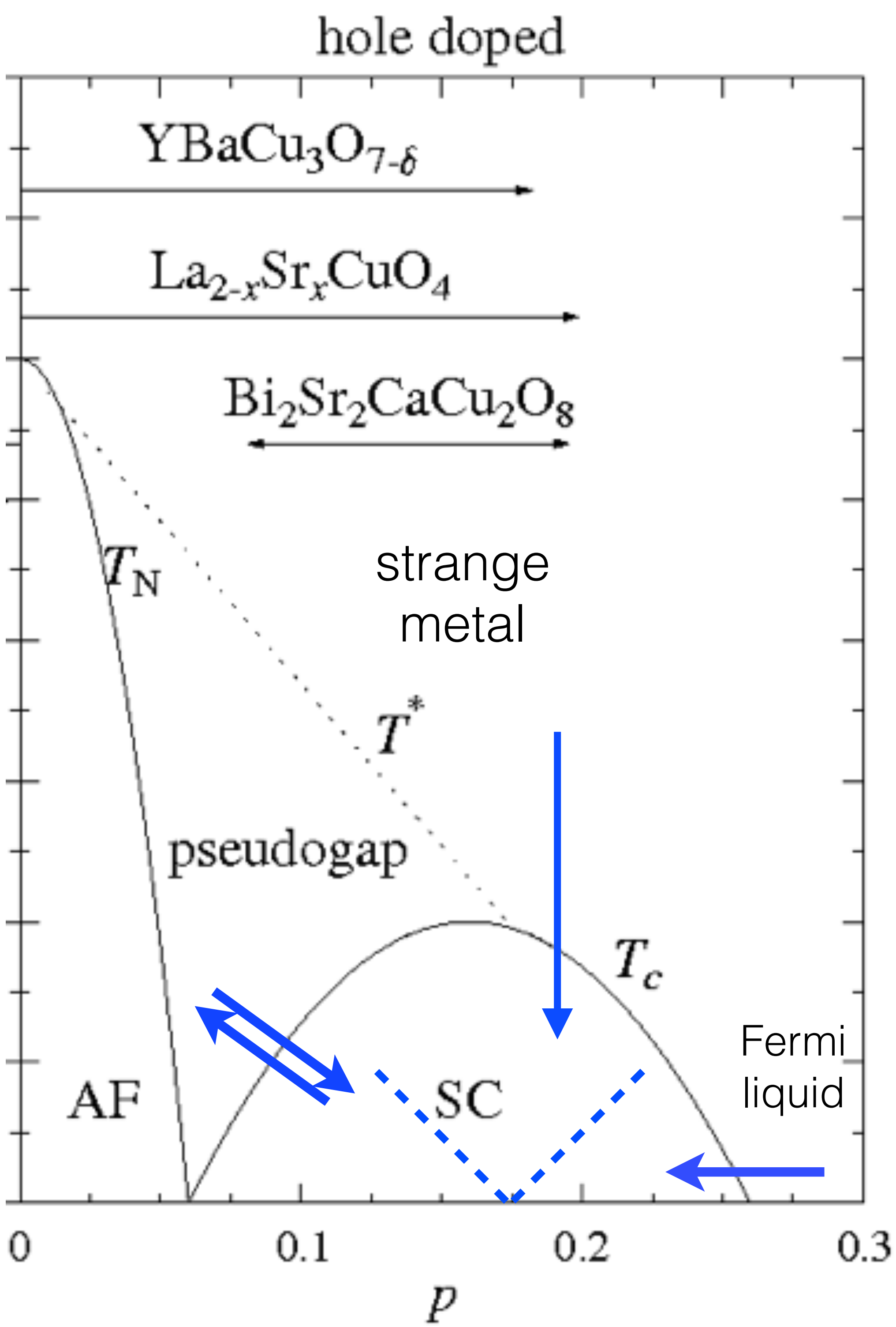
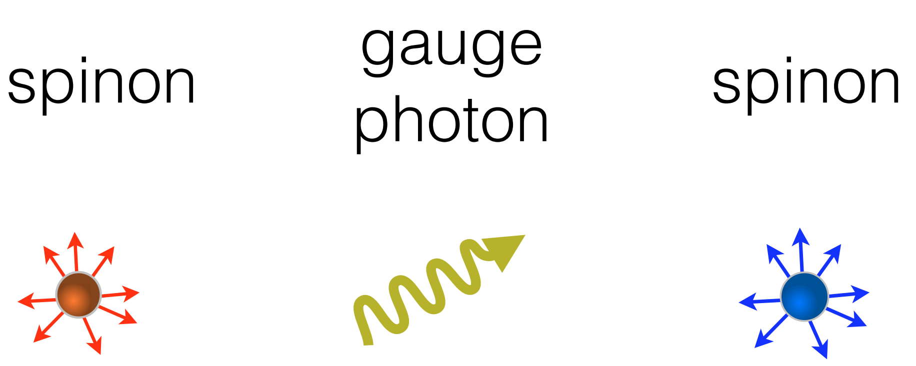


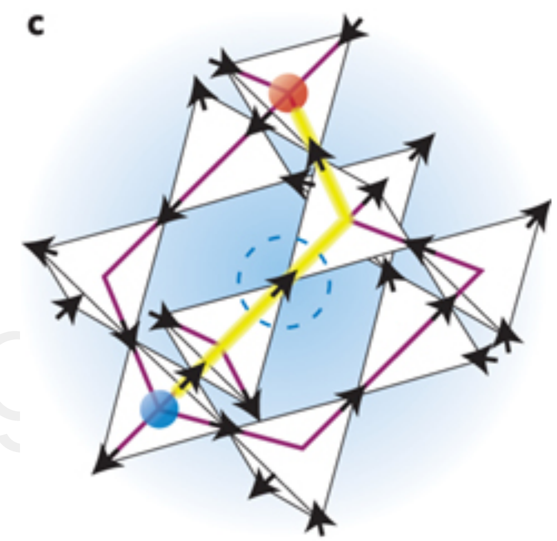
Figure from wiki

One important question is to understand the relationship between different phases (and/or orders)

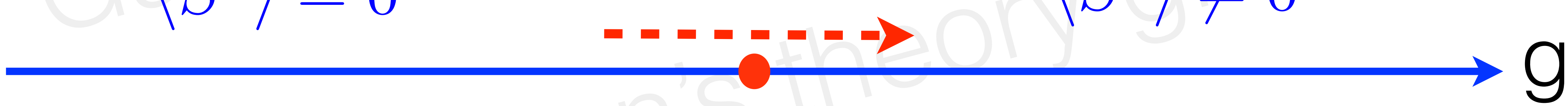
1. Perturbative treatment (not interesting): instability of Fermi liquid;
2. Attack from top: instability of non-Fermi liquid;
3. Attack from Left, attack from Right: what is PG (Z2 topological order?) ? (Senthil, Balents, Nayak, Fisher 2000-2002);
4. Attack from bottom: some quantum criticality under the SC dome?

Attack from left (quantum spin ice)





$\langle S^z \rangle = 0$ $\langle S^z \rangle \neq 0$



featureless disordered state
=quantum spin ice??

magnetic order

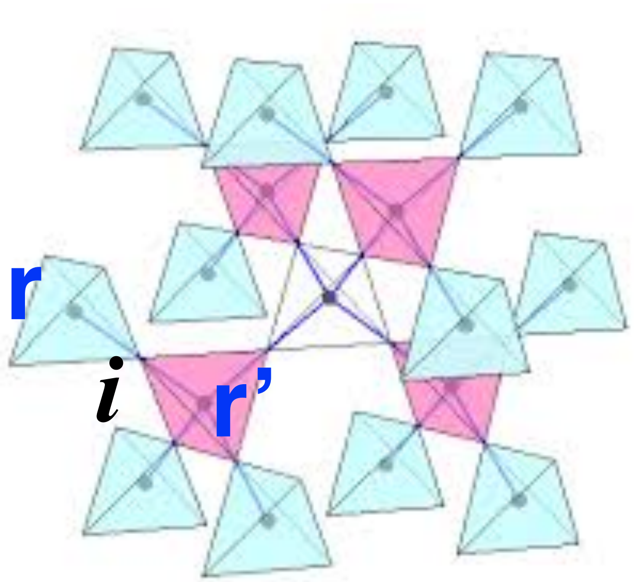
Spinons are deconfined.

