Quantum spin ice

nic shannon

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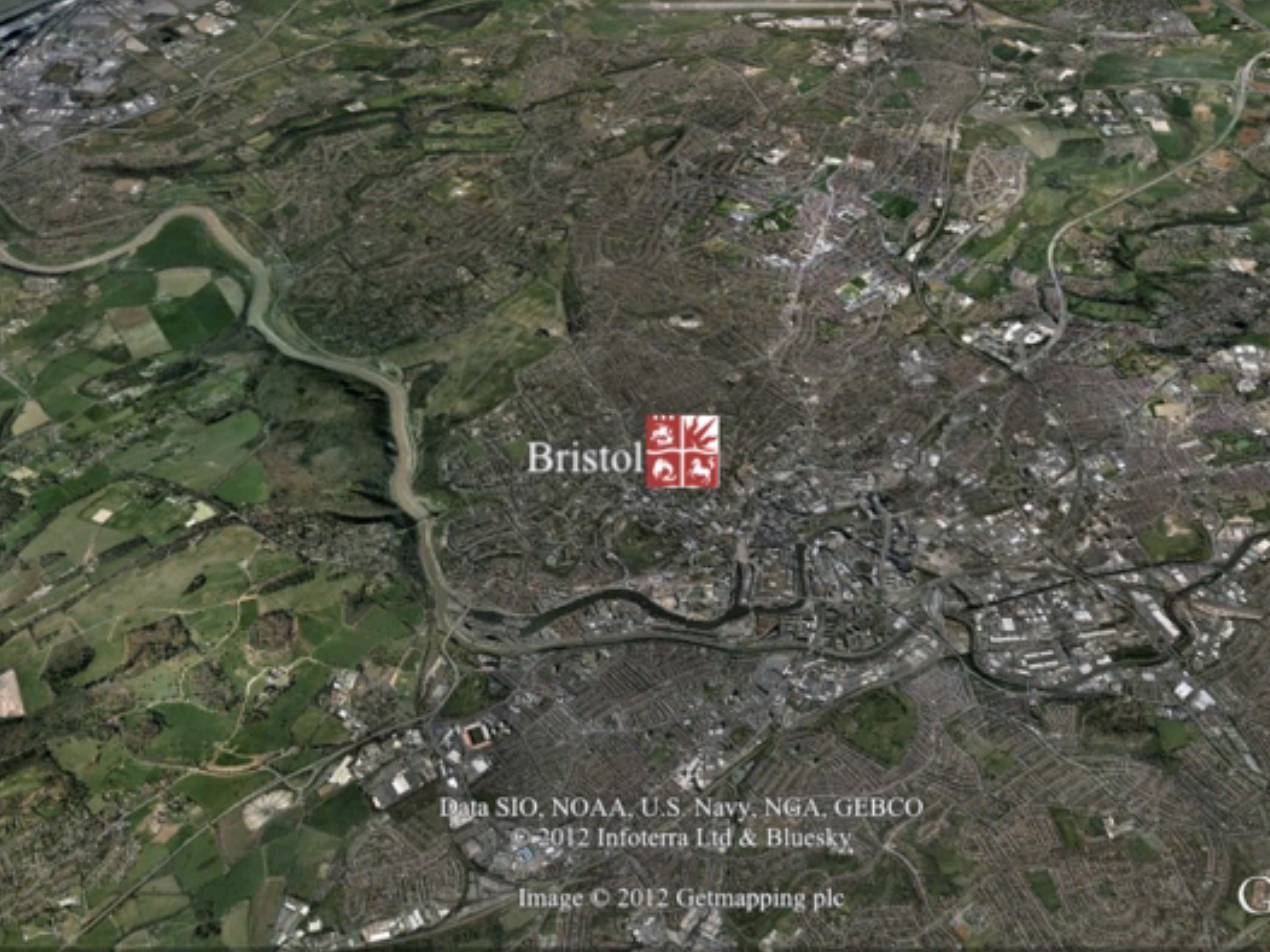
Bristol
Data SIO, NOAA, U.S. Navy, NGA, GEBCO
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English-language graduate University,
in Japan, with international faculty and students

spin ice 101

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what is spin ice ?

consider e.g.

$(Dy^{3+})_2\,(Ti^{4+})_2(O^{2-})_7$

↑

magnetic ion

$Dy^{3+} = [Xe]\ 4f^9$

↑

9 electrons in 7 orbitals

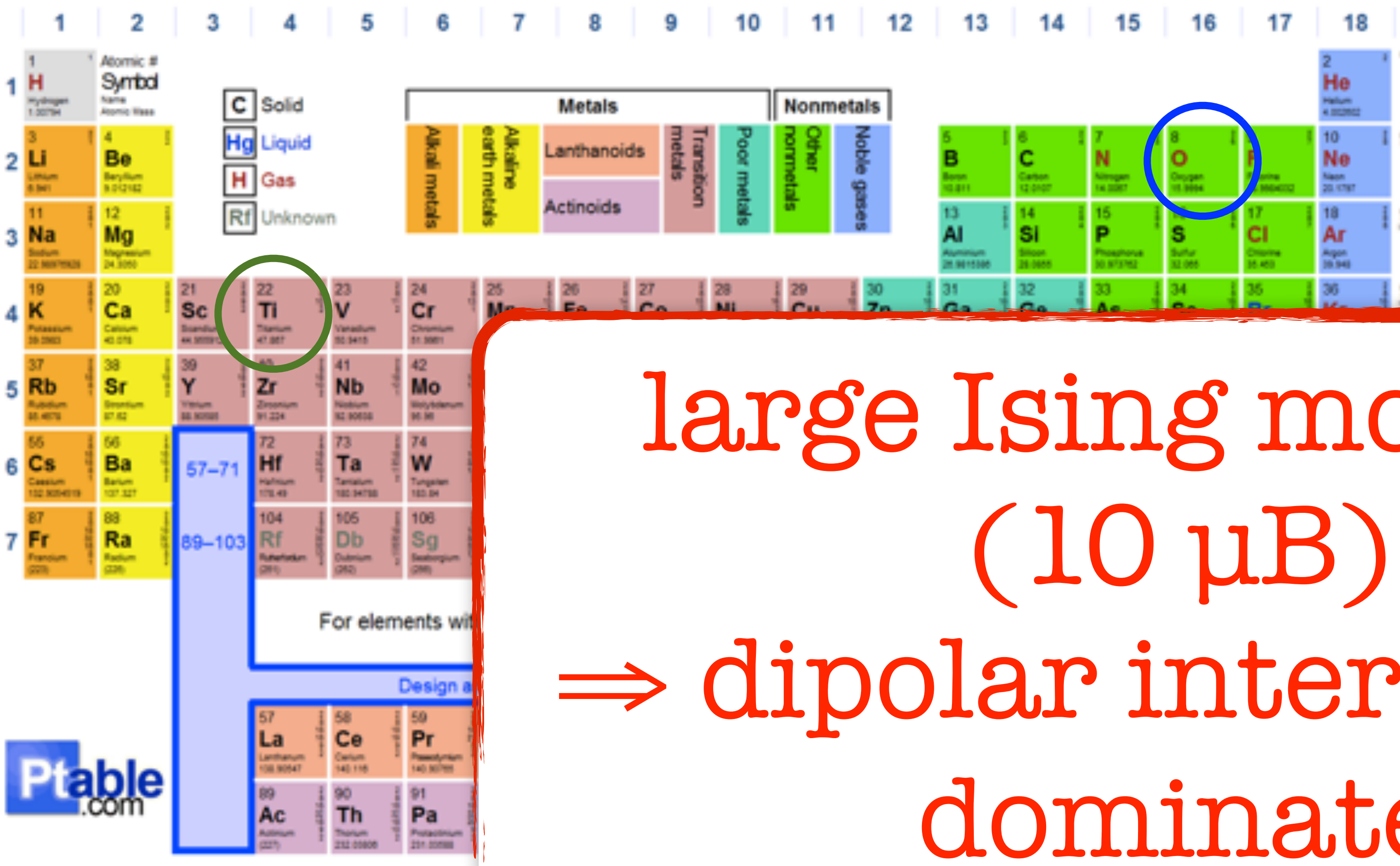
expect strong spin-orbit coupling for 4f electrons...

...need to think about $|\mathbf{J}| = |\mathbf{L}+\mathbf{S}|$ in **crystal field**

odd number of electrons

⇒ grounds state of Dy^{3+} is a Kramers doublet (effective spin-1/2)

what is spin ice ?



consider e.g.

$(Dy^{3+})_2\,(Ti^{4+})_2(O^{2-})_7$

[Xe] $4f^9$

s in 7 orbitals

large Ising moment (10 μB)
⇒ dipolar interactions dominate

expect strong spin-orbit coupling for 4f electrons...

...need to think about |**J**| = |**L**+**S**| in **crystal field**

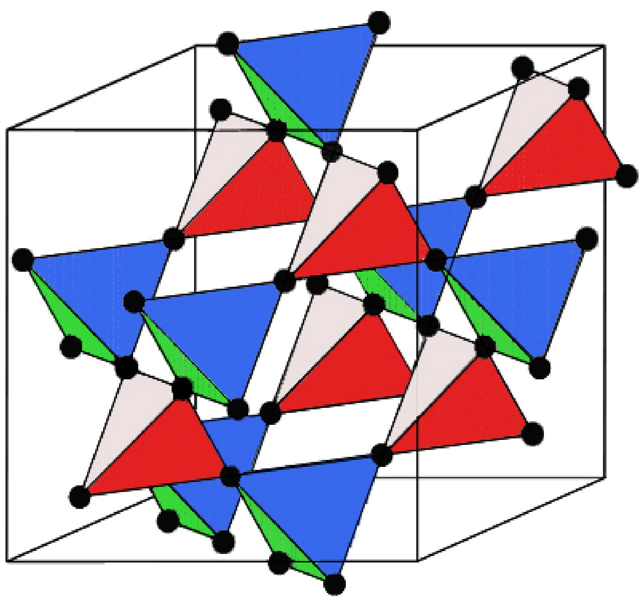
odd number of electrons

⇒ grounds state of Dy^{3+} is a Kramers doublet (effective spin-1/2)

what makes it spin ice ?

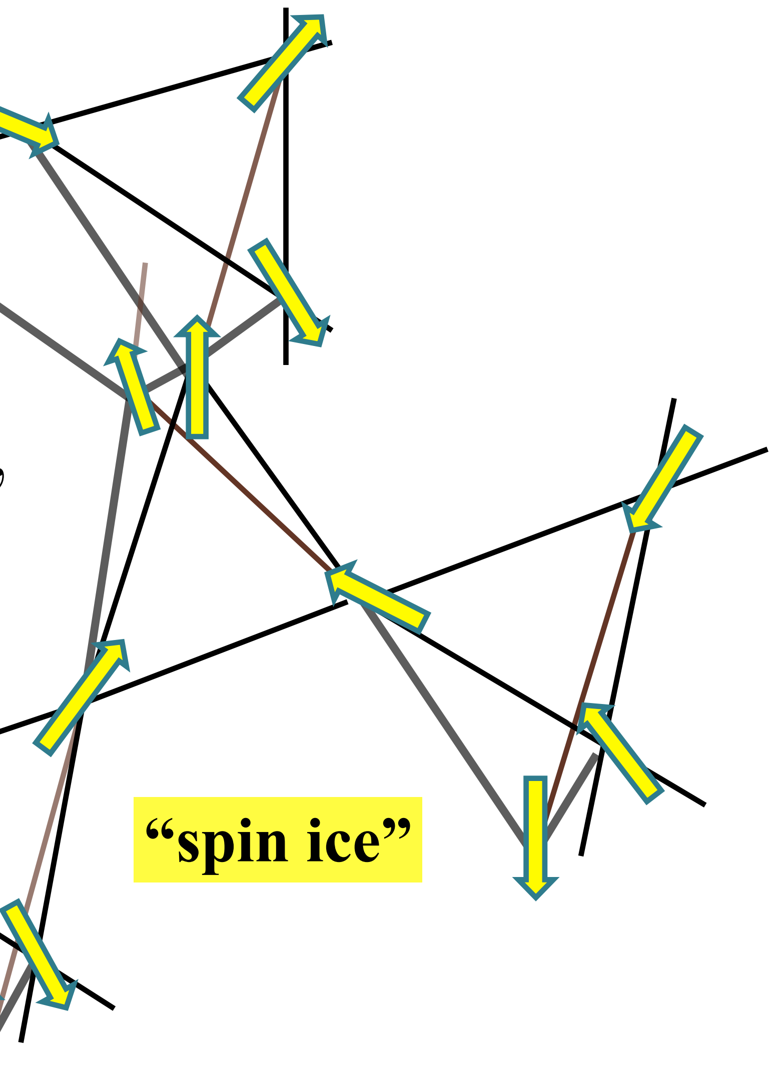
$Ho_2Ti_2O_7$
$Dy_2Ti_2O_7$

ferromagnetic nearest-neighbour interactions select an **extensive** number of states with **two in and two out** spins per tetrahedron



magnetic Ho^{8+} or Dy^{8+} ions live on a **pyrochlore lattice**

"$\nabla \cdot \mathbf{B} = 0$"

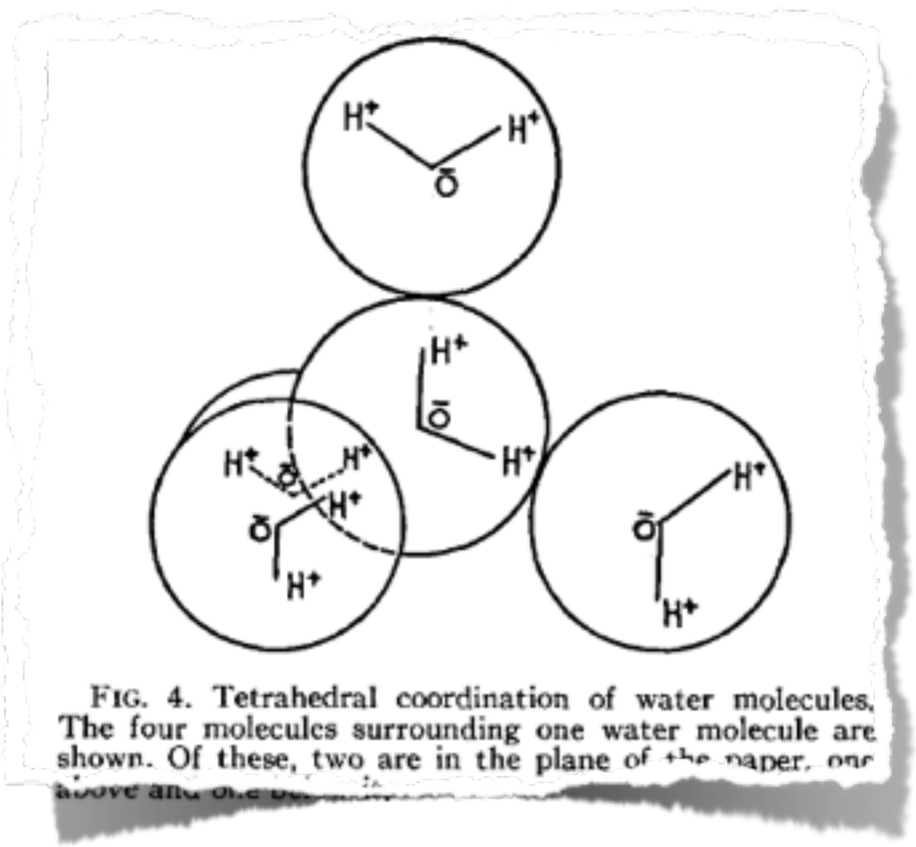


strong easy-axis anisotropy forces spins to point in or out of tetrahedron

M.J. Harris et al., Phys. Rev. Lett. **79**, 2554 (1997)

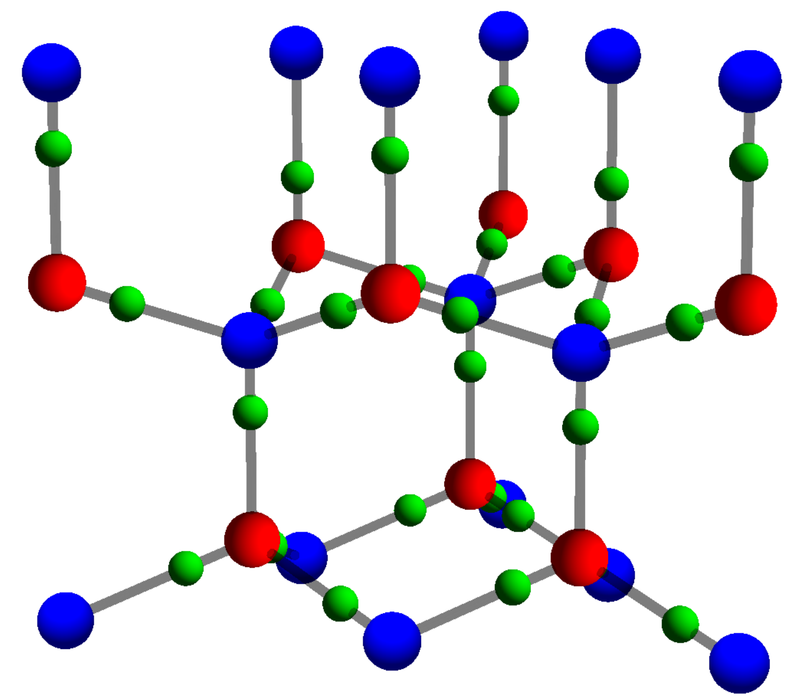
what's this got to do with water ?

water ice is composed of hydrogen-bonded water molecules, with each water molecule forming two hydrogen bonds



J. D. Bernal and R. H. Fowler,
J. Chem. Phys. **1**, 515 (1933)

in Ih water ice, O^{2-} form a hexagonal crystal lattice, but H^{+} do not order !

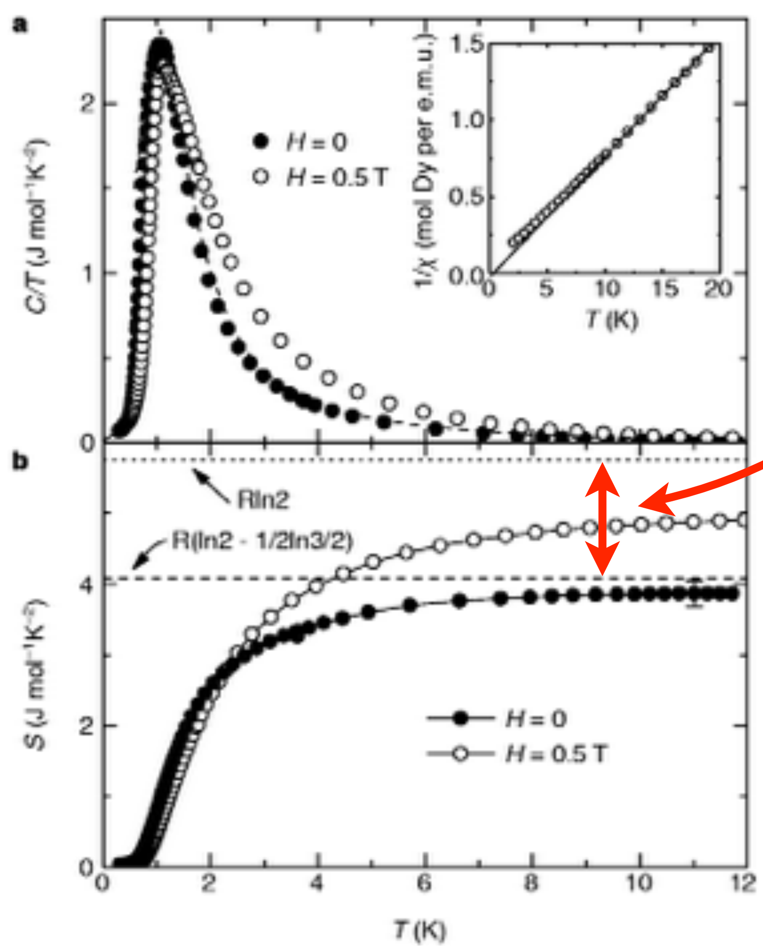


$\Omega \sim 1.5^{N/2}$
different proton configurations !

L. Pauling,
J. Am. Chem. Soc. **27**, 2680 (1935)

why should you believe in spin ice ?

heat capacity of $Dy_2Ti_2O_7$



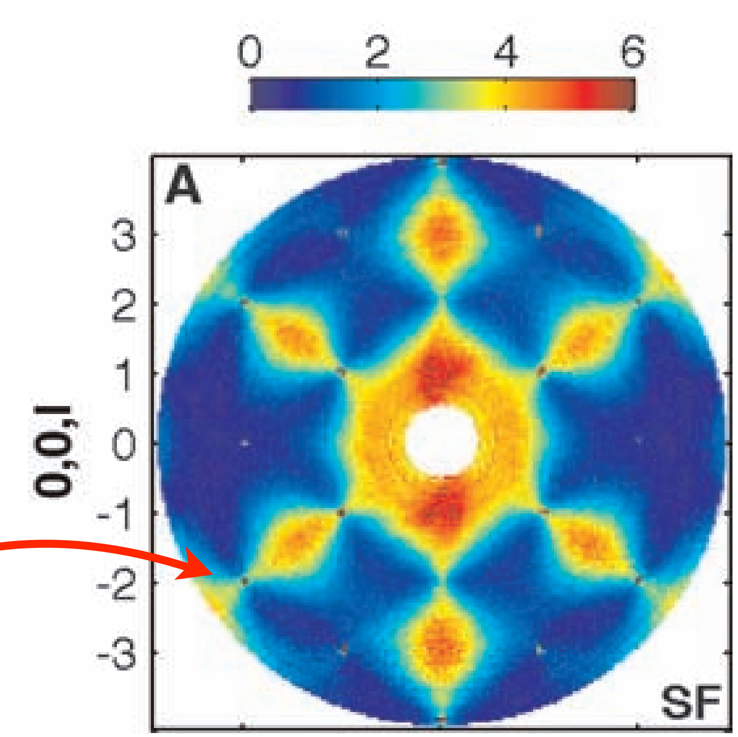
A.P. Ramirez et al.,
Nature **399**, 333 (1999)

Pauling Ice entropy

pinch point

"$\nabla \cdot \mathbf{B} = 0$"

neutron scattering on $Ho_2Ti_2O_7$



T. Fennell et al,
Science **326**, 415 (2009).

direct (thermodynamic) and indirect (scattering) evidence for extensive ground state manifold

why all the fuss ?

THE JOURNAL
OF
CHEMICAL PHYSICS

VOLUME 1 AUGUST, 1933 NUMBER 8

A Theory of Water and Ionic Solution, with Particular Reference to Hydrogen and Hydroxyl Ions

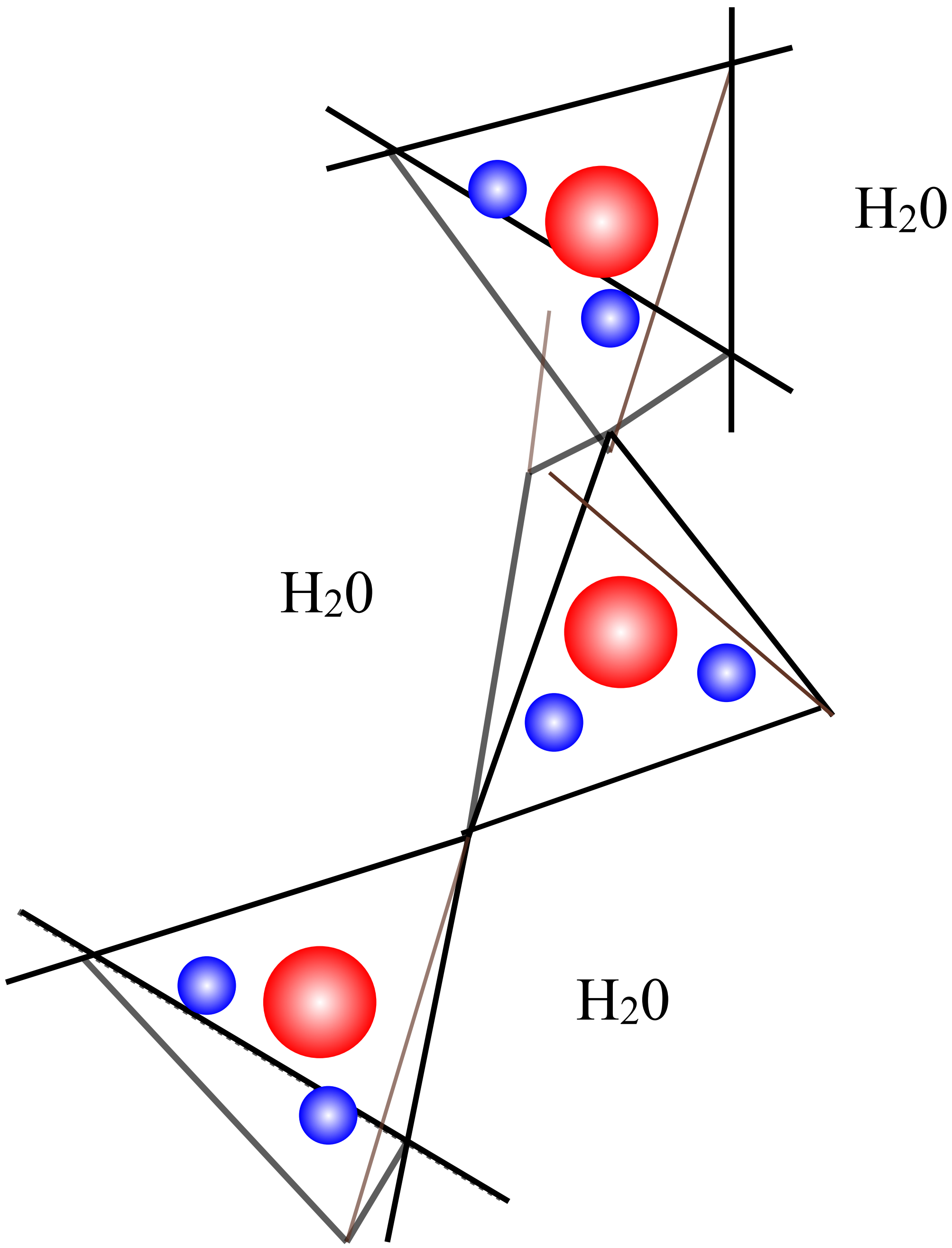
J. D. BERNAL AND R. H. FOWLER, *University of Cambridge, England*

(Received April 29, 1933)

from bodily transport through the solution. It is suggested that this different mechanism is the transfer by a jump of one proton from one water molecule to another when favourable configurations are presented. Such an idea has also

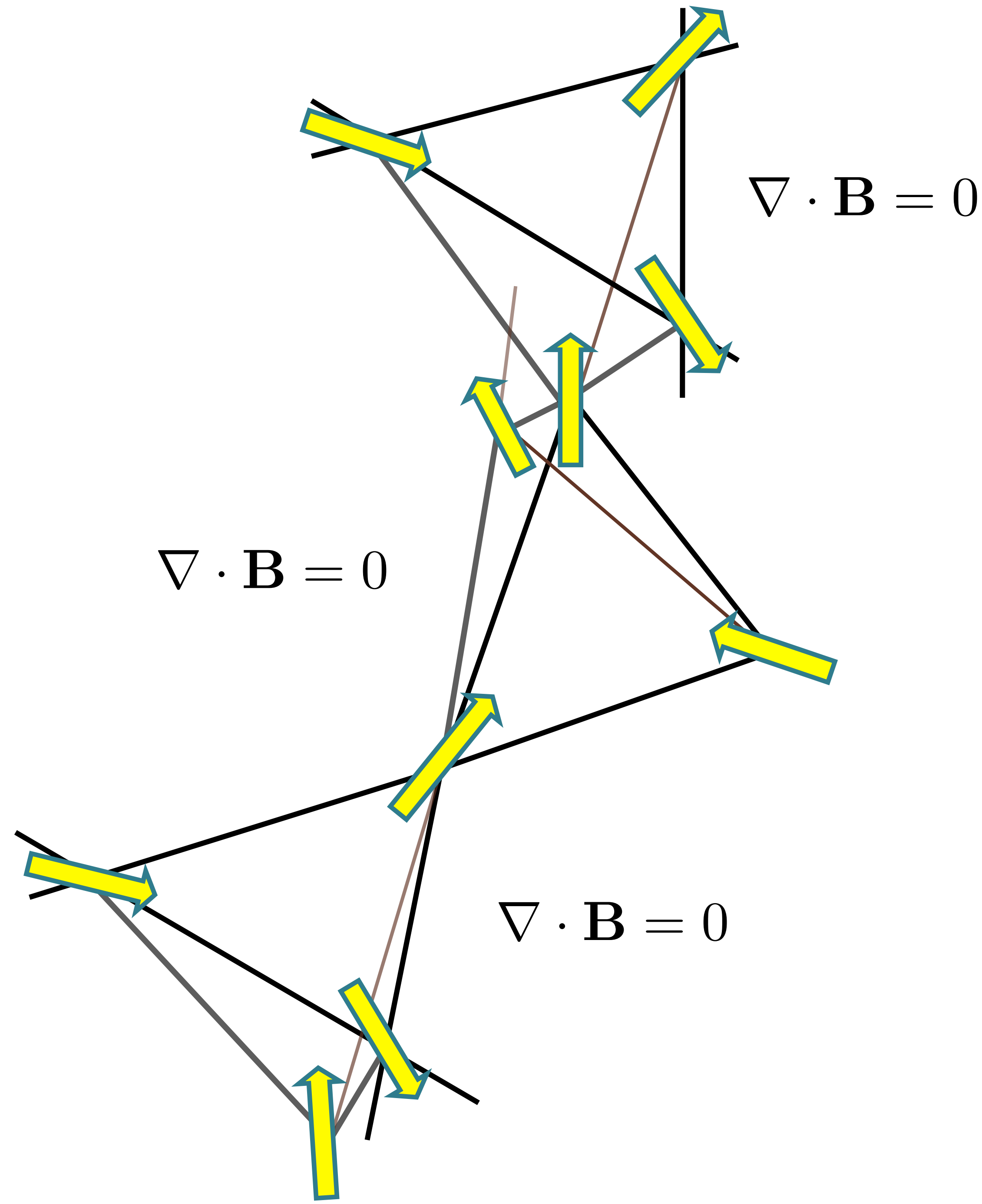
water ice

(H_20 in Ih cubic form)



