Title: Frustrating quantum spin ice: a tale of three spin liquids and hidden order

Date: Jun 08, 2017 03:45 PM

URL: http://pirsa.org/17060054

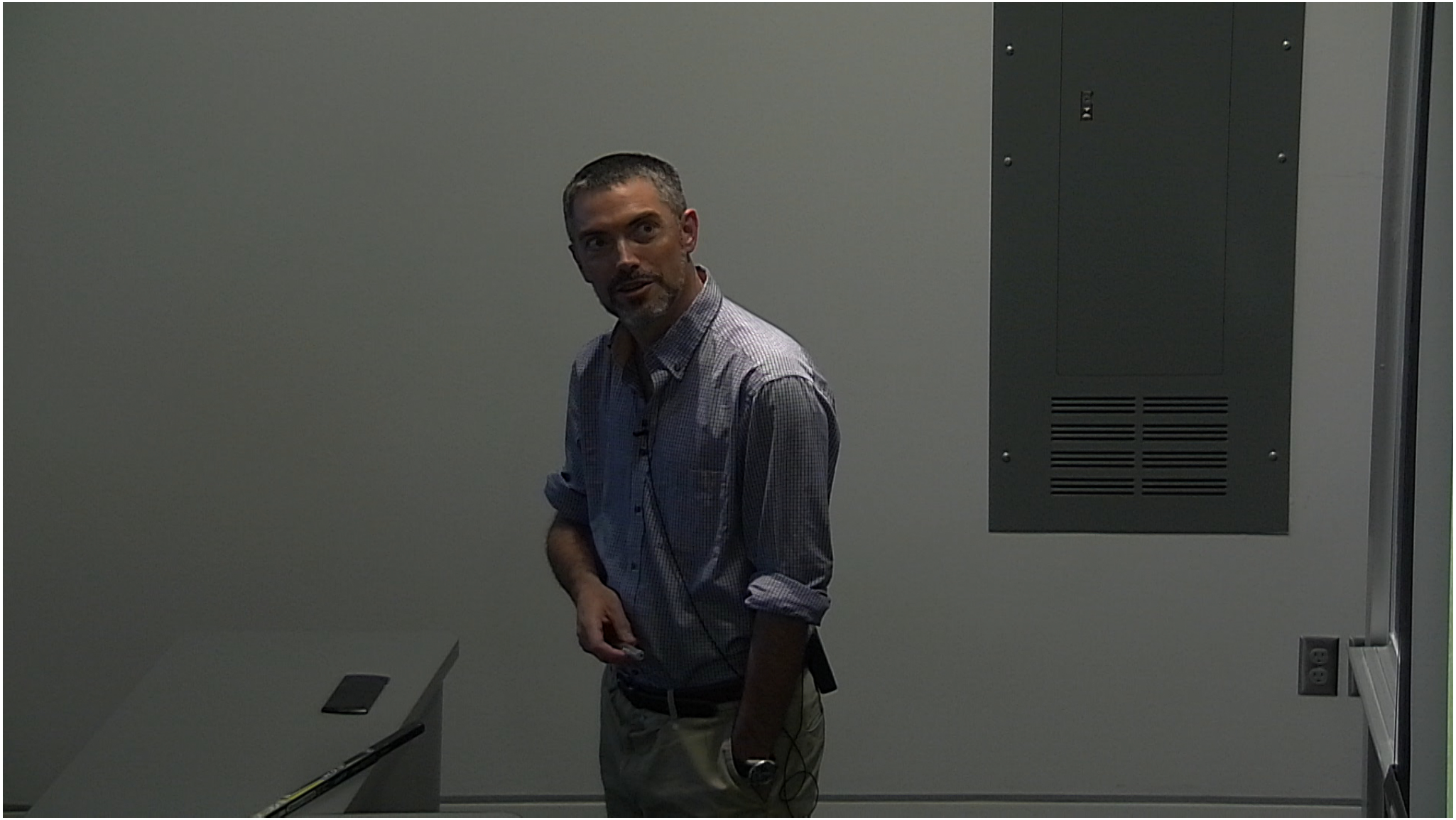
Abstract: "Quantum spin ice" materials have been widely discussed in terms of an XXZ model on a pyrochlore lattice, which is accessible to quantum Monte Carlo simulation for unfrustrated interactions J_\pm > 0. Here we argue that the properties of this model may become even more interesting once it is "frustrated". Using a combination of large-scale classical Monte Carlo simulation, semi-classical molecular dynamics, symmetry analysis and analytic field theory we explore the new phases which arise for J_\pm < 0. We find that the model supports not one, but three distinct forms of spin liquid: spin ice, a U(1) spin liquid; a disguised version of the U(1) x U(1) x U(1) spin-liquid found in the Heisenberg antiferromagnet on a pyrochlore lattice; and another entirely new form of spin liquid described by a U(1) x U(1) gauge group. At low temperatures this novel spin liquid undergoes a thermodynamic phase transition into a ground state with hidden, spin-nematic order. We present explicit predictions for inelastic neutron scattering experiments carried out on the three different spin liquids [M. Taillefumier et al., arXiv:1705.00148].

Frustrating quantum spin ice : a tale of three spin liquids (and hidden order…)

nic shannon

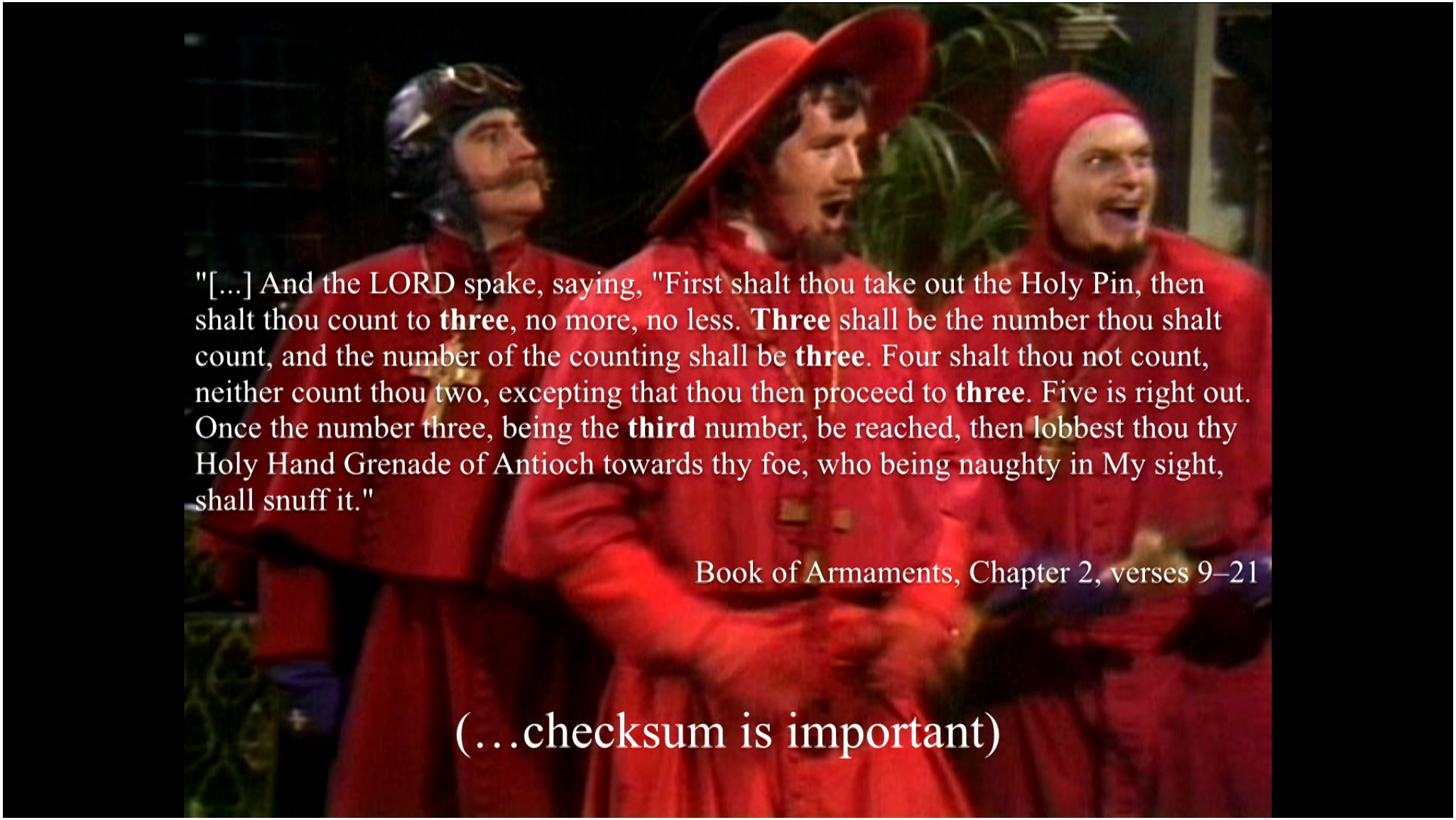
OIST
OKINAWA INSTITUTE OF SCIENCE AND TECHNOLOGY GRADUATE UNIVERSITY


“All good things come in threes.”




IN CONGRESS, JULY 4, 1776.
The unanimous Declaration of the thirteen united States of America,
...life, liberty and the pursuit of happiness.


(…checksum is important)


"[...] And the LORD spake, saying, "First shalt thou take out the Holy Pin, then shalt thou count to **three**, no more, no less. **Three** shall be the number thou shalt count, and the number of the counting shall be **three**. Four shalt thou not count, neither count thou two, excepting that thou then proceed to **three**. Five is right out. Once the number three, being the **third** number, be reached, then lobbest thou thy Holy Hand Grenade of Antioch towards thy foe, who being naughty in My sight, shall snuff it."
Book of Armaments, Chapter 2, verses 9–21
(…checksum is important)

spin ice is a good thing…

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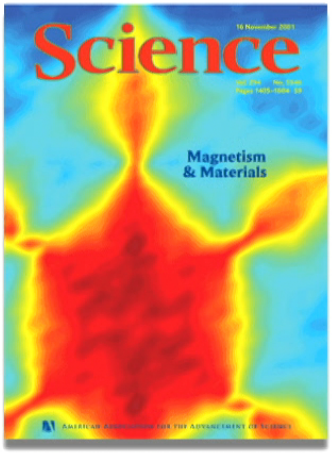


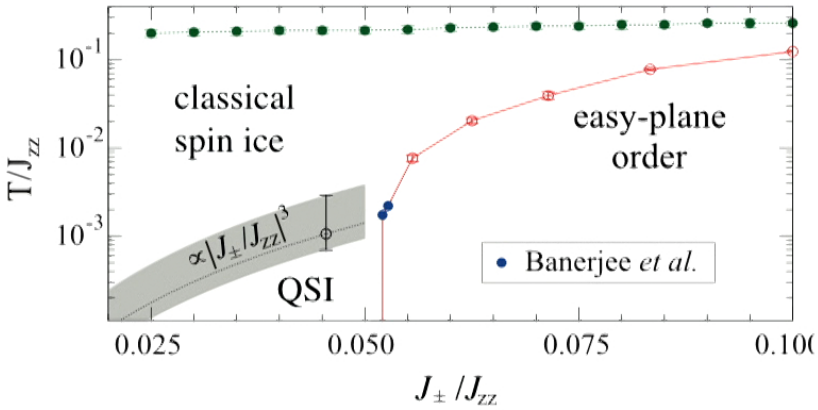
story for today

minimal model of quantum spin ice

$$\mathcal{H}_{\mathrm{QSI}} = \sum_{\langle ij \rangle} J_{zz} \mathsf{S}_i^z \mathsf{S}_j^z - J_{\pm} \left(\mathsf{S}_i^+ \mathsf{S}_j^- + \mathsf{S}_i^- \mathsf{S}_j^+ \right)$$

phase diagram from quantum Monte Carlo simulation

$(J_{\pm} > 0)$



Y. Kato and S. Onoda, Phys. Rev. Let. **115**, 077202 (2015)
[cf. A. Banerjee *et al*. Phys. Rev. Lett. **100**, 047208 (2008)]