Spinons are confined !

Remark: for non-Kramers' doublet, the magnetic transition out of QSI must be a confinement transition.

Theoretical framework: compact QED and electromagnetic duality

Lattice gauge theory formalism: technical part



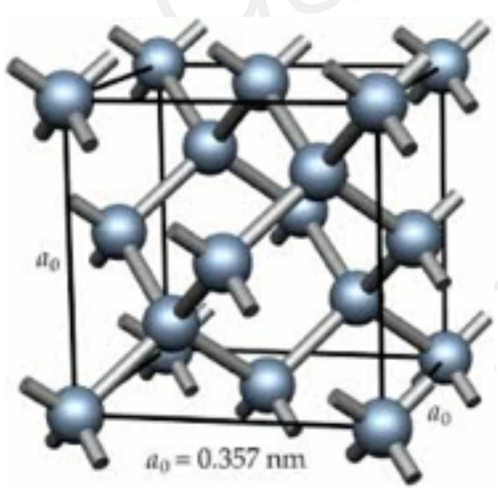
$$E_{\mathbf{rr}'} \sim S_i^z, \quad e^{iA_{\mathbf{rr}'}} \sim S_i^+.$$

Hermele etc, 2004

$$H_{\rm Ring} \sim -K \sum_{hexagon} [S_1^+ S_2^- S_3^+ S_4^- S_5^+ S_6^- + h.c.]$$

$$H_{\rm LGT} = \sum_{\langle \mathbf{rr}' \rangle} \frac{U}{2} (E_{\mathbf{rr}'} - \frac{\epsilon_{\mathbf{r}}}{2})^2 - \sum_{\hexagon_d} K \cos(curl\ A),$$

$H_{\rm LGT}$ captures the universal properties of QSI.



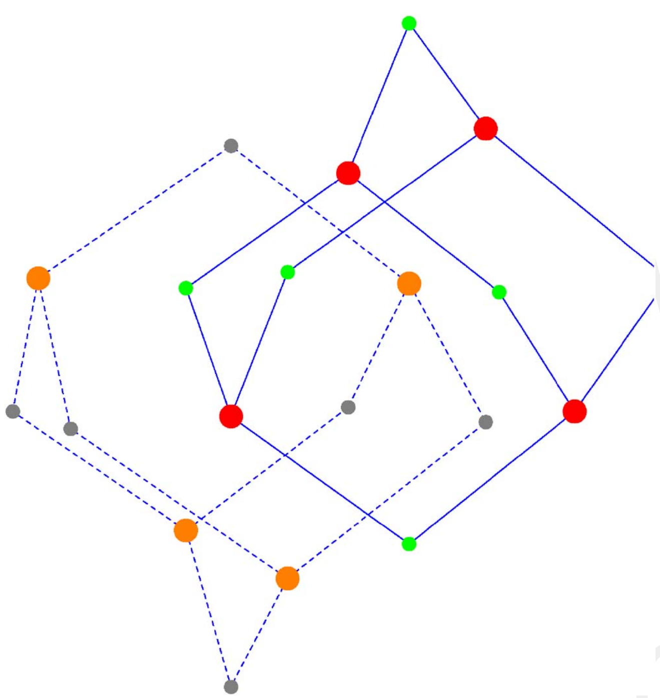
diamond lattice

- In an ordered state, <Sz>!=0, <S+> is strongly fluctuating.
- In the gauge language, **E field** is static, **B magnetic field** is strongly fluctuating, the magnetic monopole (carrying magnetic charge) is condensed, which confines the electric charge carriers (spinons).

Electromagnetic duality

Monopole lives on dual diamond lattice, carry magnetic charge or dual U(1) gauge charge.

To study monopole physics, we need to use a technique called "duality" to make it explicit.



diamond (dotted) and
dual diamond lattice
(Bergman, Fiete, Balents, PRB 2006)

$$curl\, a \equiv \sum_{\mathbf{rr'} \in \hexagon^*_d} a_{\mathbf{rr'}} \equiv E_{\mathbf{rr'}} - E^0_{\mathbf{rr'}},$$ dual U(1) gauge

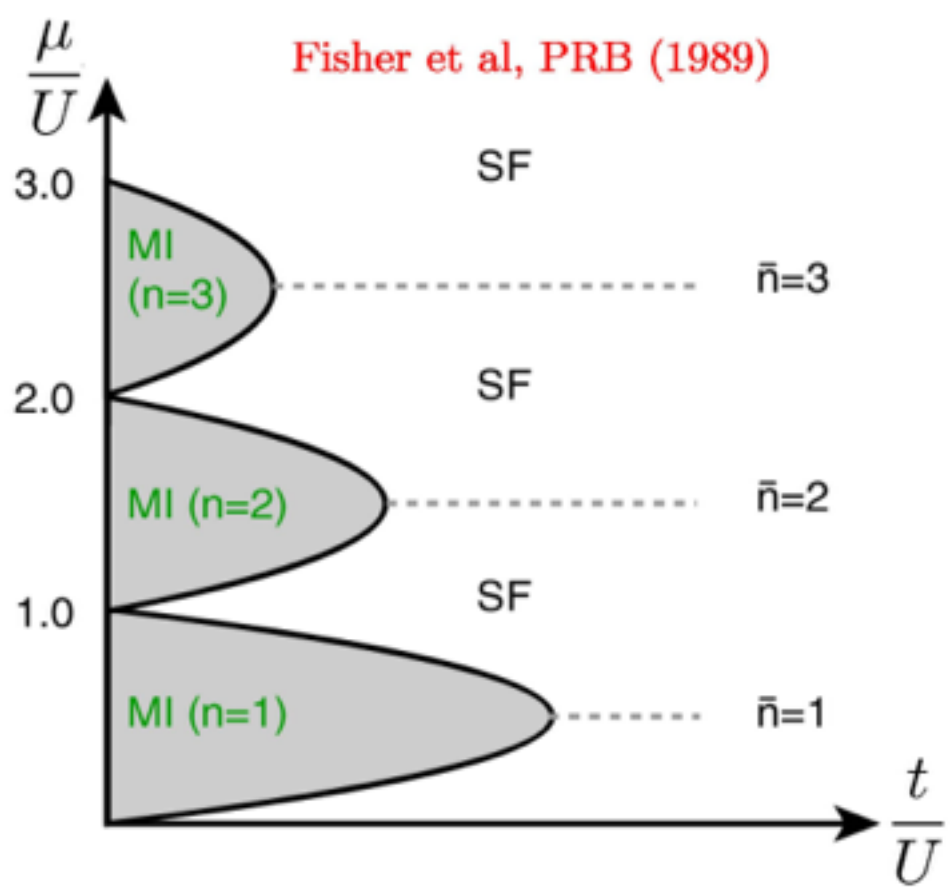
$$H_{\rm dual} = \sum_{\hexagon^*_d} \frac{U}{2} (curl\, a - \bar{E})^2 - \sum_{\mathbf{r},\mathbf{r'}} K \cos B_{\mathbf{rr'}},$$