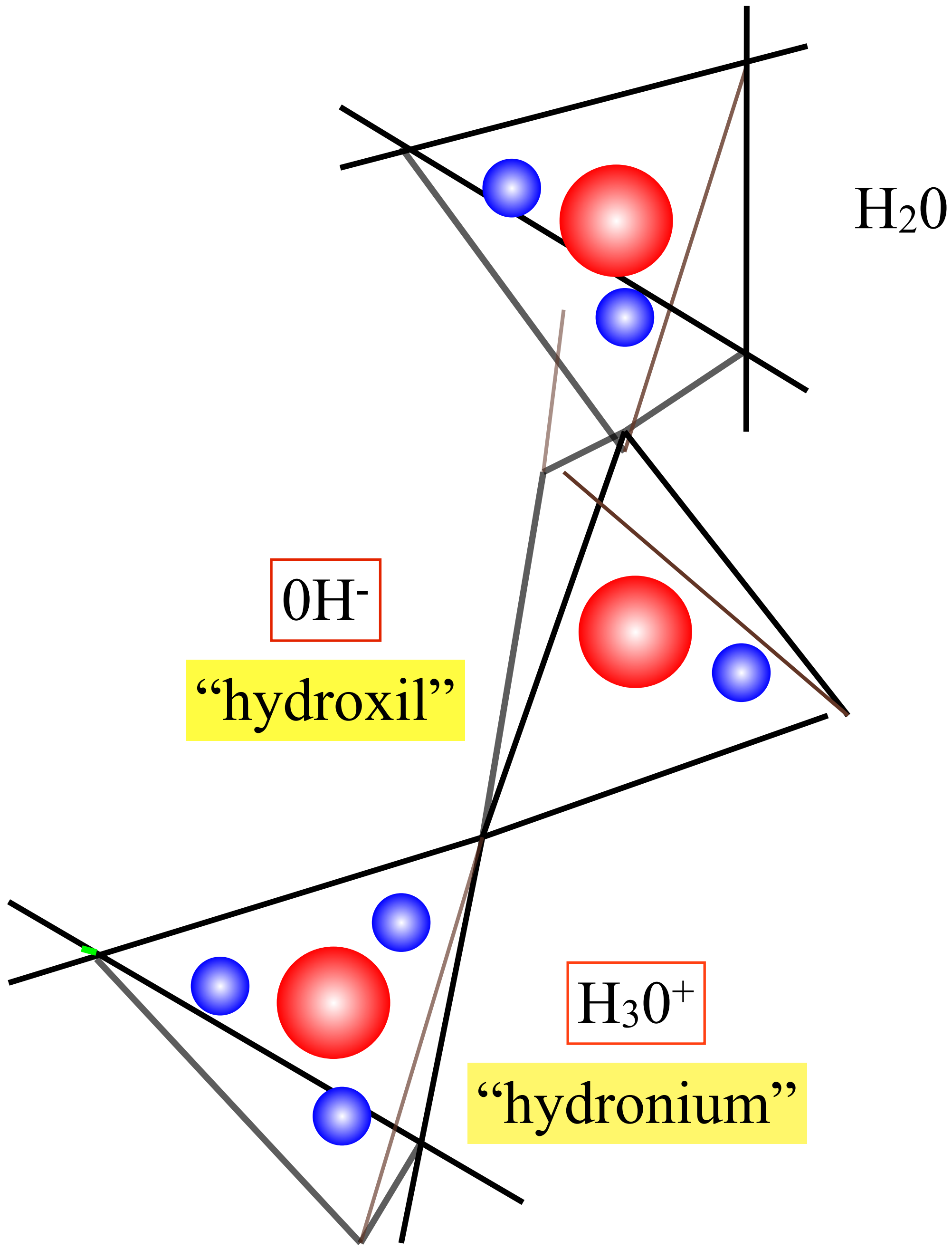
spin ice

($Ho_2Ti_2O_7$, $DyTi_2O_7$)



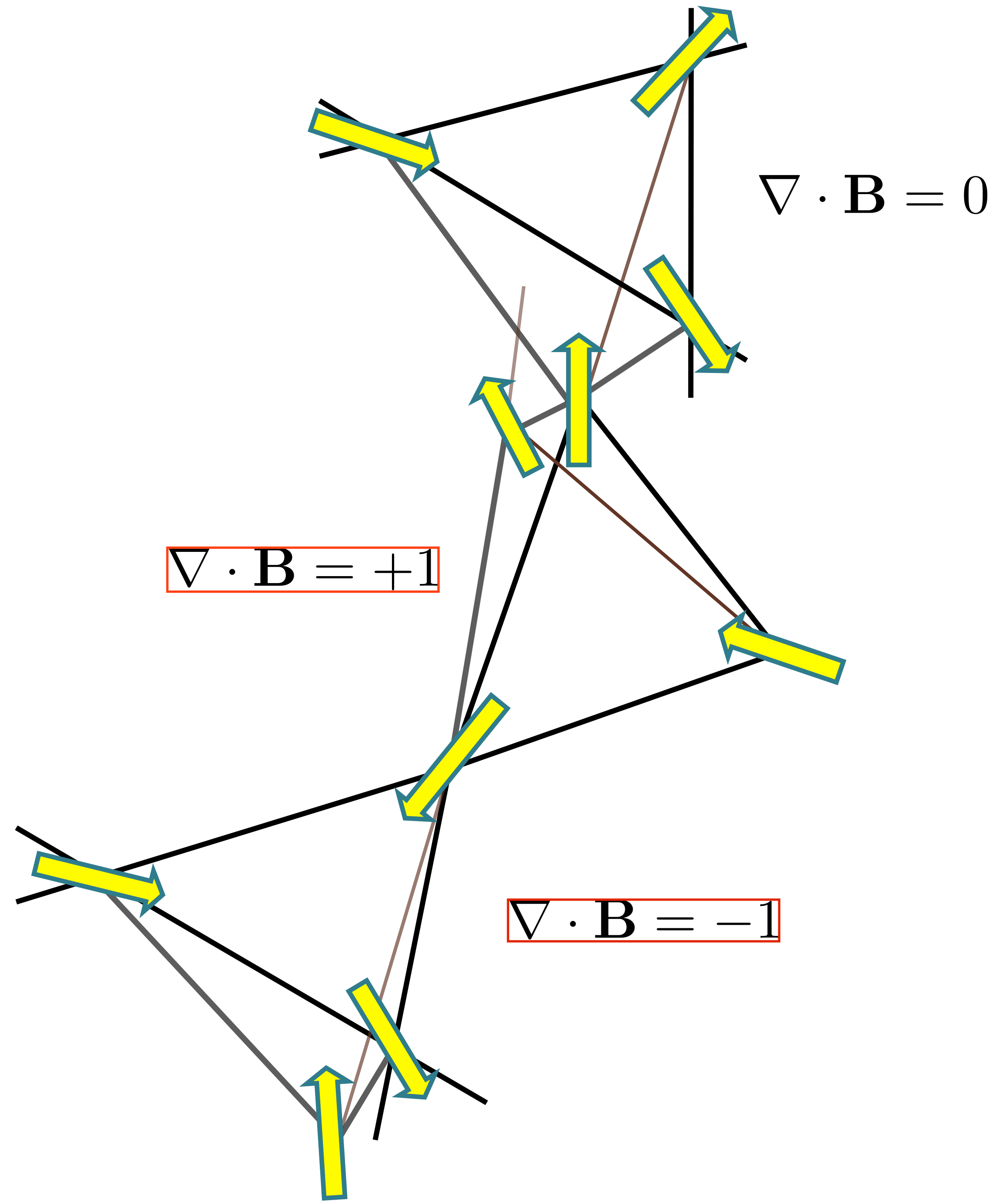
water ice

(H_20 in Ih cubic form)



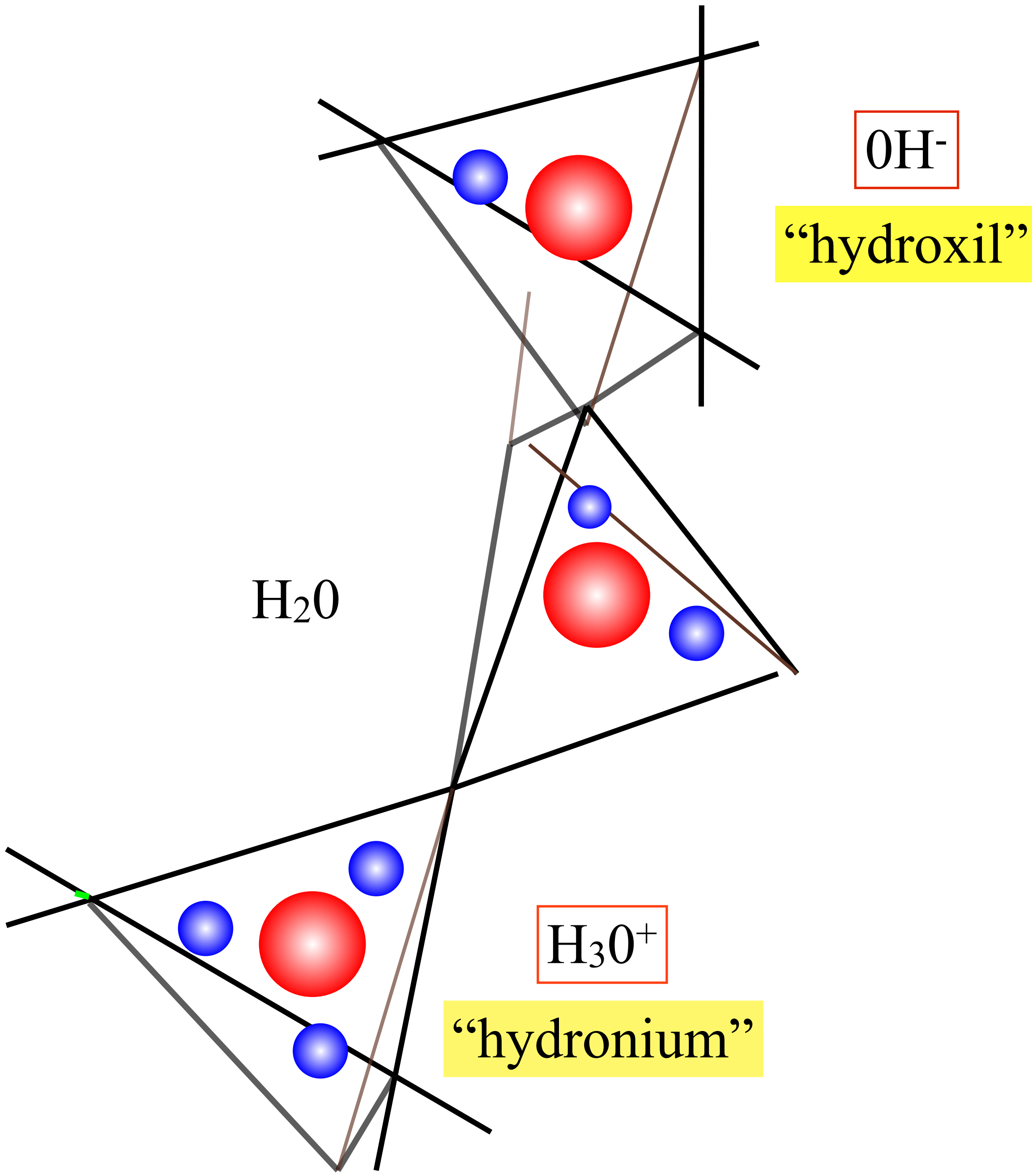
spin ice

($Ho_2Ti_2O_7$, $DyTi_2O_7$)



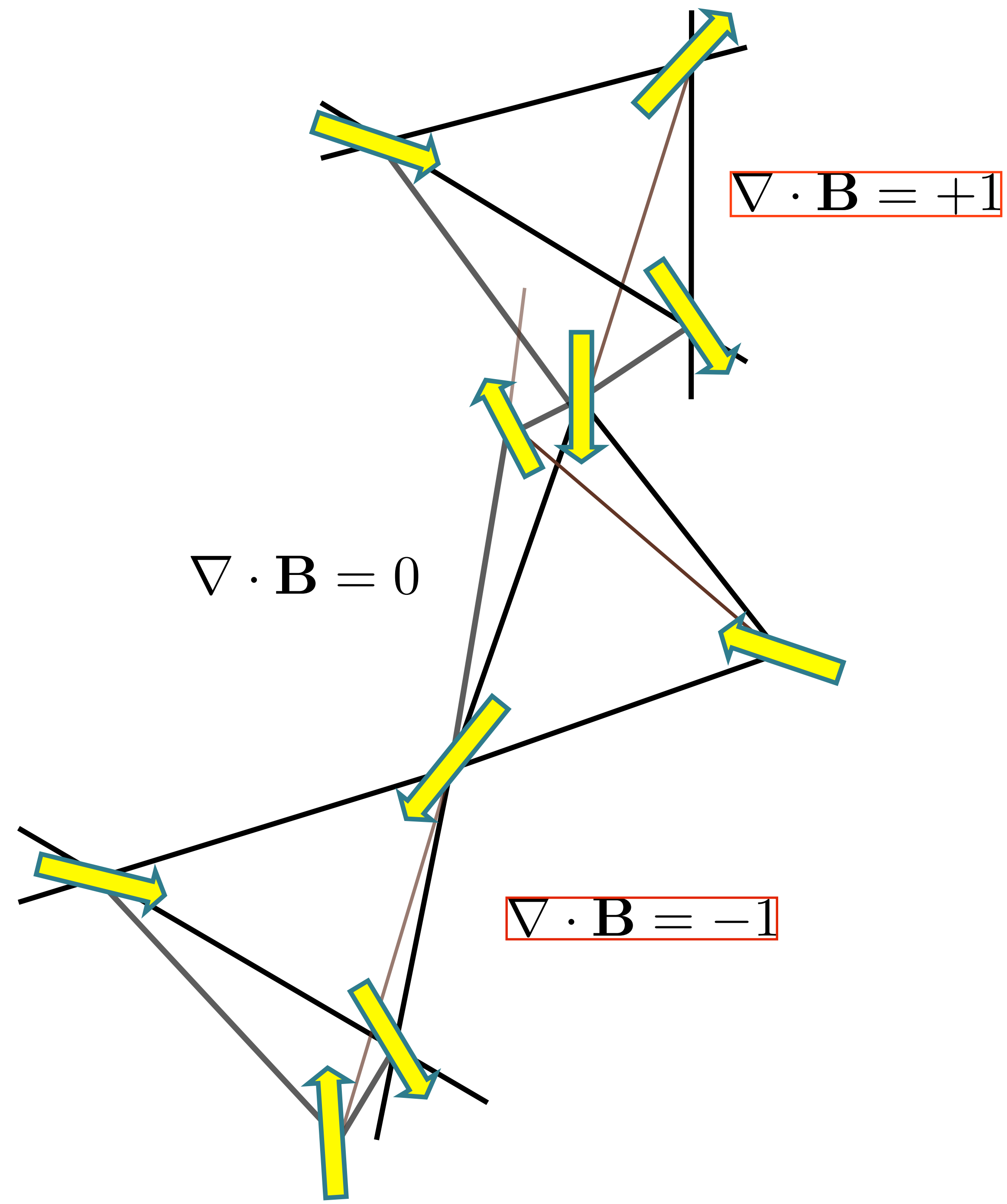
water ice

(H_20 in Ih cubic form)

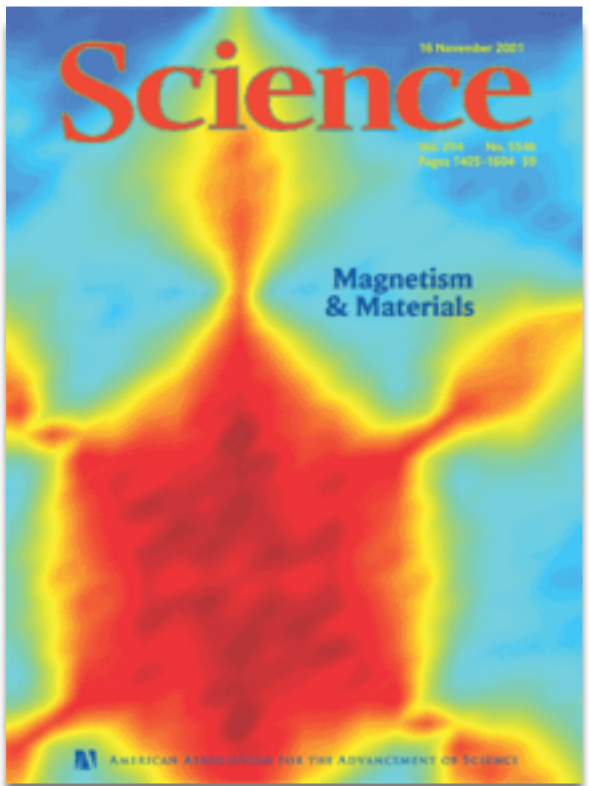


spin ice

($Ho_2Ti_2O_7$, $DyTi_2O_7$)

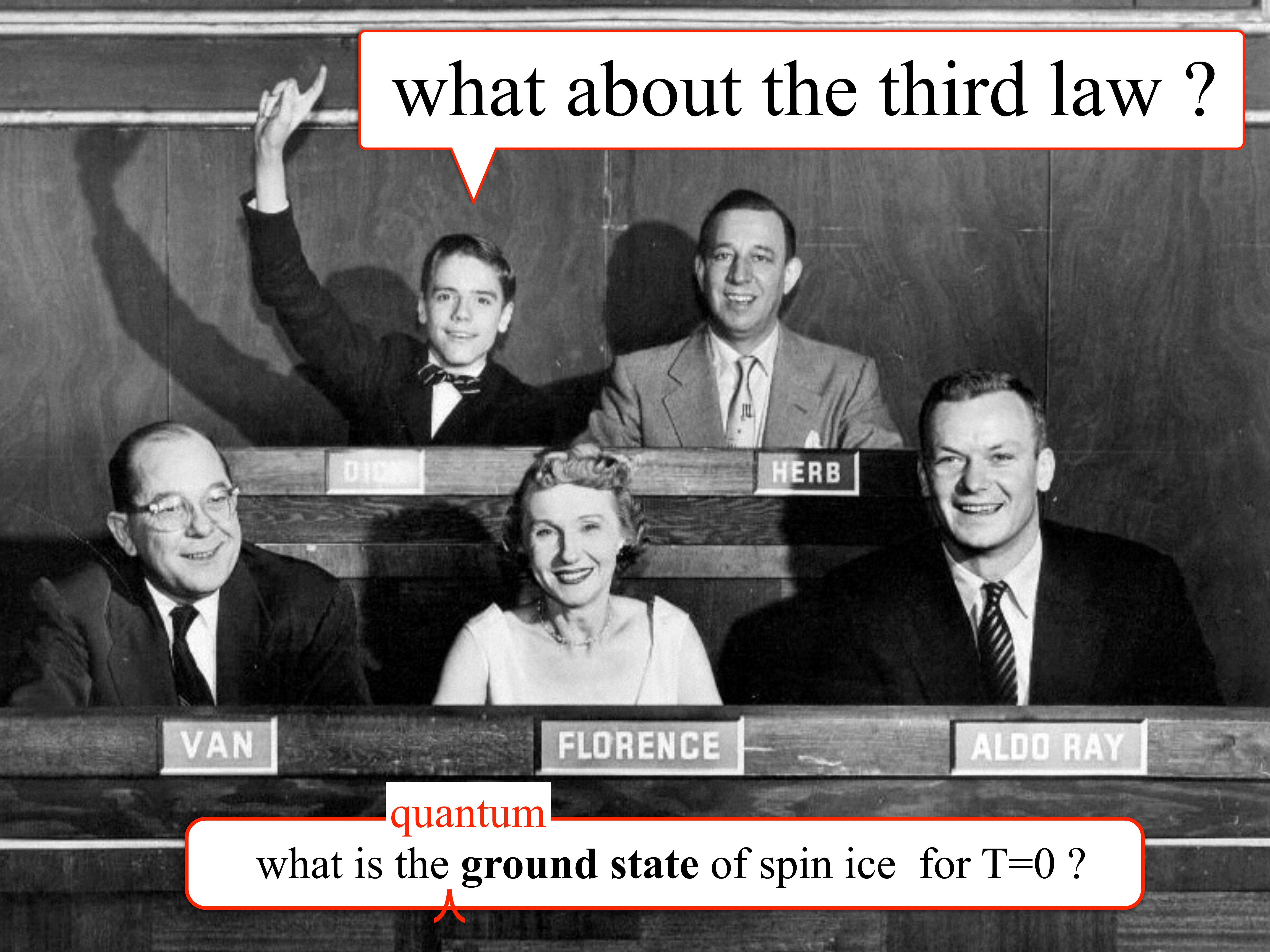


spin ice and its monopoles...



...discussed in all the most reputable sources of scientific information !

so what don’t we understand ?

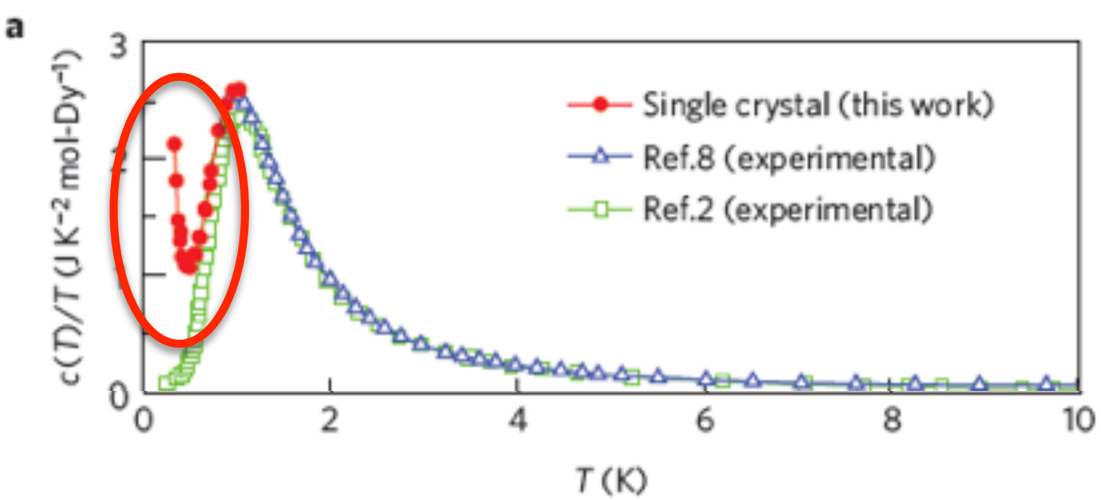

what about the third law ?
HERB
VAN
FLORENCE
ALDO RAY
quantum
what is the **ground state** of spin ice for T=0 ?

nature physics
LETTERS
PUBLISHED ONLINE: 7 APRIL 2013 | DOI: 10.1038/NPHYS2591

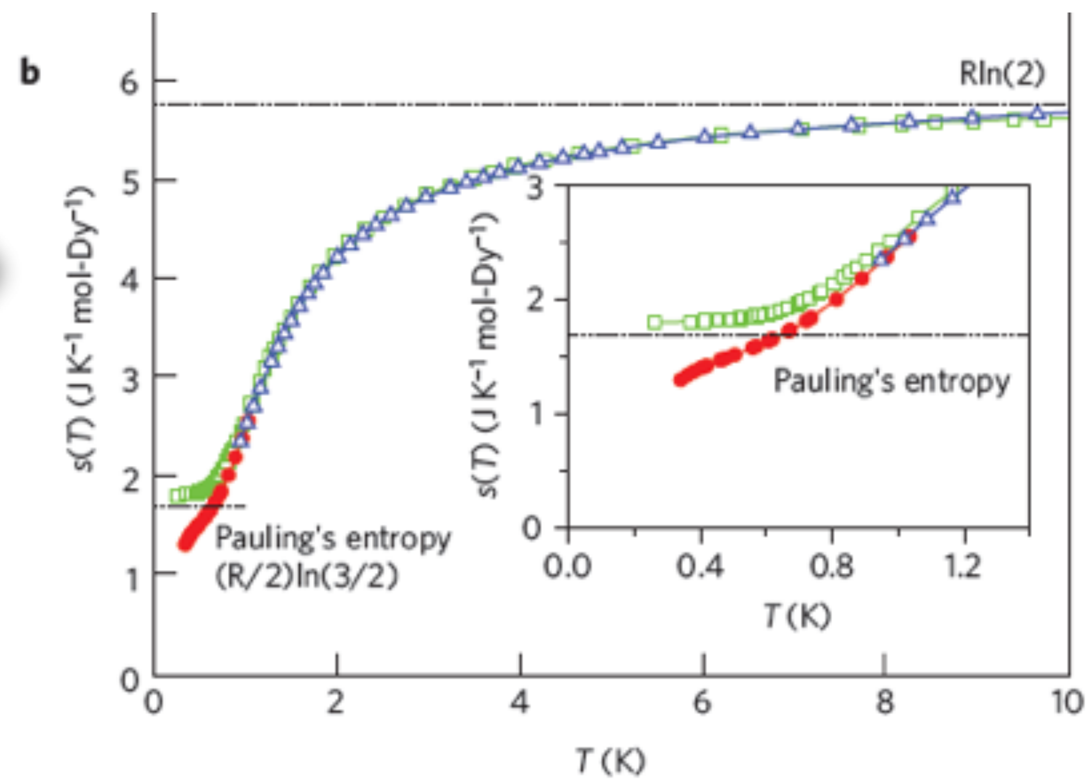
Absence of Pauling's residual entropy in thermally equilibrated $Dy_2Ti_2O_7$

D. Pomaranski[1,2,3], L. R. Yaraskavitch[1,2,3], S. Meng[1,2,3], K. A. Ross[4,5], H. M. L. Noad[4,5], H. A. Dabkowska[4,5], B. D. Gaulin[4,5,6] and J. B. Kycia[1,2,3]★

measurements of heat capacity of $Dy_2Ti_2O_7$ allowing up to one week (!) for thermalization at each temperature..



upturn in heat capacity below 500mK
⇒ onset of order ?



what is the **quantum** ground state of spin ice (in equilibrium) ?

what else is new ?

PRL 106, 187202 (2011) PHYSICAL REVIEW LETTERS 6 MAY 2011

Rods of Neutron Scattering Intensity in $Yb_2Ti_2O_7$: Compelling Evidence for Significant Anisotropic Exchange in a Magnetic Pyrochlore Oxide

Jordan D. Thompson,[1] Paul A. McClarty,[1] Henrik M. Rønnow,[2] Louis P. Regnault,[3] Andreas Sorge,[4,5] and Michel J. P. Gingras[1,5,6]

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,*]

ARTICLE
Received 27 Jan 2012 | Accepted 5 Jul 2012 | Published 7 Aug 2012 DOI: 10.1038/ncomms1989

Higgs transition from a magnetic Coulomb liquid to a ferromagnet in $Yb_2Ti_2O_7$

Lieh-Jeng Chang[1,2], Shigeki Onoda[3], Yixi Su[4], Ying-Jer Kao[5], Ku-Ding Tsuei[6], Yukio Yasui[7,8], Kazuhisa Kakurai[2] & Martin Richard Lees[9]

PRL 109, 097205 (2012) PHYSICAL REVIEW LETTERS week ending 31 AUGUST 2012

Vindication of $Yb_2Ti_2O_7$ as a Model Exchange Quantum Spin Ice

R. Applegate,[1] N. R. Hayre,[1] R. R. P. Singh,[1] T. Lin,[2] A. G. R. Day,[2,3] and M. J. P. Gingras[1,2,4]

ARTICLE
Received 4 Apr 2014 | Accepted 12 Aug 2014 | Published 18 Sep 2014 DOI: 10.1038/ncomms5970

Low-energy electrodynamics of novel spin excitations in the quantum spin ice $Yb_2Ti_2O_7$

LiDong Pan[1], Se Kwon Kim[1], A. Ghosh[1], Christopher M. Morris[1], Kate A. Ross[1,2], Edwin Kermarrec[3], Bruce D. Gaulin[3,4,5], S.M. Koohpayeh[1], Oleg Tchernyshyov[1] & N.P. Armitage[1]

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

Quantum Excitations in Quantum Spin Ice

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ARTICLE

Received 27 Jan 2012 | Accepted 5 Jul 2012 | Published

Higgs transition from ... to a ferromagnet in Y...

Lieh-Jeng Chang[1,2], Shigeki Onoda[3], Yixi Su[4] ... Kazuhisa Kakurai[2] & Martin Richard Lees[9]

spin ice goes quantum...

...ETTERS week ending 31 AUGUST 2012

...ange Quantum Spin Ice

R. Applegate,[1] N. R. Hayre,[1] R. R. P. Singh,[1] T. Lin,[2] A. G. R. Day,[2,3] and M. J. P. Gingras[1,2,4]

ARTICLE

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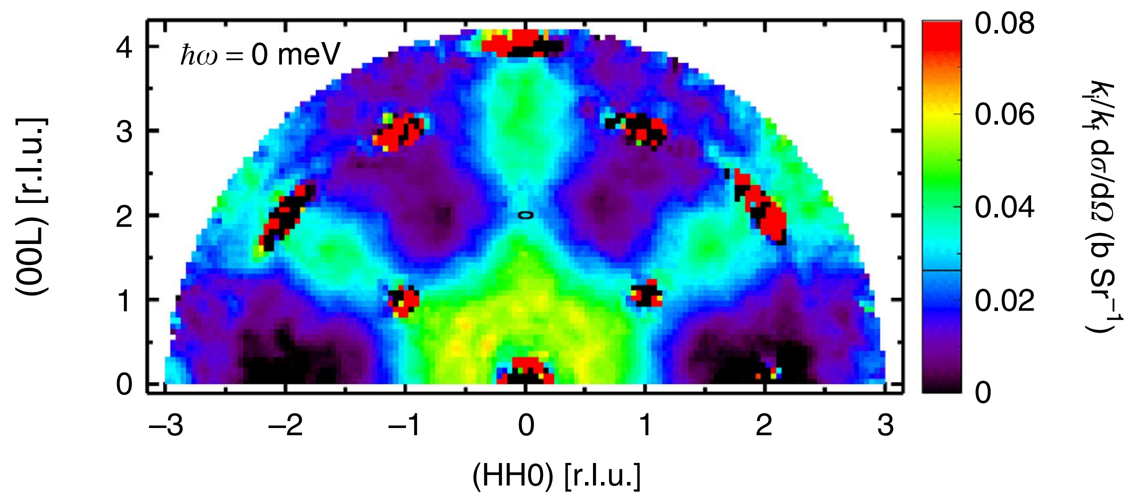
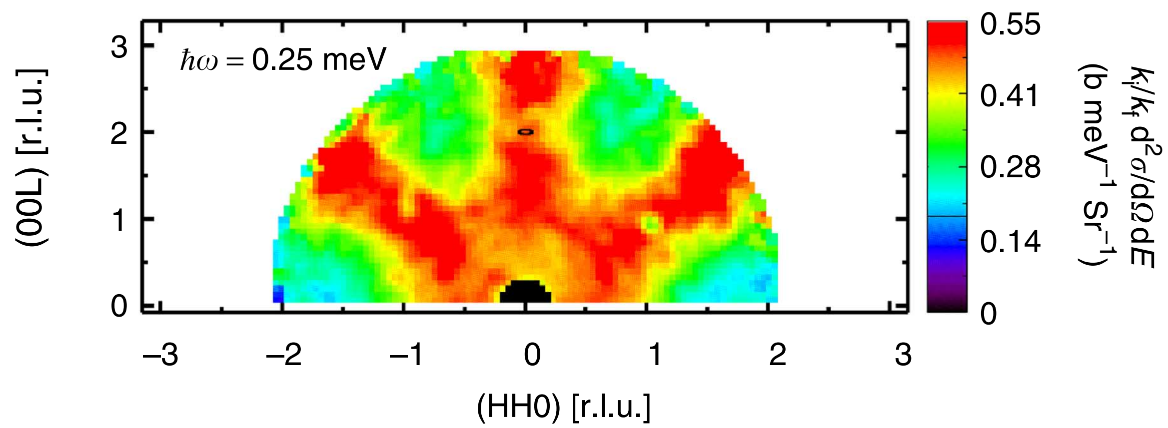
ARTICLE
Received 20 Sep 2012 | Accepted 18 Apr 2013 | Published 17 Jun 2013
DOI: 10.1038/ncomms2914

Quantum fluctuations in spin-ice-like $Pr_2Zr_2O_7$

K. Kimura[1], S. Nakatsuji[1,2], J.-J. Wen[3], C. Broholm[3,4,5], M.B. Stone[5], E. Nishibori[6] & H. Sawa[6]



elastic scattering suggests spin-ice correlations



but most scattering is inelastic - evidence of quantum monopole-dynamics ?

K. Kimura *et al*., Nat. Communs. **4**, 1934 (2013) possibility of a quantum spin-liquid with artificial light ?!!

possibility of a quantum spin-liquid with artificial light ?!!