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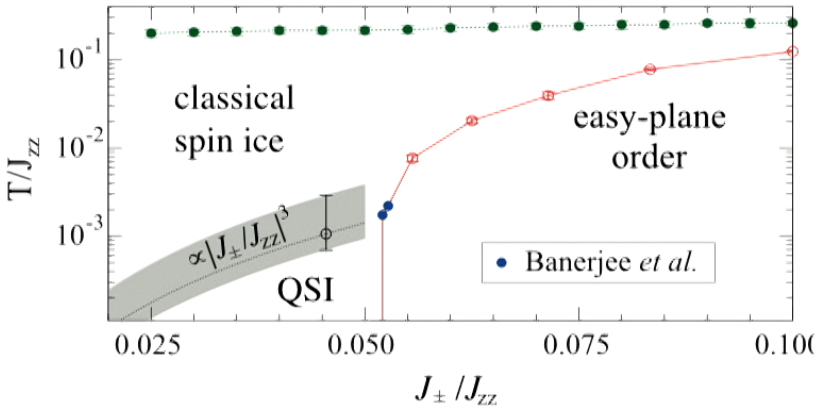

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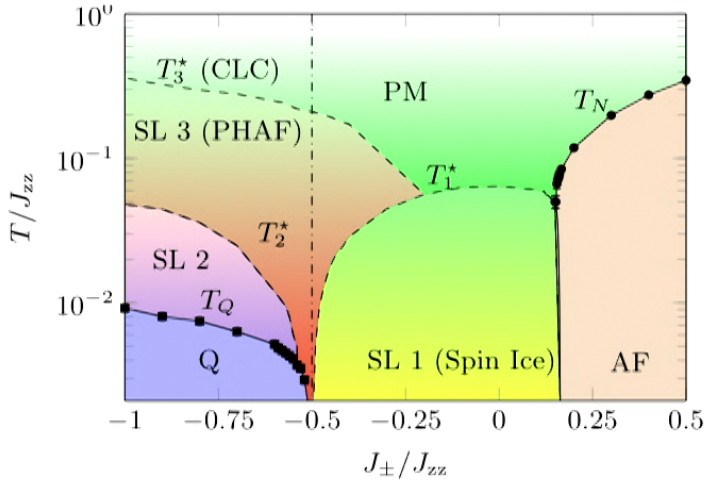
change sign of $J_{\pm}$

phase diagram from classical Monte Carlo simulation



M. Taillefumier *et al.*, arXiv:1705.00148

story for today

minimal model of quantum spin ice

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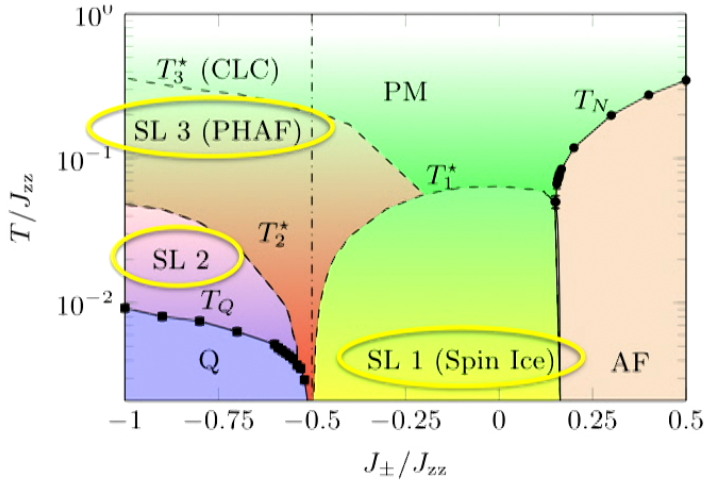
change sign of $J_{\pm}$

3 spin liquids
+ hidden spin-nematic order !

phase diagram from classical Monte Carlo simulation



M. Taillefumier *et al.*, arXiv:1705.00148

wouldn’t have happened without…

Mathieu Taillefumier
(OIST→ ETH)

Owen Benton
(Bristol/OIST
→ RIKEN)

Han Yan
(OIST)

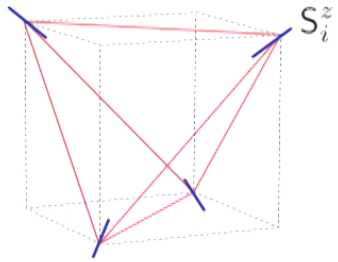
Ludovic Jaubert
(OIST → CNRS)

minimal model of a QSI

minimal model of a QSI

general model of nearest-neighbor exchange in local basis (Kramers ion) :

$$\mathcal{H}_{\text{ex}} = \sum_{\langle ij \rangle} \left\{ J_{zz} \mathsf{S}_i^z \mathsf{S}_j^z - J_{\pm}(\mathsf{S}_i^+ \mathsf{S}_j^- + \mathsf{S}_i^- \mathsf{S}_j^+) + J_{\pm\pm} \left[\gamma_{ij} \mathsf{S}_i^+ \mathsf{S}_j^+ + \gamma_{ij}^* \mathsf{S}_i^- \mathsf{S}_j^- \right] + J_{z\pm} \left[\mathsf{S}_i^z (\zeta_{ij} \mathsf{S}_j^+ + \zeta_{ij}^* \mathsf{S}_j^-) + i \leftrightarrow j \right] \right\}$$



local S^z axis rotates from site to site

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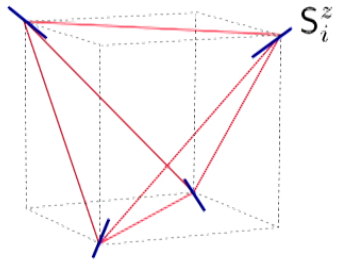
favors spin-ice ($J_{zz} > 0$)

introduces dynamics

cf. most of the talks in this workshop !

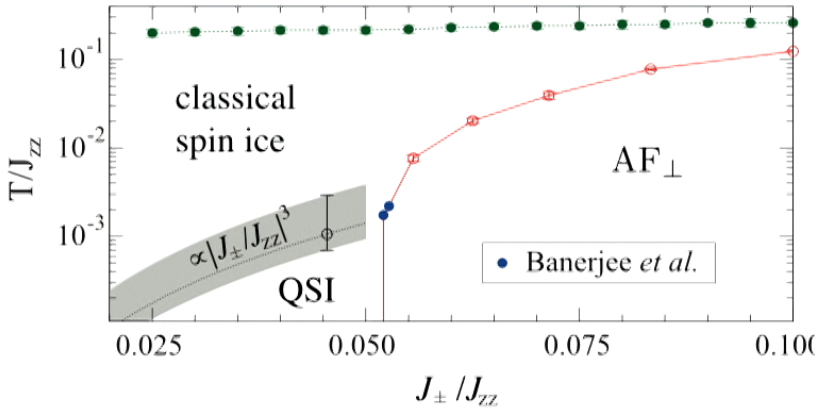


local S^z axis rotates from site to site

many authors (in many notations), with papers including :

S. Curnoe, Phys. Rev. B **78**, 094418 (2007); McClarty et al., J. Phys. Conf. Series **14**, 012032 (2009)
J. D. Thompson et al,, Phys. Rev. Lett. **106**, 187202 (2011); Ross et al., Phys. Rev. X **1**, 021002 (2011);
S. Onoda et al., Phys. Rev. B **83**, 094411 (2011); L. Savary and L. Balents, Phys. Rev. Lett **108**, 037202 (2012);

what happens for $J_\pm > 0$?



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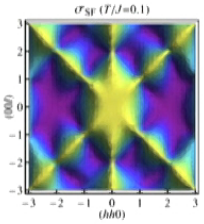
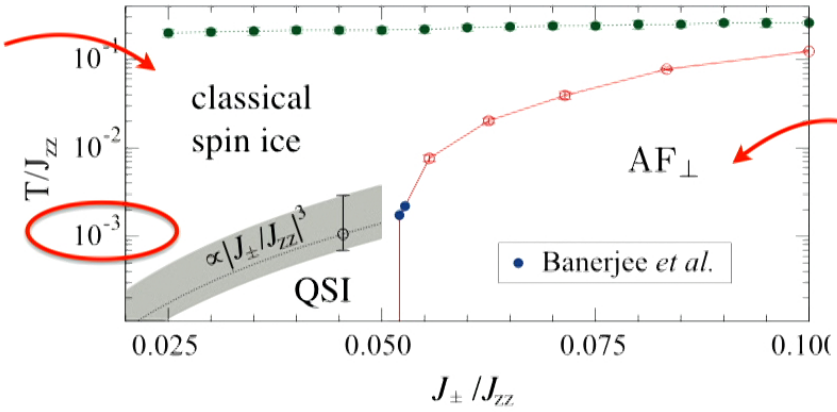
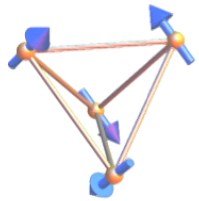


pinch points in S(**q**)





easy-plane AF order

QMC results taken from : Y. Kato and S. Onoda, Phys. Rev. Let. **115**, 077202 (2015)
A. Banerjee *et al*. Phys. Rev. Lett. **100**, 047208 (2008)

what happens for $J_{\pm} < 0$?

QMC "frustrated", i.e. suffers from (severe) sign problems

what do we know ?

1. quantum spin ice ground state perturbatively stable

M. Hermele *et al.*, Phys. Rev. B **69**, 064404 (2004)

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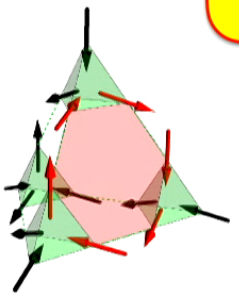

$$\mathcal{H}_{\text{tunneling}} = -g \sum_{\hexagon} |\circlearrowright\rangle\langle\circlearrowleft| + |\circlearrowleft\rangle\langle\circlearrowright| \qquad g = \frac{12 J_\pm^3}{J_{zz}^2}$$

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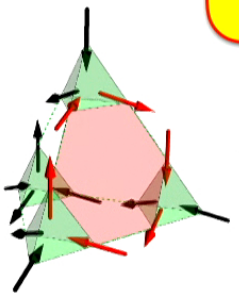

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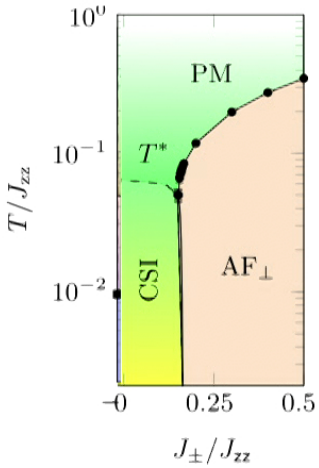
can swap sign using "gauge" transformation

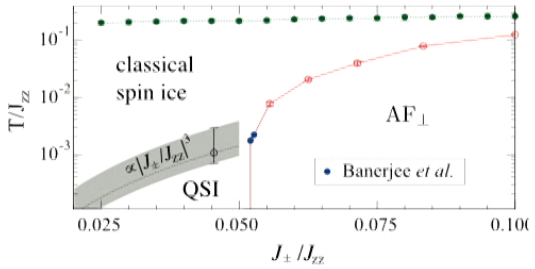
2. spinon dispersion is modified; gauge MFT predicts broad QSI regime