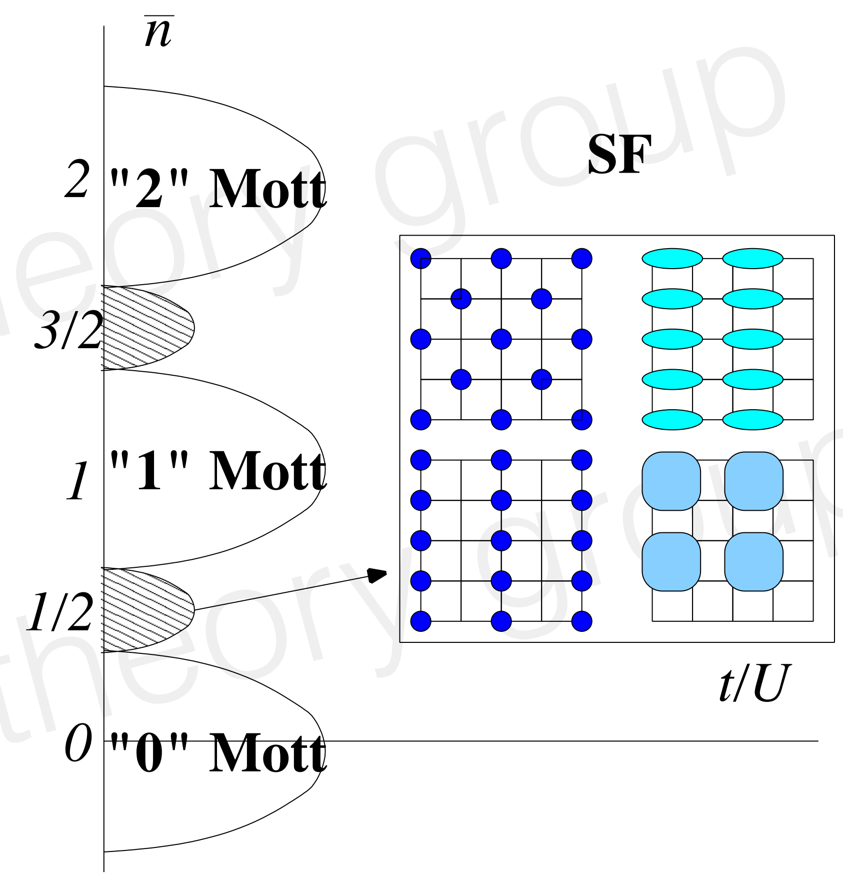
insert monopole variables

$$H_{\rm dual} = \sum_{\hexagon^*_d} \frac{U}{2} (curl\, a - \bar{E})^2 - \sum_{\mathbf{r},\mathbf{r'}} K \cos B_{\mathbf{rr'}} - \sum_{\mathbf{r},\mathbf{r'}} t \cos(\theta_{\mathbf{r}} - \theta_{\mathbf{r'}} + 2\pi a_{\mathbf{rr'}}).$$

- **B magnetic field** is strongly fluctuating, the fluctuation of dual U(1) gauge field is weak.

Analogy with Boson-vortex duality





Balents, et al, 2005

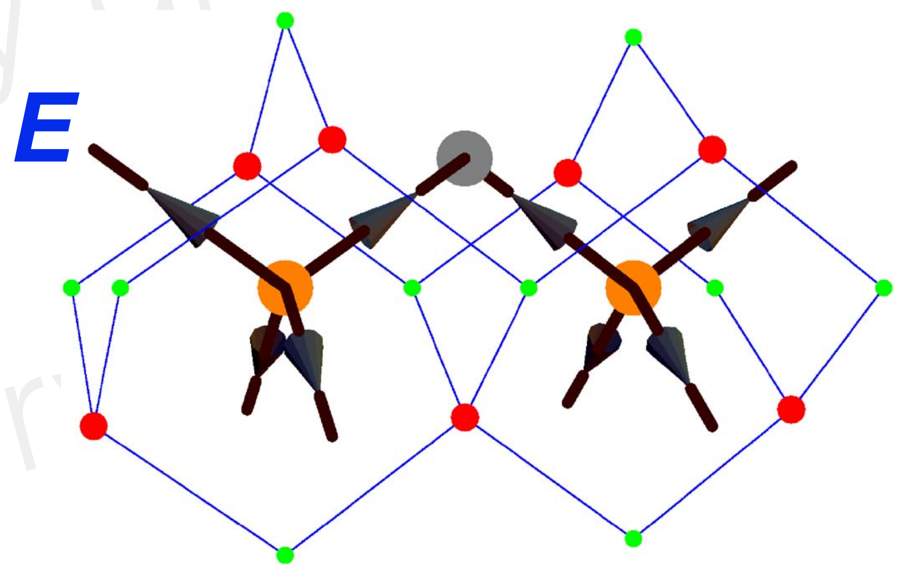
Physical observables are gauge invariant

- Monopole loop current defines the magnetic order

$$\text{curl}\ \vec{E} = -\frac{\partial \vec{B}}{\partial t} + \vec{J}_b,$$ **(Maxwell's equation)**

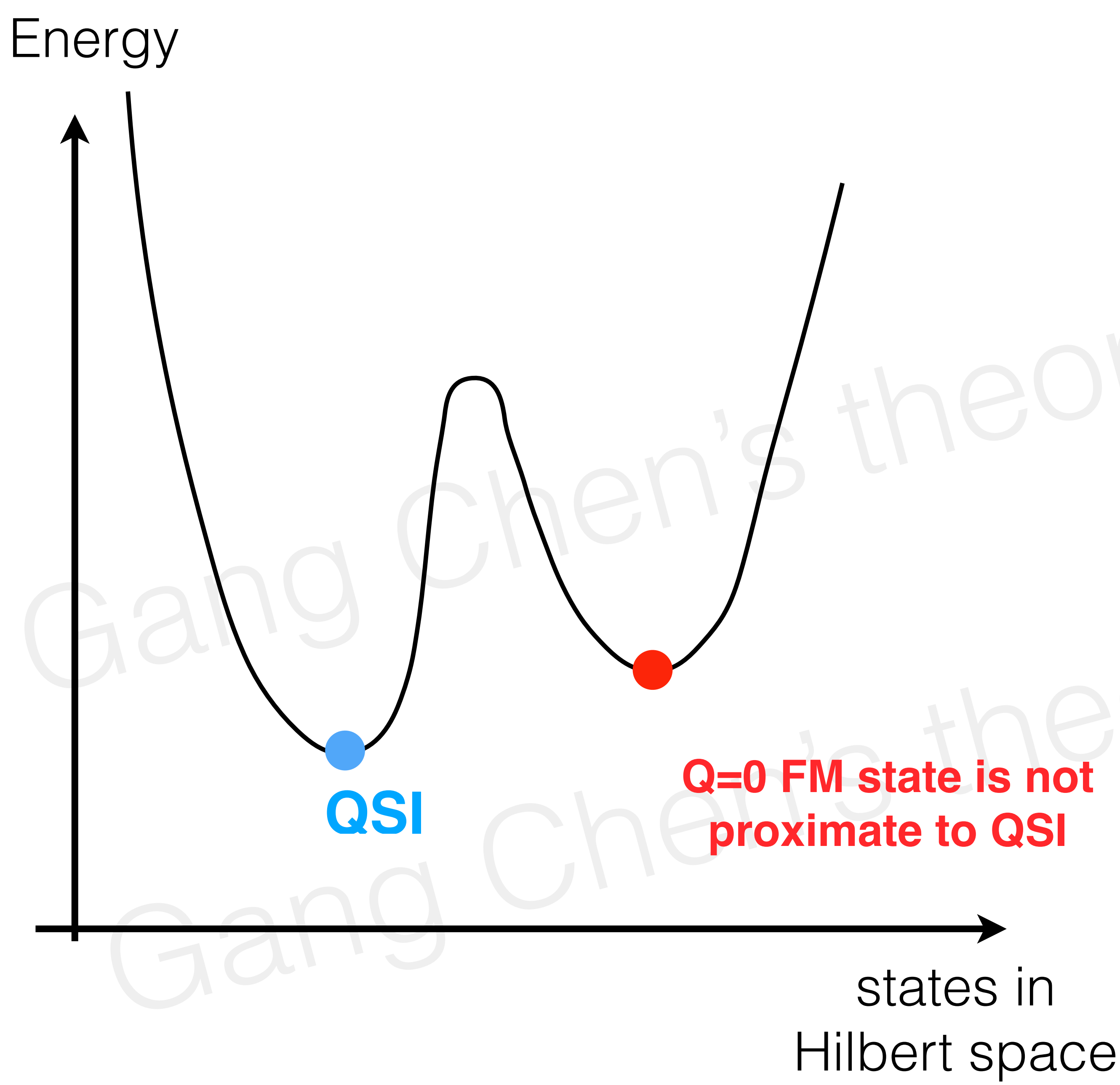
$$\oint_C \vec{J}_b \cdot d\vec{\ell} = \oint_C \text{curl}\ \vec{E} \cdot d\vec{\ell} = \int_S \vec{E} \cdot d\vec{A}.$$

$$S_i^z \sim E_{\mathbf{rr}'} \sim \sum_{\mathbf{rr}' \in \hexagon_d^*} \mathsf{J}_{\mathbf{rr}'}$$