PHYSICAL REVIEW B **69**, 064404 (2004)

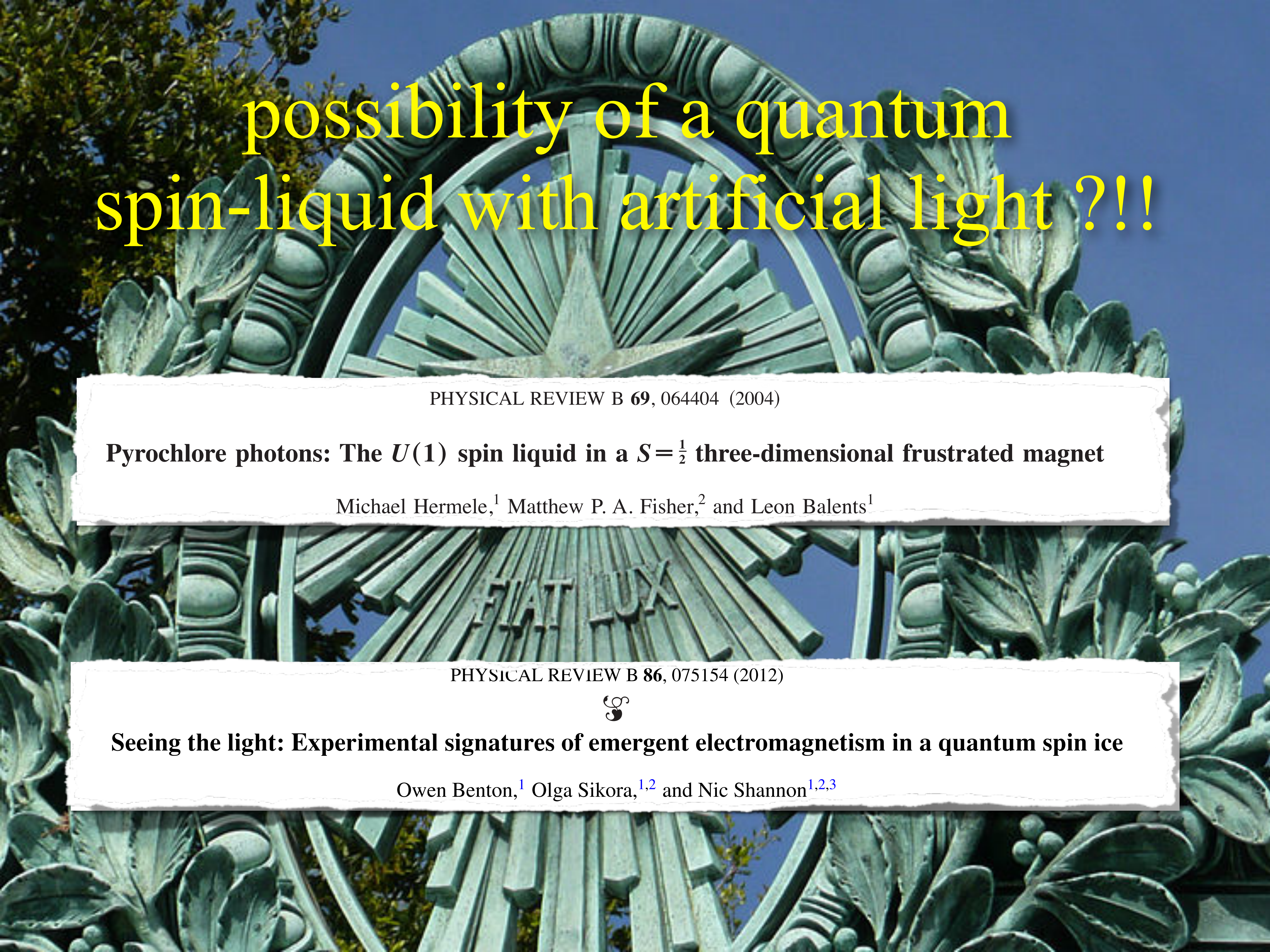
Pyrochlore photons: The $U(1)$ spin liquid in a $S=\frac{1}{2}$ three-dimensional frustrated magnet

Michael Hermele,[1] Matthew P. A. Fisher,[2] and Leon Balents[1]

PHYSICAL REVIEW B **86**, 075154 (2012)

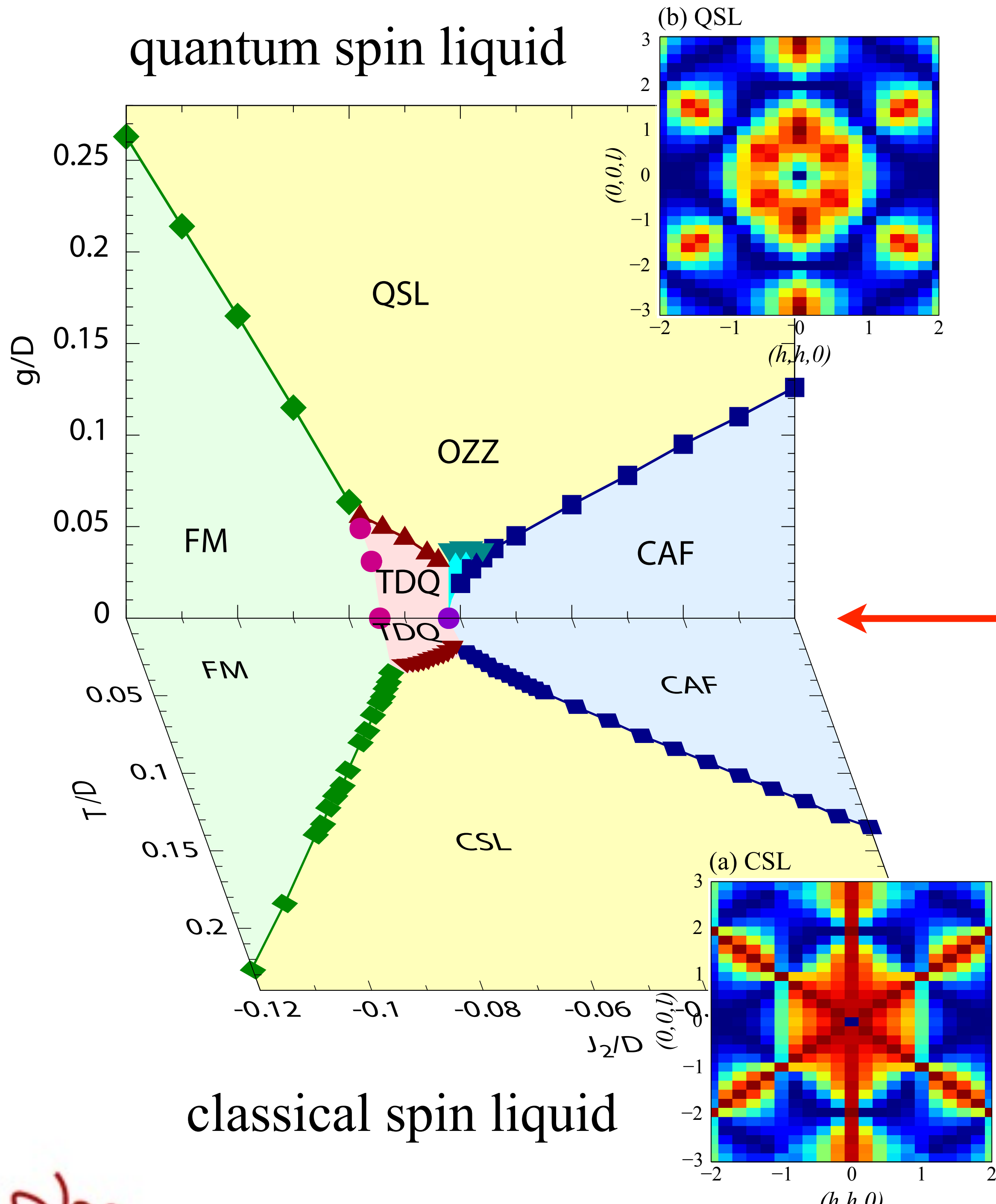
Seeing the light: Experimental signatures of emergent electromagnetism in a quantum spin ice

Owen Benton,[1] Olga Sikora,[1,2] and Nic Shannon[1,2,3]



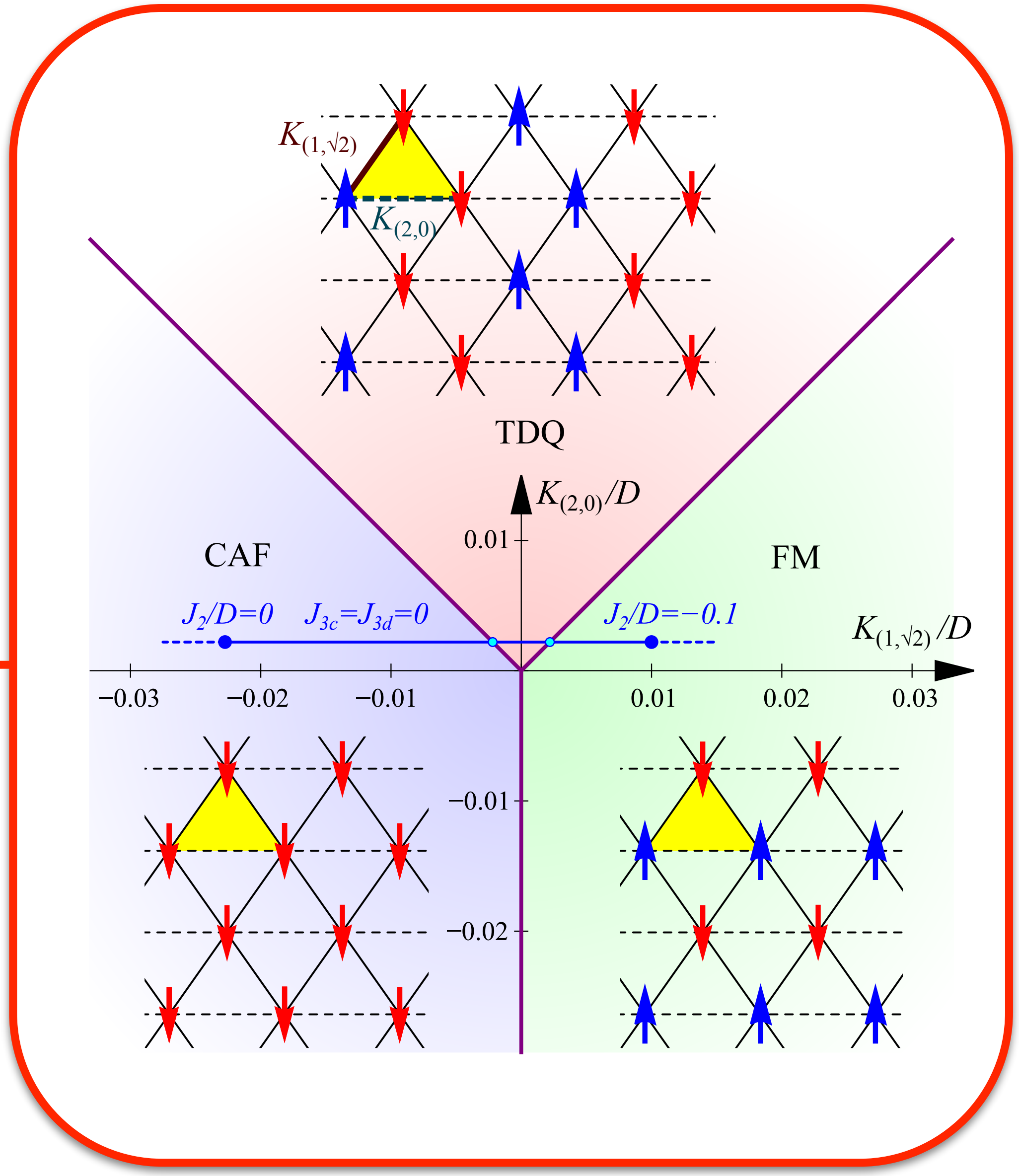
story for today : spin ice can do it all !

quantum spin liquid



classical spin liquid

ordered ground states



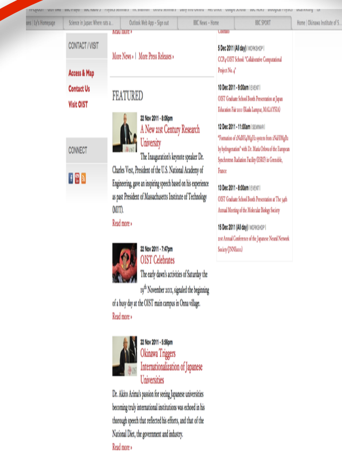
T=0, g=0

P. McClarty *et al.*, arXiv.1410.0451v1

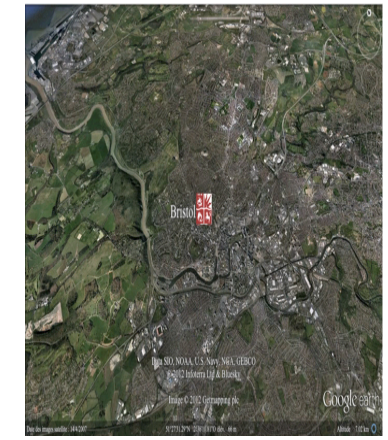
wouldn't have happened without…

Owen Benton
Bristol/OIST

Peter Fulde
MPI-PKS

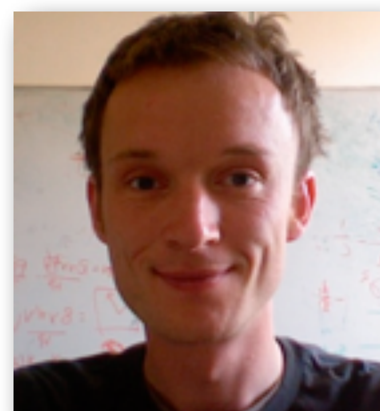


Paul McClarty
RAL



Roderich Moessner
MPI-PKS

Karlo Penc
Budapest



Frank Pollmann
MPI-PKS

Olga Sikora
NTU

EPSRC Engineering and Physical Sciences Research Council

OTKA

OIST OKINAWA INSTITUTE OF SCIENCE AND TECHNOLOGY GRADUATE UNIVERSITY

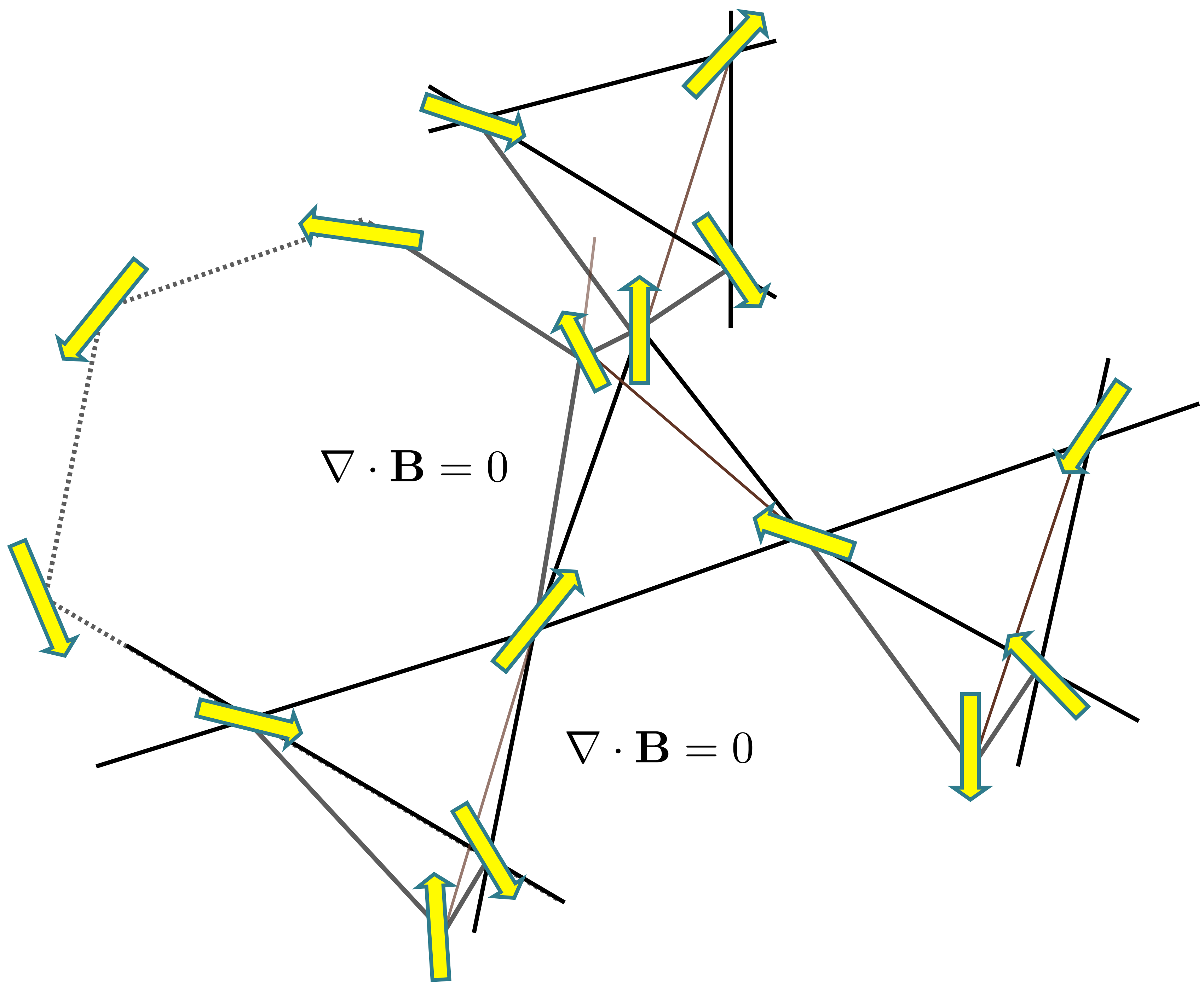
what effect does quantum mechanics have on ice ?

$$\hbar \neq 0$$

$\Rightarrow$ tunnelling between ice states


there are many flavours of ice...
leading
...but, within the ice manifold, only one form
^
of dynamics

what kind of dynamics are there in ice ?



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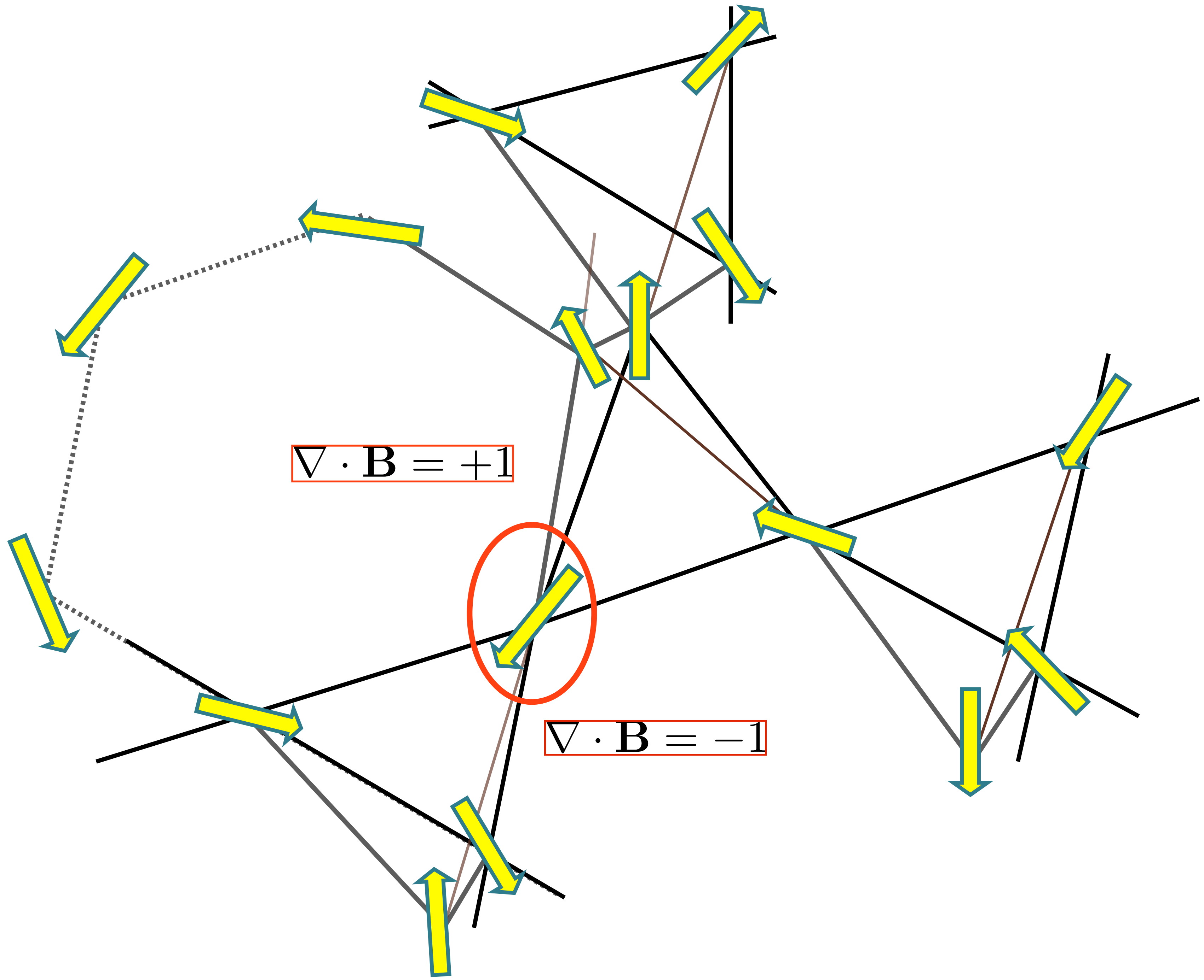

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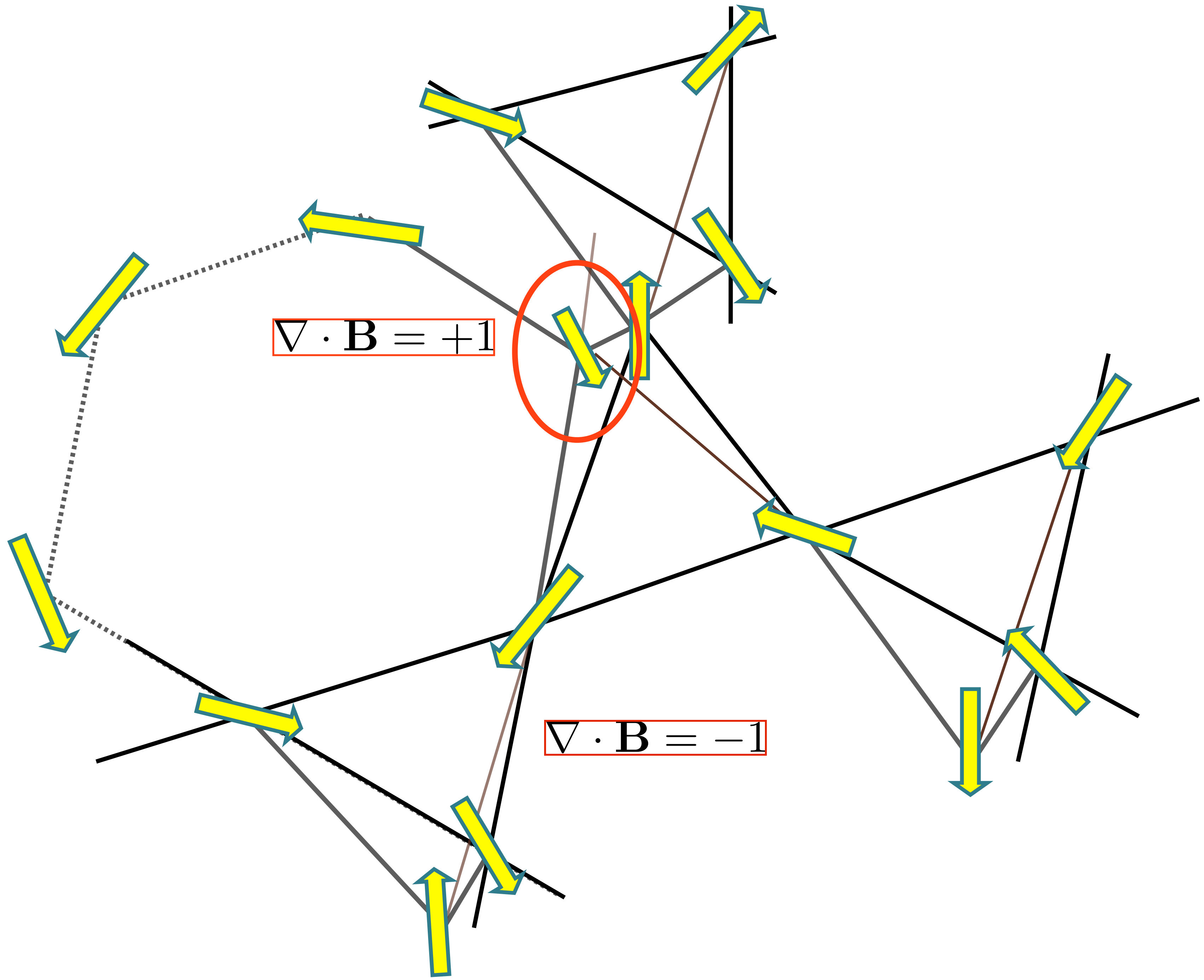

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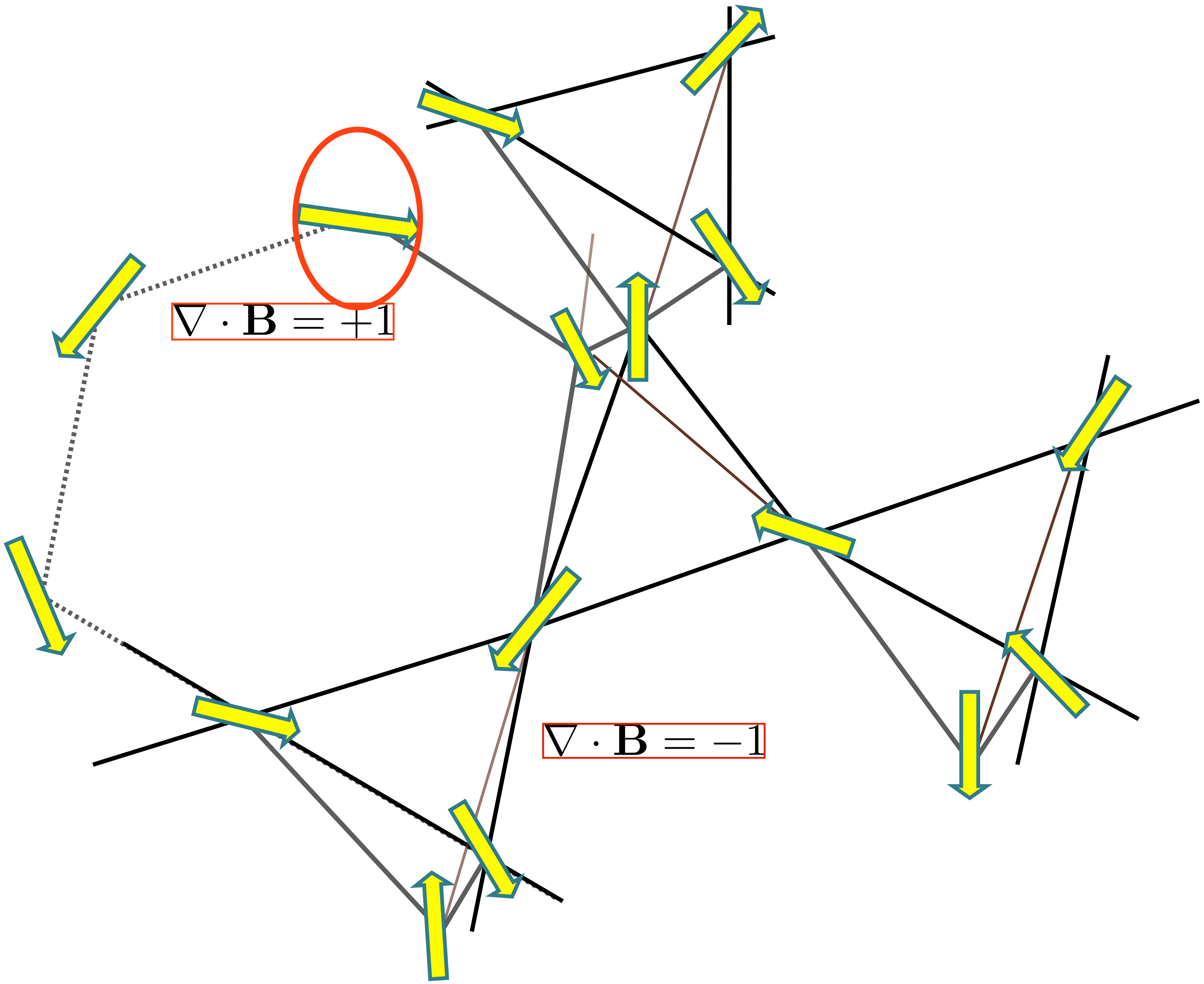

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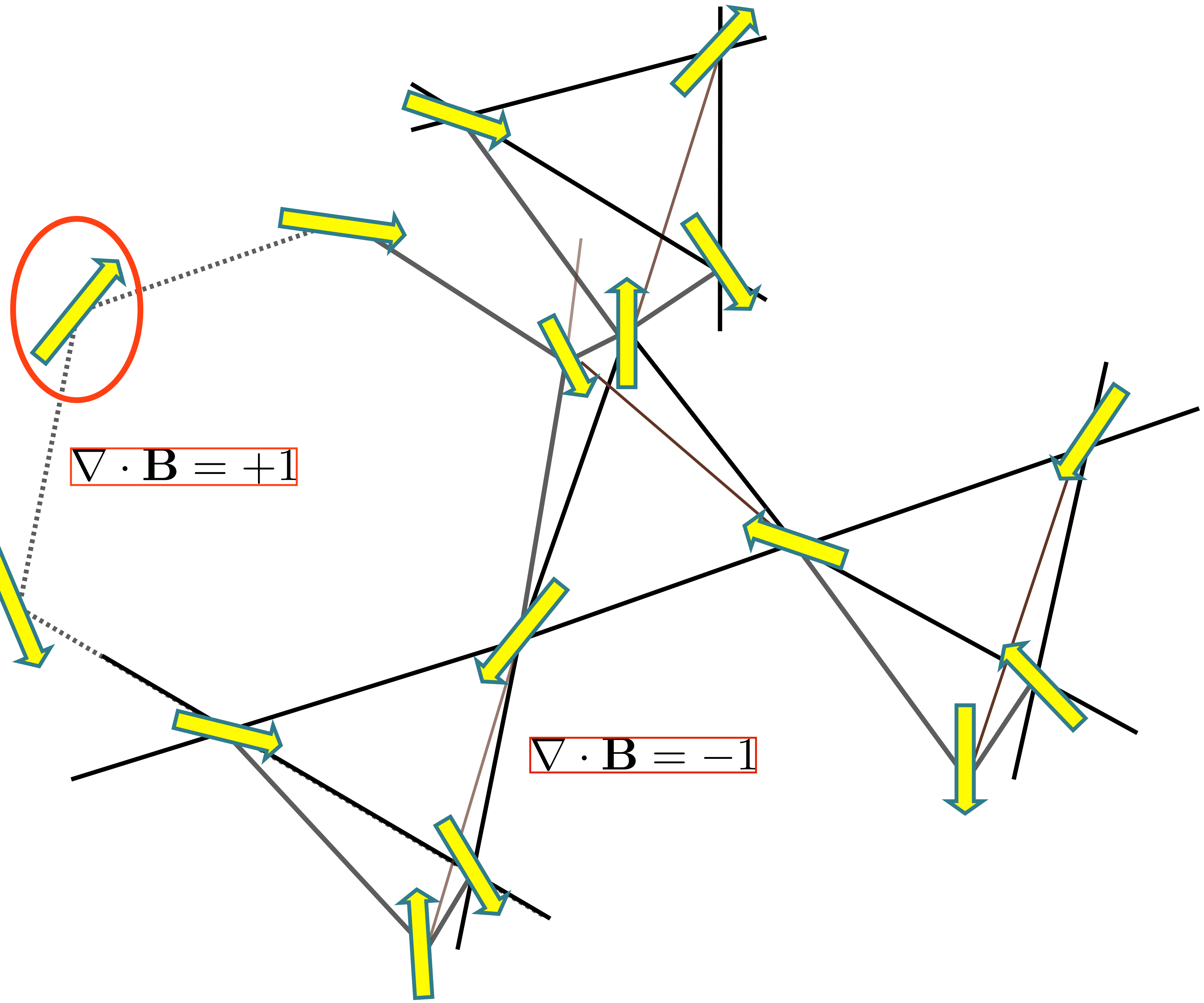