S.-B. Lee *et al.*, Phys. Rev. B **86**, 104412 (2012)

can classical simulations help ?

cf. QMC for $J_\pm > 0$





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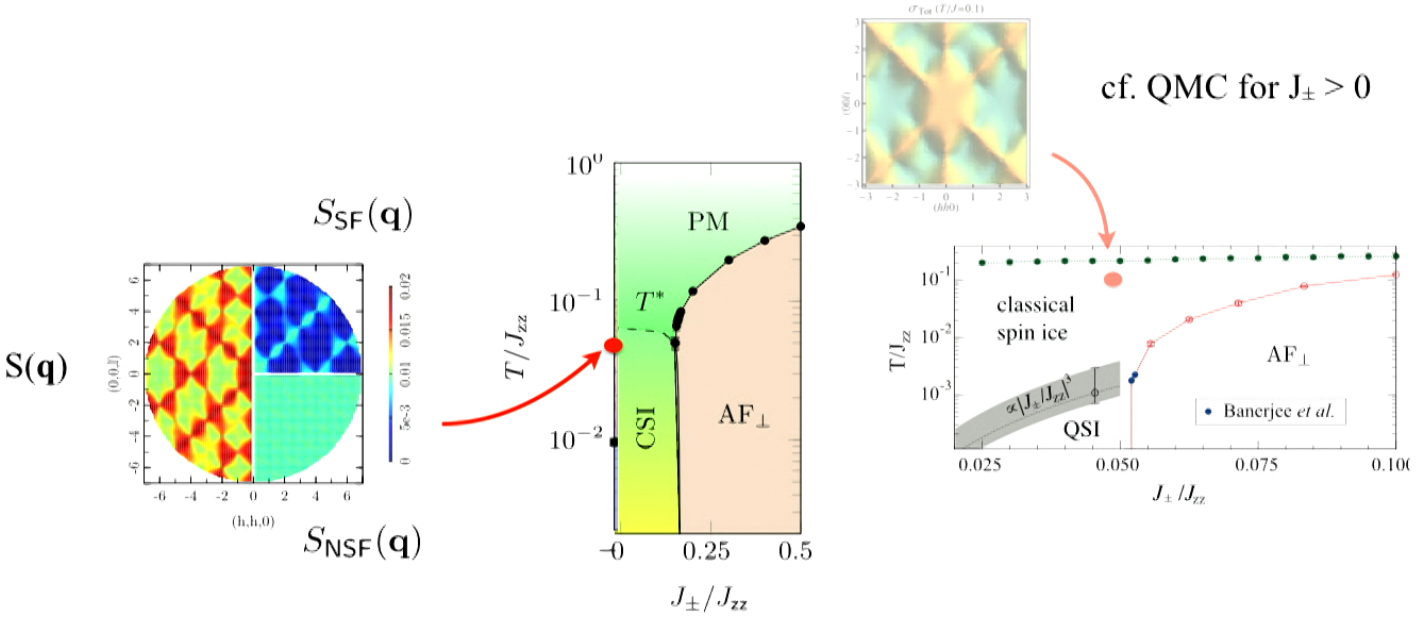

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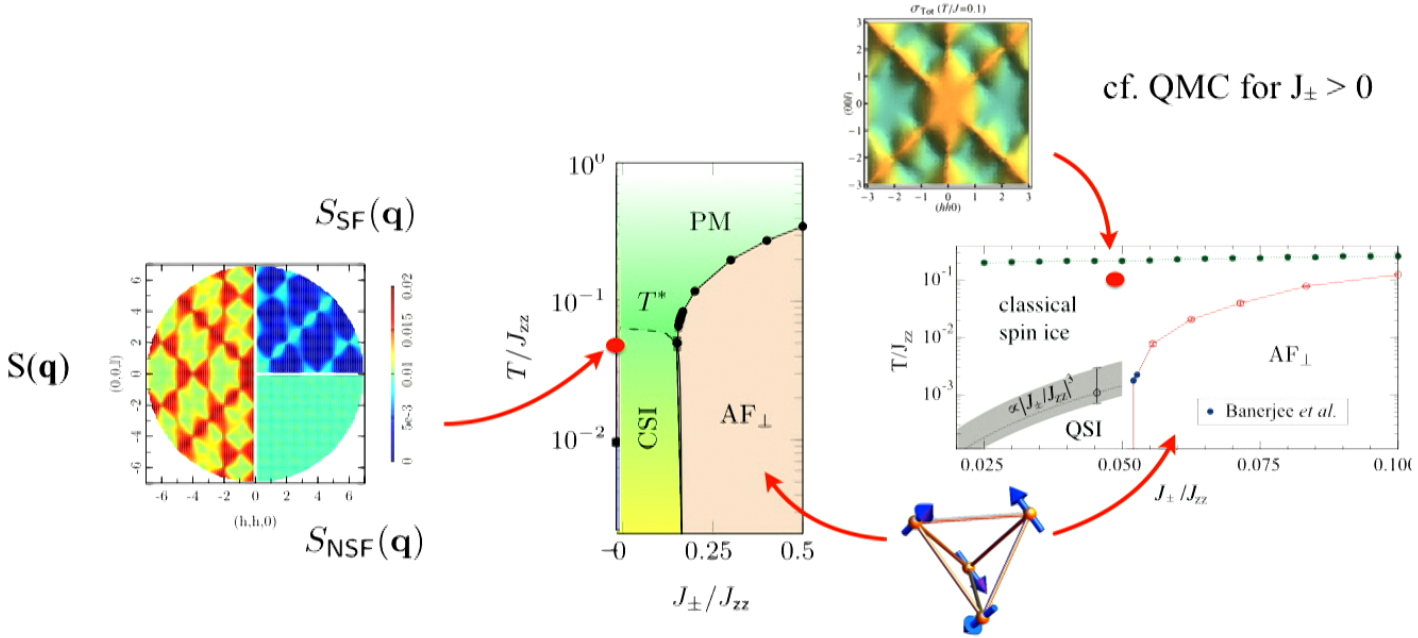

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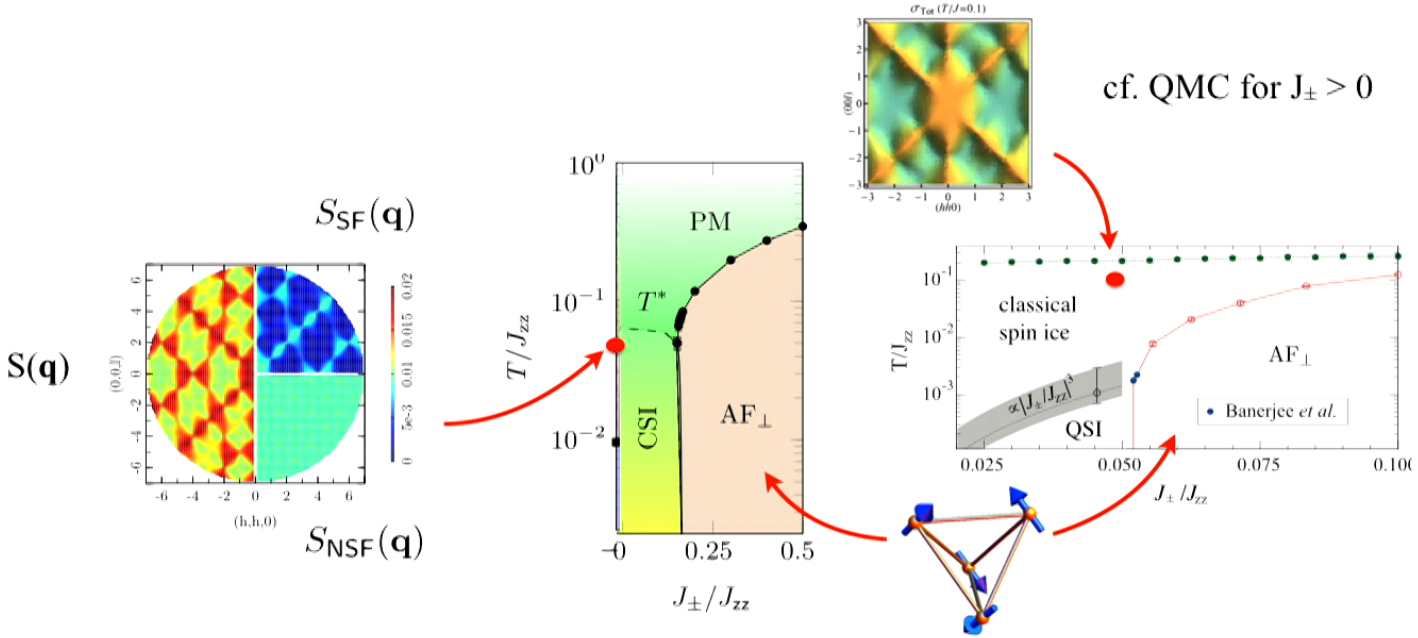

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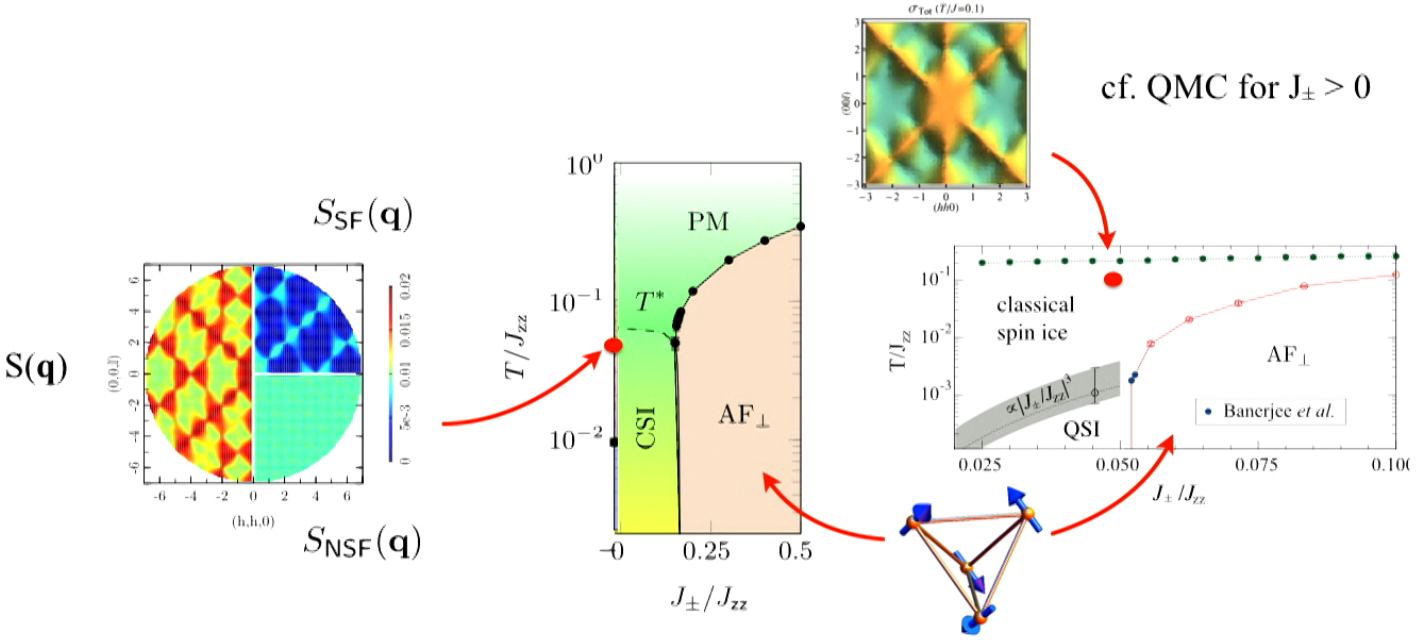


qualitatively identical phase diagram (apart from absence of low-T QSI regime)

quantitative differences in T^*, T_N, and critical value of $J_\pm/J_{zz}$

classical ground states ?