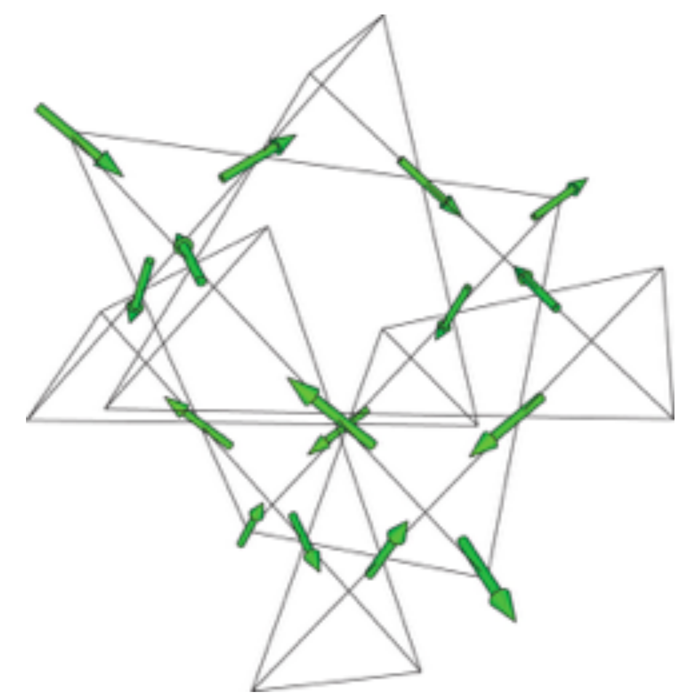


(Bergman, Fiete, Balents, PRB 2006)

Proximate and un-proximate magnetic states



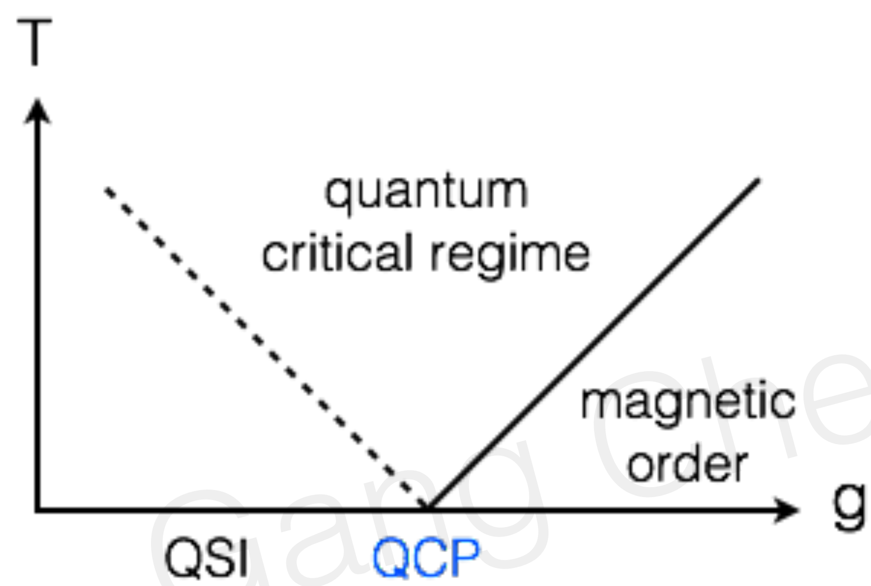
Un-proximity implies a strong
1st order transition!



Q=2Pi(001) AFM state is
the simplest **proximate** state.

Critical theory for proximate ordering transition

Standard Landau-Ginzburg expansion in the monopole fields



$$\Phi_{\mathbf{r}} = \sum_{a=1}^{12} \varphi_a(\mathbf{r})\,\phi_a,$$

determined by **projective symmetry group**

$$L = \sum_a \left[|(\partial_\mu - i\tilde{a}_\mu)\phi_a|^2 + m^2|\phi_a|^2 \right] + \frac{{F_{\mu\nu}}^2}{2}$$
$$+u_0\Big(\sum_a |\phi_a|^2\Big)^2 + \cdots,$$

The critical theory is described by multicomponent bosons coupled with a fluctuating U(1) gauge field in 3+1D.

a unusual weak divergence $\chi(Q) \sim -\ln T$ "subsidiary order"

Implication for experiments

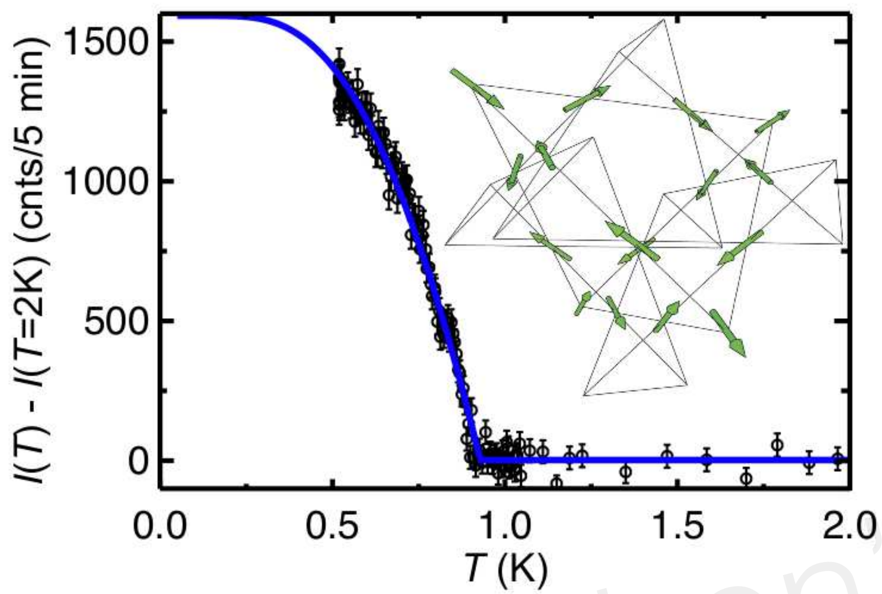


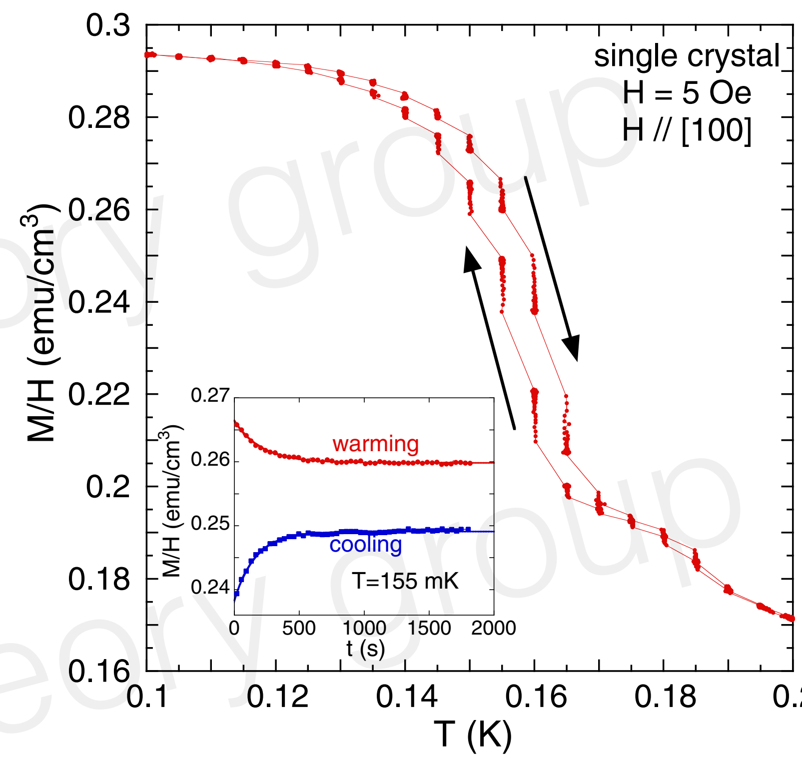
FIG. 2. (color online) Temperature dependence of elastic neutron scattering intensity of $Pr_{2+x}Ir_{2-x}O_{7-\delta}$ at the position of the $\mathbf{q}_m = (100)$ reflection. The intensity measured at $T = 2$ K was subtracted as a background. Curve: Ising mean-field theory fit to the data, which yields a transition temperature of $T_M = 0.93(1)$ K. Inset: sketch of the 2-in/2-out magnetic structure.