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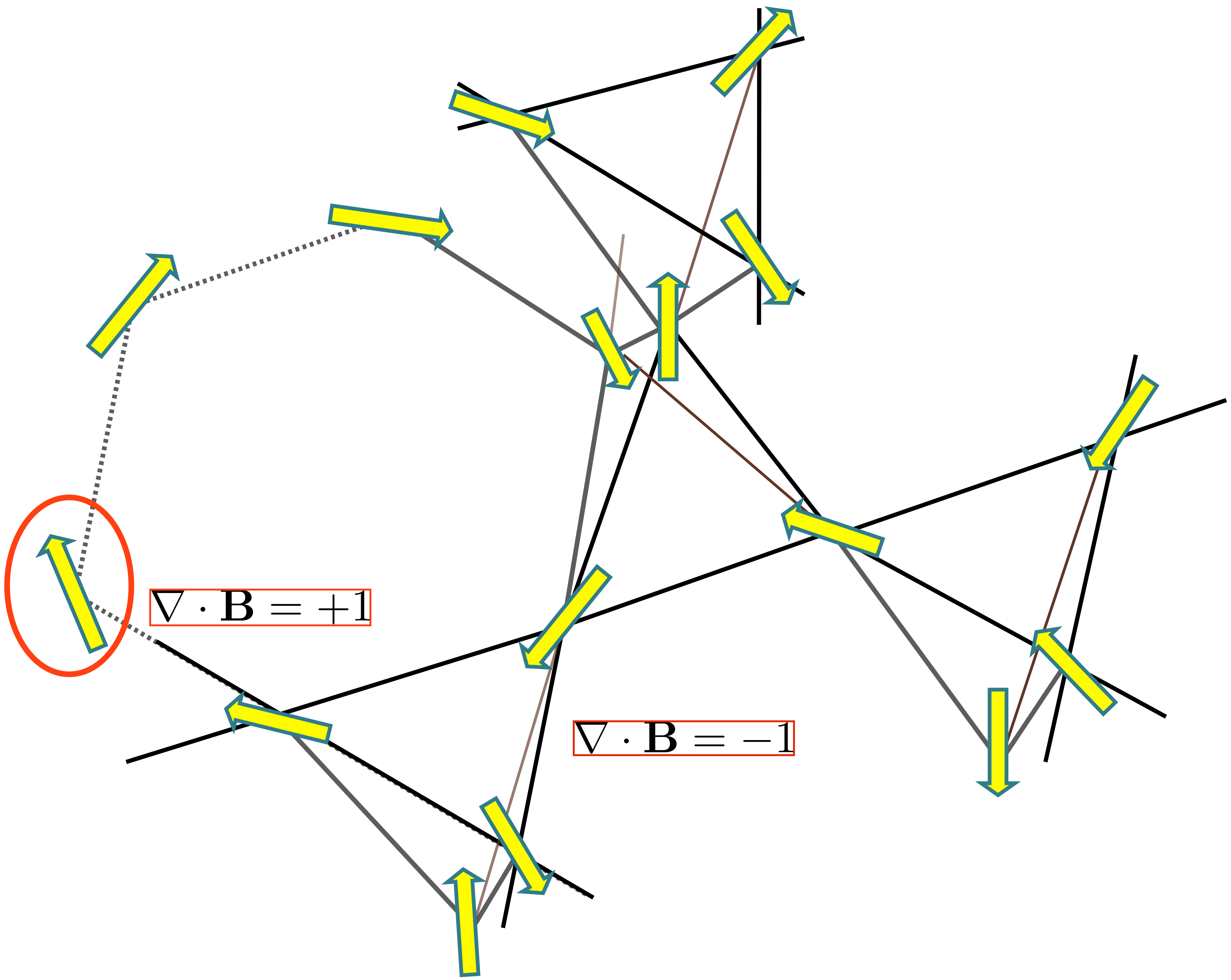

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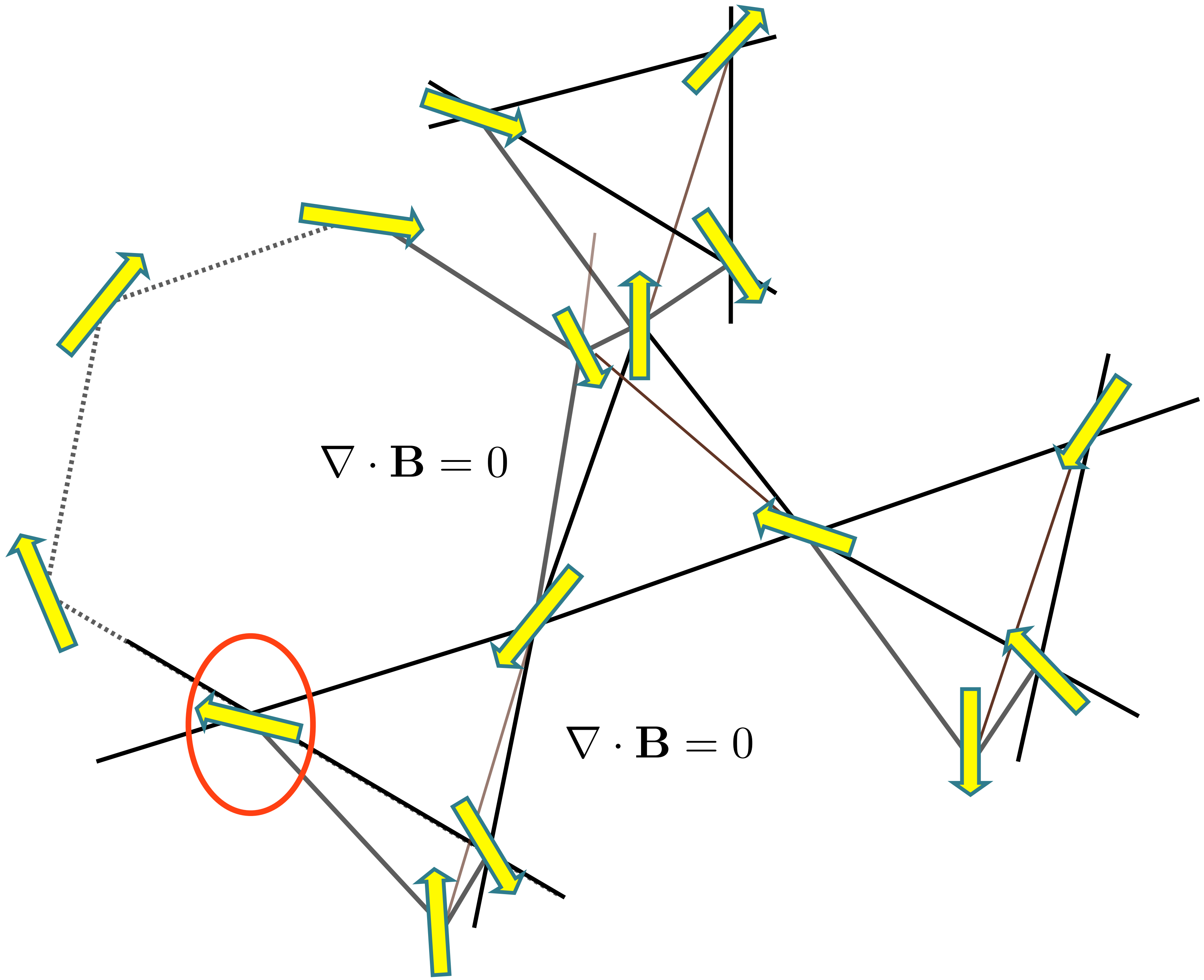
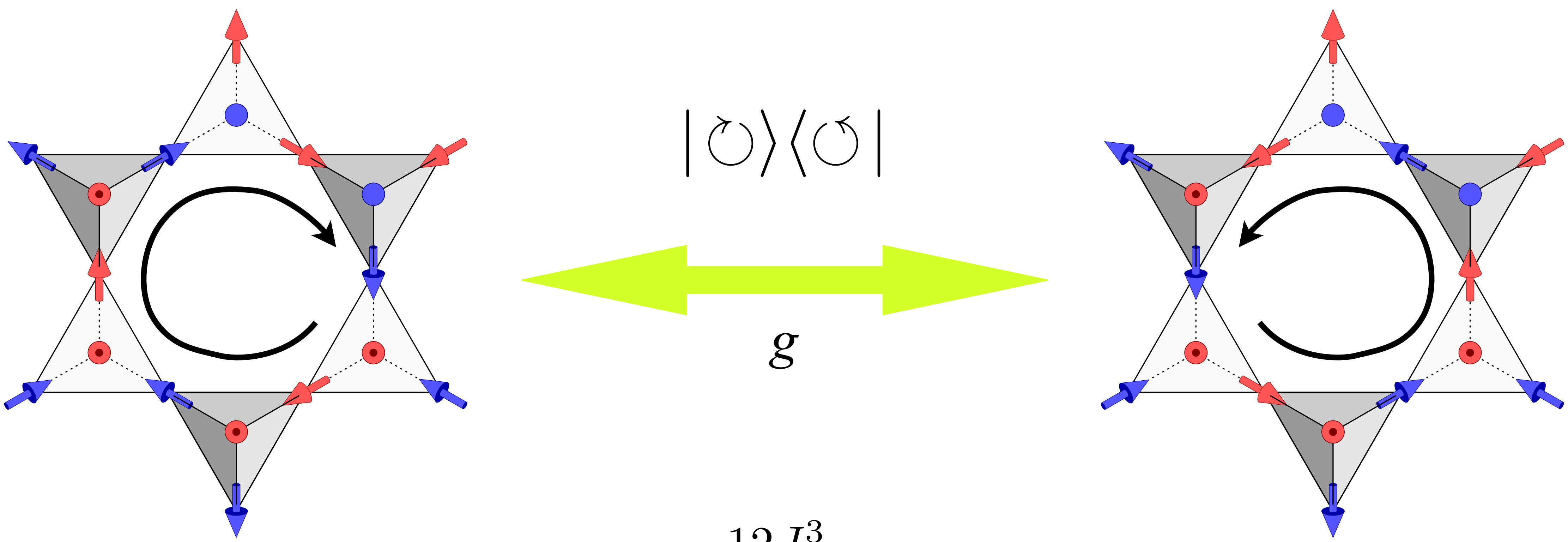


what kind of dynamics are there in ice ?

circulation of “magnetic” field on hexagon swaps sense



$$g_{\mathrm{Yb_2Ti_2O_7}} \approx \frac{12J_{\pm}^3}{J_{zz}^2} \approx 0.05\mathrm{meV}$$

what is the effect of this tunnelling ?

PHYSICAL REVIEW B **69**, 064404 (2004)

Pyrochlore photons: The $U(1)$ spin liquid in a $S=\frac{1}{2}$ three-dimensional frustrated magnet

Michael Hermele,[1] Matthew P. A. Fisher,[2] and Leon Balents[1]

S=1/2 easy-axis magnet on a pyrochlore lattice...

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

strong anisotropy

$$J_{zz} \gg J_{\pm}$$

selects ice manifold

Hamiltonian acting on ice states...

$$\mathcal{H} = -g \sum_{\hexagon} |\circlearrowright\rangle\langle\circlearrowleft| + |\circlearrowleft\rangle\langle\circlearrowright| + \mu \sum_{\hexagon} |\circlearrowright\rangle\langle\circlearrowright| + |\circlearrowleft\rangle\langle\circlearrowleft|$$

degenerate perturbation theory

$$g = \frac{12 J_{\pm}^3}{J_{zz}^2}$$

...add extra term which makes model exactly soluble for μ=g

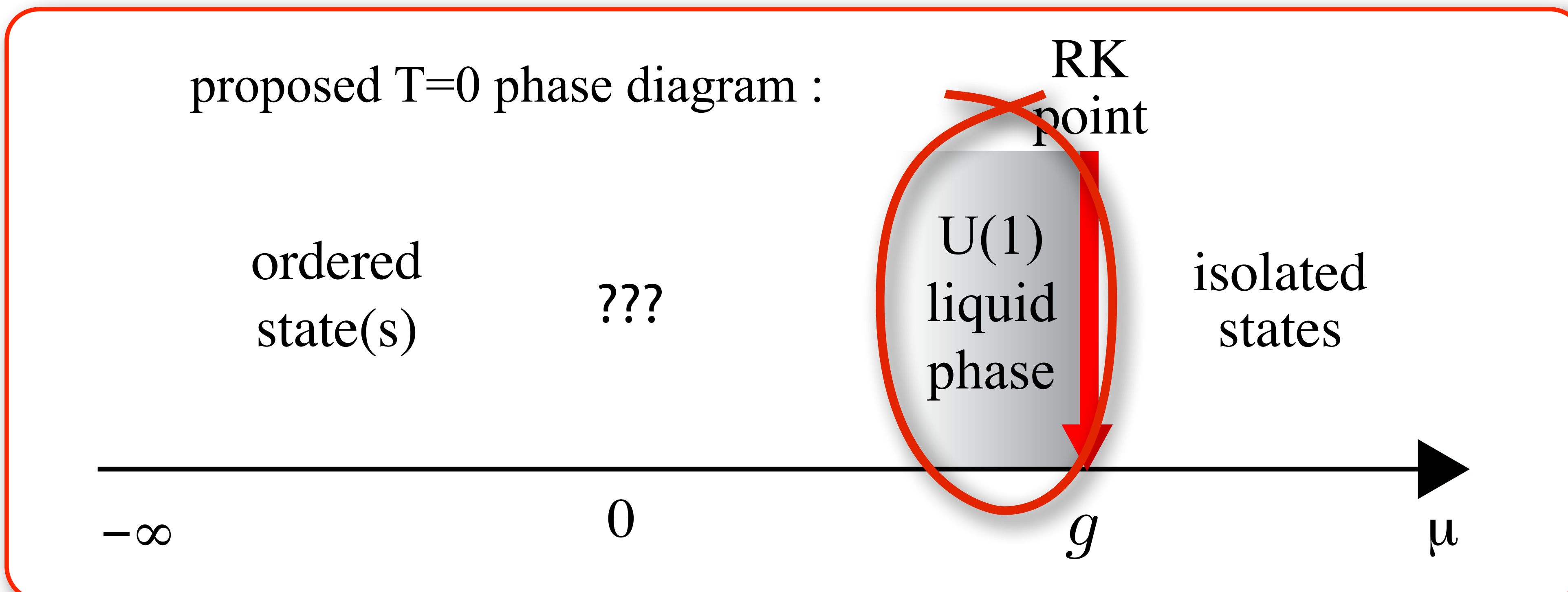
PHYSICAL REVIEW B **69**, 064404 (2004)

Pyrochlore photons: The $U(1)$ spin liquid in a $S=\frac{1}{2}$ three-dimensional frustrated magnet

Michael Hermele,[1] Matthew P. A. Fisher,[2] and Leon Balents[1]

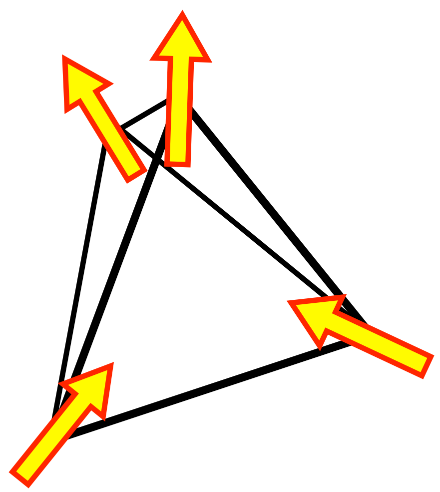
$$\mathcal{H}_\mu = -g\sum_{\hexagon} |\circlearrowright\rangle\langle\circlearrowleft| + |\circlearrowleft\rangle\langle\circlearrowright| + \mu\sum_{\hexagon} |\circlearrowright\rangle\langle\circlearrowright| + |\circlearrowleft\rangle\langle\circlearrowleft|$$

…argue for U(1)-liquid phase, based on properties of **exactly soluble point** μ=g



...equivalent proposal for 3D Quantum Dimer Model :
R. Moessner and S Sondhi, Phys. Rev. B **68**, 184512 (2003)

so what's a quantum U(1) liquid ?



$\nabla.\mathbf{B} = 0$ ...by **explicit construction**

solve as : $\mathbf{B} = \nabla \times \mathbf{A}$ and chose Coulomb gauge : $\nabla.\mathbf{A} = 0$

quantum ice has **local dynamics** :

$$\mathcal{H} = -g \sum_{\hexagon} |\circlearrowright\rangle\langle\circlearrowleft| + |\circlearrowleft\rangle\langle\circlearrowright|$$

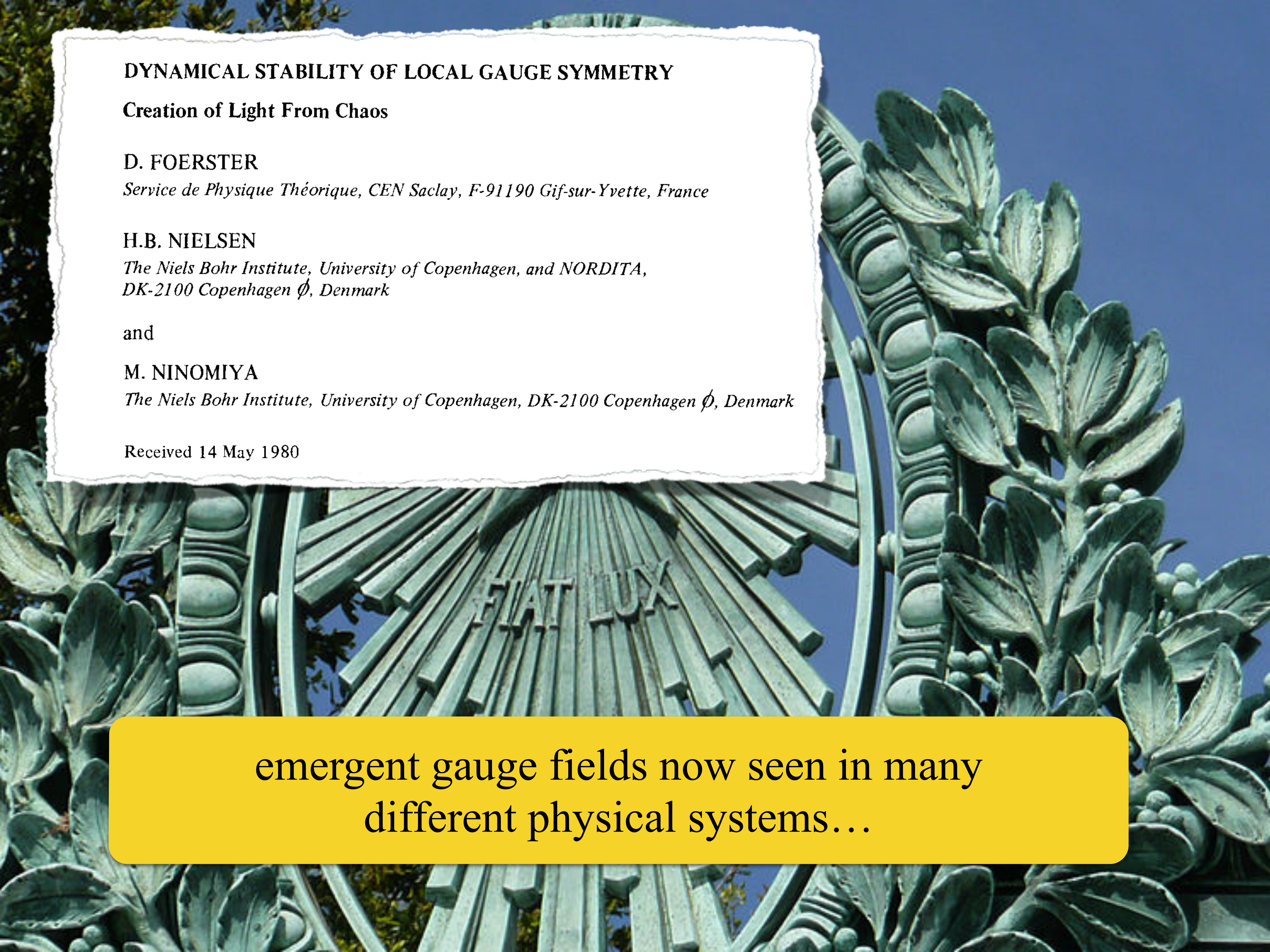
tunneling between ice states ⇒ gauge field varies in time

simplest guess for effective field theory in a liquid phase is **Maxwell** action :

$$S = \int d^3x dt \left[\mathbf{E}^2 - c^2\mathbf{B}^2\right]$$

$$\partial_t \mathbf{A} - \nabla A_0$$


FIAT LUX



DYNAMICAL STABILITY OF LOCAL GAUGE SYMMETRY

Creation of Light From Chaos

D. FOERSTER
Service de Physique Théorique, CEN Saclay, F-91190 Gif-sur-Yvette, France

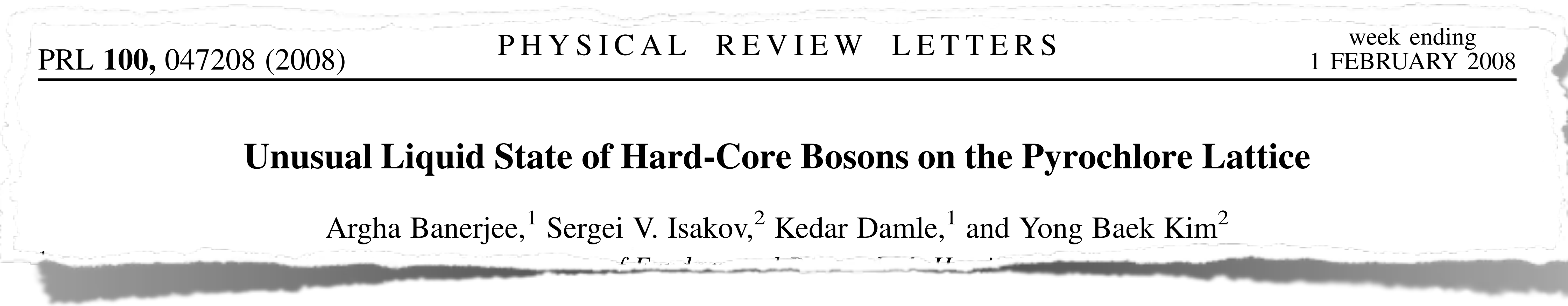
H.B. NIELSEN
The Niels Bohr Institute, University of Copenhagen, and NORDITA, DK-2100 Copenhagen Ø, Denmark

and

M. NINOMIYA
The Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen Ø, Denmark

Received 14 May 1980

so does the idea work here ?


PRL **100,** 047208 (2008) PHYSICAL REVIEW LETTERS week ending 1 FEBRUARY 2008

Unusual Liquid State of Hard-Core Bosons on the Pyrochlore Lattice

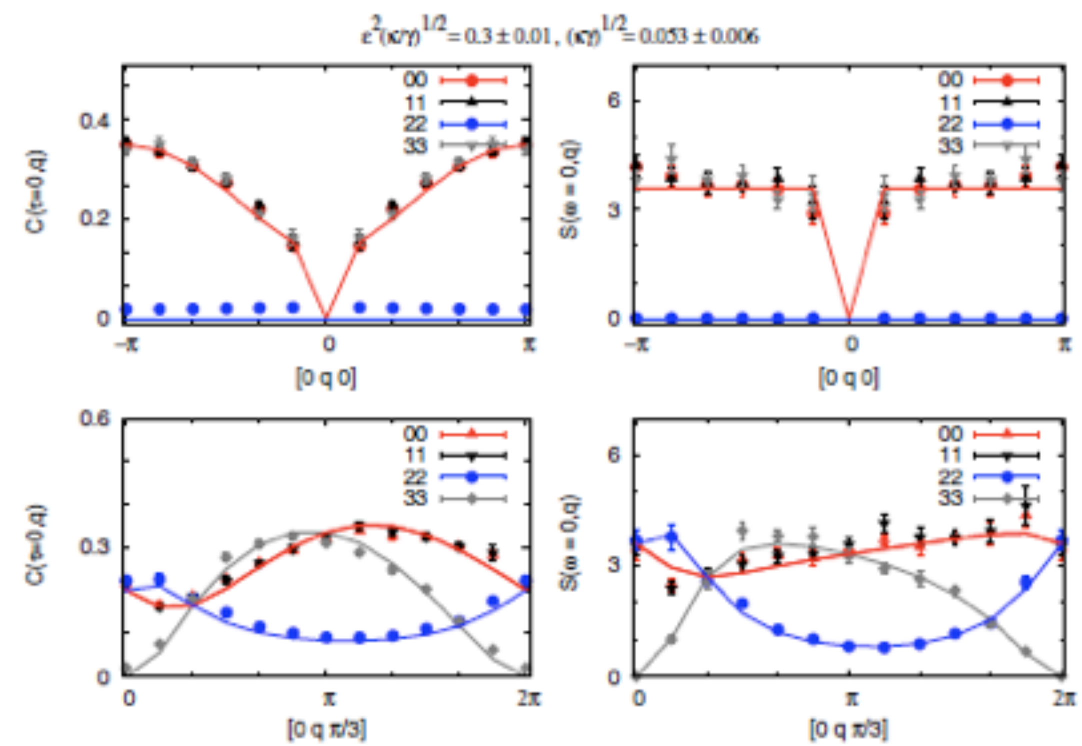
Argha Banerjee,[1] Sergei V. Isakov,[2] Kedar Damle,[1] and Yong Baek Kim[2]

consider hard-core Bosons with
strong nearest neighbour
interactions V >> t
on a pyrochlore lattice

$$\mathcal{H}_{\text{charge-ice}} = -t\sum_{\langle ij\rangle}\left(b_i^\dagger b_j + b_j^\dagger b_i\right) + V\sum_{\langle ij\rangle}\left(n_i - \frac{1}{2}\right)\left(n_j - \frac{1}{2}\right)$$

quantum charge ice with tunneling

$$g = 12t^3/V^2$$



finite temperature correlation functions, calculated using QMC [T ≈ g], and compared to the predictions of a U(1) gauge theory

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PRL **100,** 047208 (2008) PHYSICAL REVIEW LETTERS week ending 1 FEBRUARY 2008

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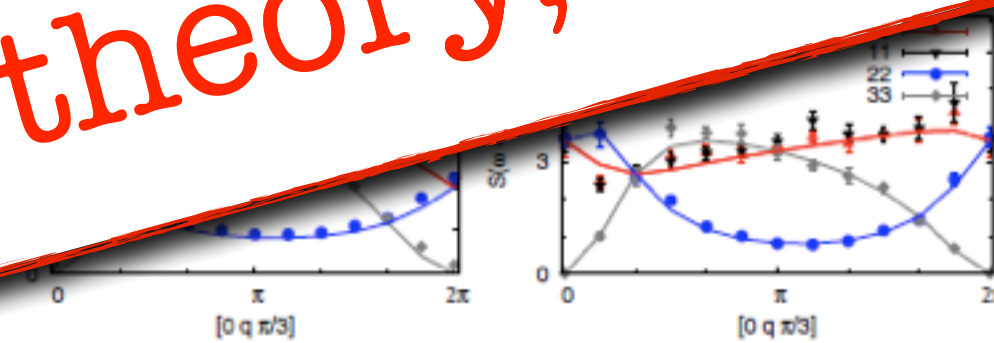
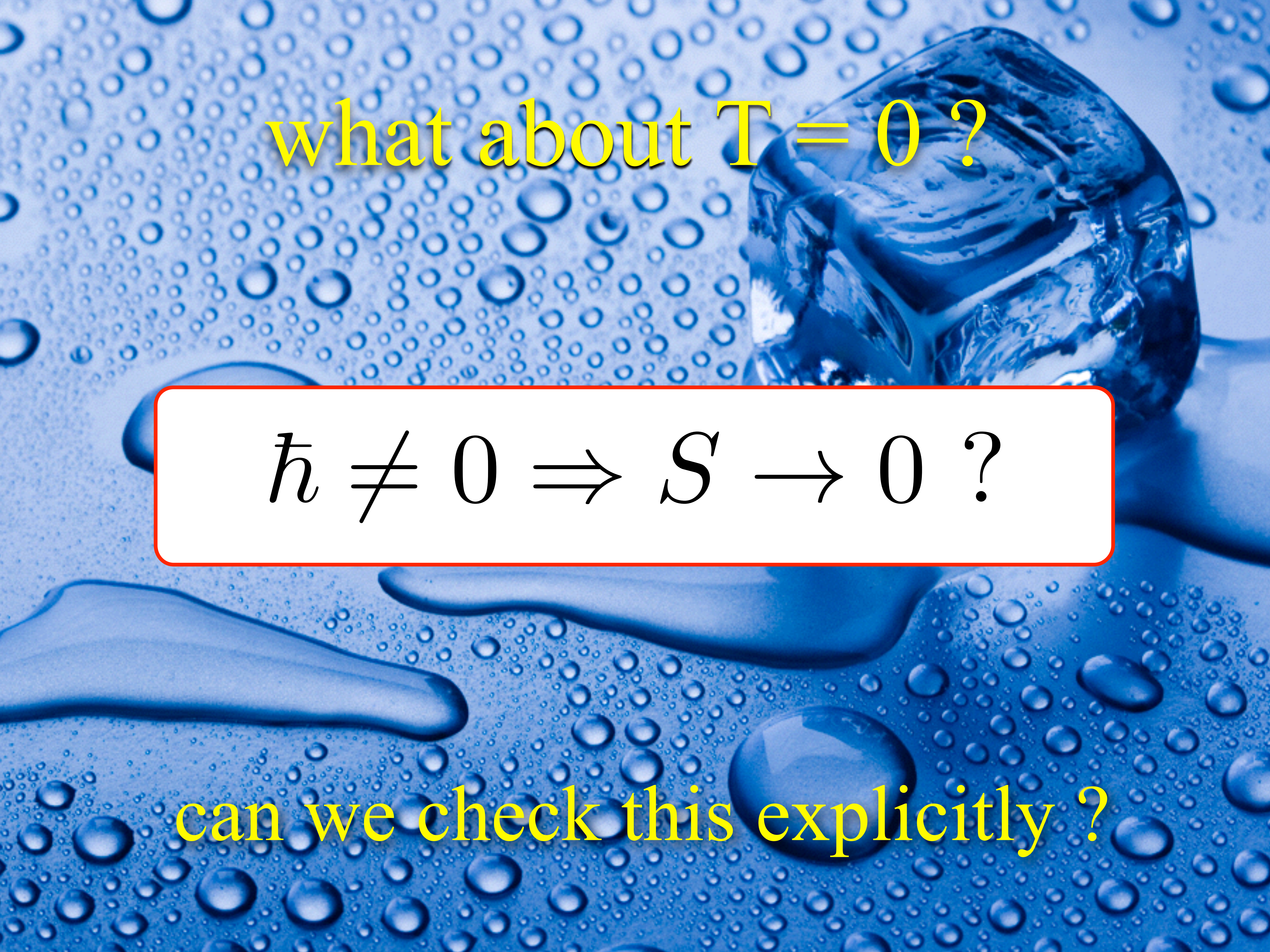
q ce with tunneling

$$g = 12t^3/V^2$$

quantitive agreement with prediction of U(1) gauge theory, T>0



finite-temperature correlation functions, calculated using QMC [T ≈ g], and compared to the predictions of a U(1) gauge theory



what about T = 0 ?

$$\hbar \neq 0 \Rightarrow S \to 0\ ?$$

can we check this explicitly ?