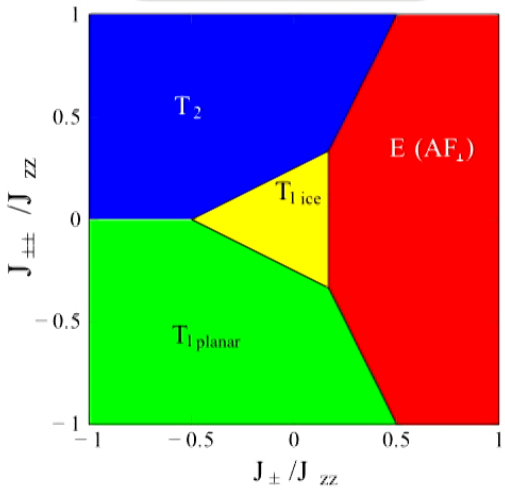
$$\mathcal{H}_{\text{ex}} = \sum_{\langle ij \rangle} \left\{ J_{zz} \mathsf{S}_i^z \mathsf{S}_j^z - J_{\pm}(\mathsf{S}_i^+ \mathsf{S}_j^- + \mathsf{S}_i^- \mathsf{S}_j^+) + J_{\pm\pm} \left[\gamma_{ij} \mathsf{S}_i^+ \mathsf{S}_j^+ + \gamma_{ij}^* \mathsf{S}_i^- \mathsf{S}_j^- \right] + J_{z\pm} \left[\mathsf{S}_i^z (\zeta_{ij} \mathsf{S}_j^+ + \zeta_{ij}^* \mathsf{S}_j^-) + i \leftrightarrow j \right] \right\}$$

rewrite in terms of irreps of T_d

$$\{\mathbf{m}_\lambda\} = \{m_{A_2}, \mathbf{m}_E, \mathbf{m}_{T_1 \text{ice}}, \mathbf{m}_{T_1 \text{planar}}, \mathbf{m}_{T_2}\}$$

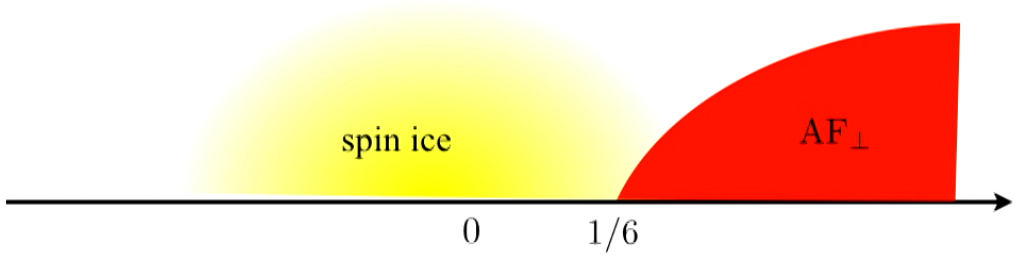
$$\mathcal{H}_{\text{ex}} = \frac{1}{2} \sum_{\text{tet},\lambda} a_\lambda \, \mathbf{m}_\lambda^2$$

spin ice is surrounded by competing forms of easy-plane AF order

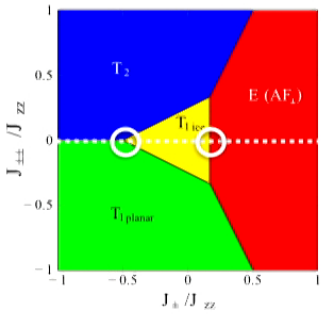


Owen Benton, PhD Thesis
H. Yan *et al.*, arXiv:1311.3501
H. Yan *et al.*, Phys. Rev. B **95**, 094422 (2017)

what do we expect at finite T ?



T=0 classical phase boundary



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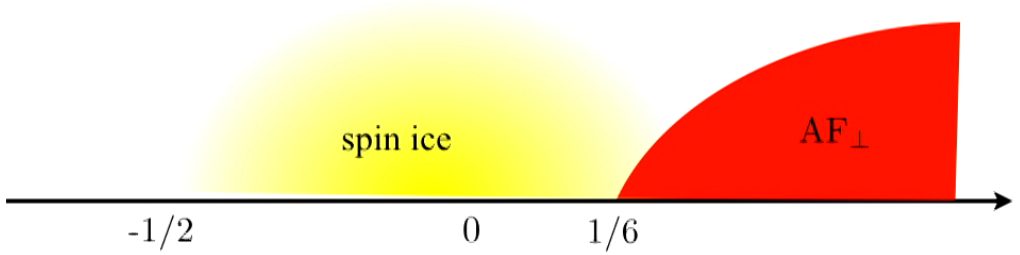

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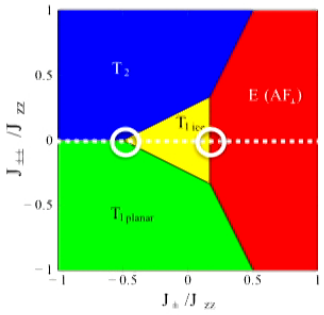
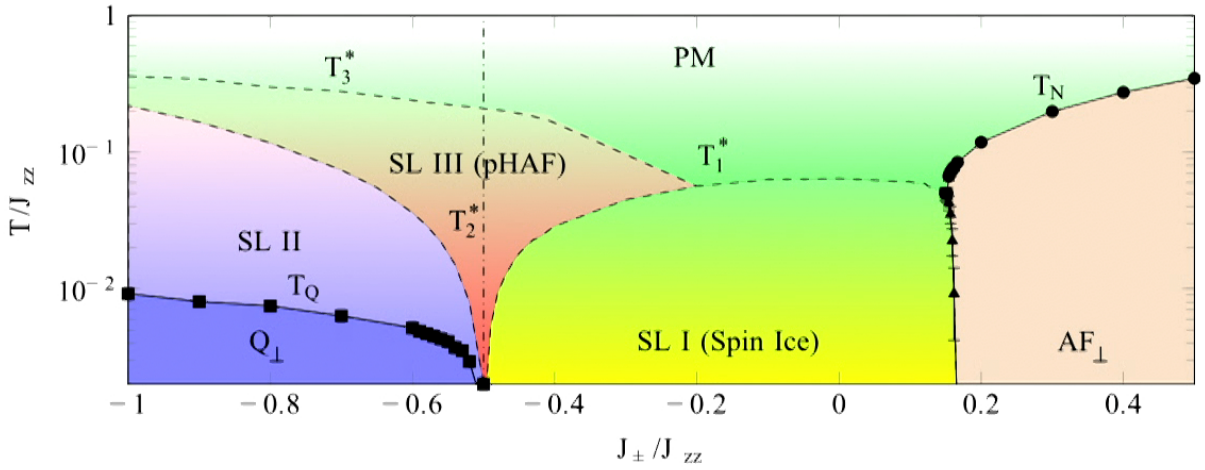
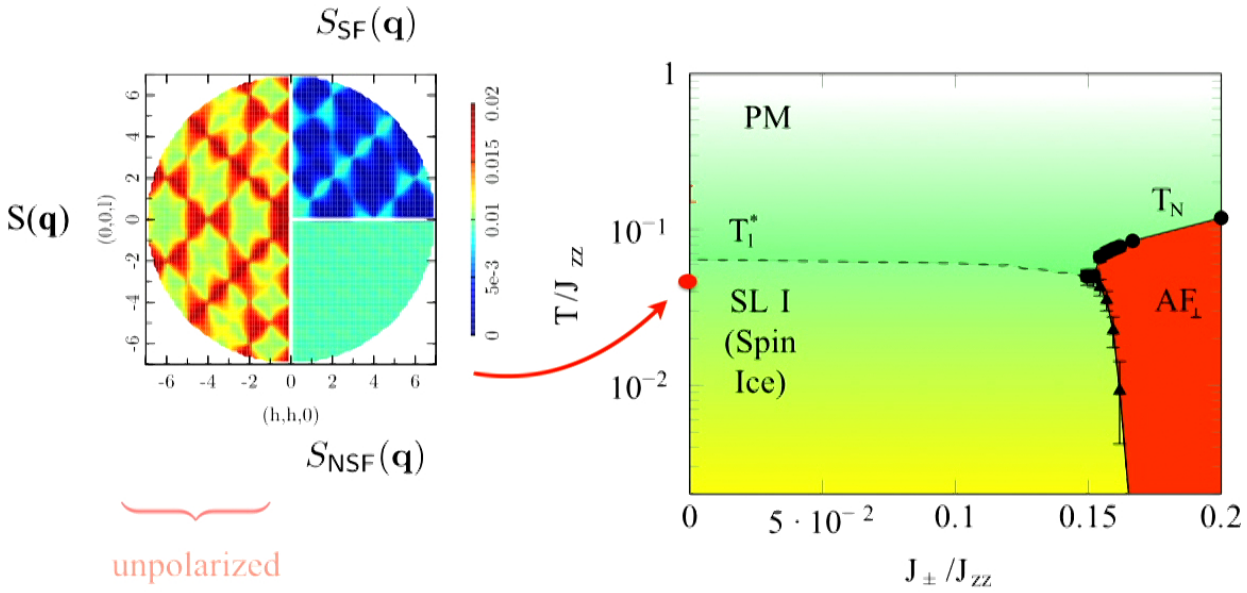


what do we find ?



M. Taillefumier *et al.*, arXiv:1705.00148

SL 1 (spin ice)



M. Taillefumier *et al.*, arXiv:1705.00148; M. Taillefumier *et al.*, in preparation.

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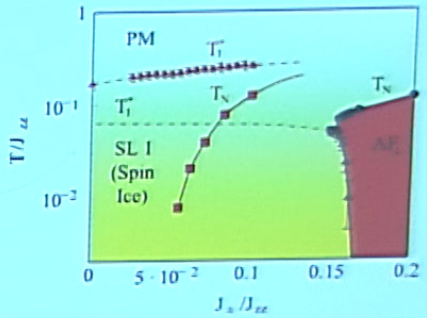

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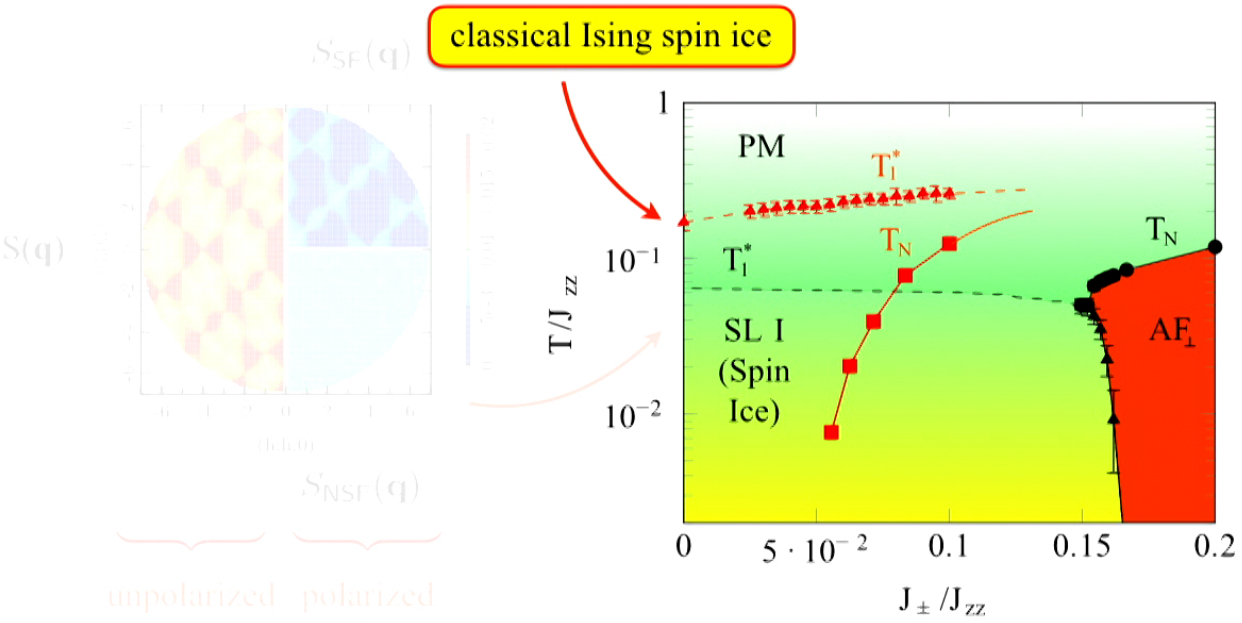