Magnetic order is discovered in some samples. (MacLaughlin, etc, 2015)

PHYSICAL REVIEW B **89**, 224419 (2014)

First-order magnetic transition in $Yb_2Ti_2O_7$

E. Lhotel,[1,*] S. R. Giblin,[2] M. R. Lees,[3] G. Balakrishnan,[3] L. J. Chang,[4] and Y. Yasui[5]



$Yb_2Ti_2O_7$

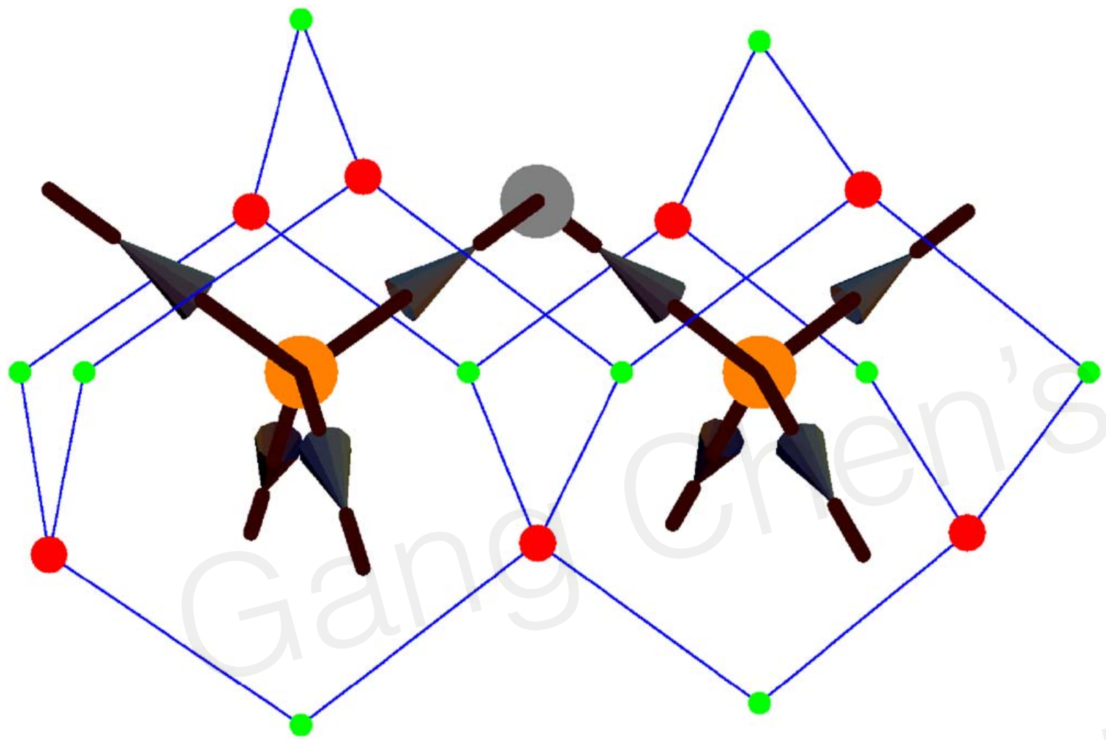
PIO: different samples have different Fermi energy -> RKKY-> **magnetic order, Q= 2Pi(001)**

YTO: First order transition to **Q=0 FM state**.

Summary for the first part

- I have studied the phase diagram near quantum spin ice.
- Using field theoretic technique, I have obtained the structure of the magnetic states and the nature of the magnetic transition.
- I use my theoretical results to explain the puzzling experiments in $Pr_2Ir_2O_7$ and $Yb_2Ti_2O_7$. It implies the disordered phase is likely to be a QSI.

Frustrated monopole bands



$$H_{\mathrm{dual}} = \sum_{\hexagon_d^*} \frac{U}{2}(curl\, a - \bar{E})^2 - \sum_{\mathbf{r},\mathbf{r}'} K \cos B_{\mathbf{r}\mathbf{r}'}$$
$$- \sum_{\mathbf{r},\mathbf{r}'} t \cos(\theta_{\mathbf{r}} - \theta_{\mathbf{r}'} + 2\pi a_{\mathbf{r}\mathbf{r}'}).$$

Fixing gauge, $curl\, \bar{a} = \bar{E}$,

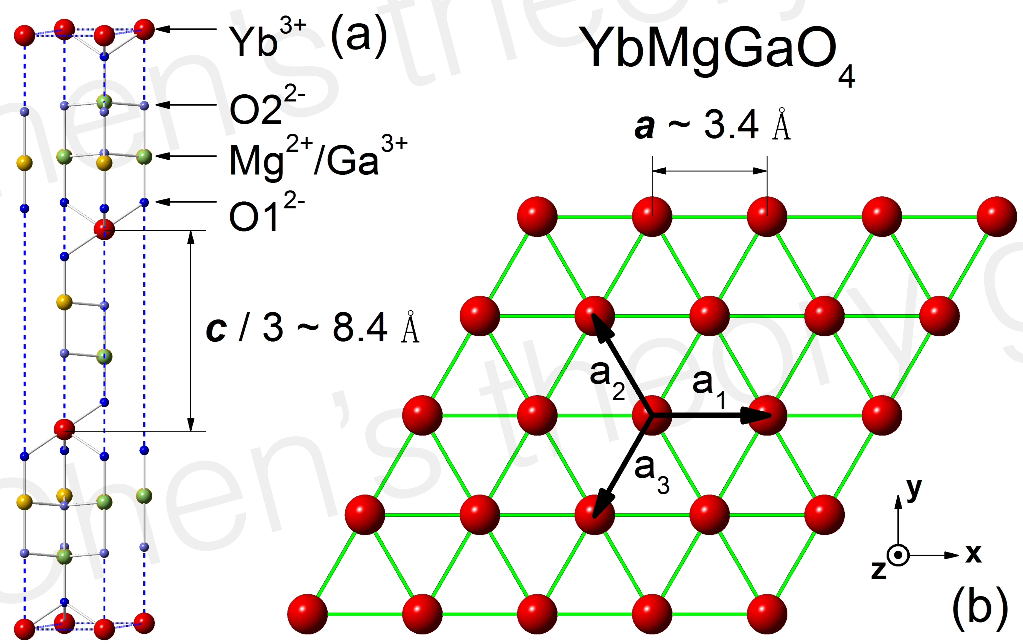
$$H_m = -\sum_{\mathbf{r},\mathbf{r}'} t\, e^{-i2\pi \bar{a}_{\mathbf{r}\mathbf{r}'}} \Phi_{\mathbf{r}}^\dagger \Phi_{\mathbf{r}'}, \qquad \Phi_{\mathbf{r}} \equiv e^{i\theta_{\mathbf{r}}}$$
$$|\Phi_{\mathbf{r}}| \equiv 1$$

The background electric field distribution creates a Pi flux experienced by the monopoles, this frustrates monopole hopping.

