Title: The spectral periodicity of spinon continuum in quantum spin ice

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Abstract: Motivated by the rapid experimental progress of quantum spin ice materials, we study the dynamical properties of pyrochlore spin ice in the U(1) spin liquid phases. In particular, we focus on the spinon excitations that appear in high energies and show up as an excitation continuum in the dynamic spin structure factor. The keen connection between the crystal symmetry fractionalization of the spinons and the spectral periodicity of the spinon continuum is emphasized and explicitly demonstrated. The enhanced spectral periodicity of the spinon continuum provides a sharp physical observable to detect the spin quantum number fractionalization and U(1) spin liquid. Our prediction can be immediately examined by inelastic neutron scattering experiments among quantum spin ice materials with Kramers' doublets. Further application to the non-Kramers' doublets is discussed. If time permits, I will present some of our recent work in this field.

The spectral periodicity of spinon continuum in quantum spin ice

Gang Chen
Fudan University

I thank Jeff and Michel for discussion and comments

复旦大学
FUDAN UNIVERSITY

Our recent works on quantum spin ice

Quantum spin ice with dipole-octupole doublet
Yi-Ping Huang, Gang Chen, M Hermele, PRL 112, 167203, 2014

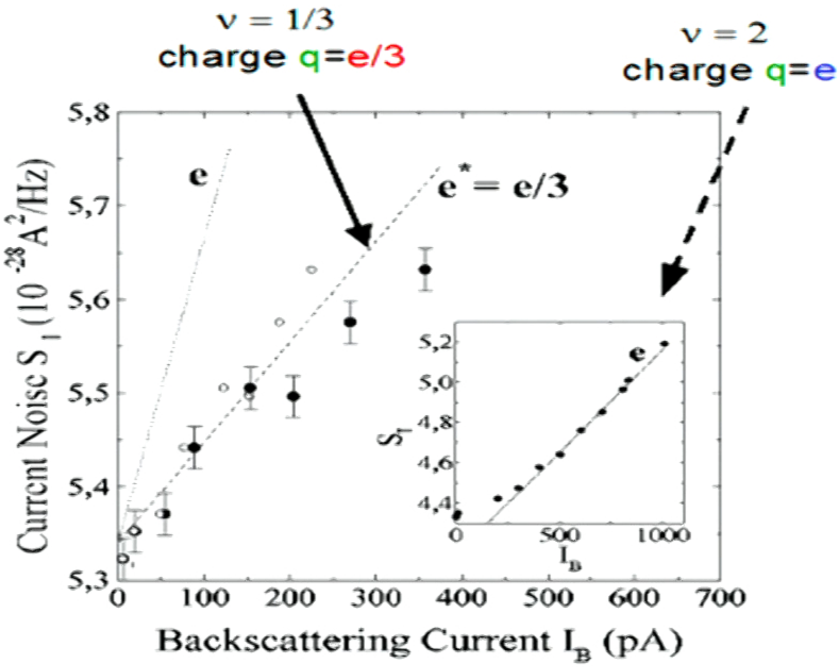
Ce2Sn2O7, symmetry enriched U(1) QSL and field-driven Anderson-Higgs transition
Yao-Dong Li, Gang Chen, PRB Rapid Comm, 95, 041106, 2017