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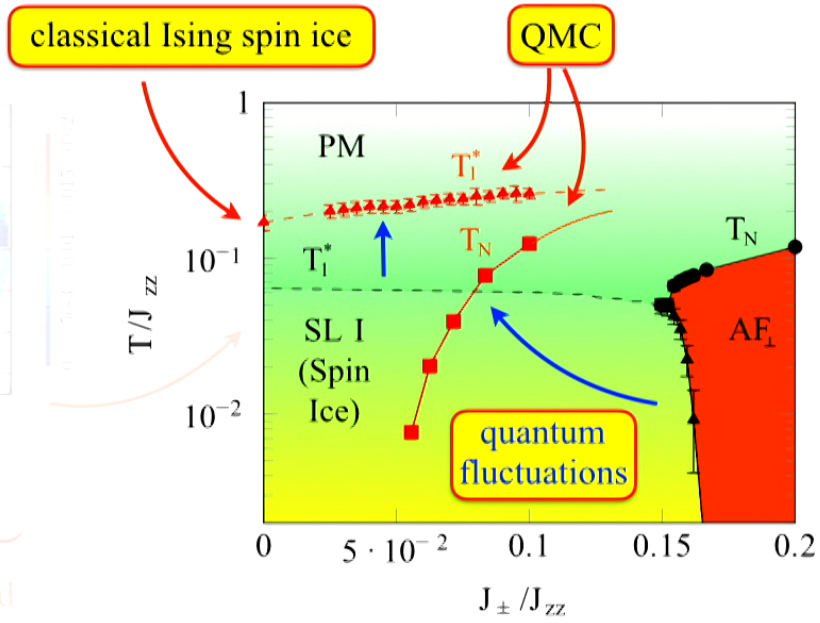

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SL 3 (“pseudo-Heisenberg AF”)

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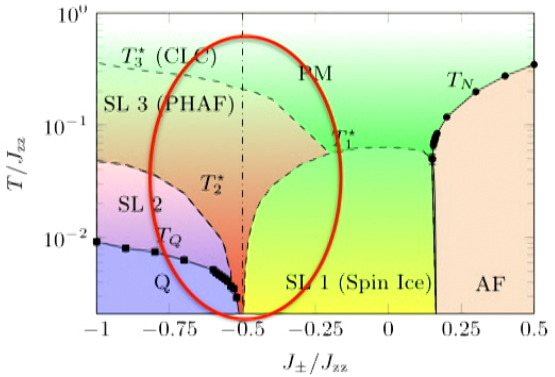

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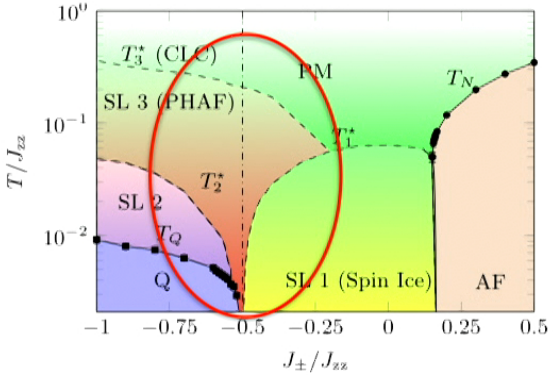
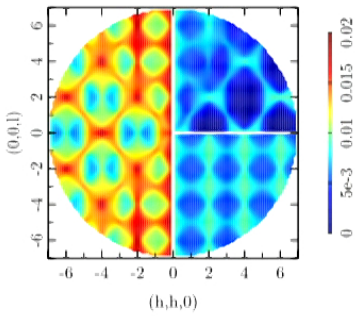
$$J_{\pm}/J_{zz} = -0.5$$

$$\mathcal{H}_{\mathsf{pHAF}} = J \sum_{\langle ij \rangle} \mathsf{S}_i \cdot \mathsf{S}_j$$



$S(\mathbf{q})$



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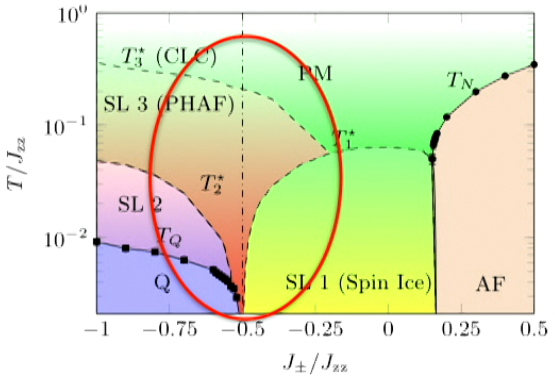
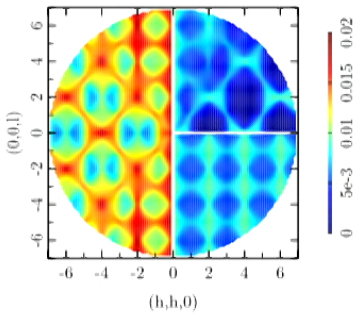
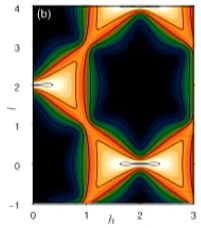


$S(\mathbf{q})$



local spin rotation

Heisenberg AF :



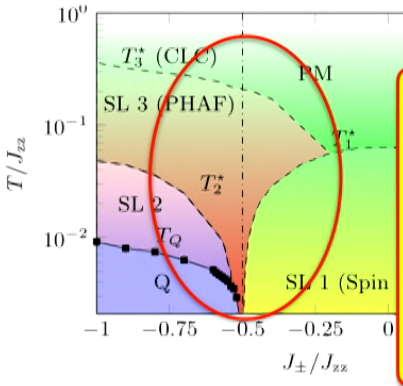
P.H. Conon and J. Chalker,
Phys. Rev B **81**, 224413 (2010)

SL 3 ("pseudo-Heisenberg AF")

$$\mathcal{H}_{\mathsf{QSI}} = \sum_{\langle ij \rangle} J_{zz} \mathsf{S}_i^z \mathsf{S}_j^z - J_{\pm} \left(\mathsf{S}_i^+ \mathsf{S}_j^- + \mathsf{S}_i^- \mathsf{S}_j^+ \right)$$

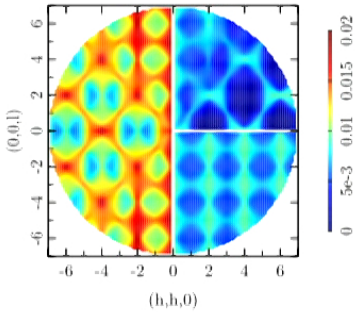
$$J_{\pm}/J_{zz} = -0.5$$

$$\mathcal{H}_{\mathsf{pHAF}} = J \sum_{\langle ij \rangle} \mathsf{S}_i \cdot \mathsf{S}_j$$



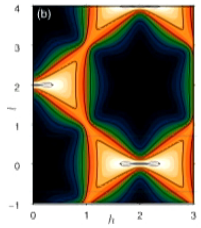
N.B. HAF on pyrochlore lattice has a long history (Reimers, Berlinsky, Moessner…)

$S(\mathbf{q})$



local spin rotation

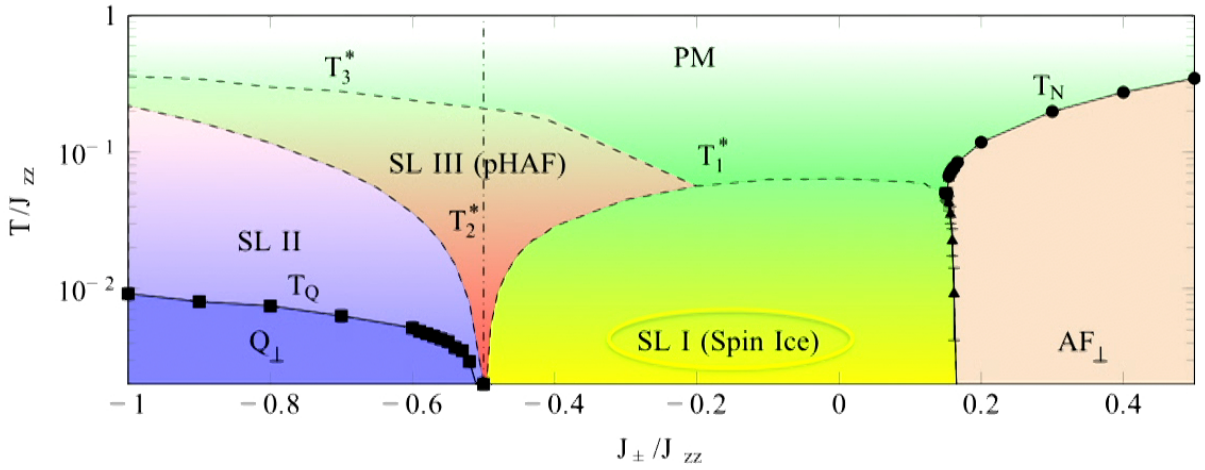
Heisenberg AF :



P.H. Conon and J. Chalker, Phys. Rev B **81**, 224413 (2010)

C. Henley, Phys. Rev B **71**, 014424 (2005) : U(1)× U(1)× U(1) gauge theory

SL 2 (something completely different)



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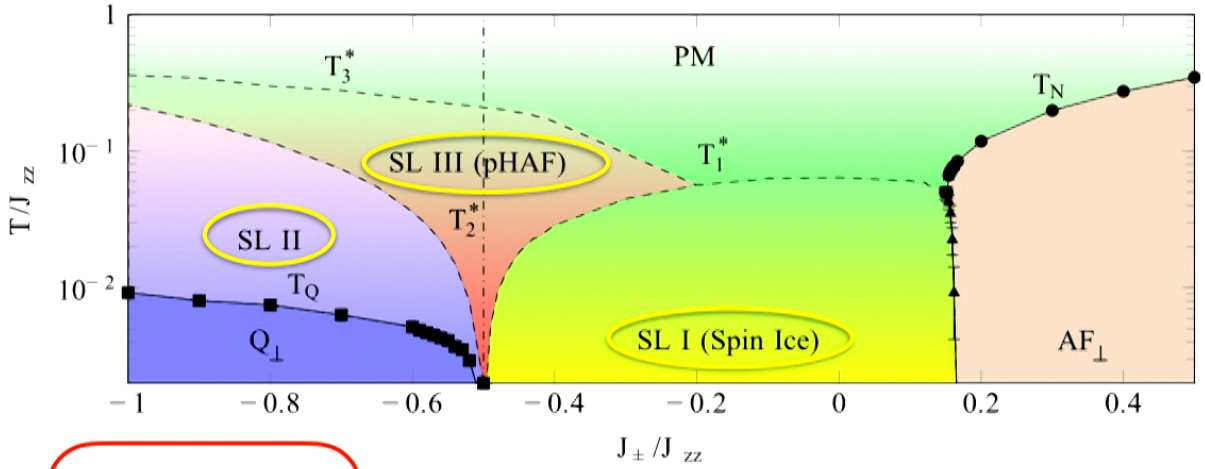
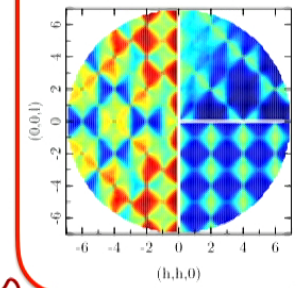
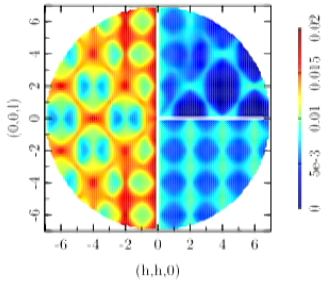