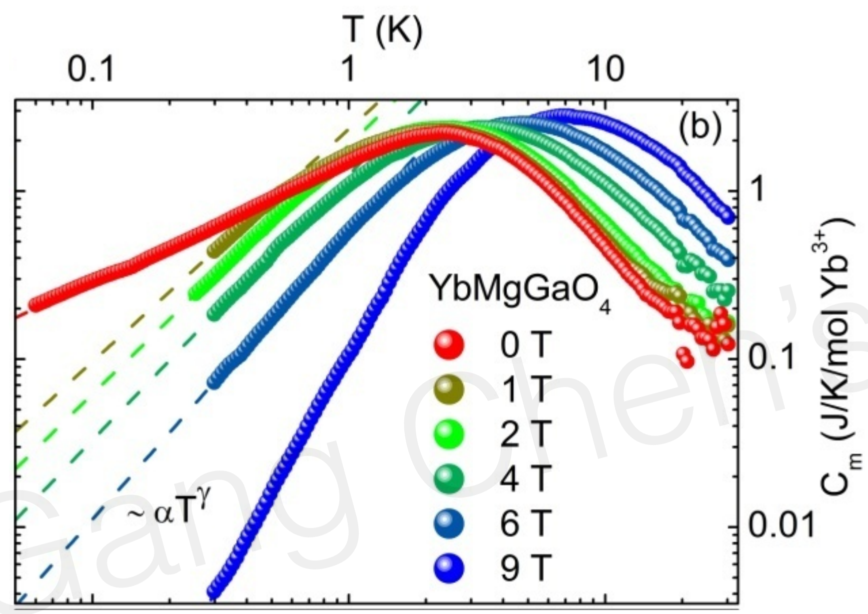
The monopole band minima have a line degeneracy in k space.

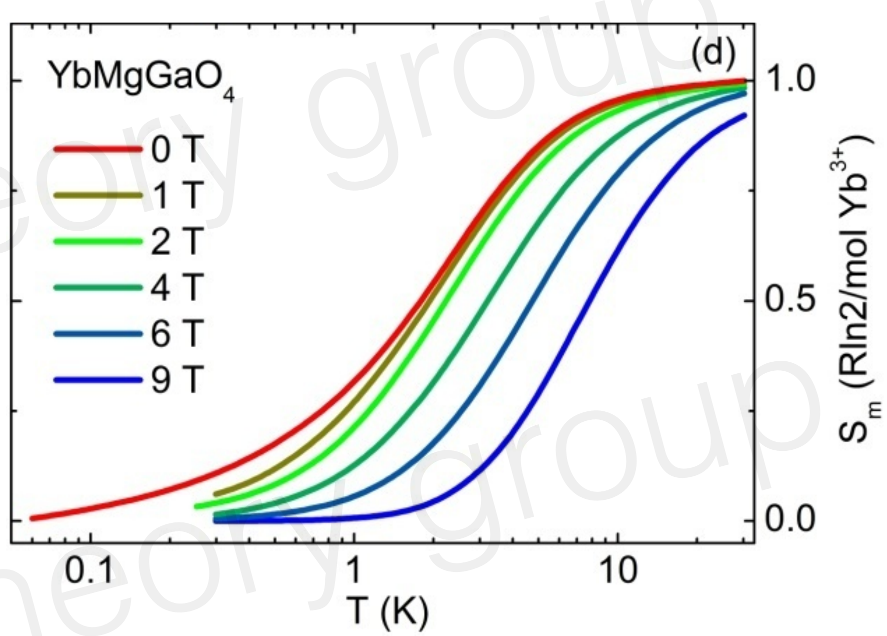
2. A rare-earth triangular lattice quantum spin liquid: **$YbMgGaO_4$**

ArXiv **1509.06766**, accepted by **PhysRevLett**



YbMgGaO$_4$

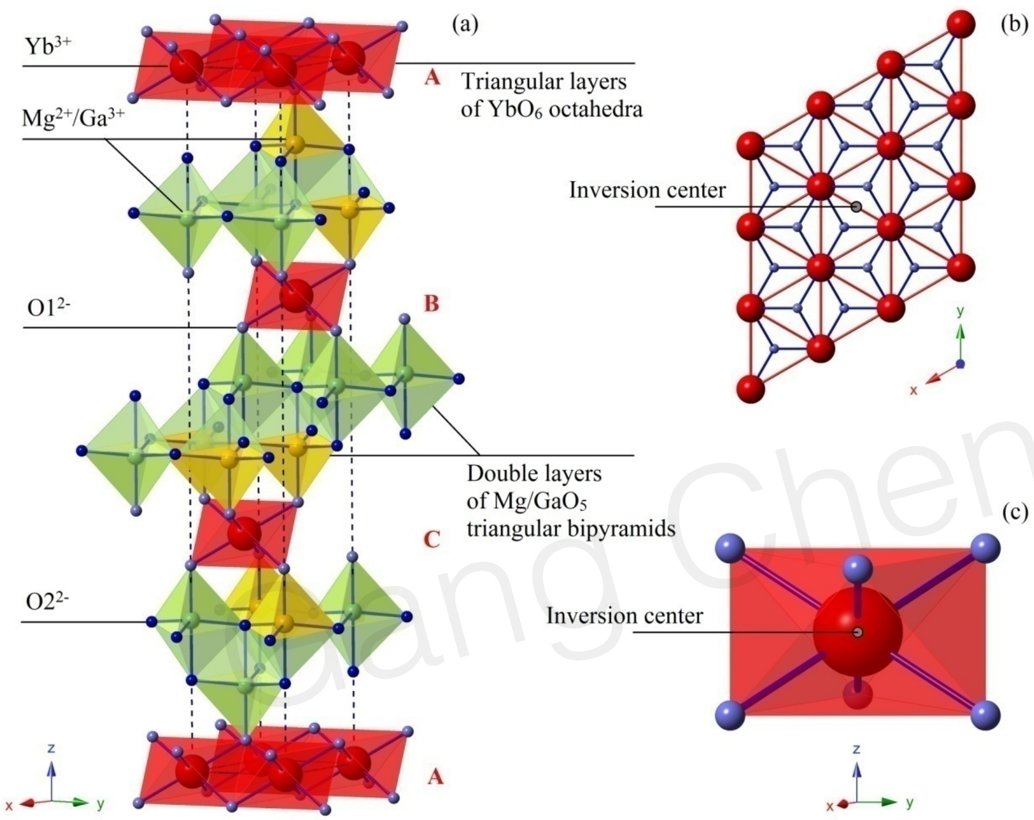




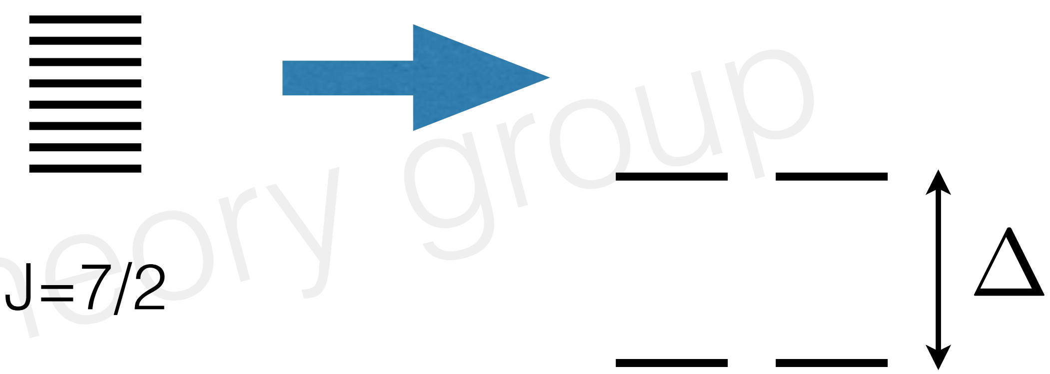
- observation of $T^{2/3}$ heat capacity
- Entropy: effective spin-1/2 local moments

Yuesheng Li, …, Qingming Zhang, 2015

Microscopics



Yb^{3+} ion: 4f^{13} has J=7/2 due to SOC.