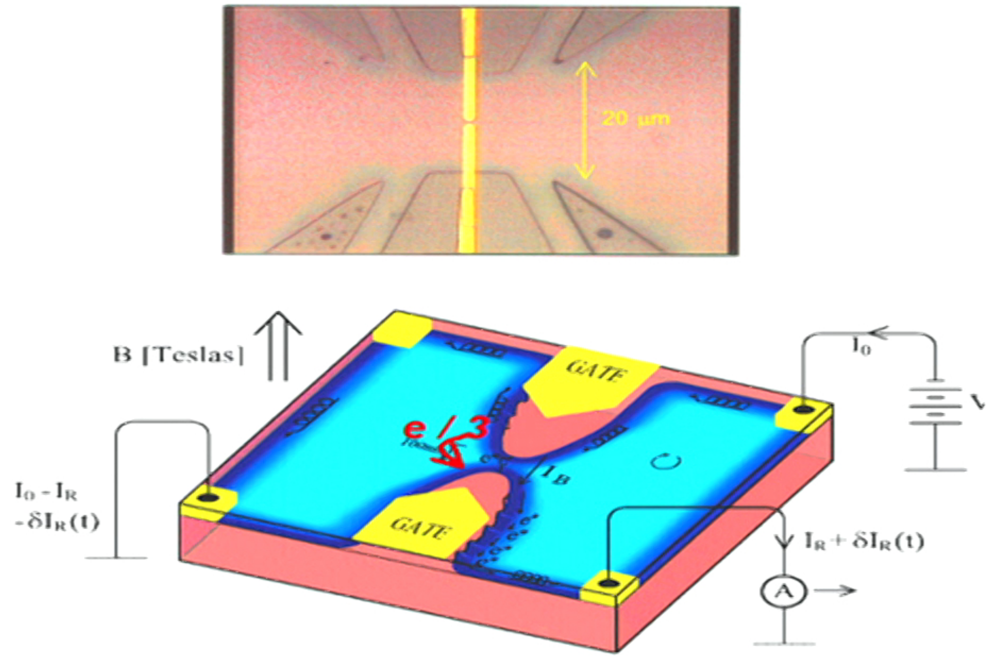
Quantum spin ice on the breathing pyrochlore lattice.
L Savary, XQ Wang, HY Kee, YB Kim, Y Yu, Gang Chen PRB 94, 205107, 2016

"Magnetic Monopole" condensation transition out of spin ice U(1) QSL: Pr2Ir2O7
Gang Chen PRB 94, 205107, 2016

The spectral periodicity of spinon continuum in quantum spin ice
Gang Chen, arXiv 1704.02734, 2017

Fractionalization in FQHE: shot-noise measurement





Etien et al, PRL 79, 2526 (1997)
also see Heiblum et al, Nature (1997)

FQHE is arguably the only existing topological order so far.

Chiral (Abelian) topological order

↓

Fractionalization: fractionalized & deconfined excitation
Chern-Simon gauge structure

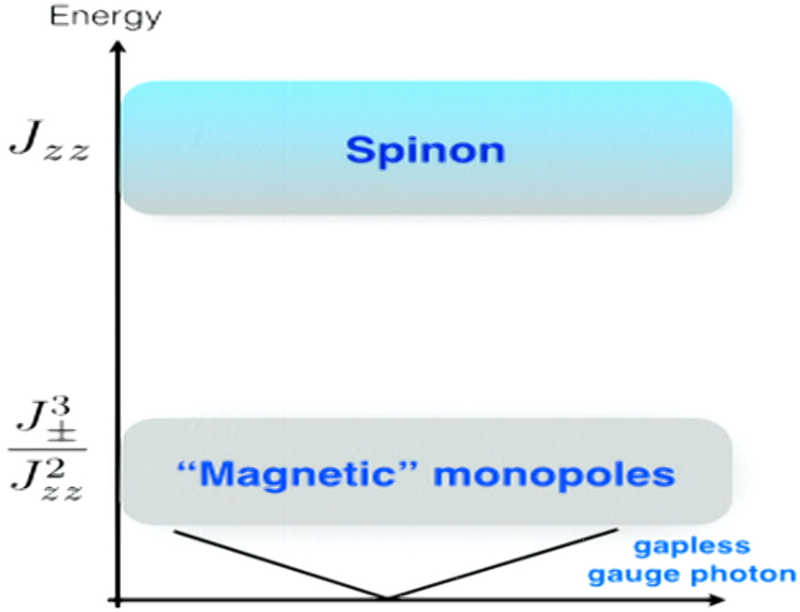
with charge U(1) **symmetry**:
charge conservation