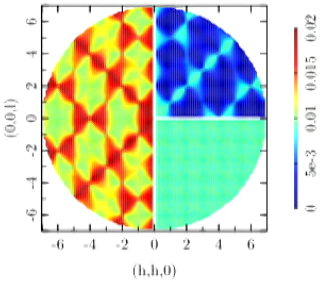
SL 2



SL 3 (pHAF)

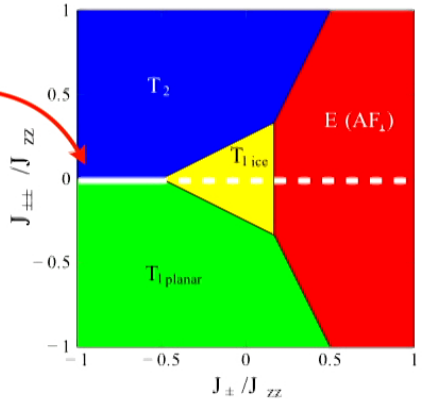


SL 1 (spin ice)



where does SL 2 come from ?

highly-degenerate manifold formed of combination of easy-plane states with T_1 and T_2 symmetry



minimal model QSI

O. Benton, PhD Thesis; M. Taillefumier *et al.*, arXiv:1705.00148

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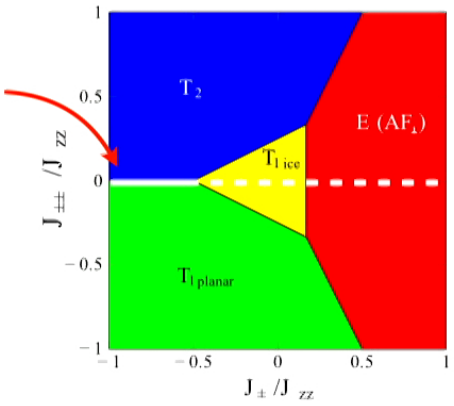

minimal model QSI

	Definition in terms of spins within tetrahedron
$\mathbf{m}_{T_{1,\text{planar}}}$	$\begin{pmatrix} \frac{1}{2}\left(S_0^x + S_1^x - S_2^x - S_3^x\right) \\ \frac{1}{4}\left(-S_0^x + \sqrt{3}S_0^y + S_1^x - \sqrt{3}S_1^y - S_2^x + \sqrt{3}S_2^y + S_3^x - \sqrt{3}S_3^y\right) \\ \frac{1}{4}\left(-S_0^x - \sqrt{3}S_0^y + S_1^x + \sqrt{3}S_1^y + S_2^x + \sqrt{3}S_2^y - S_3^x - \sqrt{3}S_3^y\right) \end{pmatrix}$
$\mathbf{m}_{T_2}$	$\begin{pmatrix} \frac{1}{2}\left(-S_0^y - S_1^y + S_2^y + S_3^y\right) \\ \frac{1}{4}\left(\sqrt{3}S_0^x + S_0^y - \sqrt{3}S_1^x - S_1^y + \sqrt{3}S_2^x + S_2^y - \sqrt{3}S_3^x - S_3^y\right) \\ \frac{1}{4}\left(-\sqrt{3}S_0^x + S_0^y + \sqrt{3}S_1^x - S_1^y + \sqrt{3}S_2^x - S_2^y - \sqrt{3}S_3^x + S_3^y\right) \end{pmatrix}$

O. Benton, PhD Thesis; M. Taillefumier *et al.*, arXiv:1705.00148

gauge structure ?

combine $\mathbf{m}_{\mathsf{T}_{1,\mathsf{planar}}}$ and $\mathbf{m}_{\mathsf{T}_2}$

into two fields satisfying zero-divergence condition

$$\mathbf{B}_1 = \frac{1}{2}(2m^x_{\mathsf{T}_1\mathsf{planar}}, -\sqrt{3}m^y_{\mathsf{T}_2} - m^y_{\mathsf{T}_1\mathsf{planar}}, \sqrt{3}m^z_{\mathsf{T}_2} - m^z_{\mathsf{T}_1\mathsf{planar}}) \qquad \nabla \cdot \mathbf{B}_1 = 0$$

$$\mathbf{B}_2 = \frac{1}{2}(2m^x_{\mathsf{T}_1\mathsf{planar}}, -m^y_{\mathsf{T}_2} + \sqrt{3}m^y_{\mathsf{T}_1\mathsf{planar}}, -m^z_{\mathsf{T}_2} - \sqrt{3}m^z_{\mathsf{T}_1\mathsf{planar}}) \qquad \nabla \cdot \mathbf{B}_2 = 0$$

can describe spin liquid SL 2 by
introducing two U(1) gauge
fields $\mathbf{A}_1$ and $\mathbf{A}_2$

$$\mathcal{F}_{\mathsf{SL2}} = \frac{T}{V}\int d^3r\ \lambda\left[\underbrace{(\nabla \times \mathbf{A}_1)^2}_{\mathbf{B}_1} + \underbrace{(\nabla \times \mathbf{A}_2)^2}_{\mathbf{B}_2}\right]$$

$\Rightarrow$ pinch points in $\mathbf{B}_1$ and $\mathbf{B}_2$

M. Taillefumier *et al.*, arXiv:1705.00148

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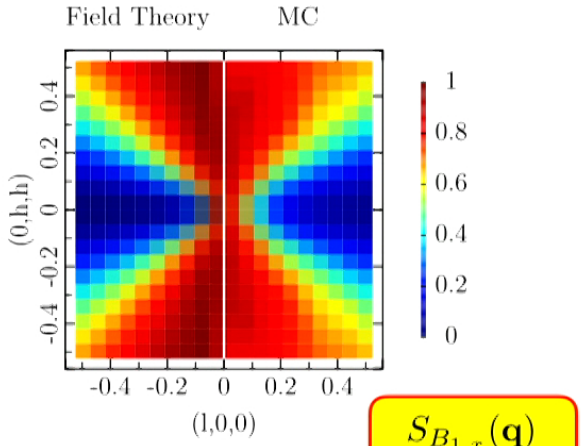
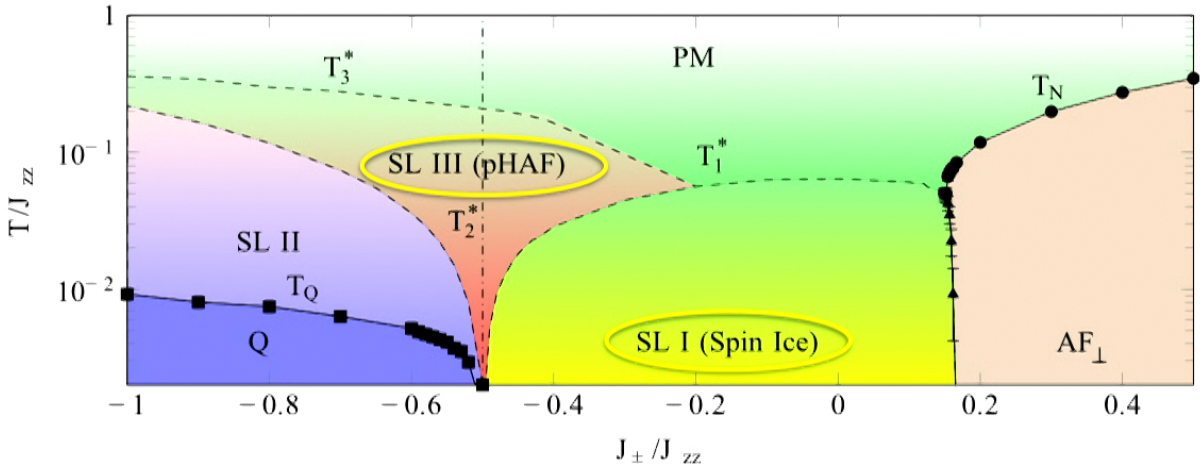


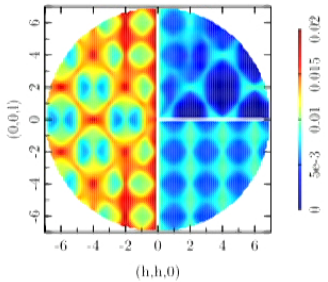
$S_{B_{1,x}}(\mathbf{q})$

M. Taillefumier *et al.*, arXiv:1705.00148

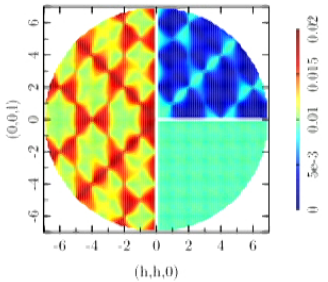
a new form of spin liquid…



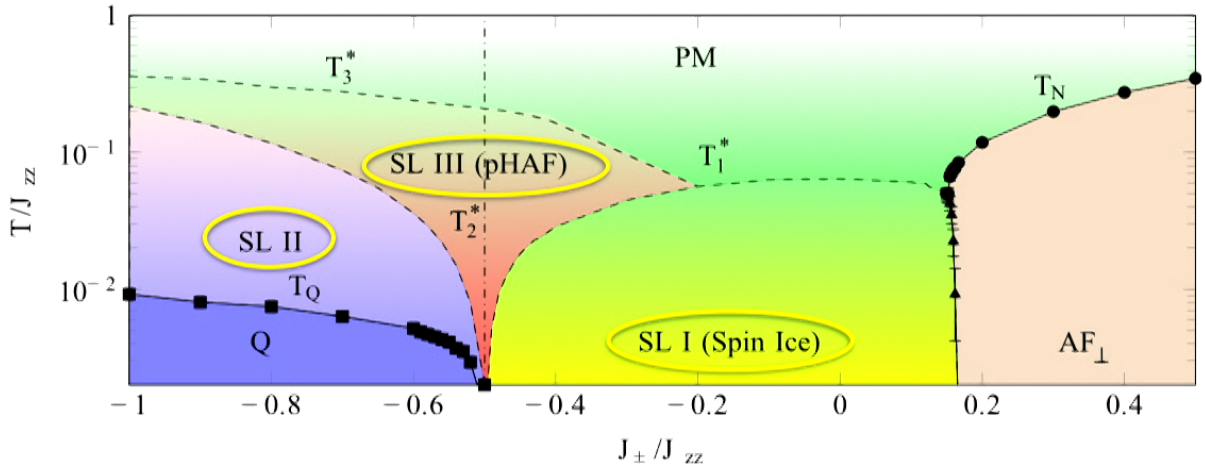
SL 3 (pHAF)