YS Li, GC, …, QM Zhang, PRL2015
YD Li, XQ Wang, GC PRB 2016

At $T \ll \Delta$, the only active DOF is the ground state doublet that gives rise to an effective spin-1/2.

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Can this kind of system support a QSL ground state? Yes.

Filling constraints for spin-orbit coupled insulators in symmorphic and non-symmorphic crystals

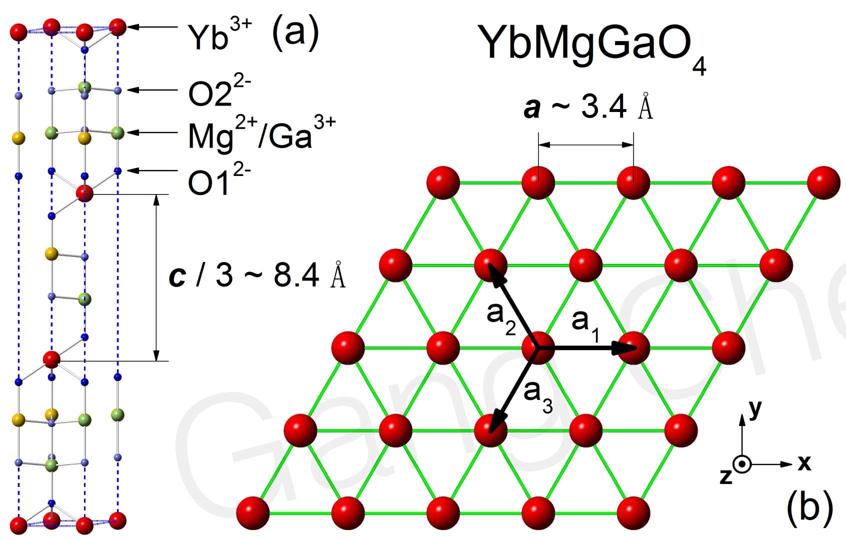
Haruki Watanabe,[1] Hoi Chun Po,[1] Ashvin Vishwanath,[1,2] and Michael P. Zaletel[3] May2015

and a crystalline lattice or a magnetic field. Mott insulators are a particularly interesting class, with an odd number of electrons in each unit cell. Their low energy physics is captured by a spin model with an odd number of $S = 1/2$ moments in the unit cell. A powerful result due to Lieb, Schultz, and Mattis in 1D[1], later extended to higher dimensions by Hastings and Oshikawa[2,3], holds that if all symmetries remain unbroken, the ground state must be 'exotic' - such as a Luttinger liquid in 1D, or a quantum spin liquid in higher dimensions, with fractional 'spinon' excitations. These exotic states cannot be represented as simple product states, as a consequence of long ranged quantum entanglement. This general re-

tirely different theoretical approaches are needed. We argue that if a spin-orbit coupled insulator at odd filling is time-reversal symmetric, its ground state must, in a precise sense, be exotic. We introduce two theoreti-

What is the nature of the QSL? What is the physical origin of the QSL?

4f electron is very localized, and dipolar interactions weak.



$$\mathcal{H} = \sum_{\langle ij \rangle} \big[J_{zz} S_i^z S_j^z + J_{\pm} (S_i^+ S_j^- + S_i^- S_j^+) + J_{\pm\pm} (\gamma_{ij} S_i^+ S_j^+ + \gamma_{ij}^* S_i^- S_j^-) - \frac{i J_{z\pm}}{2} (\gamma_{ij}^* S_i^+ S_j^z - \gamma_{ij} S_i^- S_j^z + \langle i \leftrightarrow j \rangle) \big], \quad (1)$$

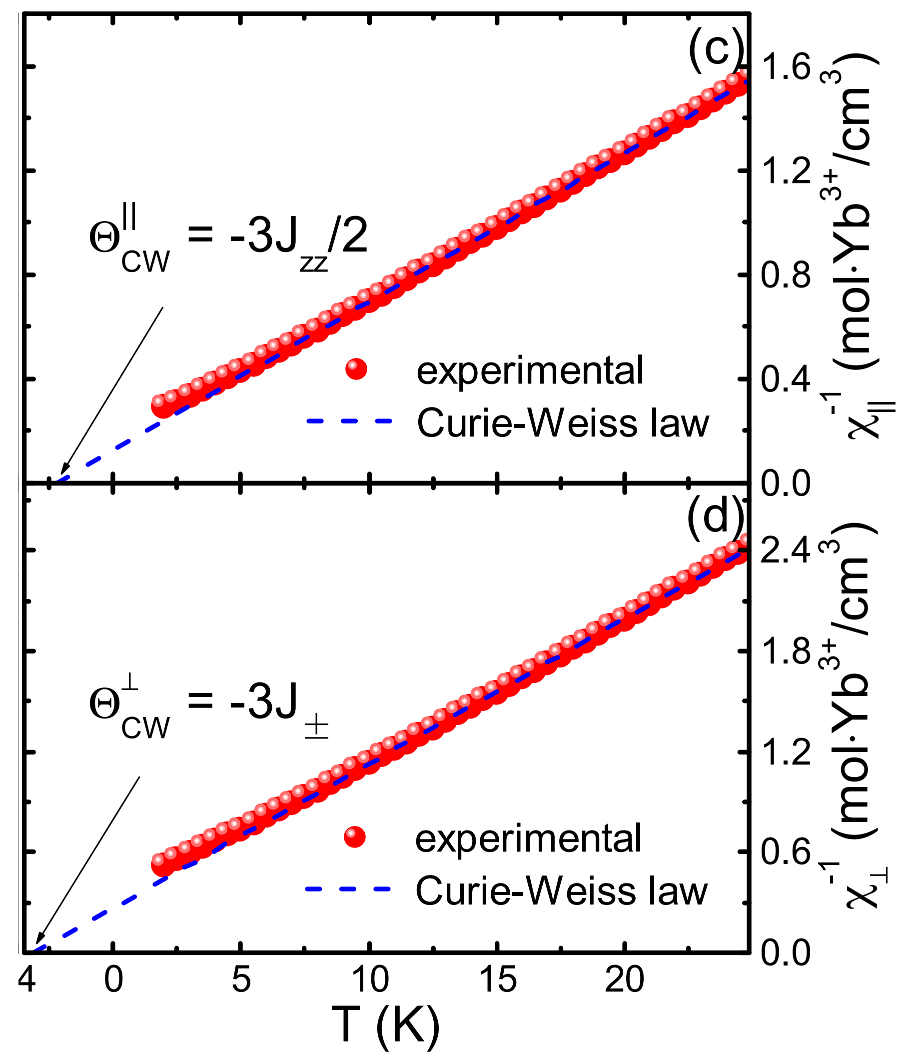
where $S_i^{\pm} = S_i^x \pm i S_i^y$, and the phase factor $\gamma_{ij} = 1, e^{i2\pi/3}, e^{-i2\pi/3}$ for the bond ij along the $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ direction (see Fig. 1), respectively. This generic Hamil-