...some CPU-centuries later

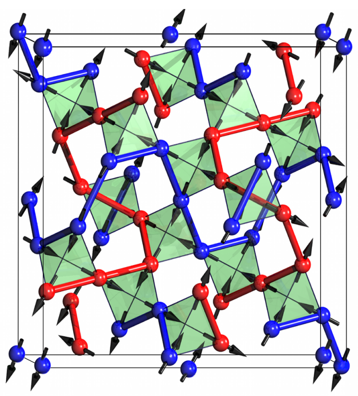
PRL **108**, 067204 (2012) PHYSICAL REVIEW LETTERS week ending 10 FEBRUARY 2012

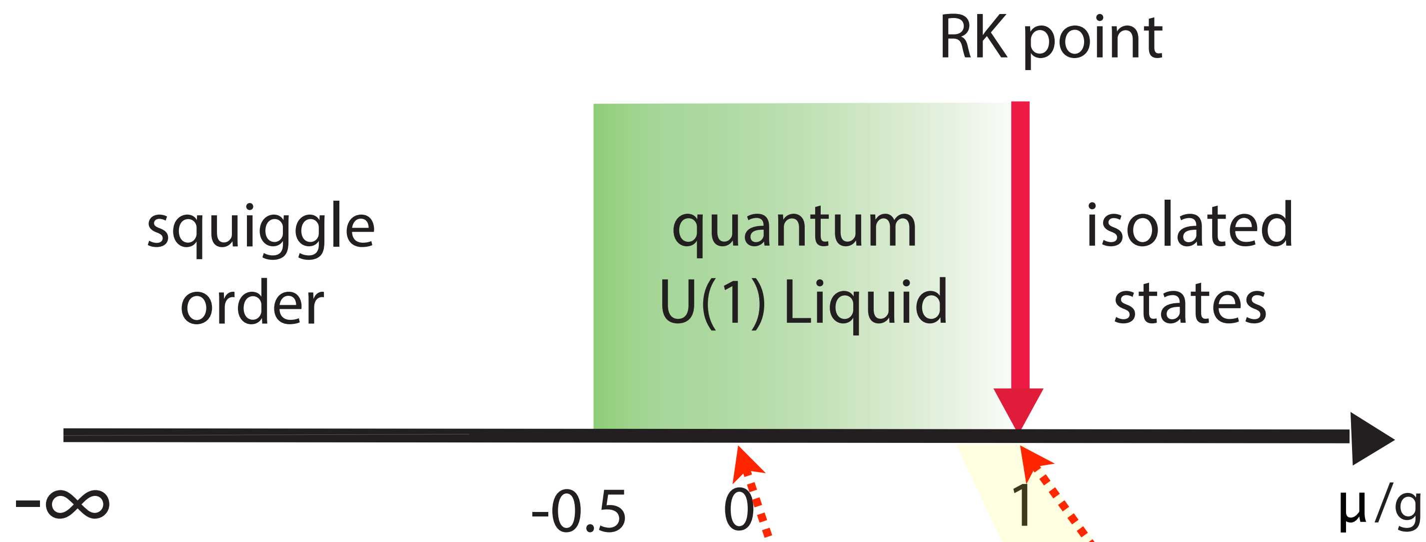
Quantum Ice: A Quantum Monte Carlo Study

Nic Shannon,[1] Olga Sikora,[1] Frank Pollmann,[2] Karlo Penc,[3] and Peter Fulde[2,4]

consider minimal model with RK-point, acting on spin-ice states…

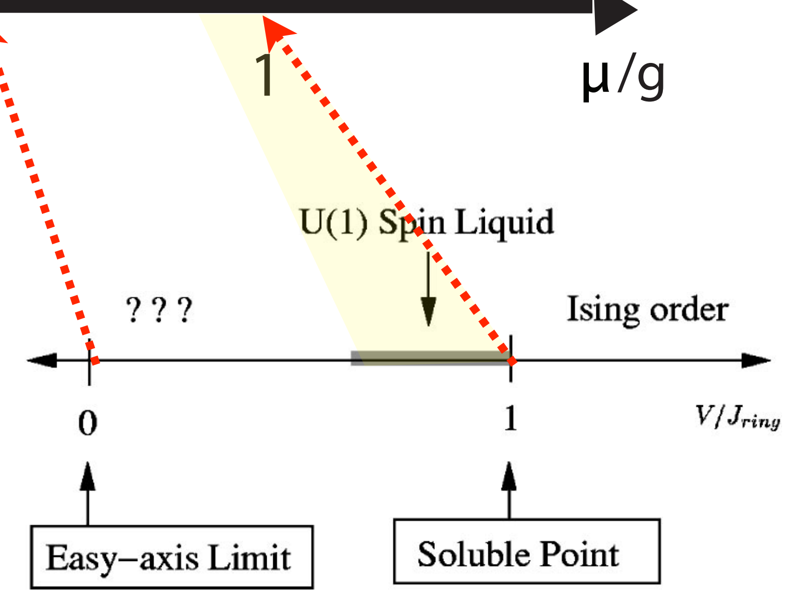
$$\mathcal{H}_\mu = -g \sum_{\hexagon} |\circlearrowright\rangle\langle\circlearrowleft| + |\circlearrowleft\rangle\langle\circlearrowright| + \mu \sum_{\hexagon} |\circlearrowright\rangle\langle\circlearrowright| + |\circlearrowleft\rangle\langle\circlearrowleft|$$





ice entropy absorbed into unique quantum ground state

cf. M. Hermele *et al.*, Phys. Rev. B **69**, 064404 (2012)



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PRL **108,** 067204 (2012) PHYSICAL REVIEW LETTERS week ending 10 FEBRUARY 2012

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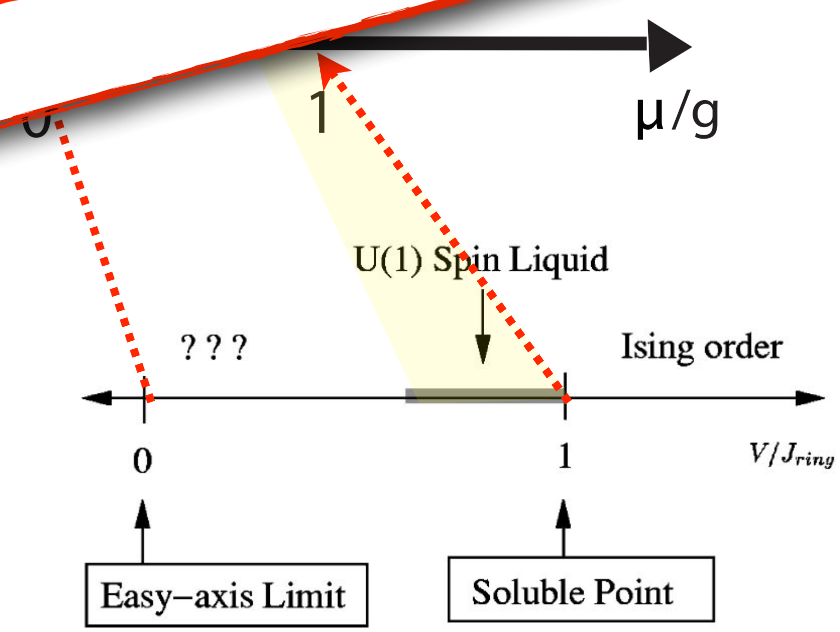
consider minimal model with RK-point, a...

$\mathcal{H}_\mu = -g \sum | \circlearrowright \rangle \langle \circlearrowleft | \ldots$

quantitive agreement with prediction of U(1) gauge theory, T=0

ic... abso... uniqu... ground state

cf. M. Hermele *et al.*, Phys. Rev. B **69**, 064404 (2012)

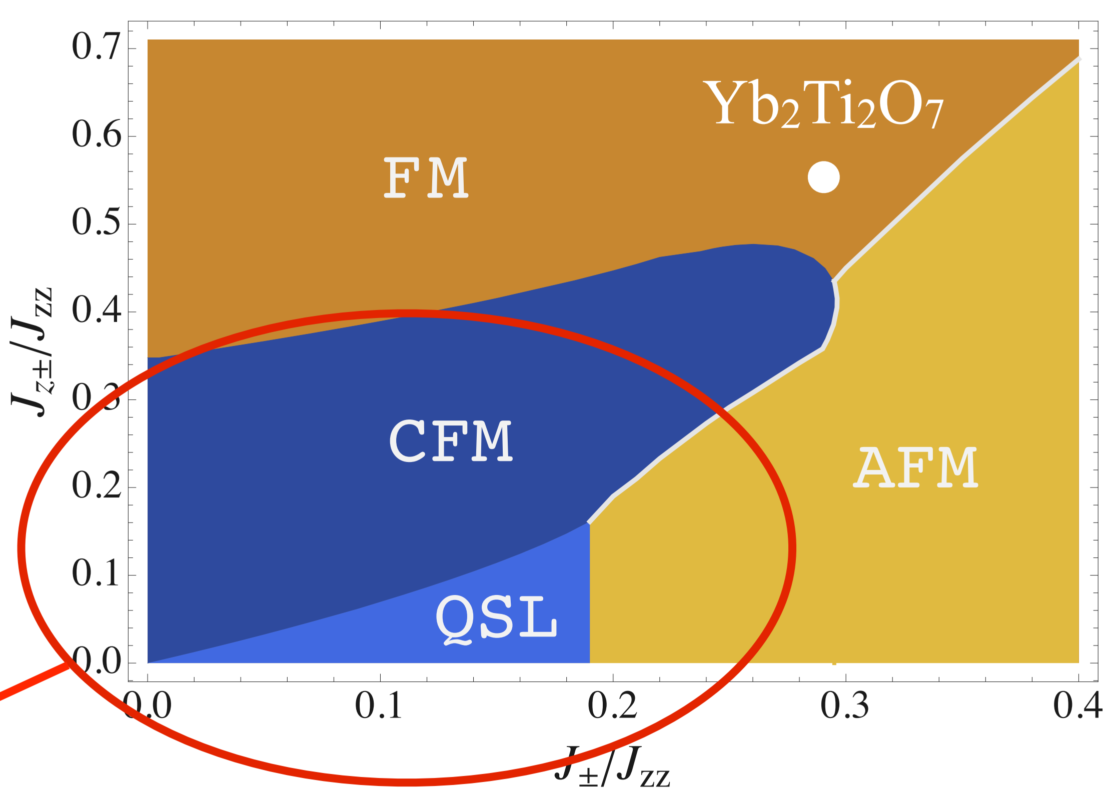


valid for more general interactions ?

general model for exchange between spin-1/2 ions on a pyrochlore lattice has 4 independent parameters

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

phase diagram within “Gauge mean field theory” :



L. Savary and L. Balents, Phys. Rev. Lett **108**, 037202 (2012)

quantum spin liquids derived from spin ice

N.B. see also :
S. Onoda *et al.*, Phys. Rev. B **83**, 094411 (2011)
S.-B. Lee *et al.*, Phys. Rev. B **86**, 104412 (2012)

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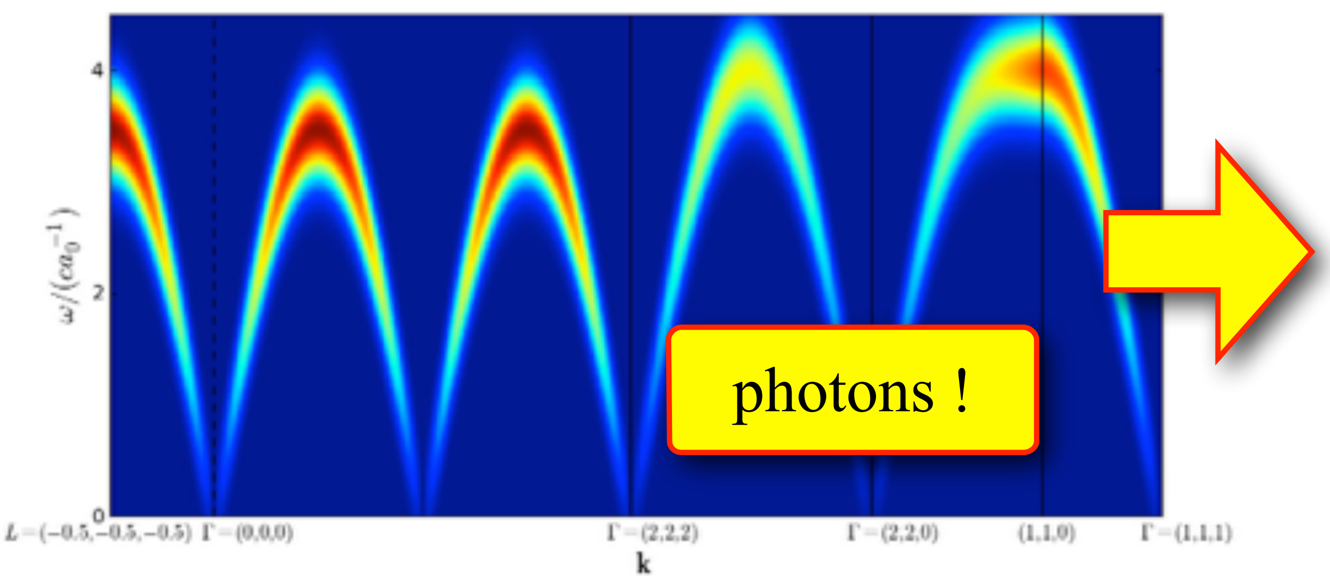
what would this look like in experiment ?

consider minimal model for a quantum spin ice…

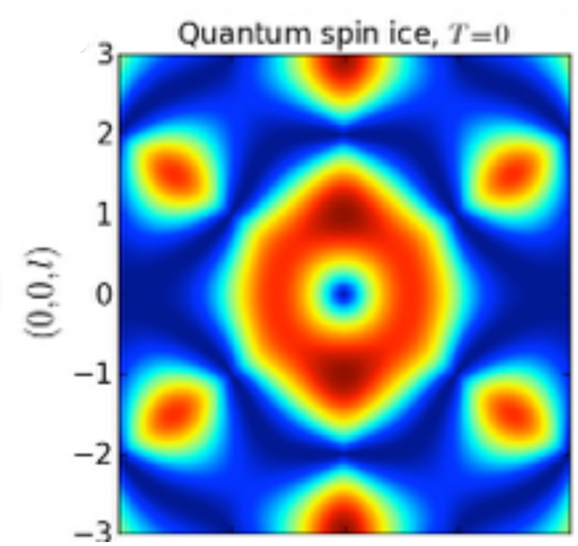
$$\mathcal{H}_{\text{tunneling}} = -g \sum_{\hexagon} |\circlearrowright\rangle\langle\circlearrowleft| + |\circlearrowleft\rangle\langle\circlearrowright| \qquad \text{(acting on spin-ice states)}$$

…parameterize lattice gauge theory from quantum Monte Carlo simulation

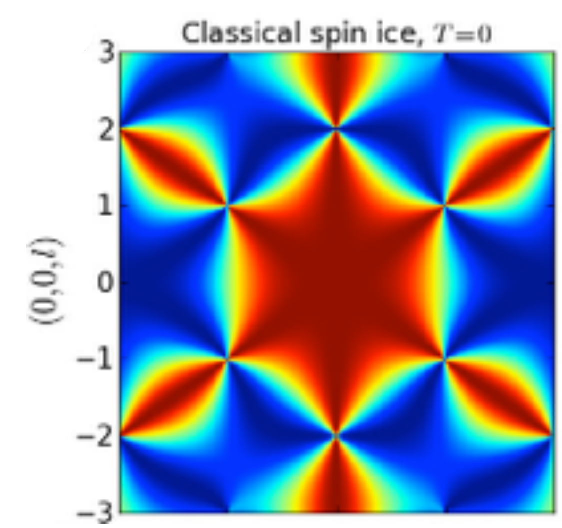
prediction for inelastic neutron scattering



prediction for quasi-elastic neutron scattering



v.



pinch points are suppressed !

O. Benton *et al.*, Phys. Rev. B. **86**, 075174 (2012) ❦

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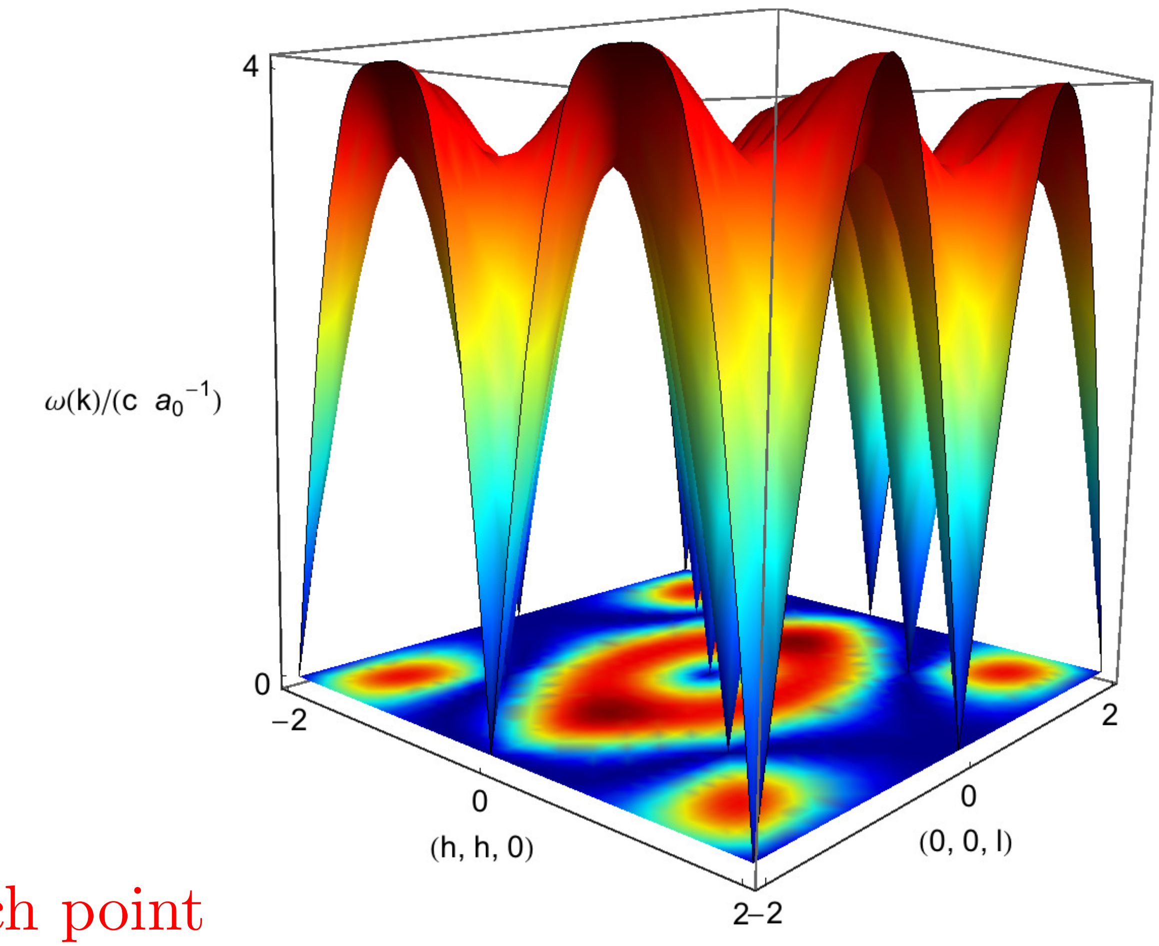
where did the pinch-points go ?

quasi-elastic neutron scattering measures the equal-time structure factor:

$$S^{\alpha\beta}(\mathbf{q}) = \int d\omega\, S^{\alpha\beta}(\mathbf{q},\omega)$$

prediction of lattice gauge theory :



additional factor of q

pinch point

$$S^{\alpha\beta}(\mathbf{q}) \propto \langle \mathcal{B}_\alpha(-\mathbf{q})\mathcal{B}_\beta(\mathbf{q})\rangle = \frac{8\pi^4 q}{c}\left[\delta_{\alpha\beta} - \frac{q_\alpha q_\beta}{q^2}\right]\coth\left(\frac{cq}{2T}\right)$$

thermal excitation of photons

O. Benton *et al.*, Phys. Rev. B. **86**, 075174 (2012) ❦

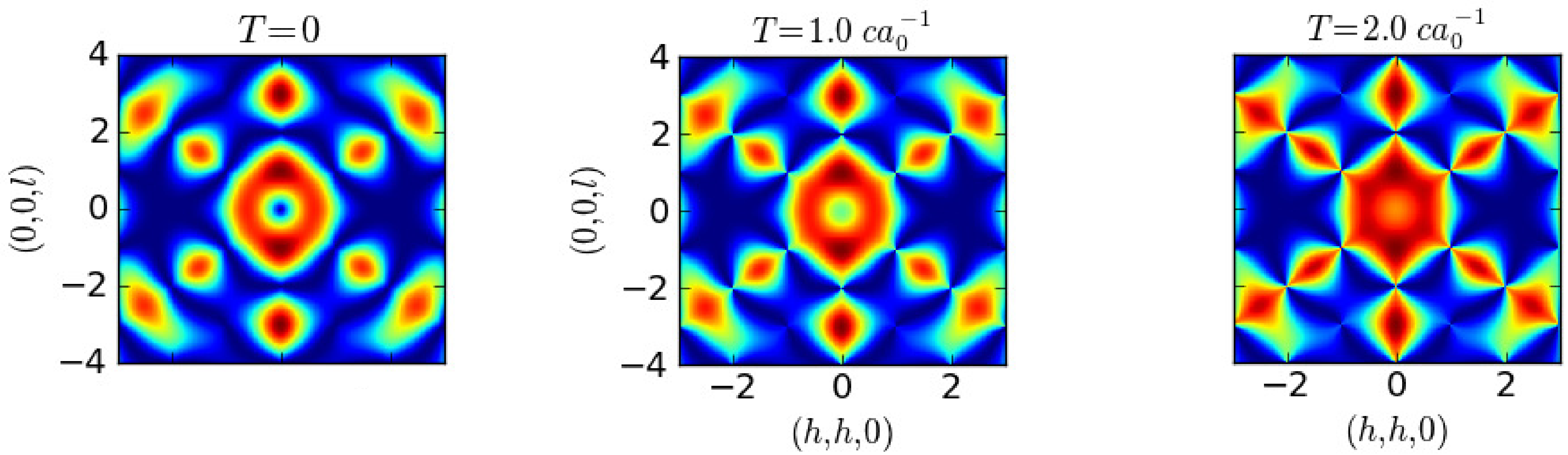
how does this connect with (classical) spin-ice ?

simplest scenario is a **crossover**, controlled by the **thermal excitation of photons**

i.e. see classical correlations for $\mathbf{q} \ll \frac{1}{\lambda_T}$ where **thermal de Broglie wavelength** $\lambda_T = \frac{\pi c}{T}$

thermal correction to quantum correlations at low T :

$$S^{\alpha\beta}(\mathbf{q} \approx 0) \propto T \left[\delta_{\alpha\beta} - \frac{q_\alpha q_\beta}{q^2}\right]$$



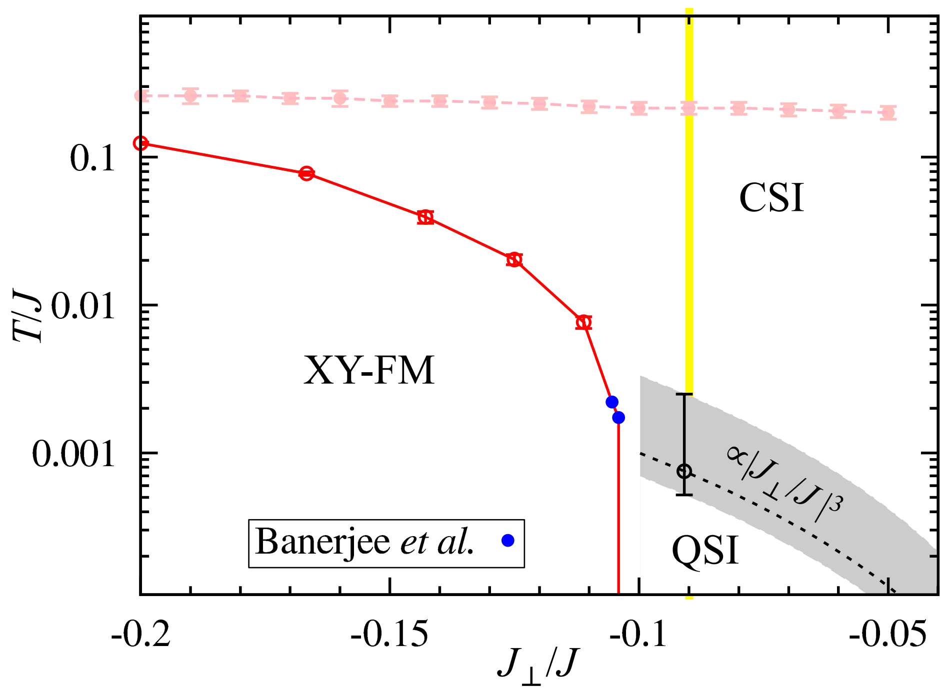
...i.e. pinch-points are progressively restored at finite T

O. Benton *et al.*, Phys. Rev. B. **83**, 075174 (2012) ❦

is this seen in simulation ?

$$\mathcal{H} = \sum_{\langle ij \rangle} \left[J S_i^z S_j^z + J_\perp \left(S_i^x S_j^x + S_i^y S_j^y \right) \right]$$

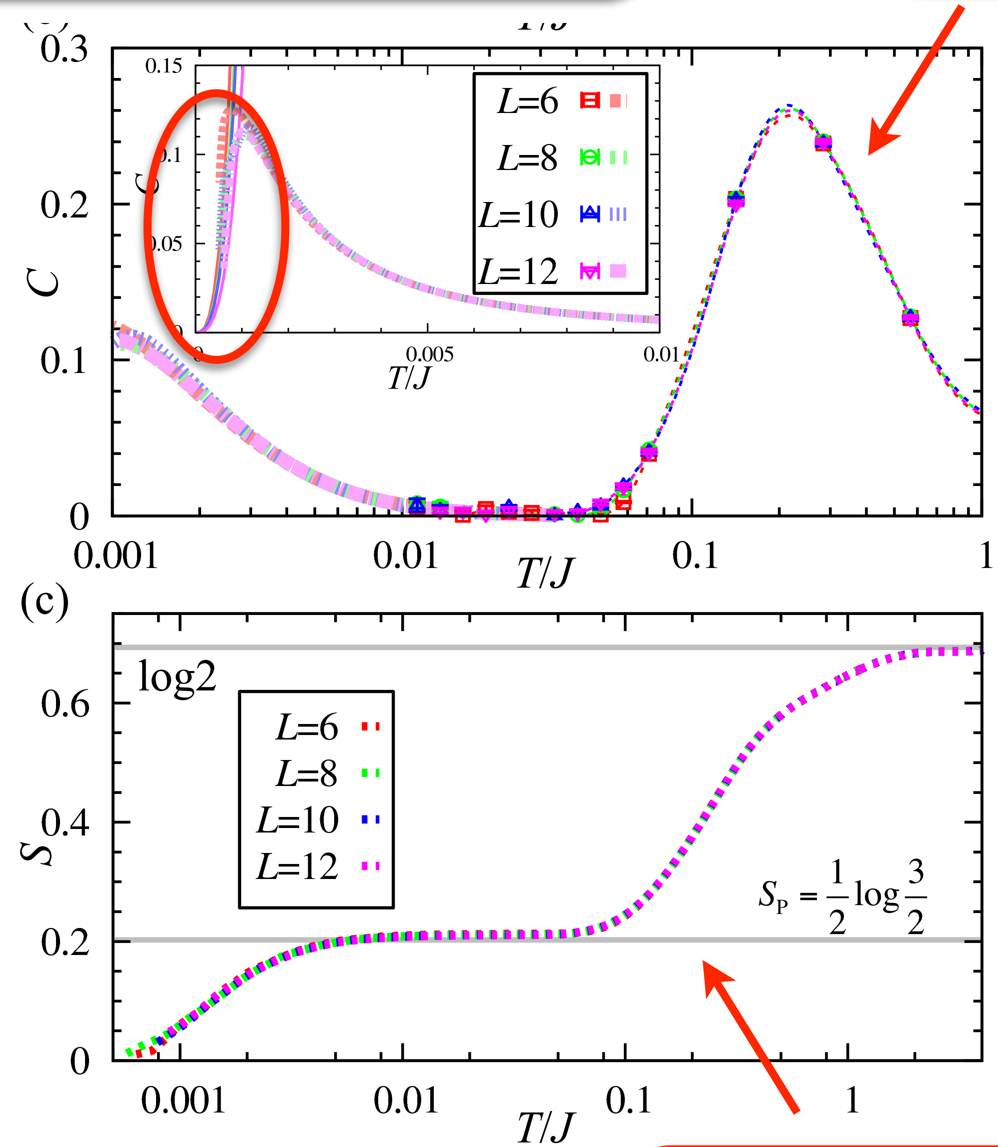
…finite-temperature QMC



$J_\perp / J = -1/11$

T^3 at low-T ⇒ photons ✓

spin-ice peak

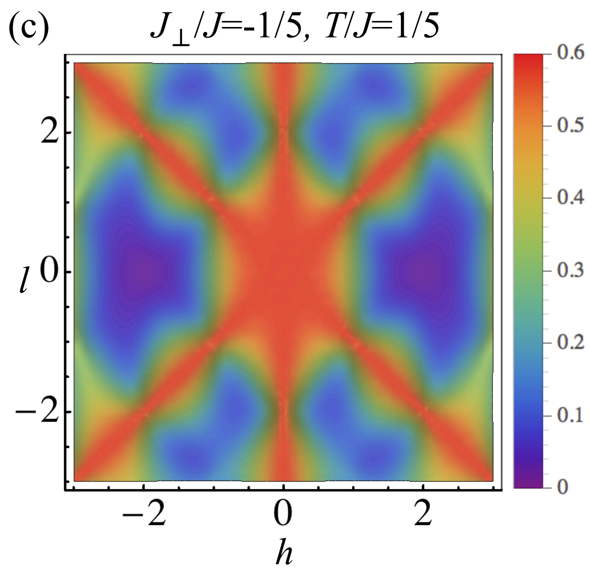


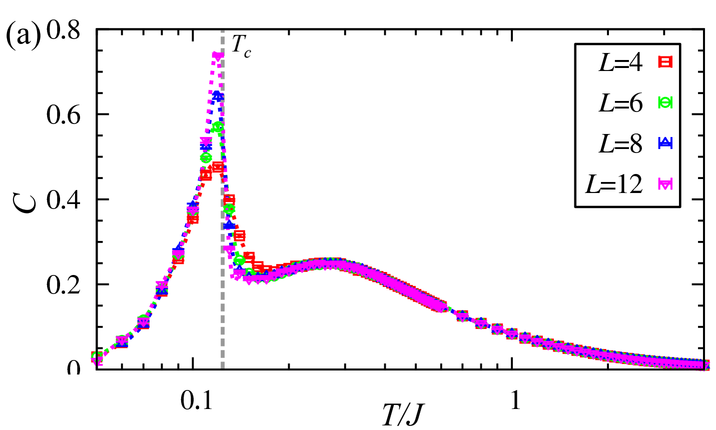
spin-ice entropy

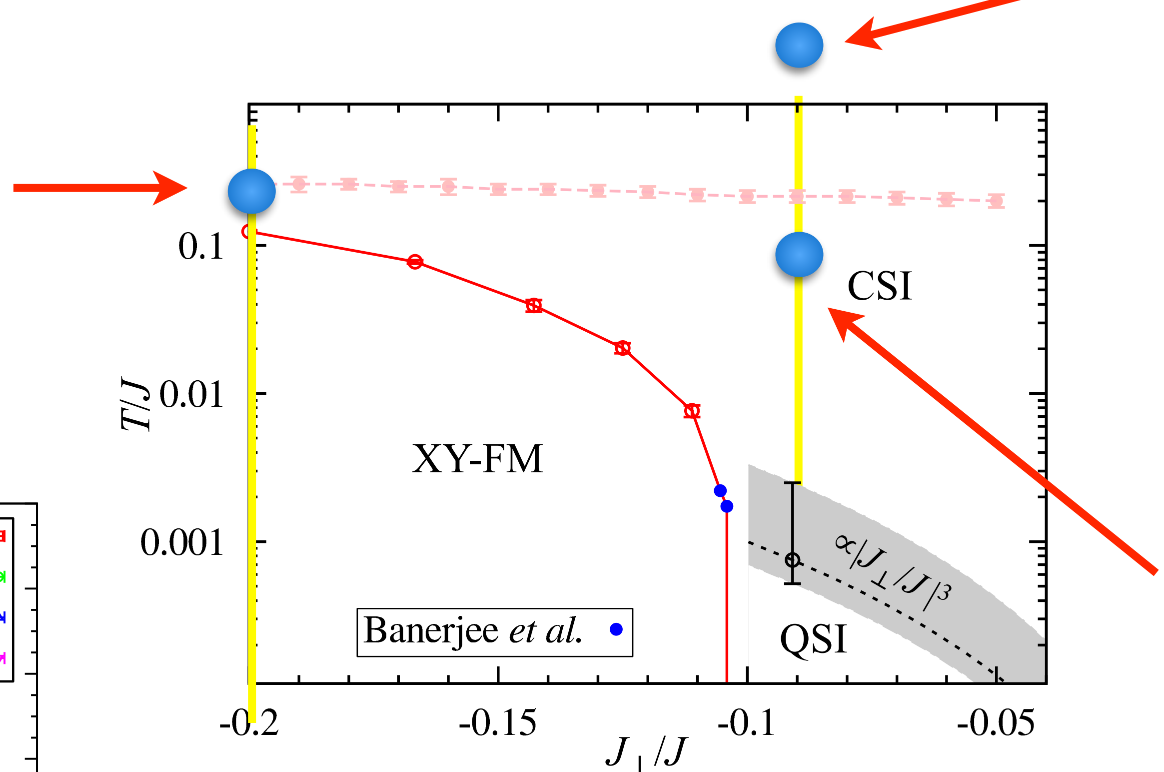
Y. Kato and S. Onoda, arXiv:1411.1981v1

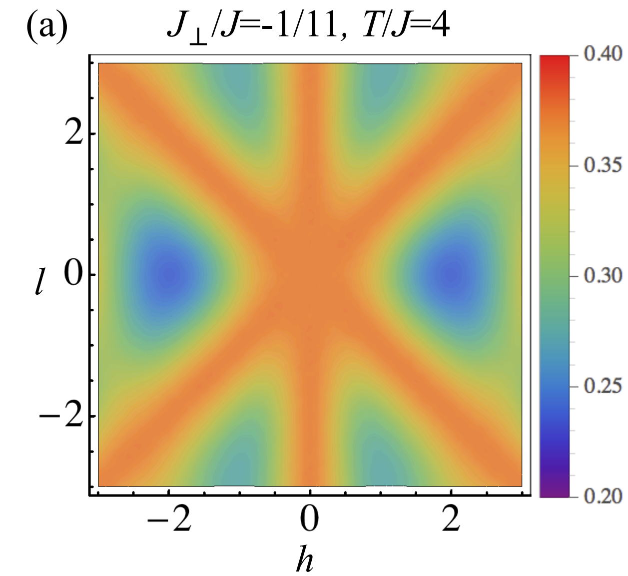
cf. Banerjee *et al*. Phys. Rev. Lett. **100**, 047208 (2008)

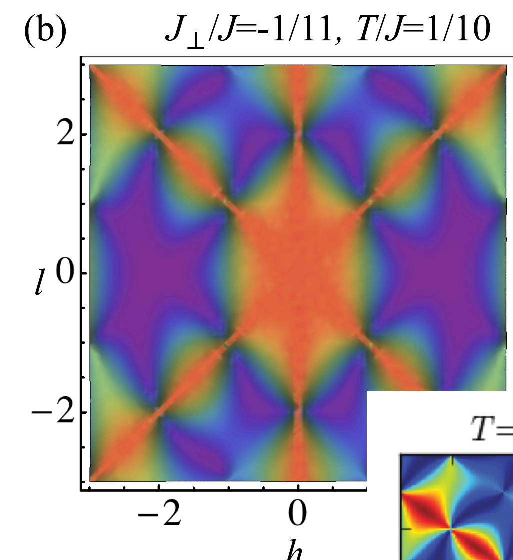
is this seen in simulation ?