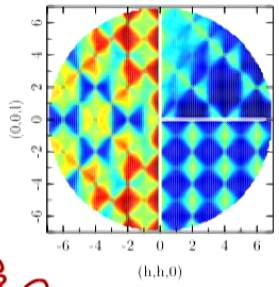
SL 1 (spin ice)



a new form of spin liquid…



SL 2



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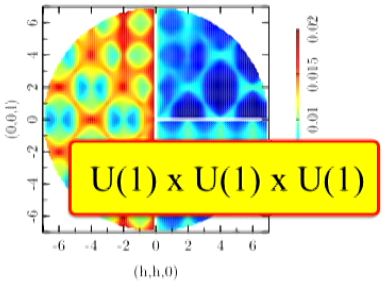

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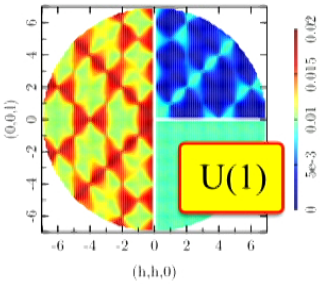
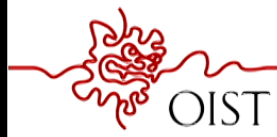
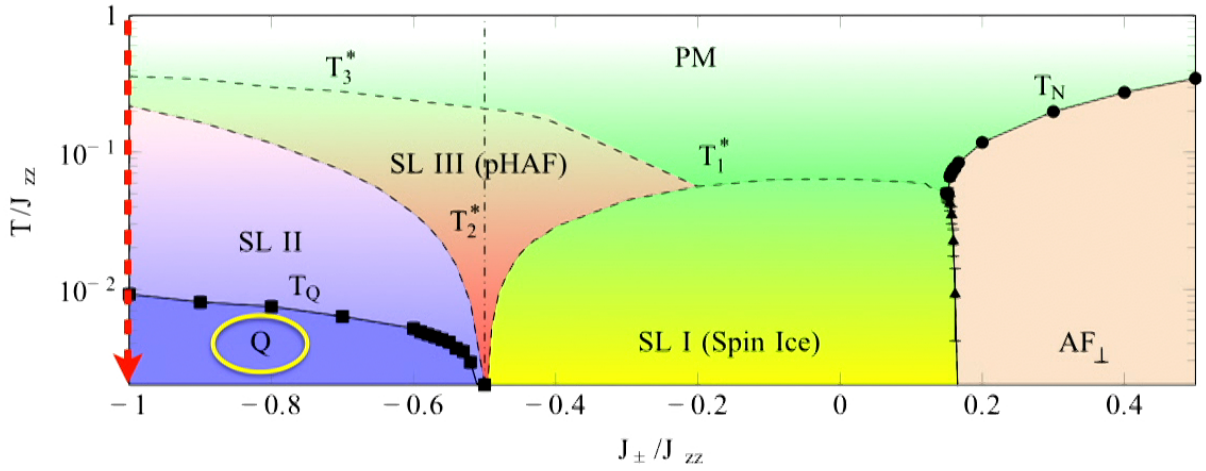


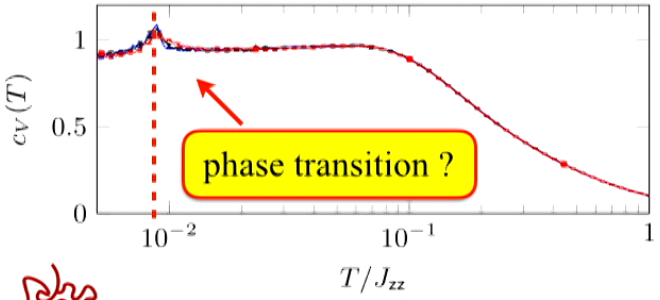
is that it ?



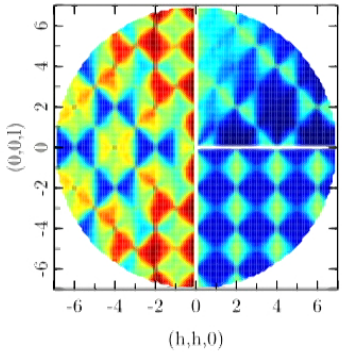
staged loss of entropy

is that it ?

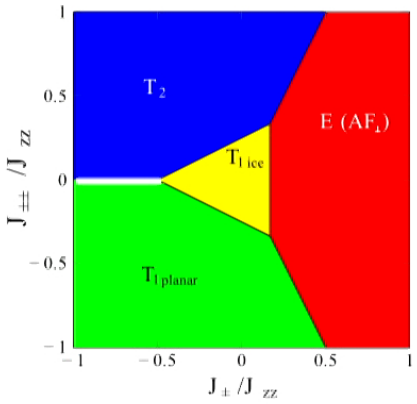




spin correlations unchanged
⇒
hidden order



hidden order…



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candidate for hidden order
is spin-nematic state
with director in easy-plane

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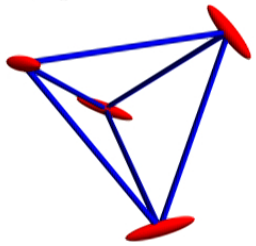

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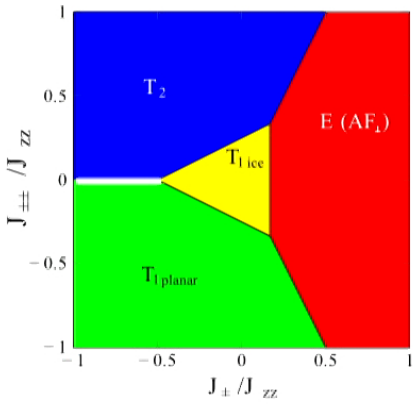

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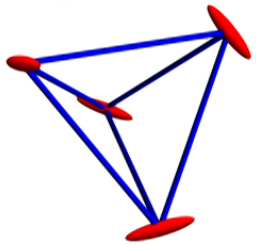

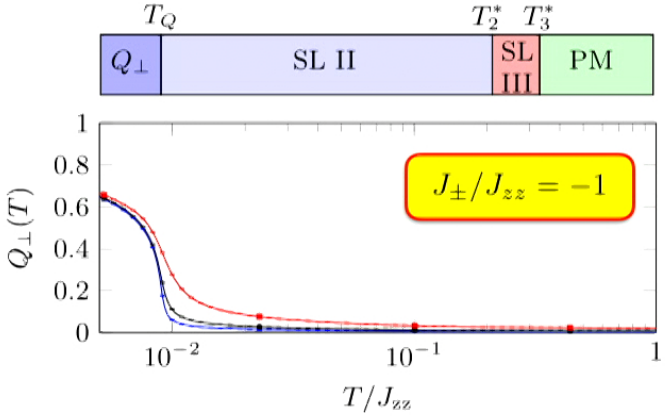

M. Taillefumier *et al.*, arXiv:1705.00148

what about spin excitations ?

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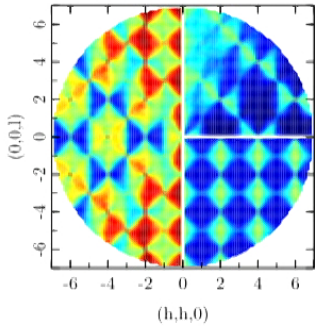
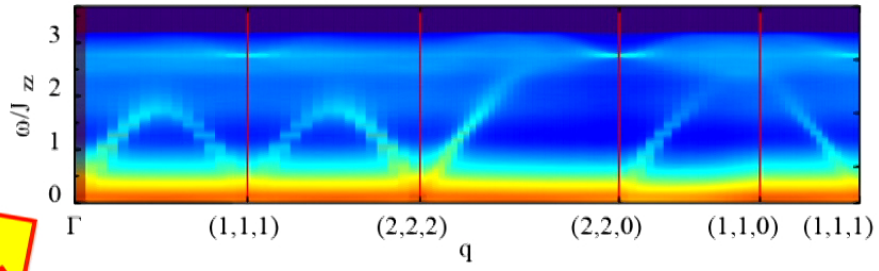
dynamical structure factor for spins : $S(\mathbf{q},\omega)$

$S(\mathbf{q})$





Q-phase

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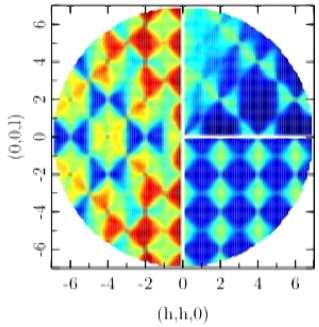
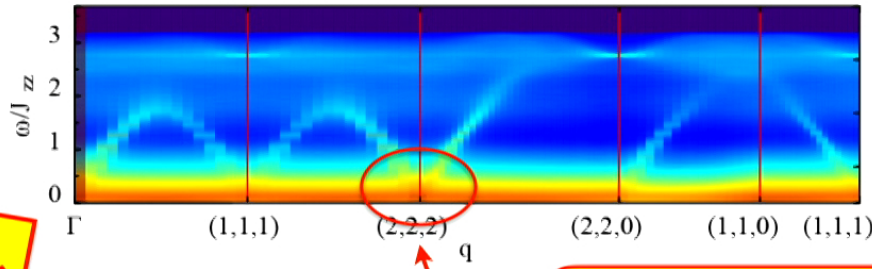
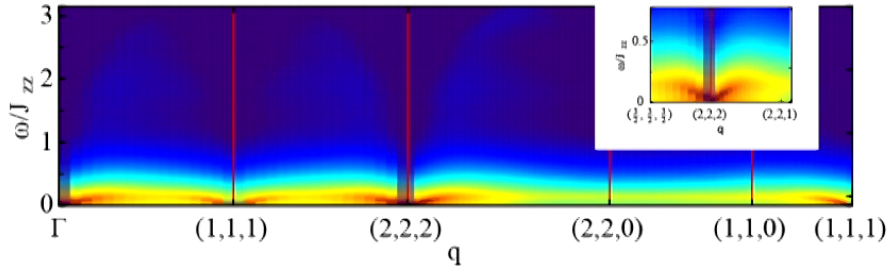


Q-phase



non-dispersing continuum

dynamical correlation function for quadrupoles : $\chi_Q(\mathbf{q},\omega)$



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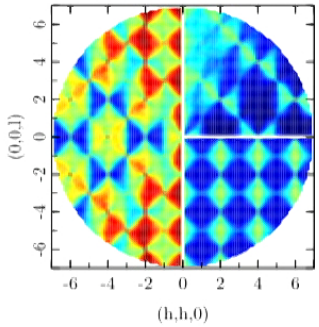
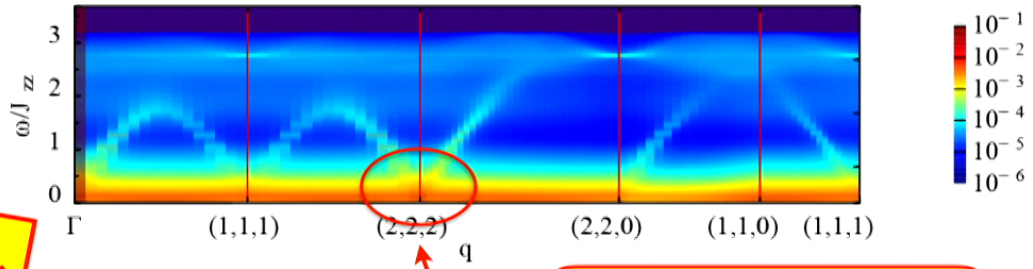
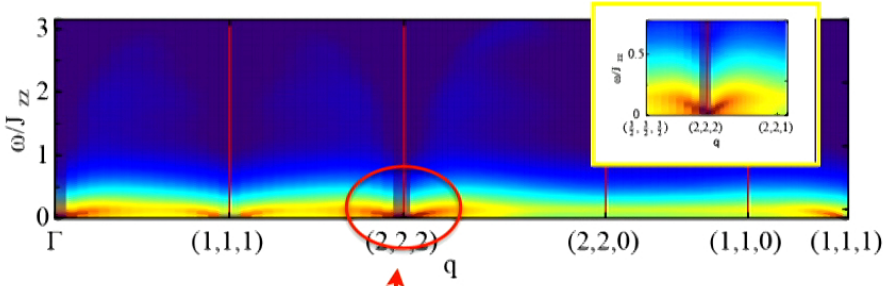