↓

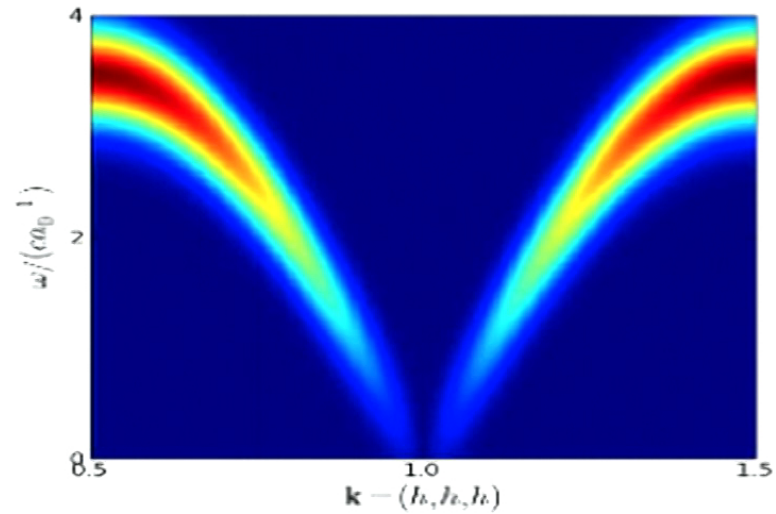
Fractionalized charge excitation

Symmetry makes topological order more visible in experiments.

What is the sharp physical observable for the U(1) QSL in quantum spin ice?



Hermele, Fisher, Balents 2004



$I(\omega) \sim \omega$

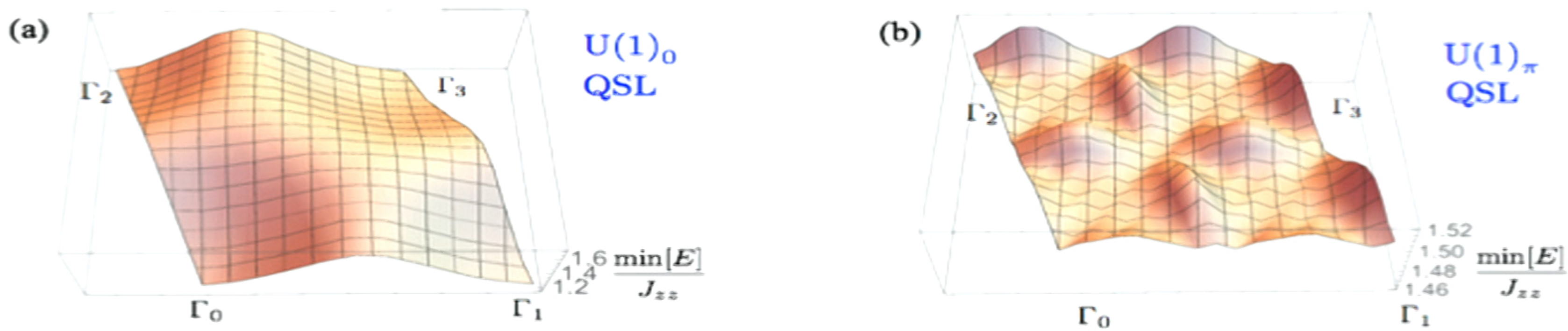
low energy scale
suppressed intensity

Nic Shannon, etc 2012,
Savary, Balents, 2012

heat capacity (Savary&Balents: 1000 times larger than phonon!) and spinon continuum

One answer:

the spectral periodicity of the spinon continuum



regular periodicity

enlarged periodicity

Enlarged periodicity is like the fractional charge in FQHE.