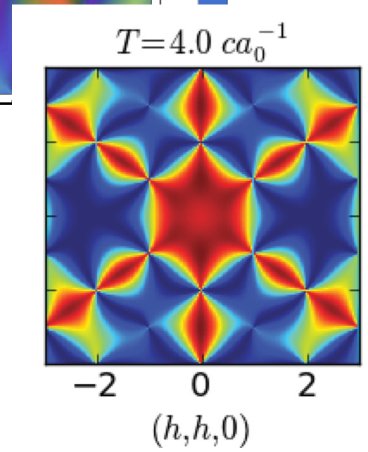












Y. Kato and S. Onoda, arXiv:1411.1981v1

cf. O. Benton *et al.*, Phys. Rev. B. **83**, 075174 (2012) ❦

so what about $Dy_2Ti_2O_7$?

nature physics

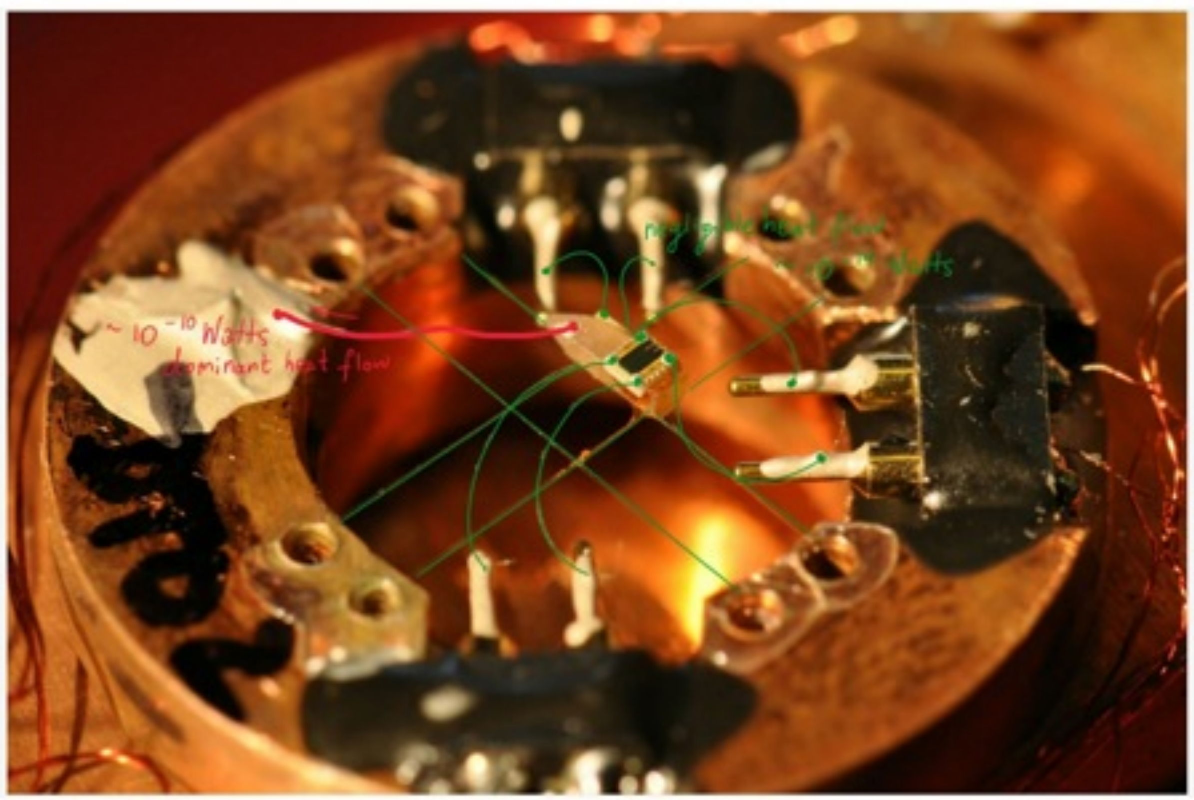
LETTERS

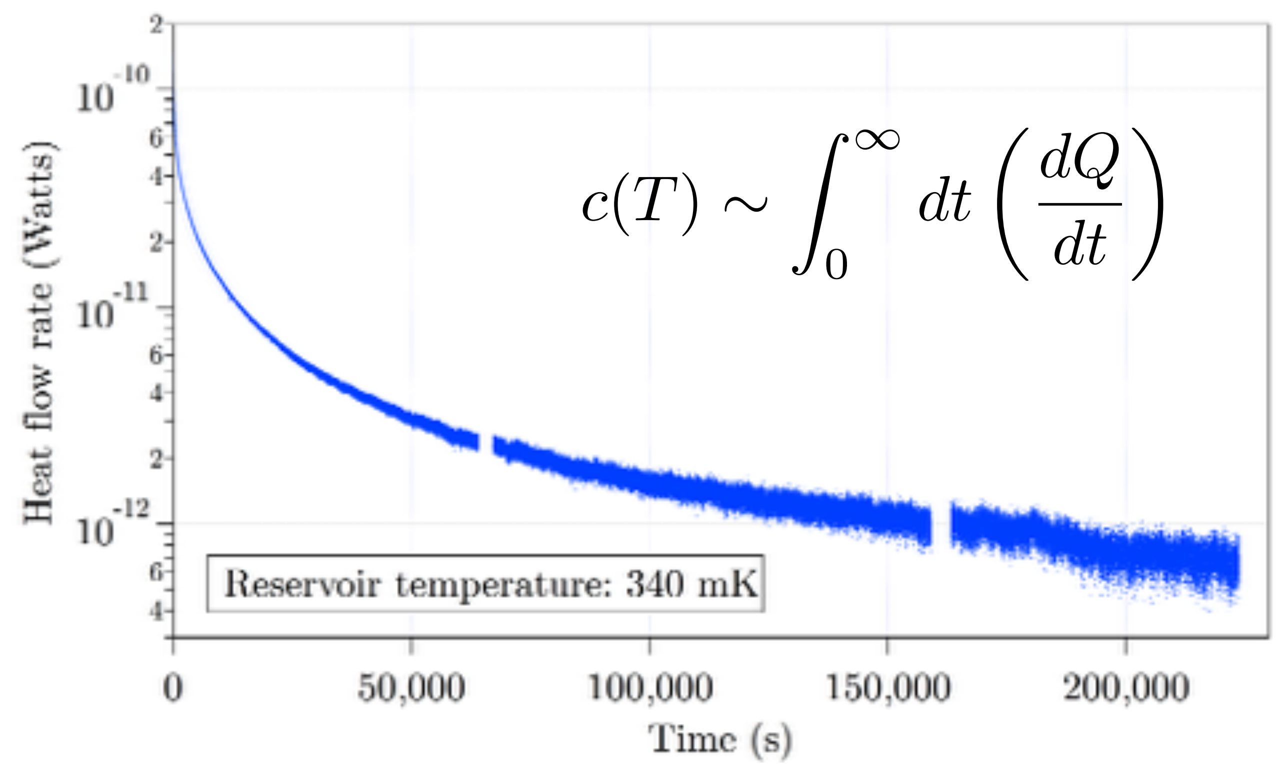
PUBLISHED ONLINE: 7 APRIL 2013 | DOI: 10.1038/NPHYS2591

Absence of Pauling's residual entropy in thermally equilibrated $Dy_2Ti_2O_7$

D. Pomaranski[1,2,3], L. R. Yaraskavitch[1,2,3], S. Meng[1,2,3], K. A. Ross[4,5], H. M. L. Noad[4,5], H. A. Dabkowska[4,5], B. D. Gaulin[4,5,6] and J. B. Kycia[1,2,3]★

measurements of heat capacity of $Dy_2Ti_2O_7$ allowing up to one week (!) for thermalization at each temperature..





nature physics | LETTERS
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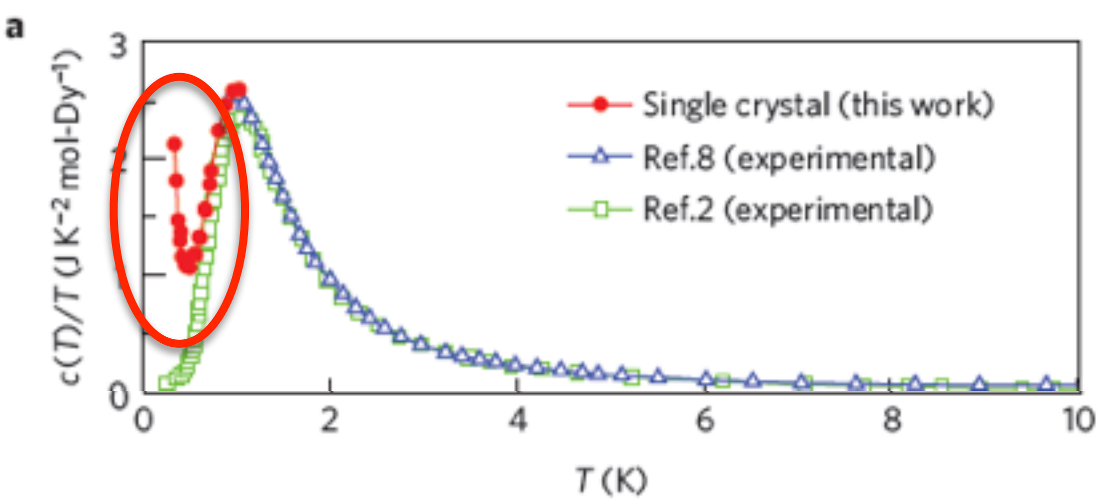
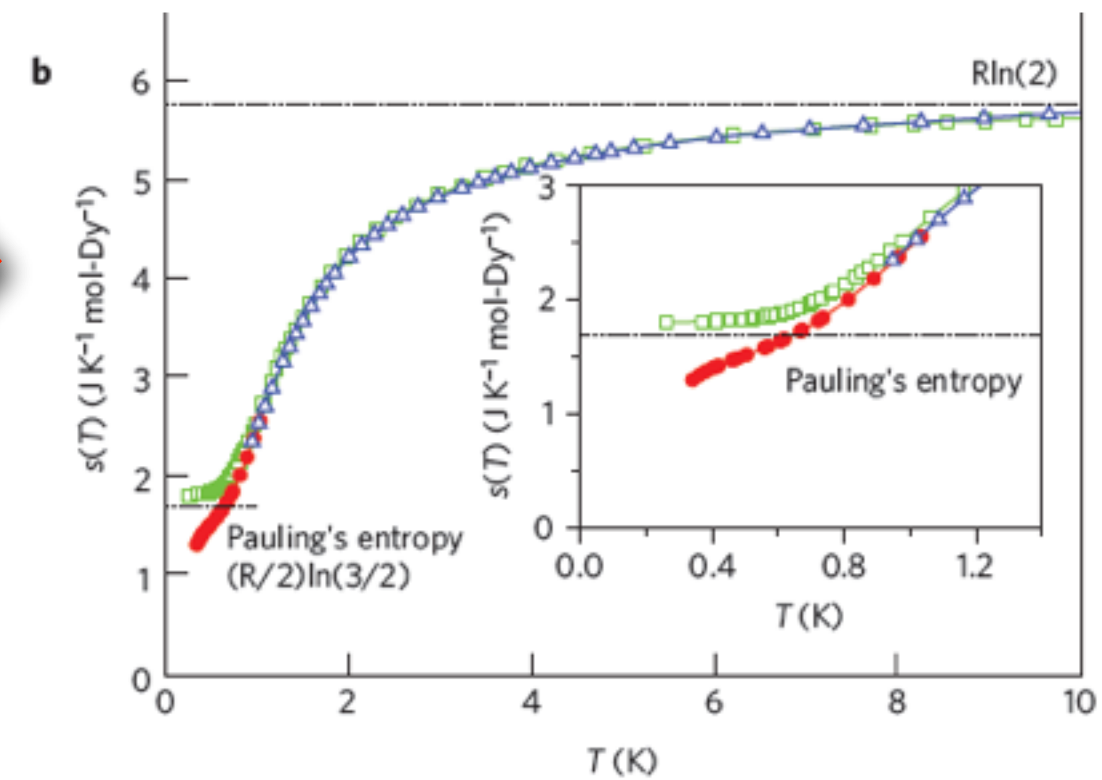


upturn in heat capacity below 500mK
⇒ onset of order ?



what is the **classical** ground state of spin ice (in equilibrium) ?

N.B. if the sample orders, the monopoles confine.

VOLUME 87, NUMBER 6 PHYSICAL REVIEW LETTERS 6 AUGUST 2001

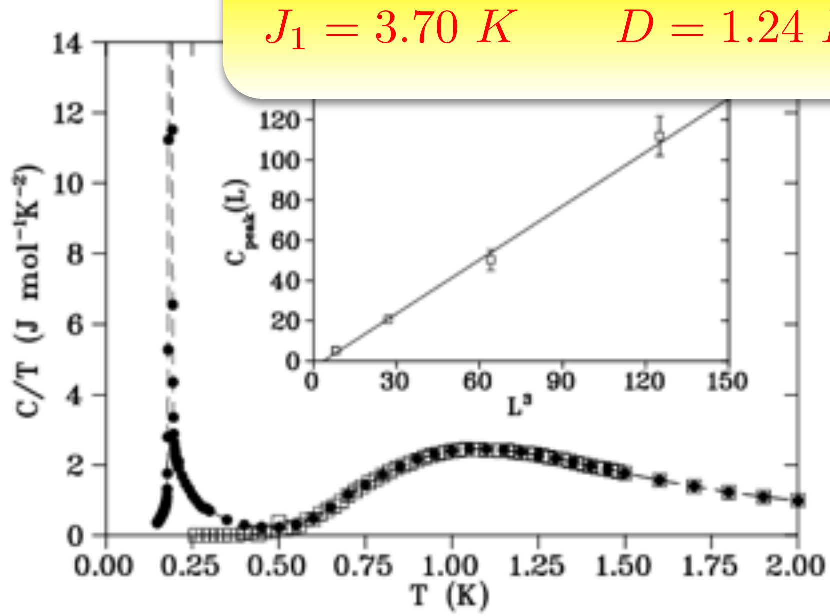
Long-Range Order at Low Temperatures in Dipolar Spin Ice

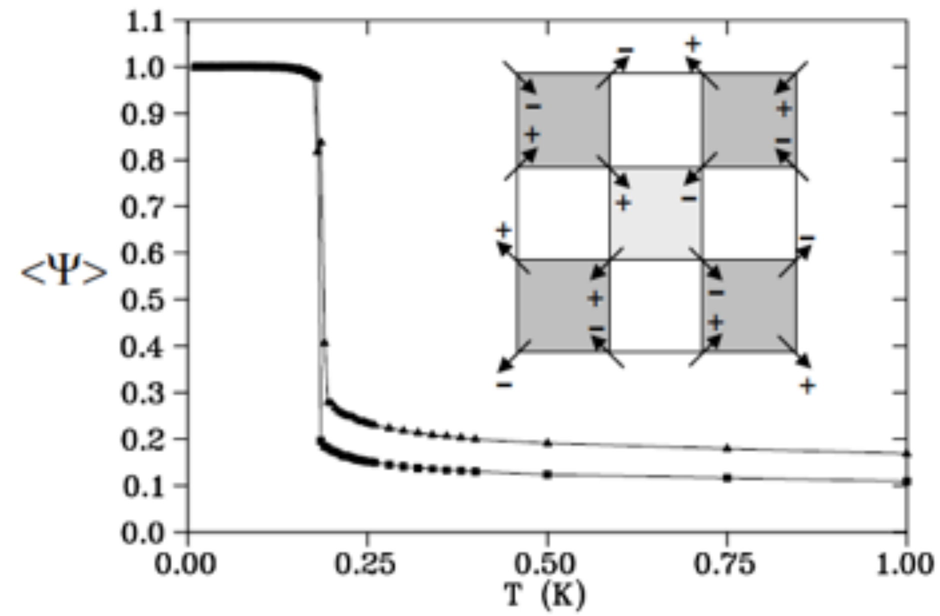
Roger G. Melko,[1] Byron C. den Hertog,[1] and Michel J. P. Gingras[1,2]
[1]Department of Physics, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1

$$\mathcal{H}_{\mathsf{minimal}} = J_1 \sum_{\langle ij \rangle_1} \sigma_i^z \sigma_j^z \; (\hat{\mathbf{z}}_i \cdot \hat{\mathbf{z}}_j) + D \sum_{i<j} \left(\frac{r_1}{r_{ij}}\right)^3 \sigma_i^z \sigma_j^z \left[(\hat{\mathbf{z}}_i \cdot \hat{\mathbf{z}}_j) - 3 \, (\hat{\mathbf{z}}_i \cdot \mathbf{r}_{ij}) \, (\hat{\mathbf{z}}_i \cdot \mathbf{r}_{ij}) \right]$$

1^{st}-neighbour exchange (FM) long-range dipolar interaction (Dy moment is $\mu \sim 10\mu_B$)

$J_1 = 3.70\ K \qquad D = 1.24\ K$





…long-range dipolar interactions select an 8-sublattice ordered state from among the spin-ice ground states

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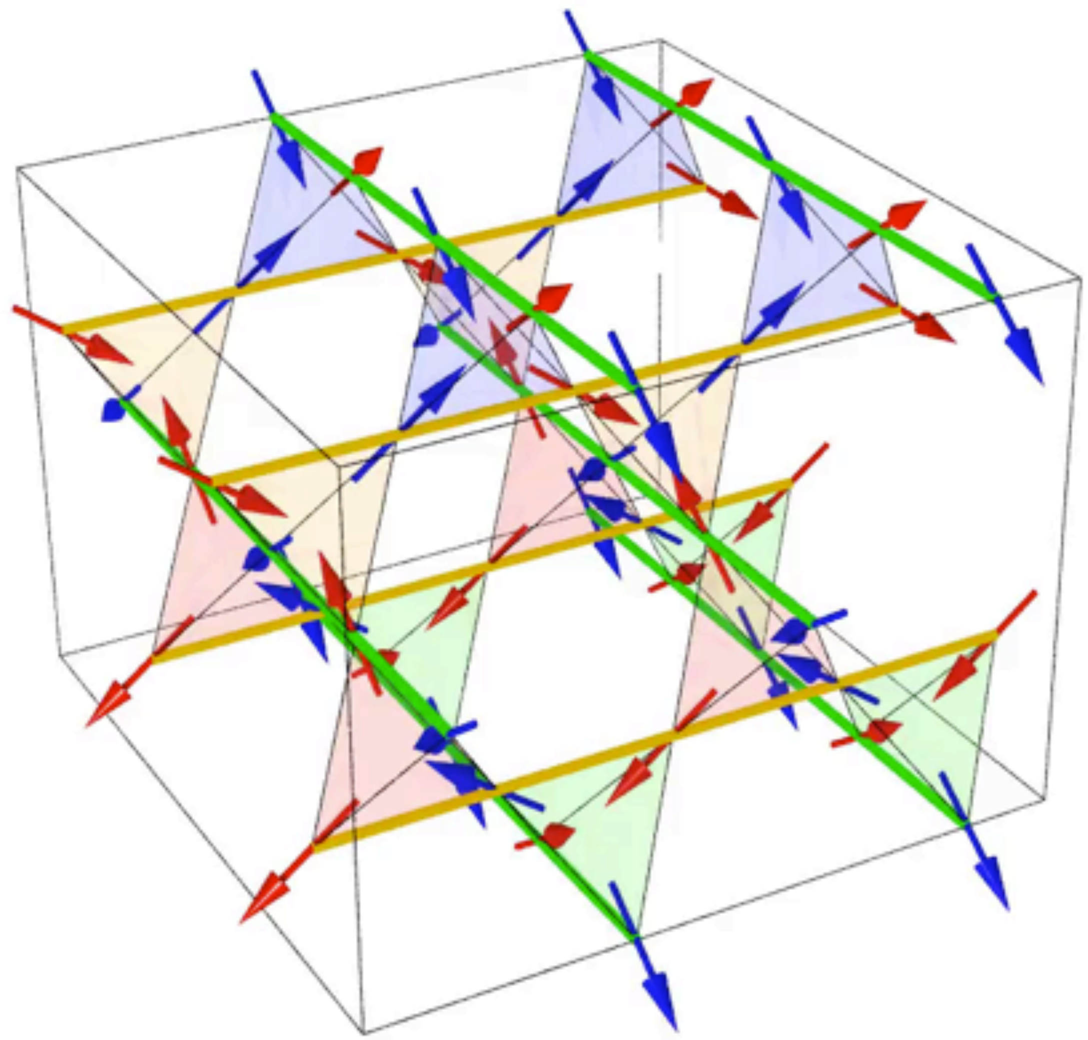
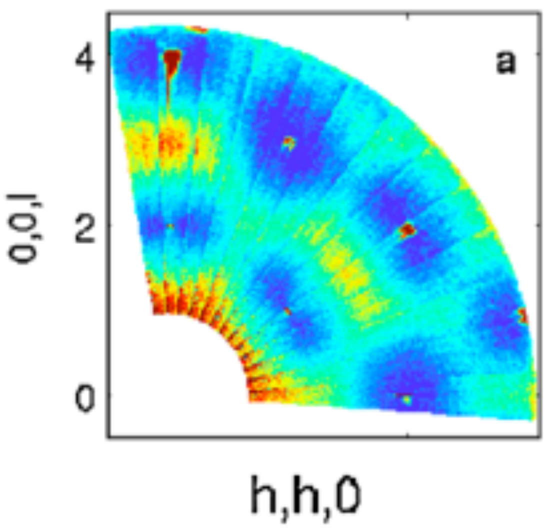
cubic antiferromagnet (CAF)



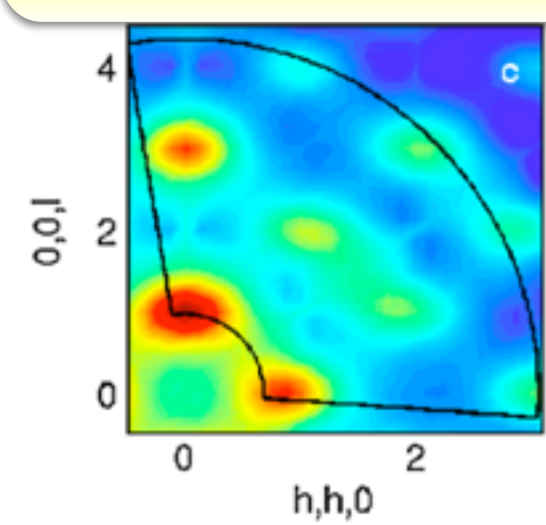
spin-ice configuration composed of **ferromagnetically-polarized chains** of spins

is this model complete ?



elastic neutron scattering at 300 mK

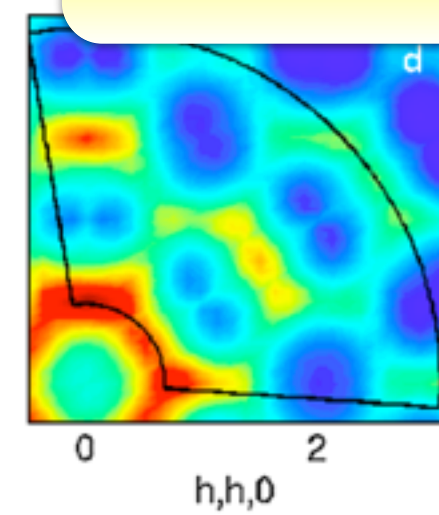
$J_1 = 3.70\ K \qquad D = 1.24\ K$

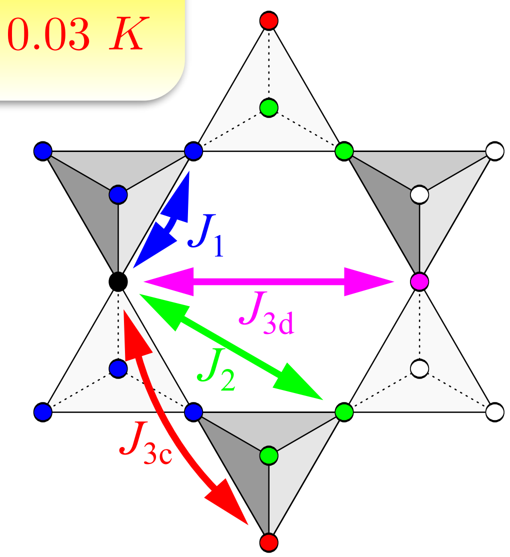


Monte Carlo simulation of minimal model (cf Melko *et al*, 2001)

$J_1 = 3.41\ K \qquad D = 1.32\ K$

$J_2 = -0.14\ K \qquad J_3 = 0.03\ K$



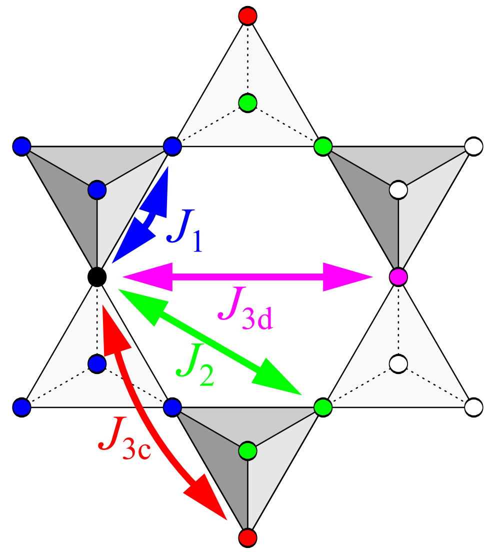


Monte Carlo simulation of model with longer-range exchange interactions

…evidence for finite 2nd neighbour exchange : $J_2/D \approx -0.1$

T. Yavorskii *et al*., Phys. Rev. Lett. **101**, 037204 (2008)

what do need to solve ?



$$\mathcal{H}_{\mathsf{DSI}} = \mathcal{H}_{\mathsf{dipolar}} + \mathcal{H}_{\mathsf{exchange}}$$

long-range dipolar interactions…

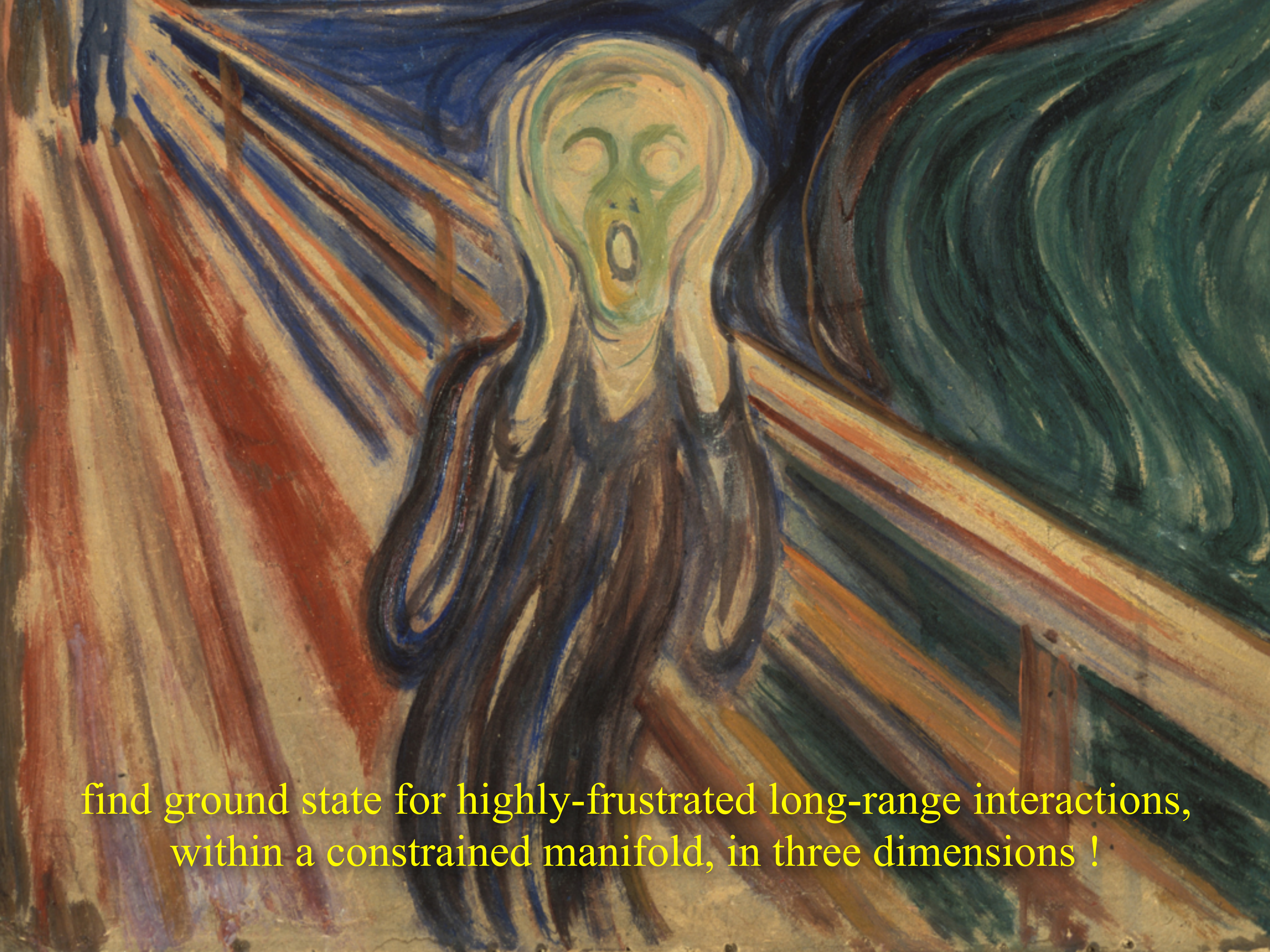
$$\mathcal{H}_{\mathsf{dipolar}} \quad = \quad 4D \sum_{i<j} \left(\frac{r_1}{r_{ij}}\right)^3 \left[\hat{\mathbf{z}}_i \cdot \hat{\mathbf{z}}_j - 3\left(\hat{\mathbf{z}}_i \cdot \hat{\mathbf{r}}_{ij}\right)\left(\hat{\mathbf{z}}_j \cdot \hat{\mathbf{r}}_{ij}\right)\right] \mathsf{S}_i^z\, \mathsf{S}_j^z$$

…no adjustable parameters !

finite-range exchange interactions…

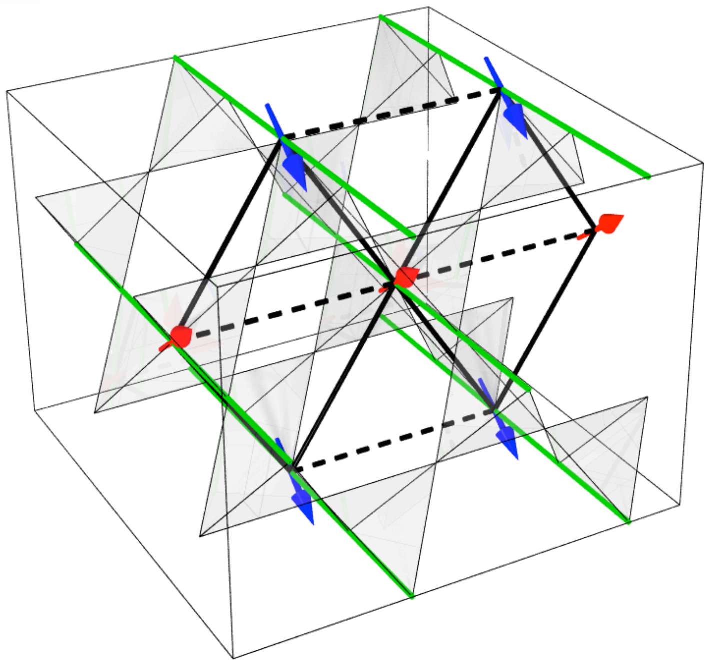
$$\mathcal{H}_{\mathsf{exchange}} = \sum_k 4J_k \sum_{\langle ij \rangle_k} \left(\hat{\mathbf{z}}_i \cdot \hat{\mathbf{z}}_j\right) \mathsf{S}_i^z\, \mathsf{S}_j^z$$

N.B. 1^{st}-neighbor exchange J_1 gives constant energy in spin-ice states.