Q-phase



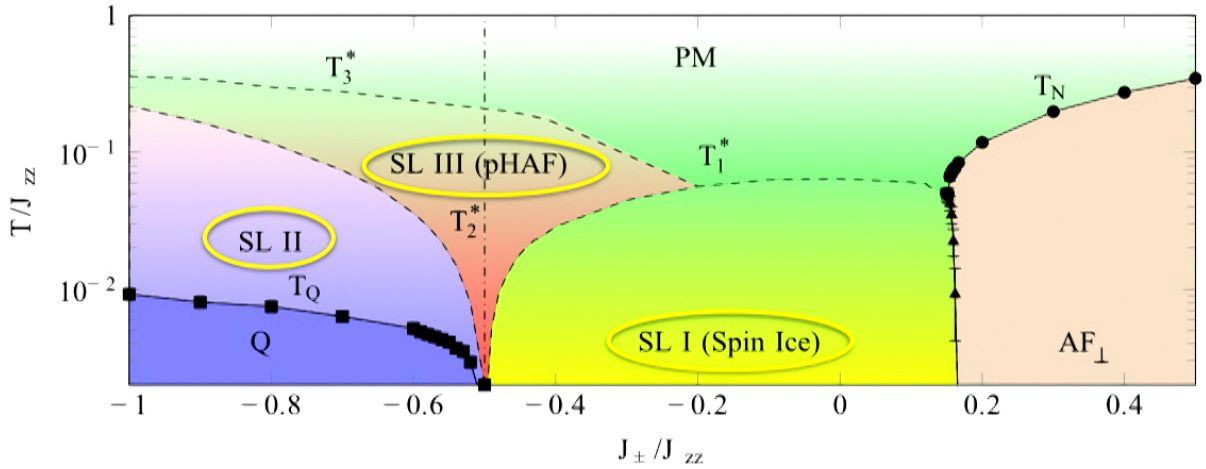
non-dispersing continuum

dynamical correlation function for quadrupoles : $\chi_Q(\mathbf{q},\omega)$

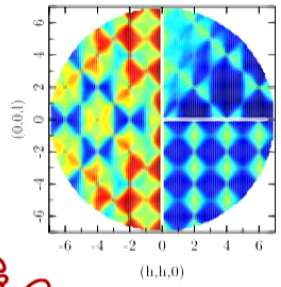


linearly-dispersing Goldstone mode

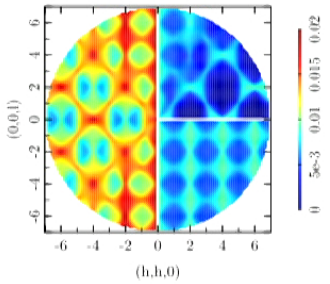
what have we learned ? (theory)



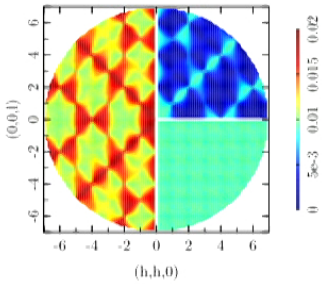
SL 2



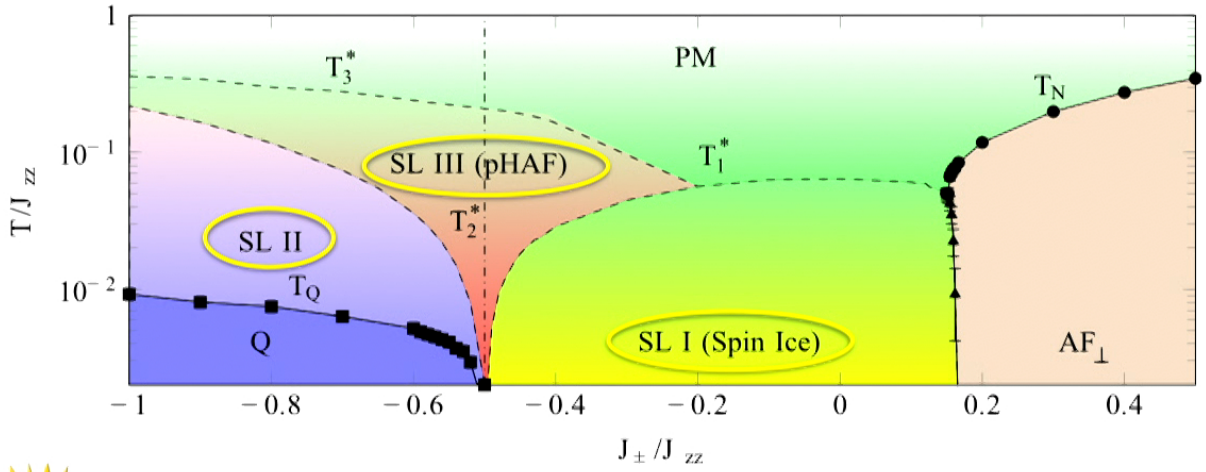
SL 3 (pHAF)



SL 1 (spin ice)

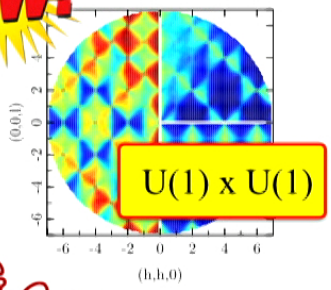


what have we learned ? (theory)

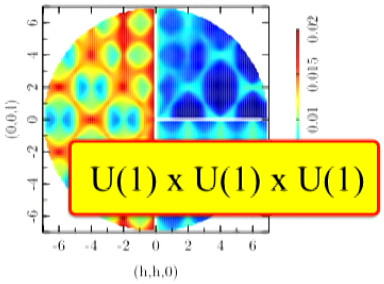


NEW!

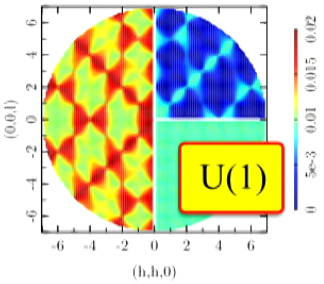
SL 2



SL 3 (pHAF)



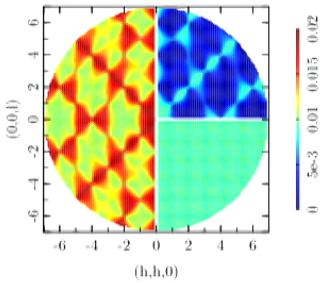
SL 1 (spin ice)



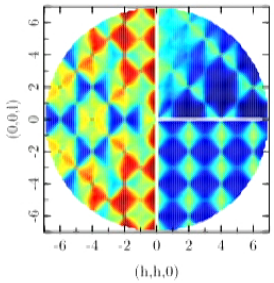
what have we learned ? (experiment)

pinch points ⇏ spin ice

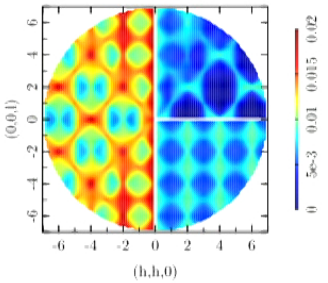
SL 1 (spin ice)



SL 2 & Q



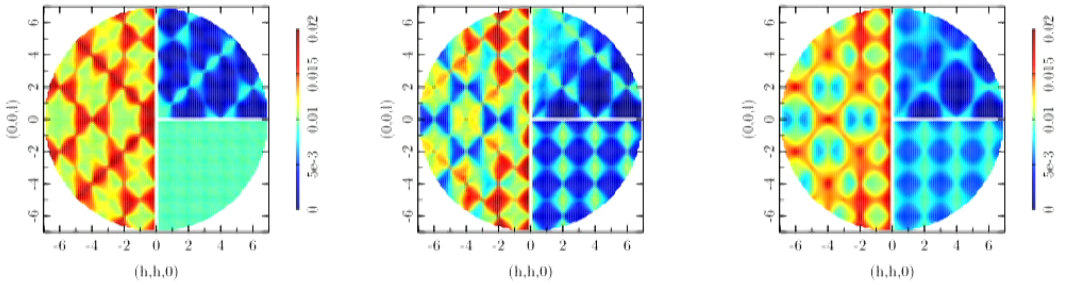
SL 3 (pHAF)



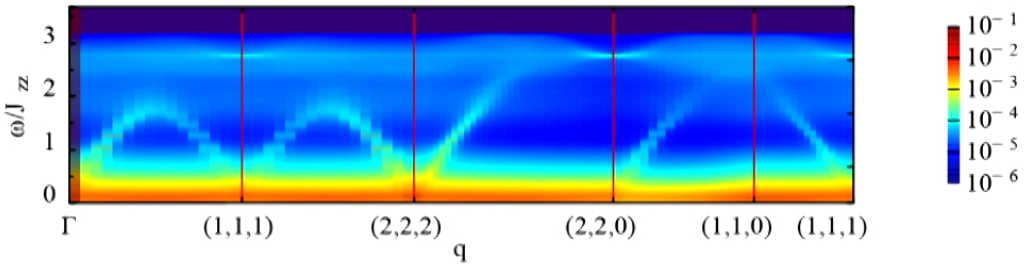
what have we learned ? (experiment)

pinch points ⇏ spin ice

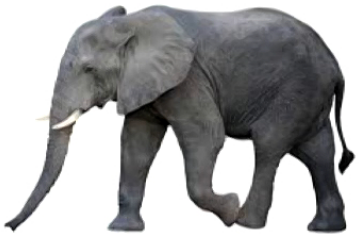
SL 1 (spin ice) SL 2 & Q SL 3 (pHAF)



non-dispersing continua may hide many secrets…



what's left ?



quantum effects !!!

the story so far…

minimal model of quantum spin ice

$$\mathcal{H}_{\mathsf{QSI}} = \sum_{\langle ij \rangle} J_{zz} \mathsf{S}_i^z \mathsf{S}_j^z - J_{\pm} \left(\mathsf{S}_i^+ \mathsf{S}_j^- + \mathsf{S}_i^- \mathsf{S}_j^+ \right)$$

change sign of $J_{\pm}$

3 spin liquids
+ hidden spin-nematic order !

the story so far…

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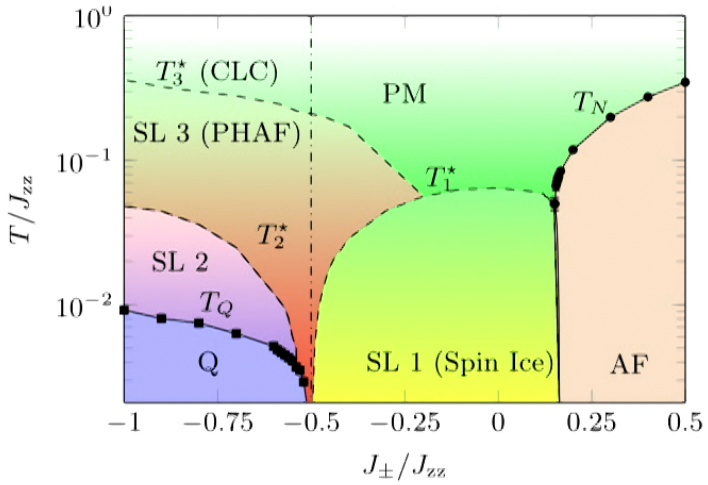
phase diagram from classical Monte Carlo simulation



omne trium perfectum !!!