Gang Chen, arXiv 1704.02734, 2017

Realistic models

- Usual Kramers' doublet and non-Kramers' doublet

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

S. H. Curnoe, PRB (2008).
Savary, Balents, PRL 2012
S. Onoda, etc, 2009, 2010
SB Lee, Onoda, Balents, 2012

- Dipole-octupole doublet

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

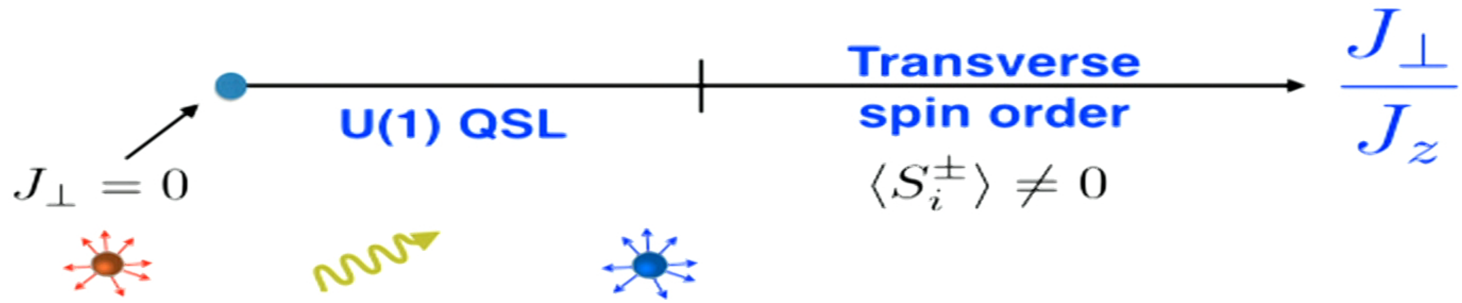

Yi-Ping Huang


Yao-Dong Li
(Fudan -> UCSB)

Y-P Huang, **Gang Chen**, M Hermele, PRL 2014
Yao-Dong Li, **Gang Chen**, PRB 2017

Use the XXZ model to illustrate the universal physics

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



Hermele, Fisher, Balents, 2004,
Banerjee, Isakov, Demle, YongBaek Kim 2008
Savary, Balents, 2012
Kato, Onoda, 2015
Nic Shannon, et al, 2012

Frustrated regime: early theoretical study

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

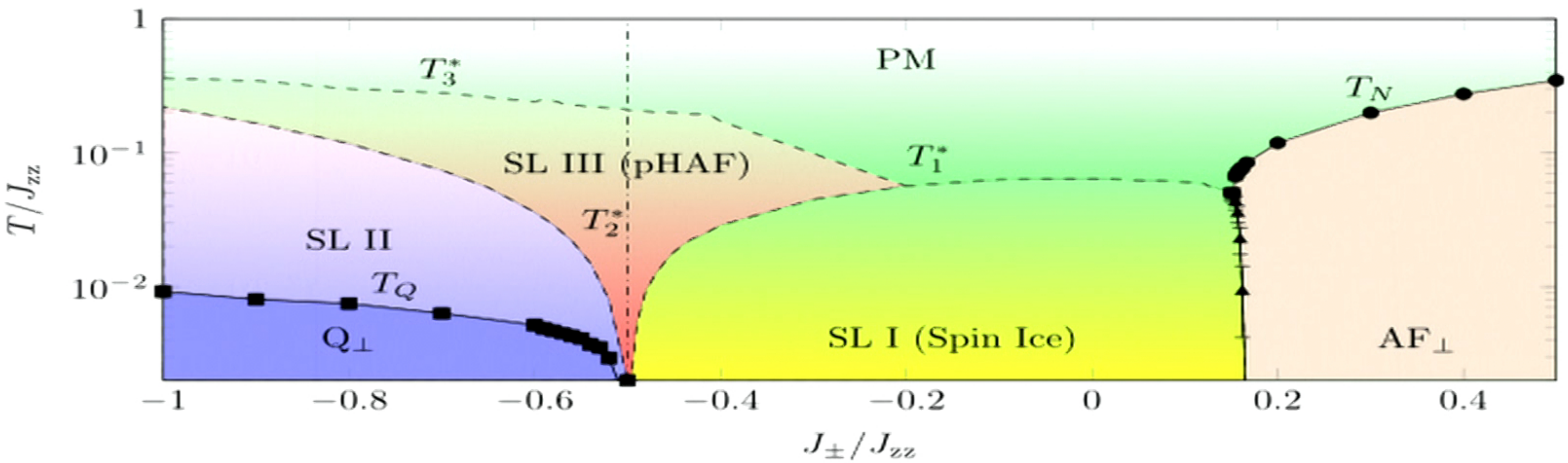
PHYSICAL REVIEW B **86**, 104412 (2012)