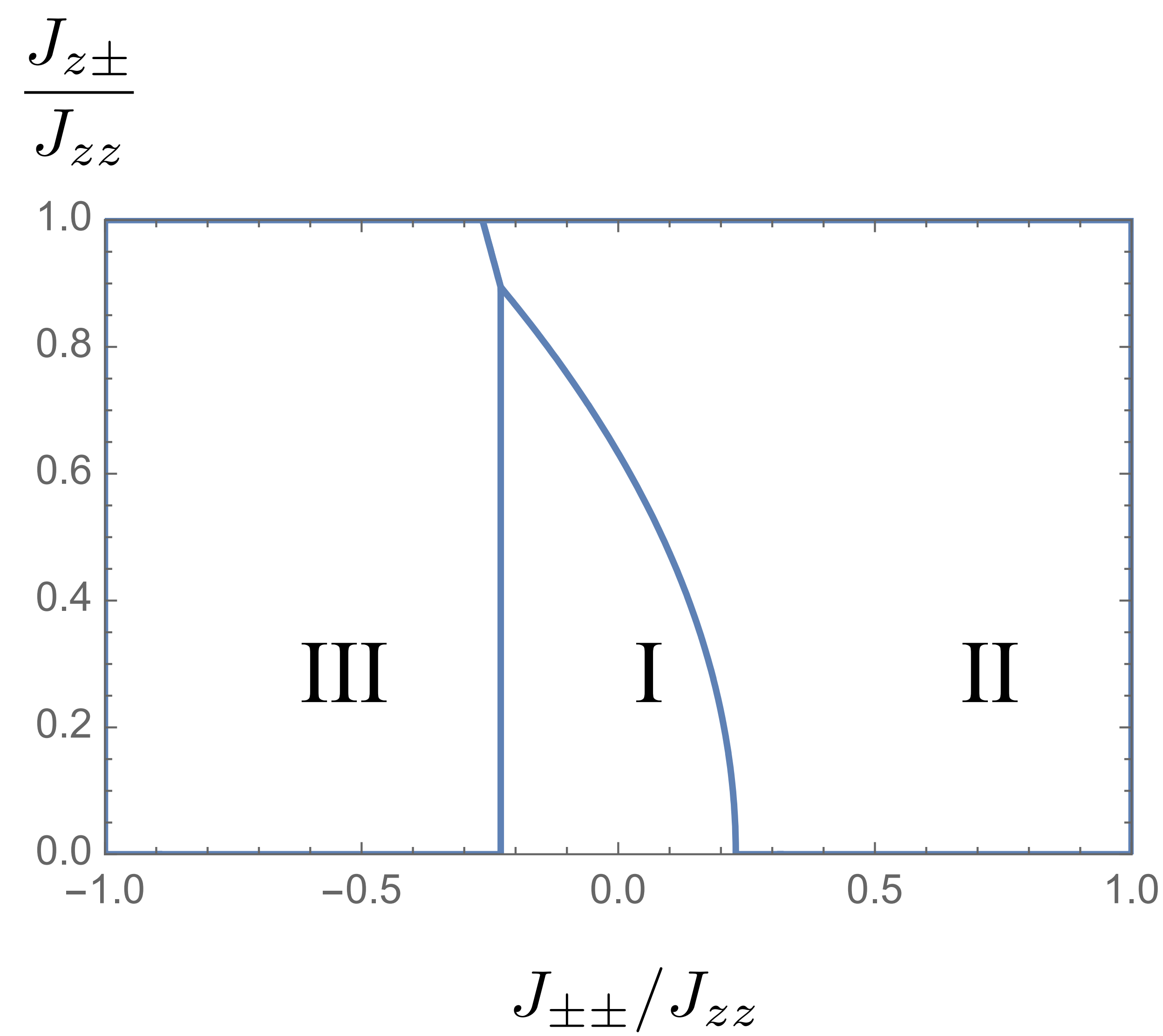
ArXiv **1509.06766**, accepted by **PhysRevLett**

The spin-1/2 XXZ model supports conventional order.

(Yamamoto, etc, PRL 2014)

Classical phase diagram





Gang Chen, working in progress

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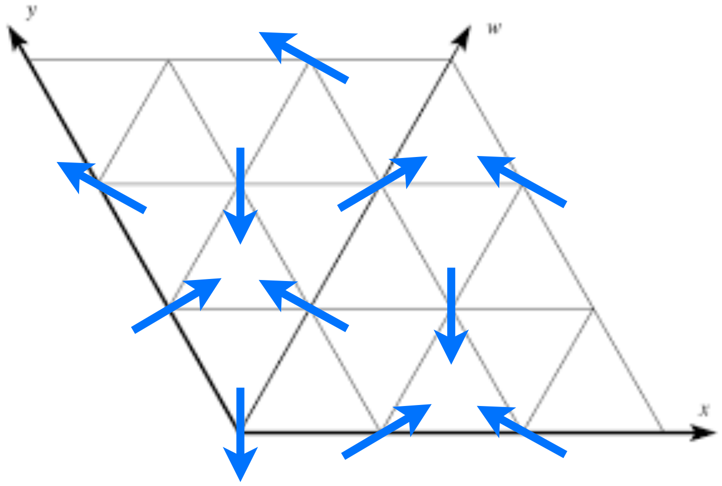
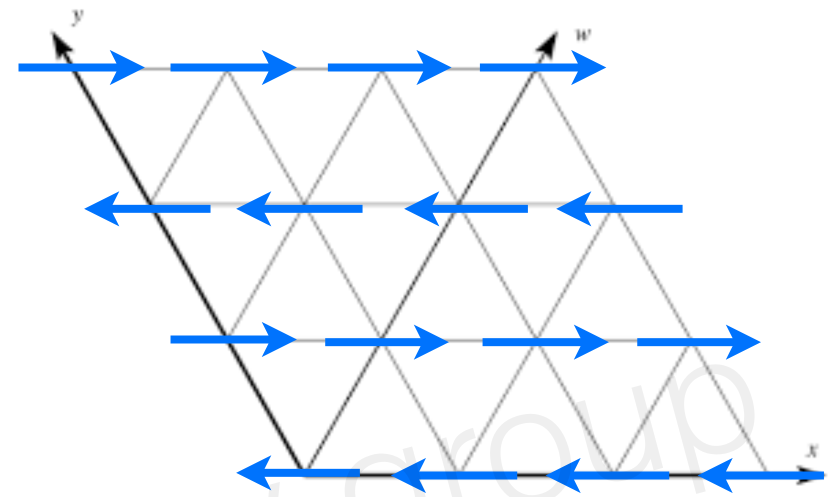
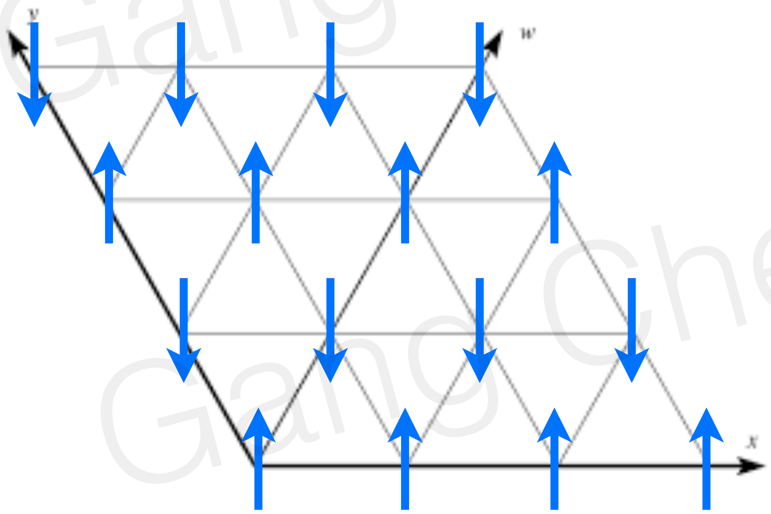


I: 120 degree state



II: stripe order in xz plane



III: stripe order along y

Many classical spin configurations have rather close energies at the phase boundaries between different ordered states, in the end, the quantum fluctuation is enhanced at these regions and may melt the magnetic order. If spin liquid exists, it can probably occur in these regions.

Future direction

- For experiments:
  1. Neutron scattering, optical, thermal transport.
  2. New materials: all the rare earth elements have the same chemical properties.
  3. Other quantum spin liquids in strong spin-orbit coupled insulators.

- For theory:
  1. Classification (beyond Xiao-Gang Wen's pioneering PSG classification in 2002)
  2. Variational Monte Carlo: projective wave function with parton construction.
  3. Other numerical methods.

Summary

1. We have studied the monopole condensation transition out of quantum spin ice.

   We applied this theory to explain the puzzling experiments in Pr2Ir2O7.

2. YbMaGaO4 is probably the first quantum spin liquid with odd electron filling and strong spin-orbit coupling.

   The QSL physics is probably originated from the anisotropic spin interaction due to SOC.