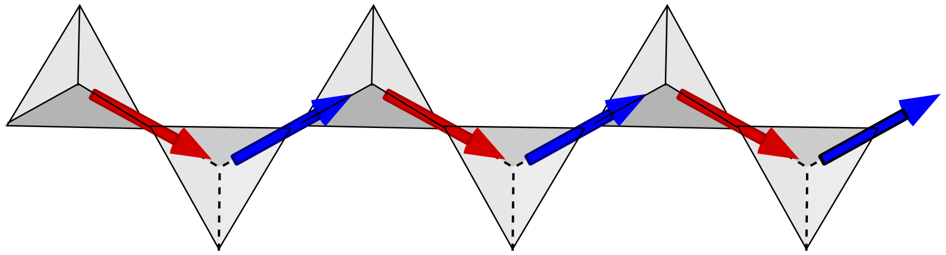

find ground state for highly-frustrated long-range interactions,
within a constrained manifold, in three dimensions !

is there a simplification ?

pyrochlore lattice can be divided into **two sets of chains**, parallel to $[110]$ and $[1\bar{1}0]$



ordered states are composed of **FM-polarised chains** of alternating "in" and "out" spins



each FM chain acts like an **Ising degree of freedom**

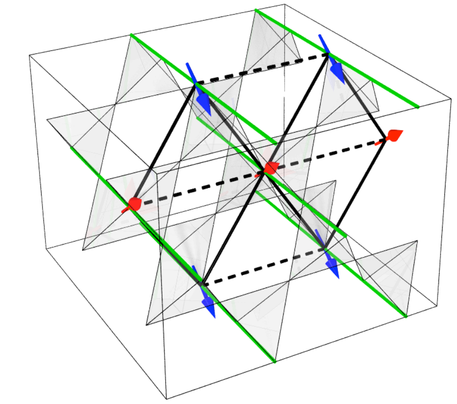
interactions between perpendicular chains **vanish**,
interactions between parallel chains are **exponentially screened**

$$\mathcal{H}_{\mathsf{DSI}} = \mathcal{H}_{\mathsf{dipolar}} + \mathcal{H}_{\mathsf{exchange}}$$

$$\mathcal{H}^{\mathsf{2D}}_{\mathsf{Ising}} = \frac{1}{2}\sum_{\boldsymbol{r},\boldsymbol{\delta}} K_{\boldsymbol{\delta}}\, \sigma_{\boldsymbol{r}}\ \sigma_{\boldsymbol{r}+\boldsymbol{\delta}}$$

P. McClarty *et al.*, arXiv.1410.0451v1

how does this work ?



dipolar interaction between FM chains of spins separated by distance $\delta = |(\delta_1, \delta_2)|$

$$K_{\boldsymbol{\delta}} = \sqrt{2}^3 D \sum_{l=-\infty}^{\infty} \left[(-1)^l \frac{2}{3} \frac{(\delta_1^2 - 2\delta_2^2 + l^2)}{2^{5/2} (\delta_1^2 + \delta_2^2 + l^2)^{5/2}} + (-1)^{\delta_1} \frac{4}{3} \frac{(\delta_1^2 + \delta_2^2 - 2l^2)}{2^{5/2} (\delta_1^2 + \delta_2^2 + l^2)^{5/2}} \right]$$

sum over infinitely-long chain

$$K_{\boldsymbol{\delta}}/D \approx \frac{4\pi}{3\delta} K_1(\pi\delta) - \frac{4\pi^2\delta_2^2}{3\delta^2} K_2(\pi\delta) \approx -\frac{2\sqrt{2}}{3} \left[\pi^2 \left(\frac{\delta_2}{\delta} \right)^2 \delta^{-1/2} - \pi\delta^{-3/2} + \cdots \right] e^{-\pi\delta}$$

modified Bessel functions

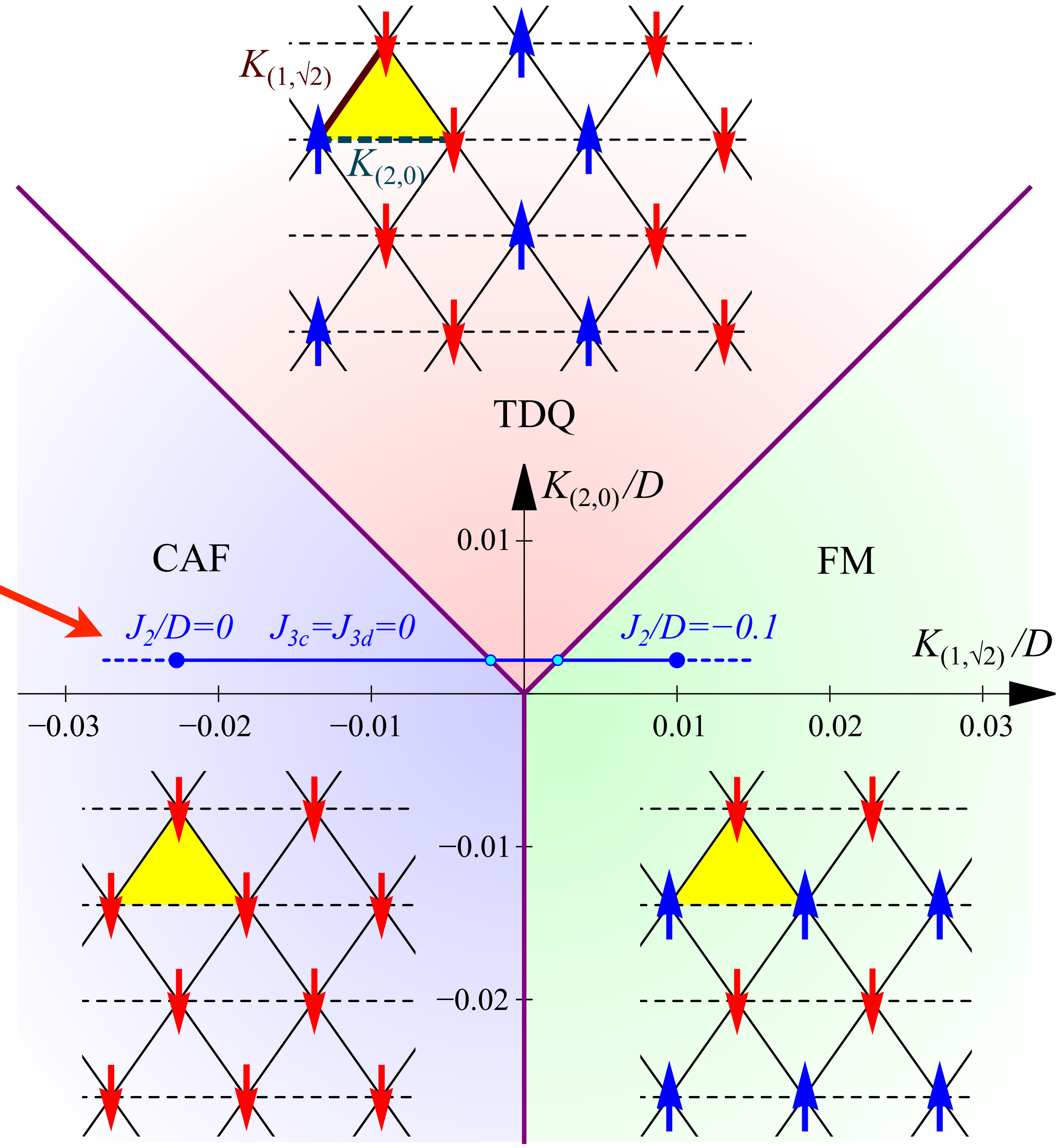
exponential decay

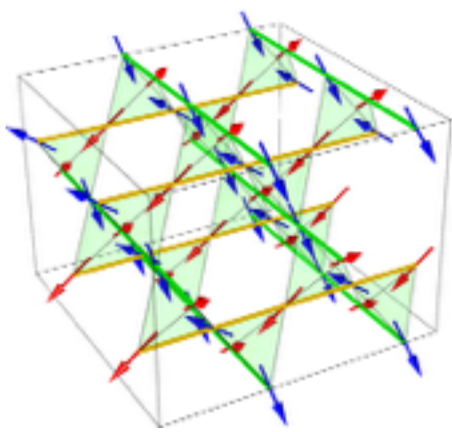
chains described by 2D Ising model with only short-range interactions !

P. McClarty *et al.*, arXiv.1410.0451v1

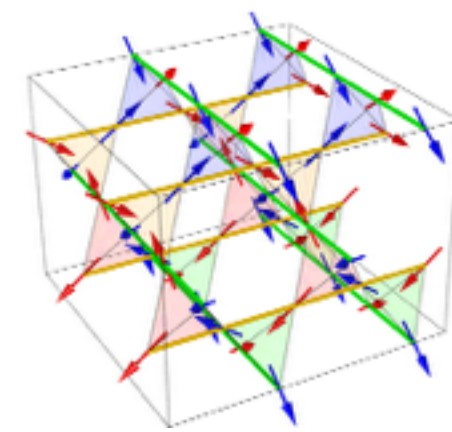
what states do we find ?

parameters used
in simulations





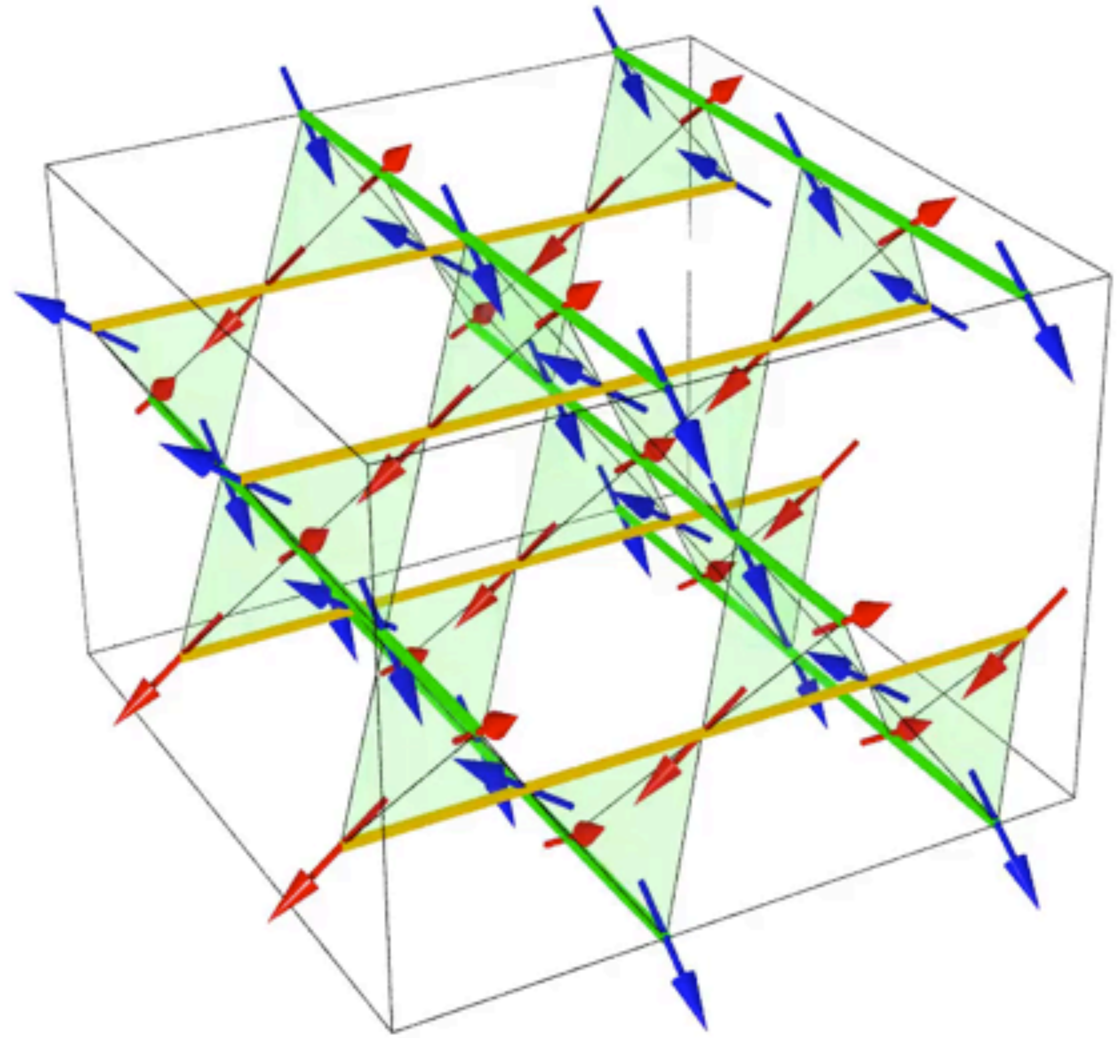
CAF



FM

P. McClarty *et al.*, arXiv.1410.0451v1

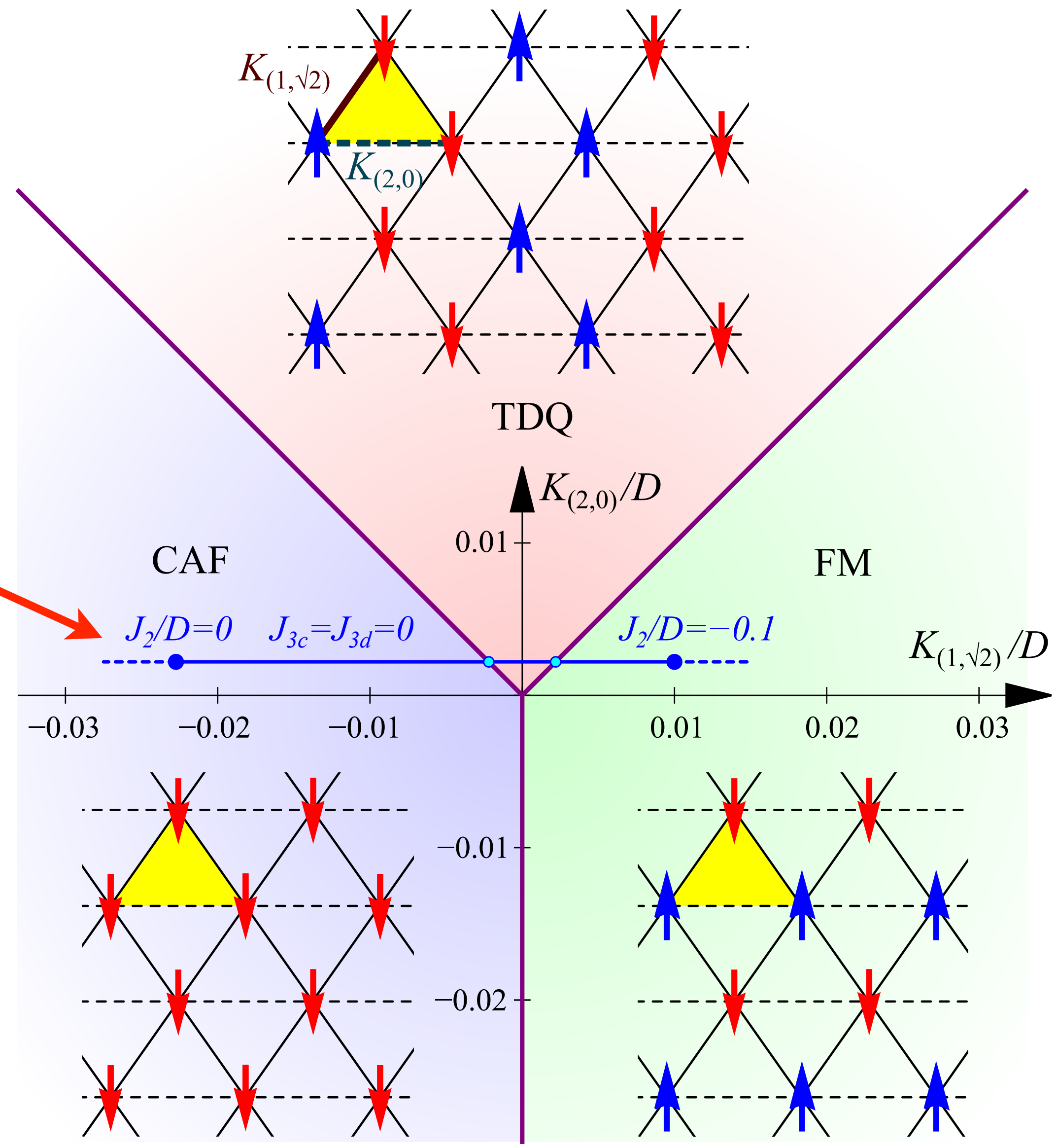
ferromagnet (FM)

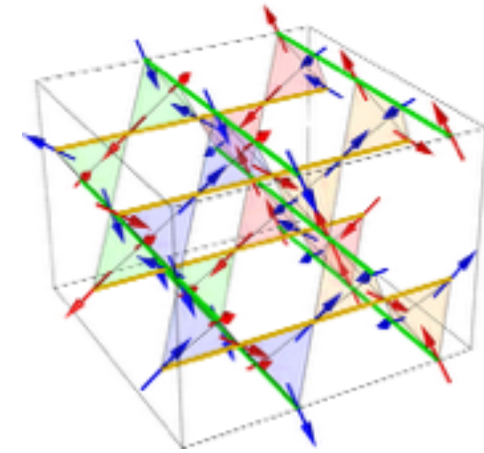


spin-ice configuration composed of **ferromagnetically-polarized chains** of spins

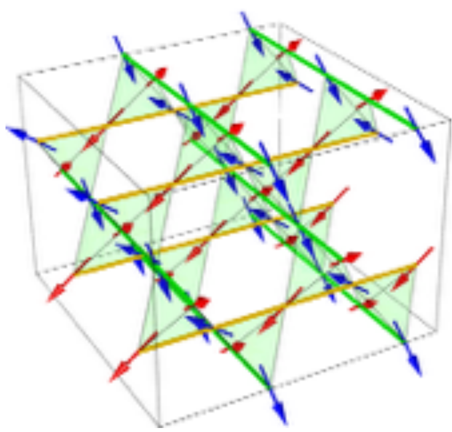
what states do we find ?

parameters used
in simulations

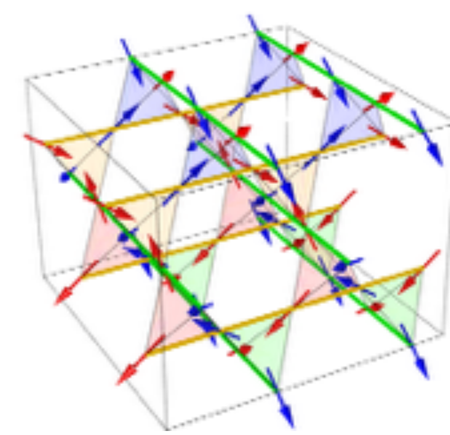




TDQ



CAF



FM

P. McClarty *et al.*, arXiv.1410.0451v1

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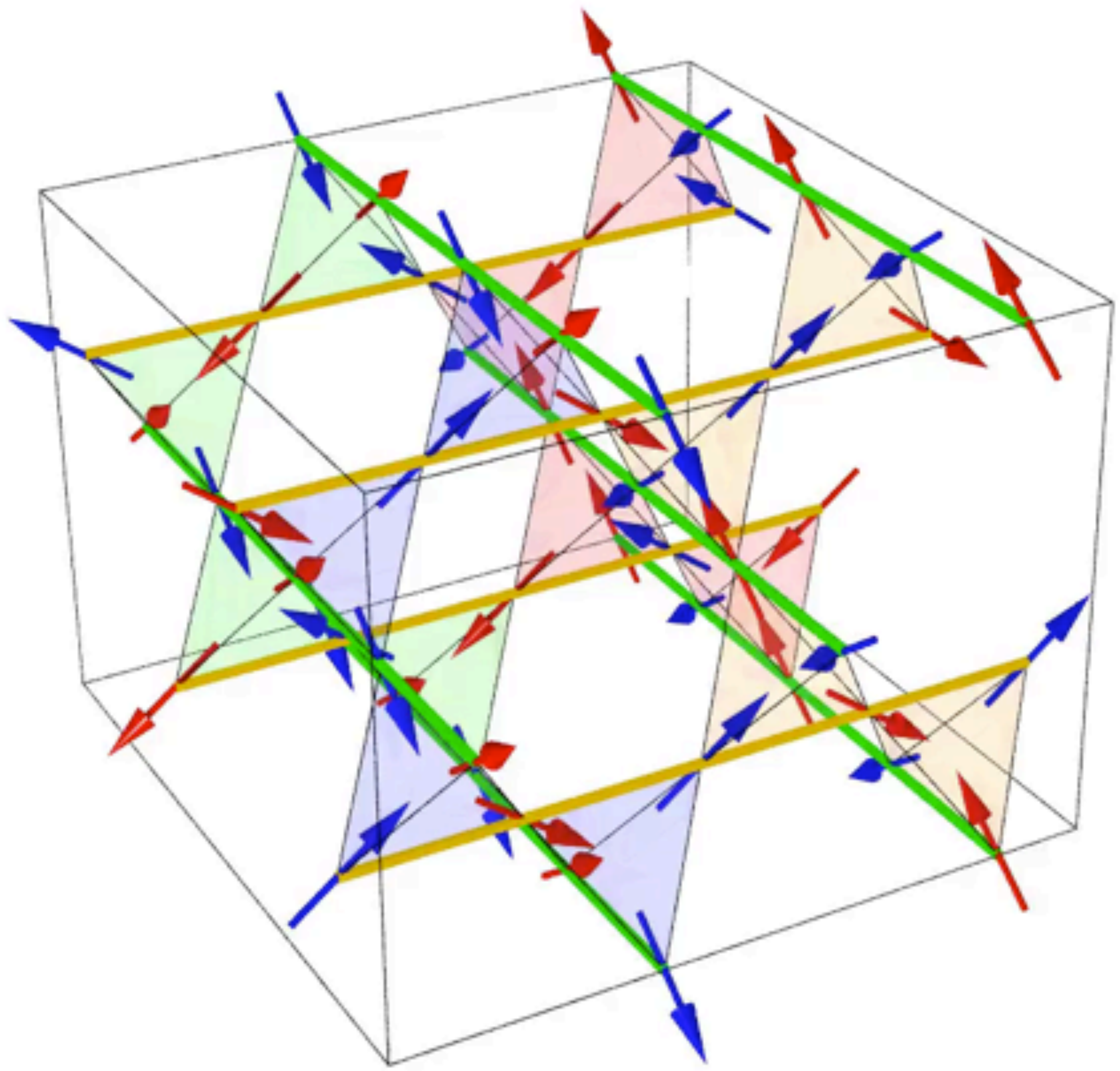
tetragonal double-q state (TQD)



spin-ice configuration composed of **ferromagnetically-polarized chains** of spins

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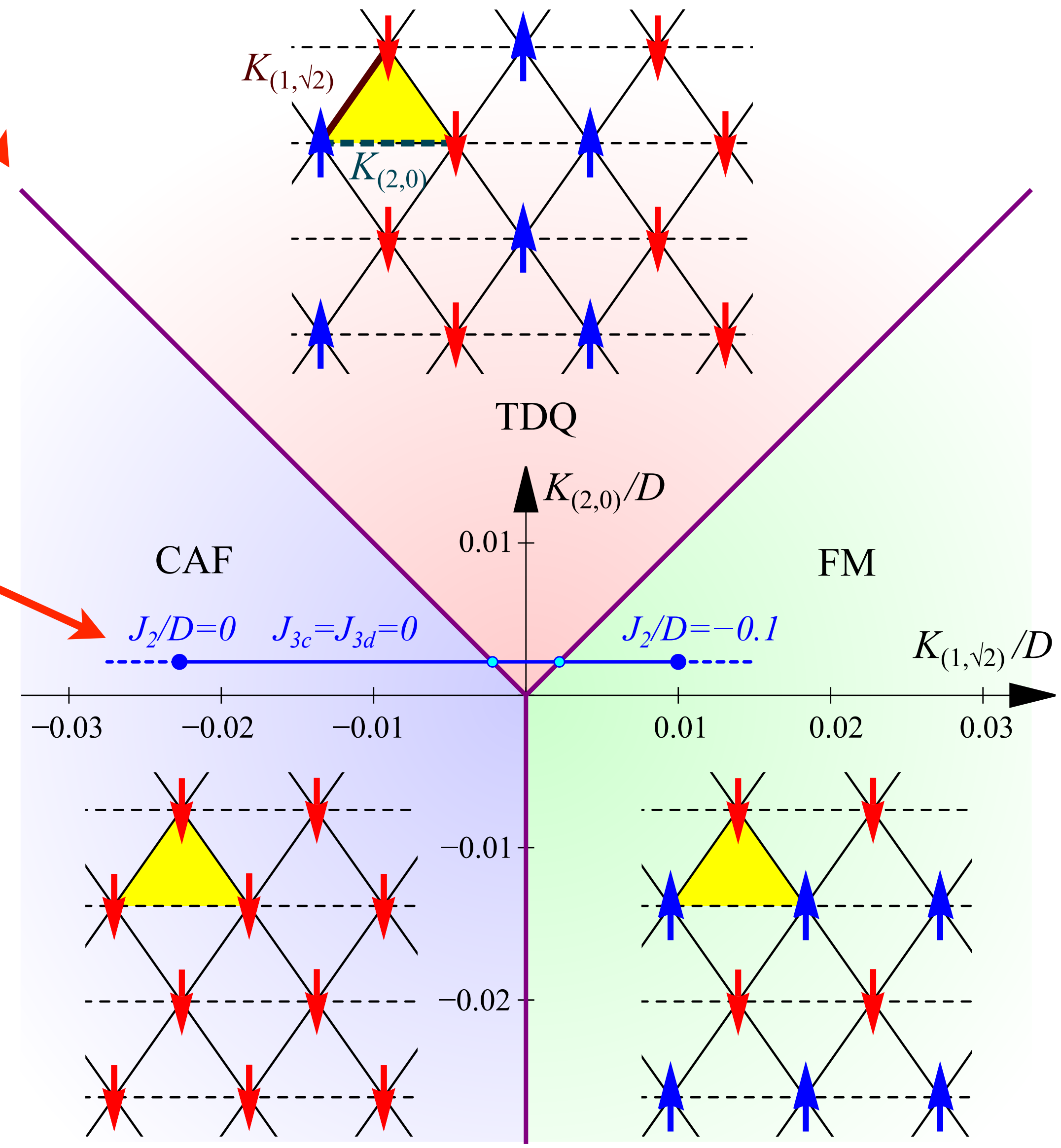
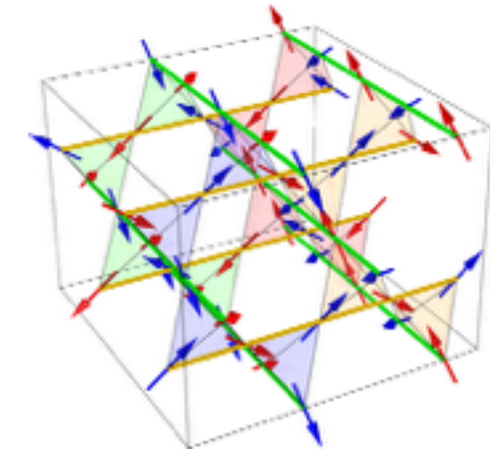
what states do we find ?