Generic quantum spin ice

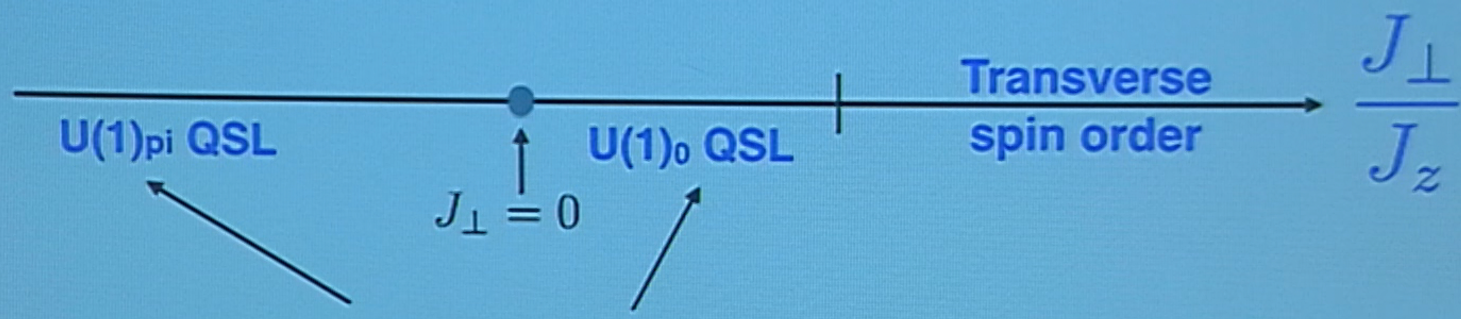
SungBin Lee,[1] Shigeki Onoda,[2] and Leon Balents[3]

one. We also consider the case of frustrated *XY* exchange, and find that it favors a π-flux QSL, with an emergent line degeneracy of low-energy spinon excitations. This feature greatly enhances the stability of the QSL with respect to classical ordering.

Nic Shannon's interesting work of semiclassic phases



complementary study in the classical regime:
three classical spin liquids



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

Besides the quantitative differences, are there sharp distinctions between the $U(1)_{pi}$ QSL on the left and the $U(1)_0$ QSL on the right?

Lattice gauge theory

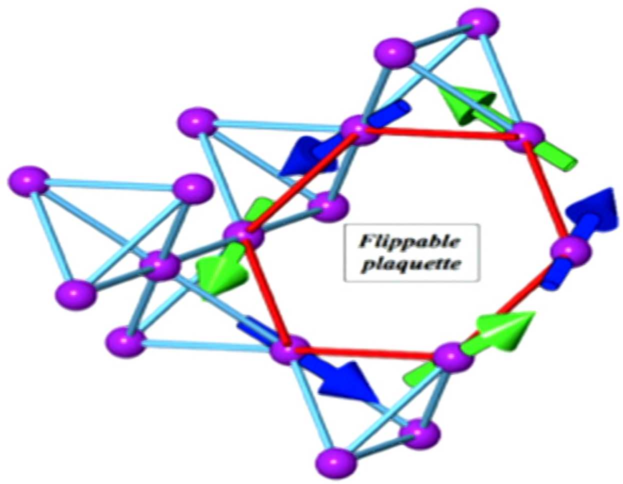


Figure from Michel Gingras' paper

Lattice gauge theory
on the dual diamond lattice

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

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

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

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

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

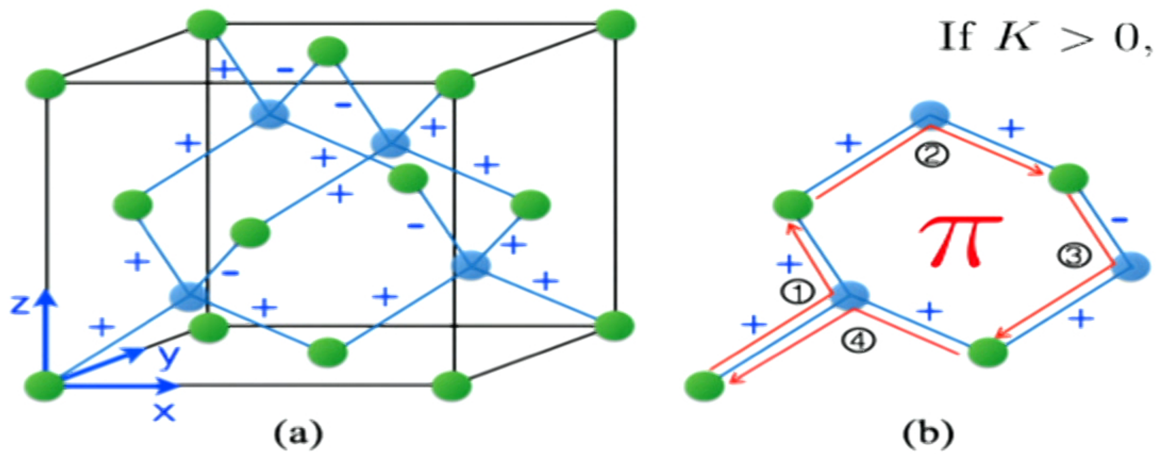
$$K = 24 J_\perp^3 / J_{zz}^2$$

Pi flux and the spinon translation

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

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

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



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

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

Pi flux means crystal symmetry fractionalization

$$T_\mu^s T_\nu^s = -T_\nu^s T_\mu^s$$

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 vector

$$|b\rangle = T_1^s(1)|a\rangle, \quad |c\rangle = T_2^s(1)|a\rangle, \quad |d\rangle = T_3^s(1)|a\rangle$$

$$\begin{aligned} T_1|b\rangle &= T_1^s(1)T_1^s(2)T_1^s(1)|a\rangle = +T_1^s(1)[T_1|a\rangle], \\ T_2|b\rangle &= T_2^s(1)T_2^s(2)T_1^s(1)|a\rangle = -T_1^s(1)[T_2|a\rangle], \\ T_3|b\rangle &= T_3^s(1)T_3^s(2)T_1^s(1)|a\rangle = -T_1^s(1)[T_3|a\rangle], \end{aligned}$$

$\Rightarrow$

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

Xiao-Gang Wen, 2001, 2002,
Andrew Essin, Michael Hermele, 2014
Gang Chen, 1704.02734

Spectral periodicity of the spinon continuum

spectral periodicity for the spinon continuum. The spectral periodicity can be reflected by the spectral intensity $\mathcal{I}(\boldsymbol{q}, E)$, the lower $\mathcal{L}(\boldsymbol{q})$ and upper excitation edge $\mathcal{U}(\boldsymbol{q})$ of the spinon continuum. For $\mathrm{U}(1)_\pi$ QSL, we have

$$
\begin{aligned}
\mathcal{I}(\boldsymbol{q}, E) &= \mathcal{I}(\boldsymbol{q} + 2\pi(100), E) = \mathcal{I}(\boldsymbol{q} + 2\pi(010), E) \\
&= \mathcal{I}(\boldsymbol{q} + 2\pi(001), E), \\
\mathcal{L}(\boldsymbol{q}) &= \mathcal{L}(\boldsymbol{q} + 2\pi(100)) = \mathcal{L}(\boldsymbol{q} + 2\pi(010)) \\
&= \mathcal{L}(\boldsymbol{q} + 2\pi(001)), \\
\mathcal{U}(\boldsymbol{q}) &= \mathcal{U}(\boldsymbol{q} + 2\pi(100)) = \mathcal{U}(\boldsymbol{q} + 2\pi(010)) \\
&= \mathcal{U}(\boldsymbol{q} + 2\pi(001)).
\end{aligned}
$$

But elastic neutron scattering will NOT see extra Bragg peak.

Xiao-Gang Wen, 2001, 2002,
Andrew Essin, Michael Hermele, 2014
Gang Chen, 1704.02734

Calculation to demonstrate the above prediction

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

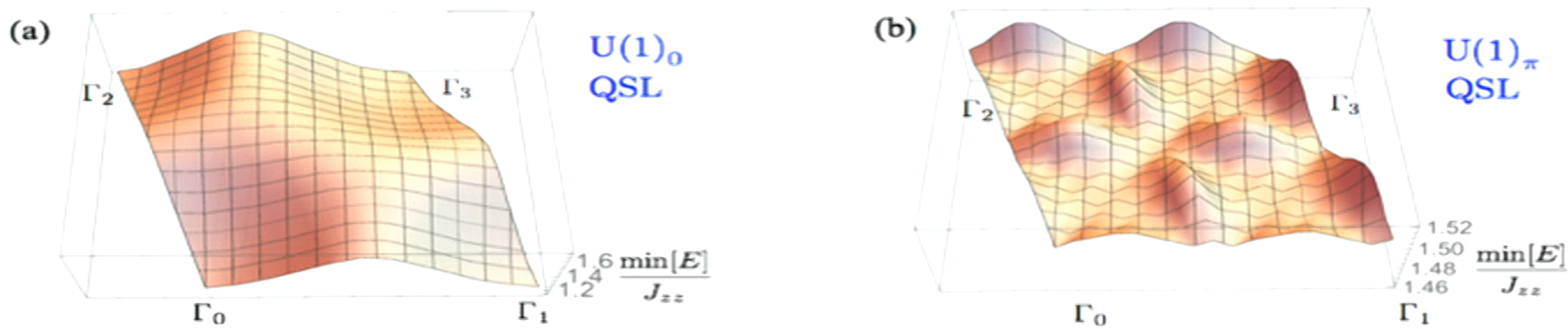
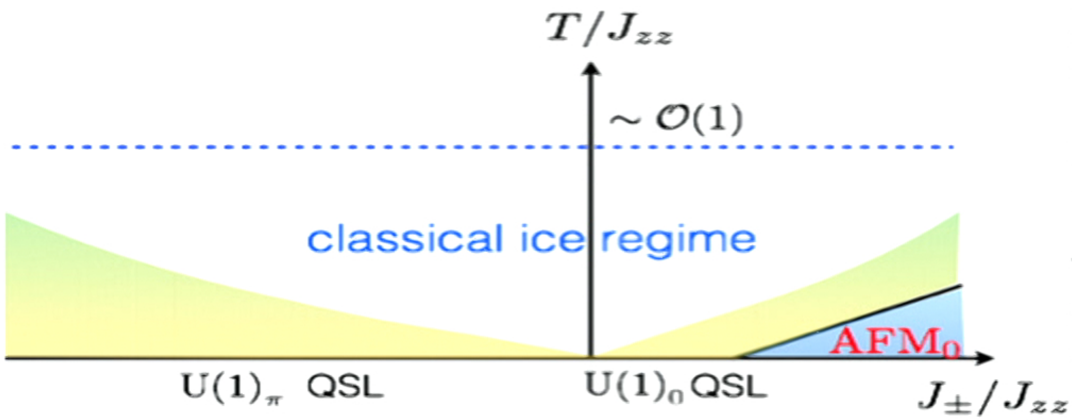


FIG. 3. (Color online.) The lower excitation edge of the spinon continuum in $U(1)_0$ and $U(1)_\pi$ QSLs. Here, $\Gamma_0\Gamma_1 = 2\pi(\bar{1}11)$, $\Gamma_0\Gamma_2 = 2\pi(1\bar{1}1)$. We set $J_\perp = 0.12 J_{zz}$ for $U(1)_0$ QSL in (a) and $J_\perp = -J_{zz}/3$ for $U(1)_\pi$ QSL in (b).

Lower excitation edge of spinon continuum within the gauge MFT calculation

Conclusion

U(1) QSLs	$U(1)_0$ QSL	$U(1)_\pi$ QSL
Background U(1) Flux	0 Flux	π Flux
Heat Capacity	$C_v \sim T^3$	$C_v \sim T^3$
Proximate XY Order	Keep Translation	Enlarged Cell
Spectral Periodicity	Not Enhanced	Enhanced



For usual Kramers' doublet, spinon continuum is detectable by INS.

Lucile & Kate: Yb2Ti2O7 is either in or proximate to 0-flux.

So Yb2Ti2O7 does not have enhanced spectral periodicity.

For non-Kramers' doublet, spinon continuum cannot be detected by INS. But the proximate quadrupolar order would break translation symmetry, and can however be detectable.

Lee, Onoda, Balents: Pi flux state is more robust. This is great !

This means it is more likely for a candidate material to have spectral periodicity enhancement.