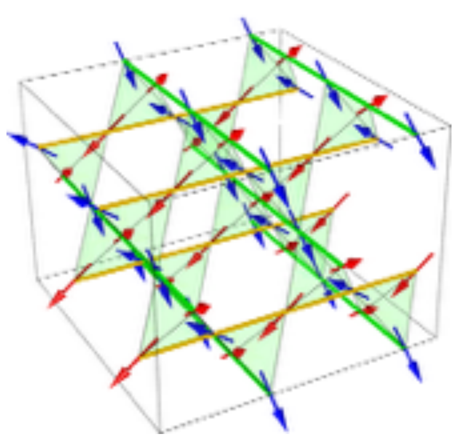
additional degeneracy
on phase boundary
cf. ANNNI model

parameters used
in simulations





TDQ



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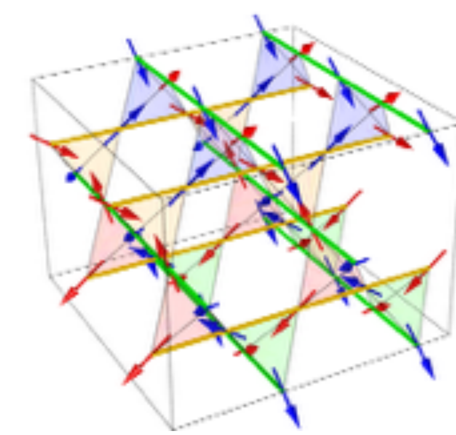


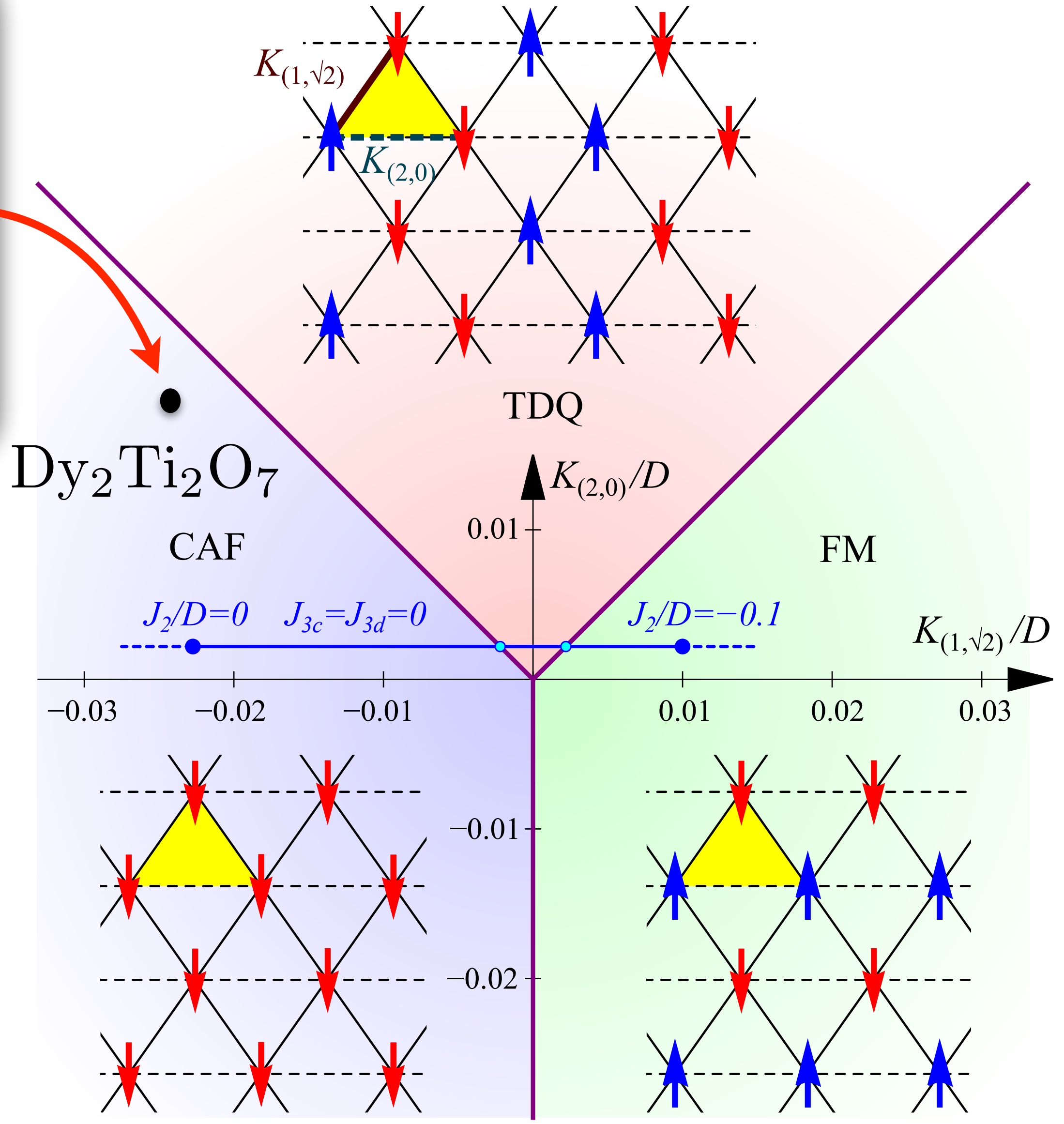
FM

P. McClarty *et al.*, arXiv.1410.0451v1

what might this mean for $Dy_2Ti_2O_7$?

parameters from Yavorskii et al. put $Dy_2Ti_2O_7$ in CAF state…

$$D = 1.32\text{ K} \qquad J_1 = 3.41\text{ K}$$
$$J_2 = -0.14\text{ K} \qquad J_3 = 0.03\text{ K}$$



P. McClarty *et al.*, arXiv.1410.0451v1

warning !

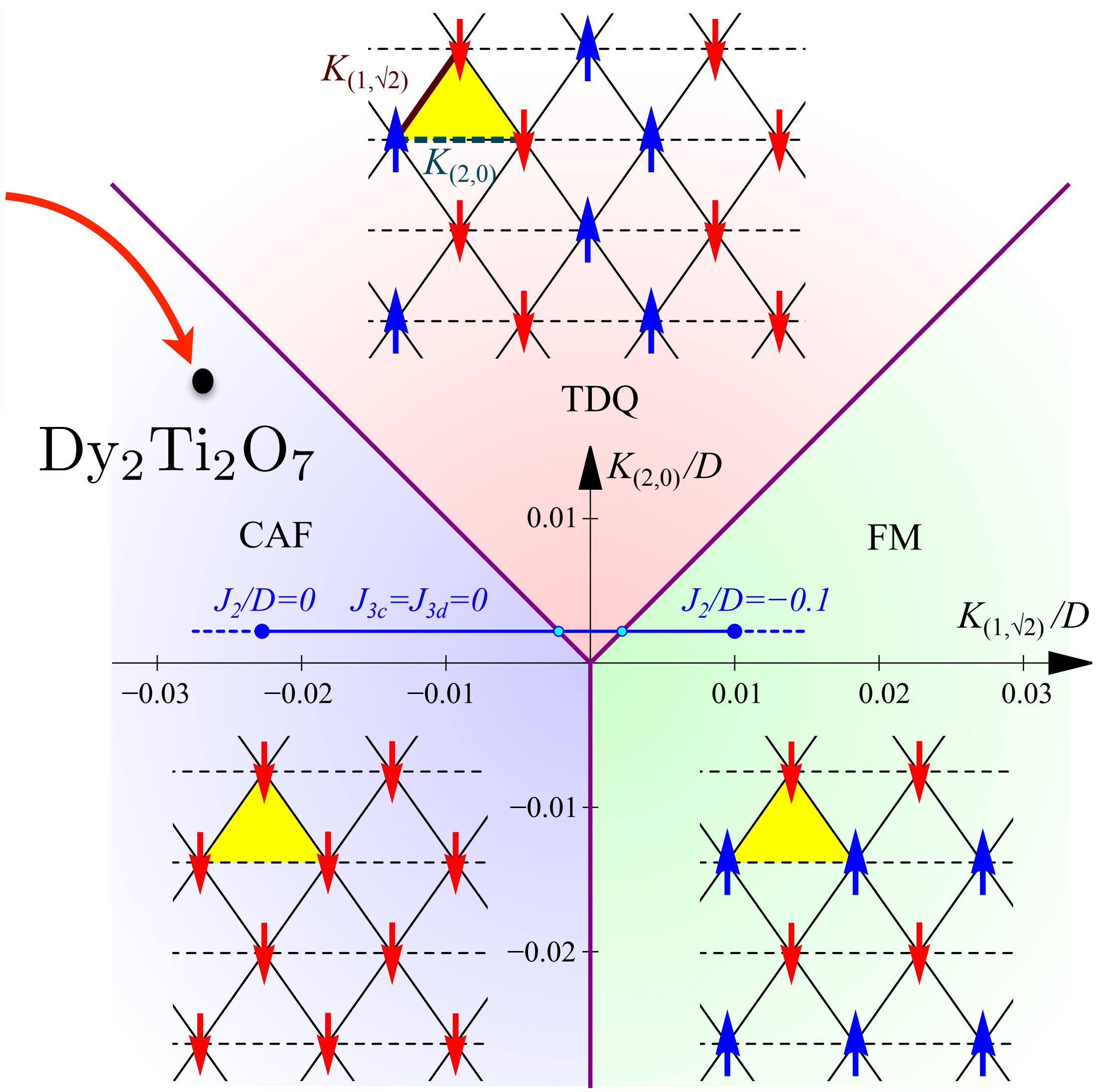
what might this mean for $Dy_2Ti_2O_7$?

parameters from Yavorskii et al. put $Dy_2Ti_2O_7$ in CAF state…

$$D = 1.32\text{ K} \qquad J_1 = 3.41\text{ K}$$
$$J_2 = -0.14\text{ K} \qquad J_3 = 0.03\text{ K}$$

..but this parameterization should be regarded as under-constrained, and ground state is *very* sensitive to small changes in parameters

$$K_{(1,\sqrt{2})} = -0.0227D - J_2/3 - J_{3c} - J_{3d}$$
$$K_{(2,0)} = 0.0022D + J_{3d}$$
$$K_{(0,2\sqrt{2})} = -0.0008D$$



P. McClarty *et al.*, arXiv.1410.0451v1

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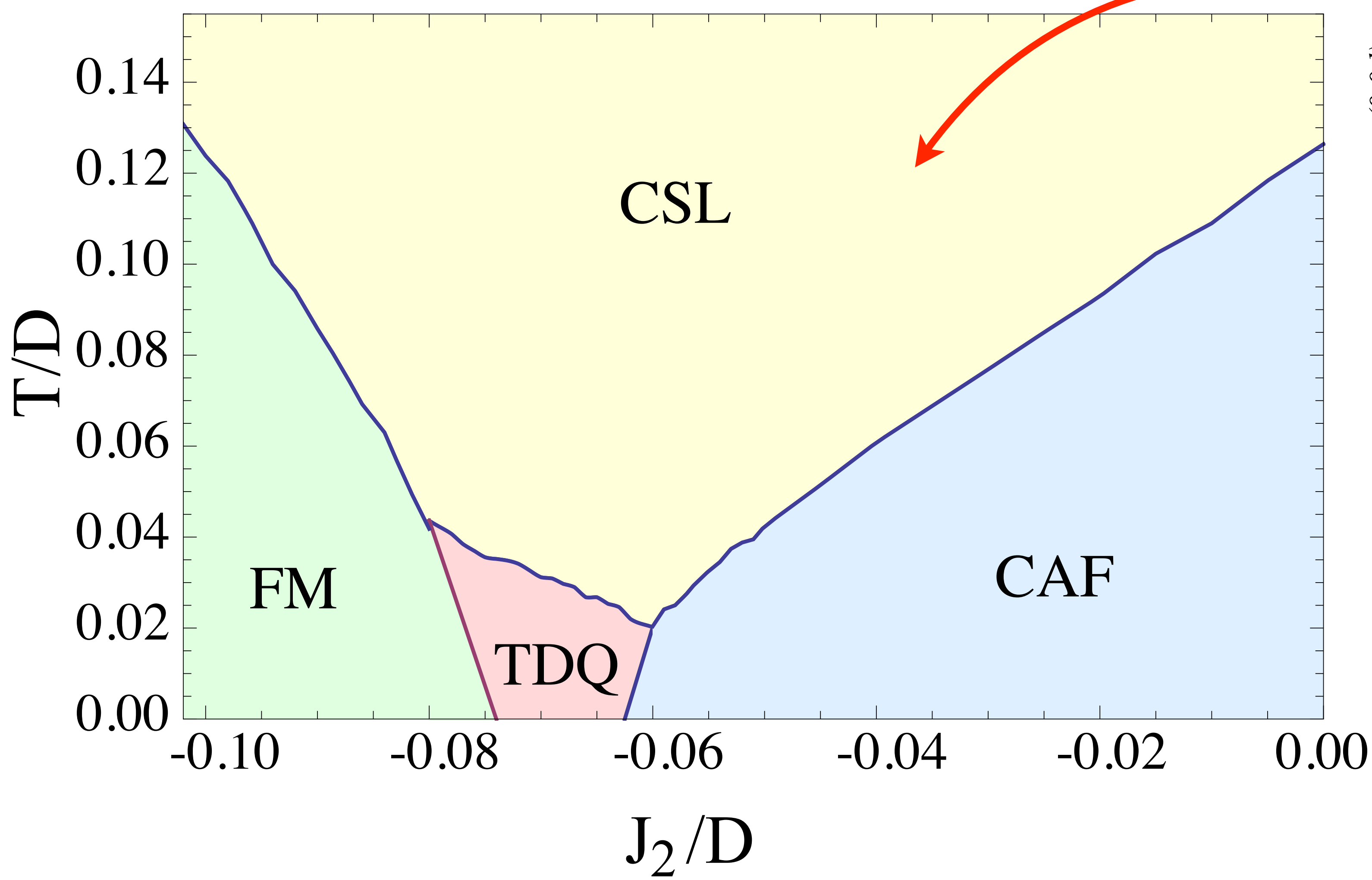
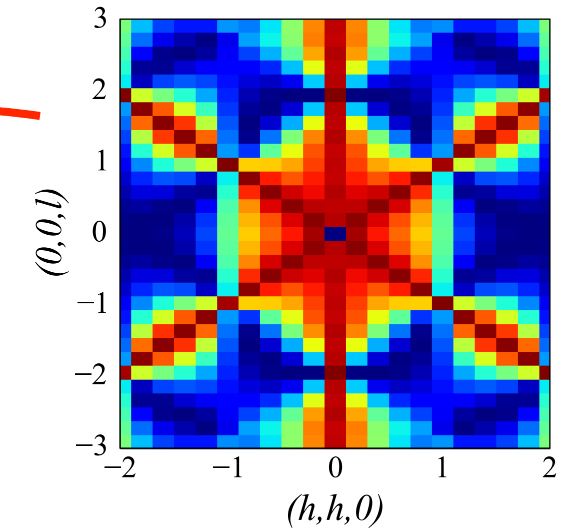
what happens at finite T ?

results of classical Monte Carlo simulation for cluster of 128 spins

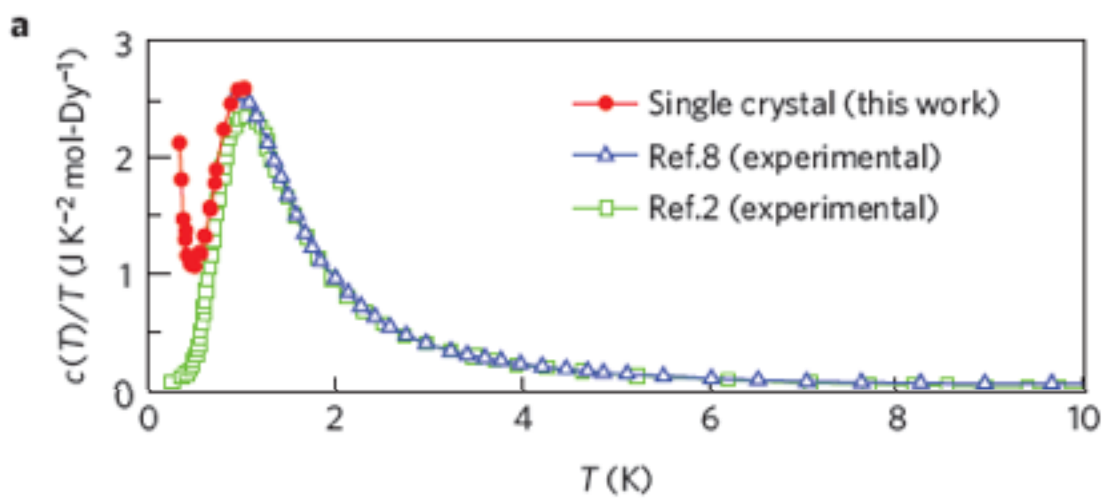




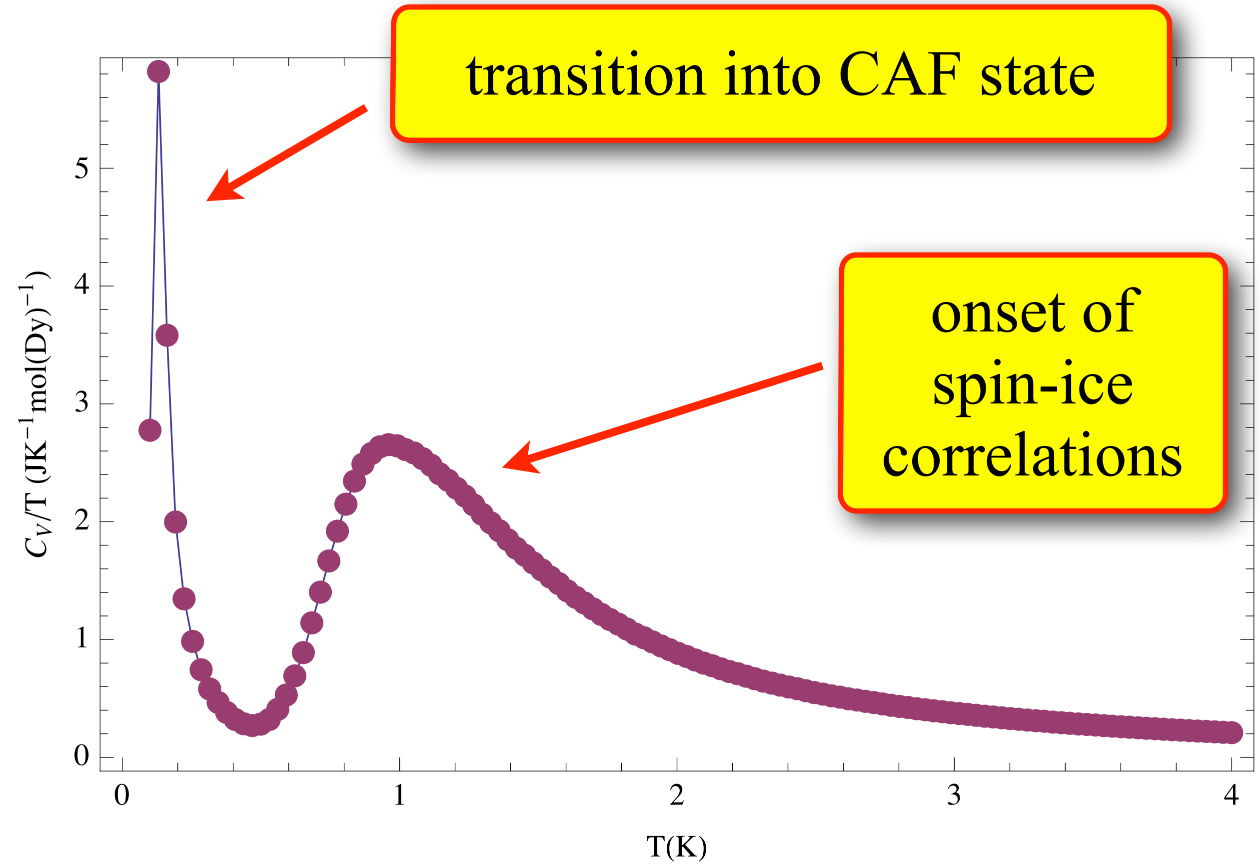
spin correlations S(q) reveal classical spin-liquid with pinch-points i.e. spin-ice

P. McClarty *et al.*, arXiv.1410.0451v1

does this look like experiment ?



D. Pomaranski *et al.*, Nature Physics **9**, 353 (2013).

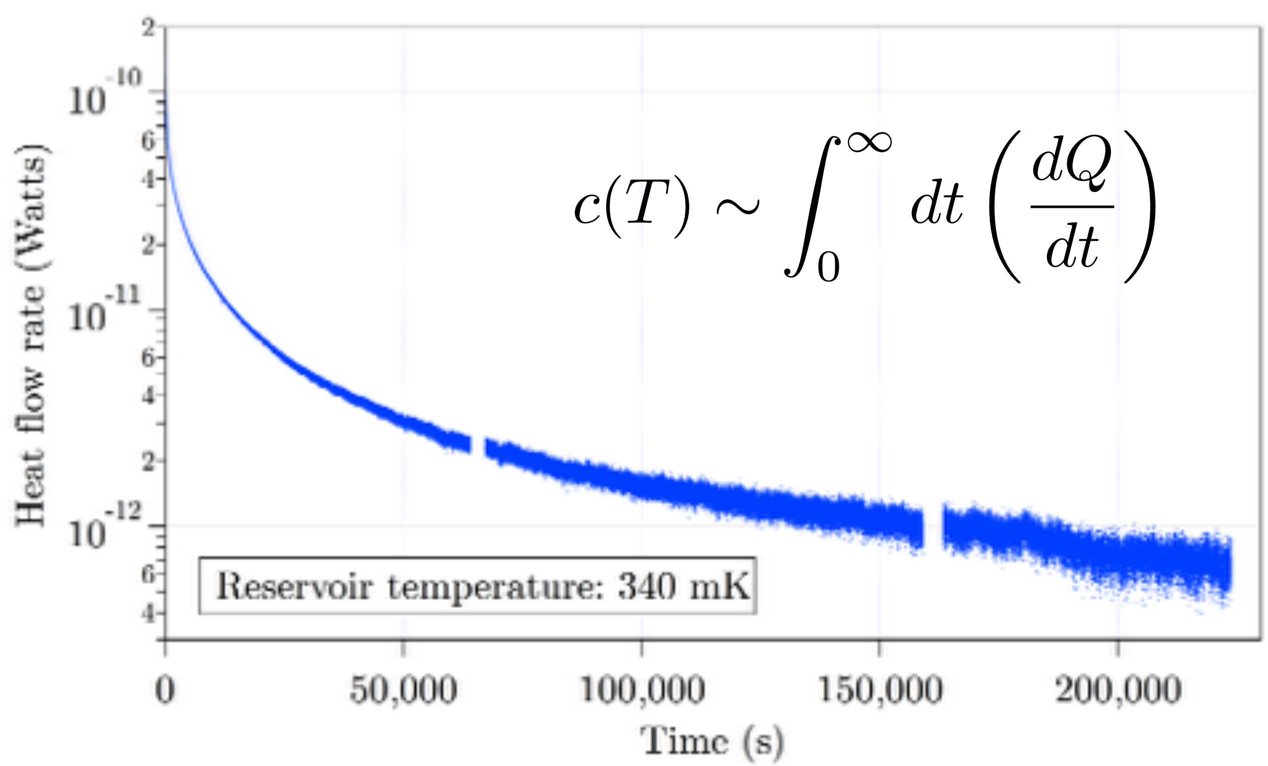


classical Monte Carlo simulation of

$$\mathcal{H}_{\mathsf{DSI}} = \mathcal{H}_{\mathsf{dipolar}} + \mathcal{H}_{\mathsf{exchange}}$$

for parameters from Yavorskii *et al.*

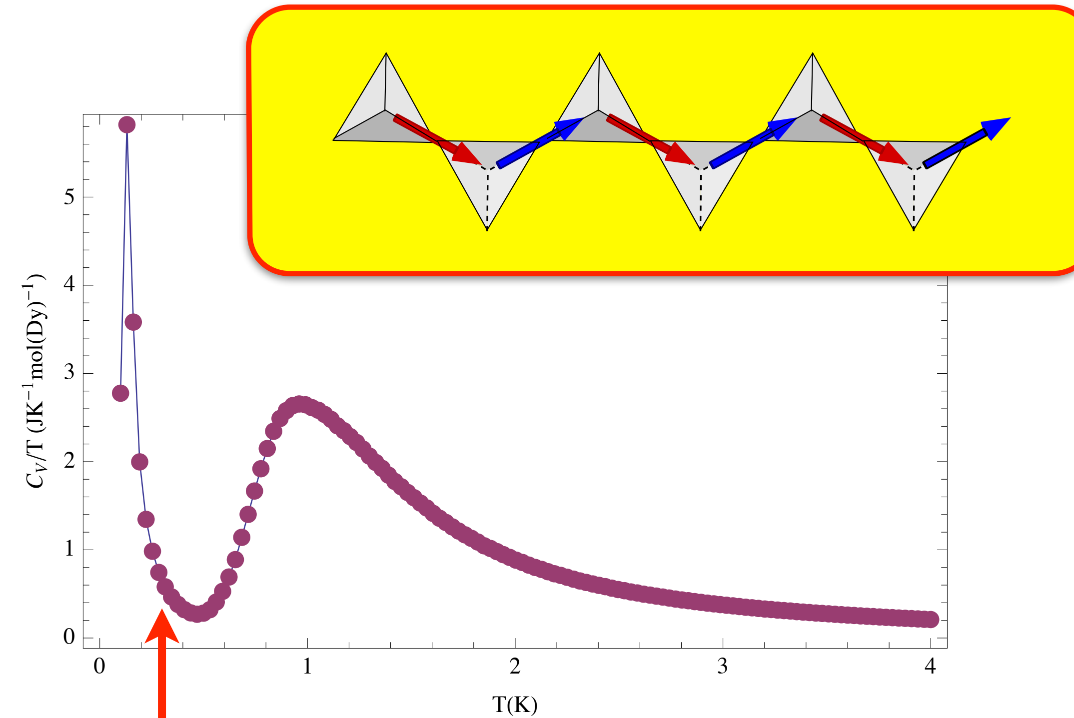
what about slow equilibration ?



$$c(T) \sim \int_0^\infty dt \left(\frac{dQ}{dt} \right)$$

D. Pomaranski *et al.*, Nature Physics **9**, 353 (2013).

for T=340 mK, sample takes
~ 1 week to reach equilibrium



T=340 mK

at T=340 mK spin-ice configurations are dominated by chain-states

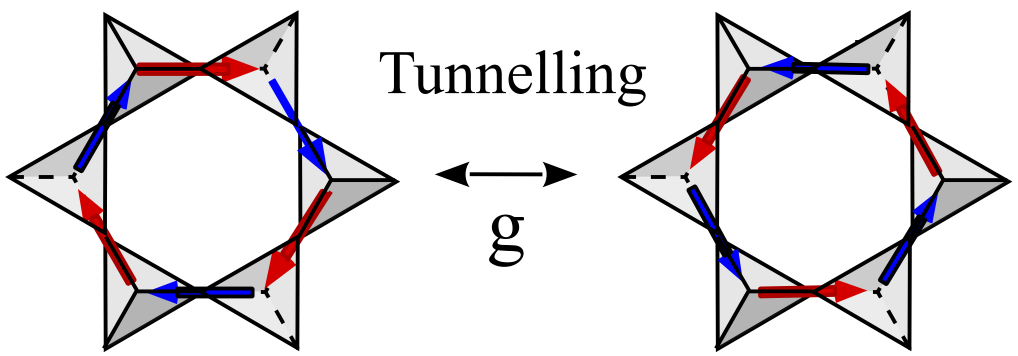
in order to reverse all the spins in a chain, a monopole must cross the entire sample !

is this the origin of the slow equilibration ?

so what about quantum tunnelling ?

quantum dipolar spin ice

new feature is quantum tunnelling between different spin-ice configurations…



$$\mathcal{H}_{\mathsf{tunnelling}} = -g \sum_{\hexagon} |\circlearrowright\rangle\langle\circlearrowleft| + |\circlearrowleft\rangle\langle\circlearrowright|$$

$$\mathcal{H}_{\mathsf{QDSI}} = \mathcal{H}_{\mathsf{dipolar}} + \mathcal{H}_{\mathsf{exchange}} + \mathcal{H}_{\mathsf{tunnelling}}$$

favours spin-ice configurations; chain-states

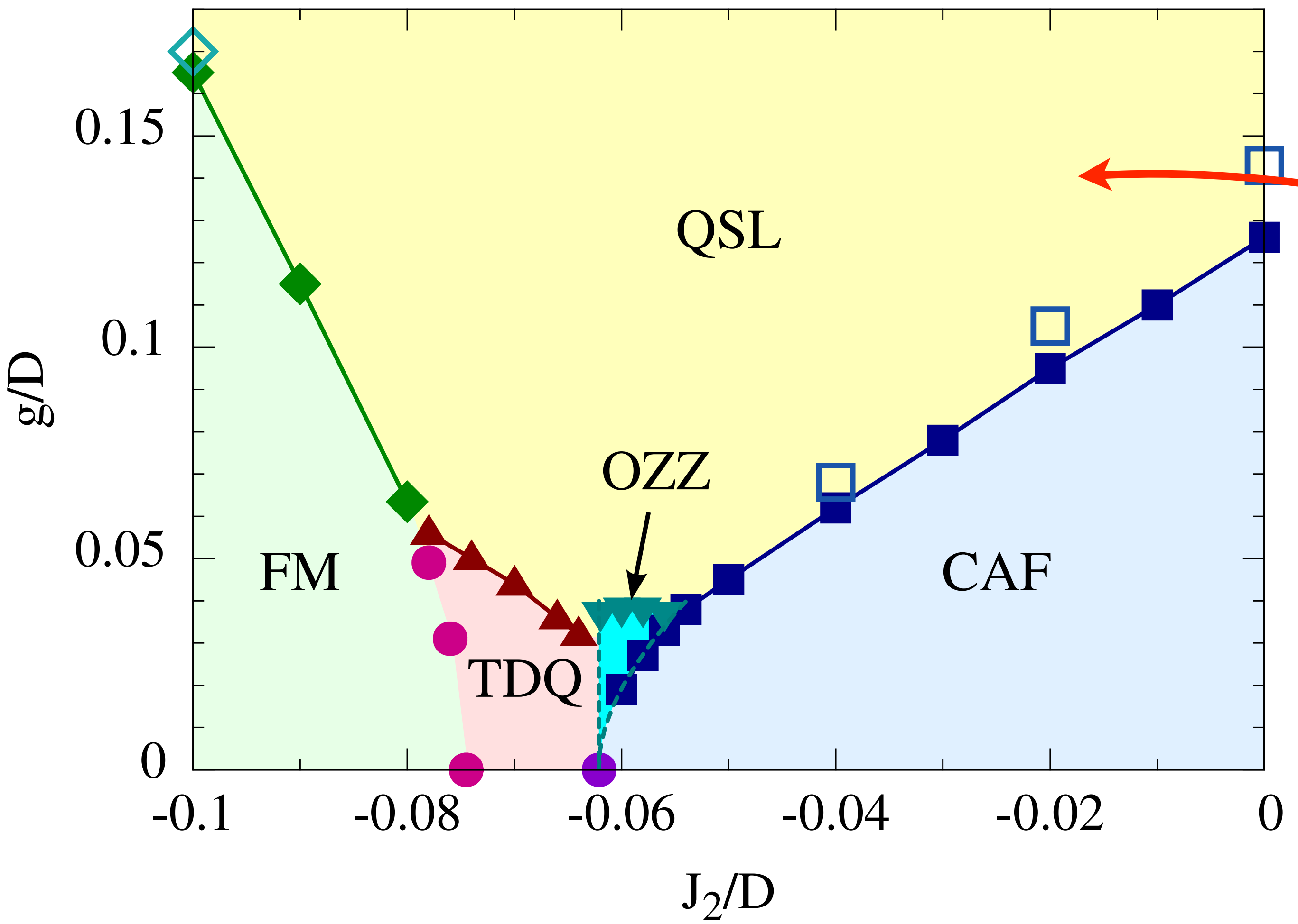
selects between chain states

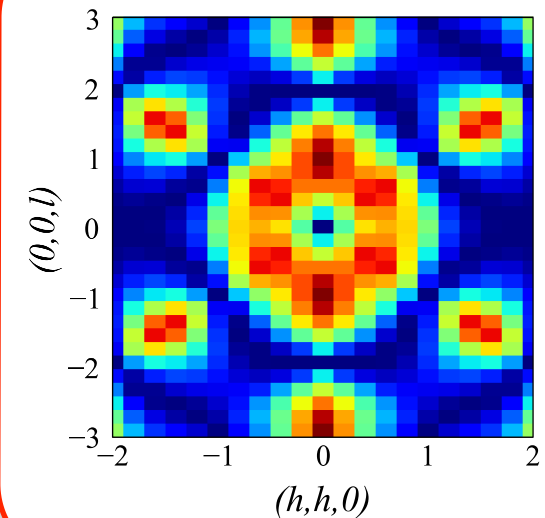
favours quantum spin liquid

…consider model as a function of (J_2/D, g/D) for T=0

quantum dipolar spin ice

$$\mathcal{H}_{\text{QDSI}} = \mathcal{H}_{\text{dipolar}} + \mathcal{H}_{\text{exchange}} + \mathcal{H}_{\text{tunneling}}$$



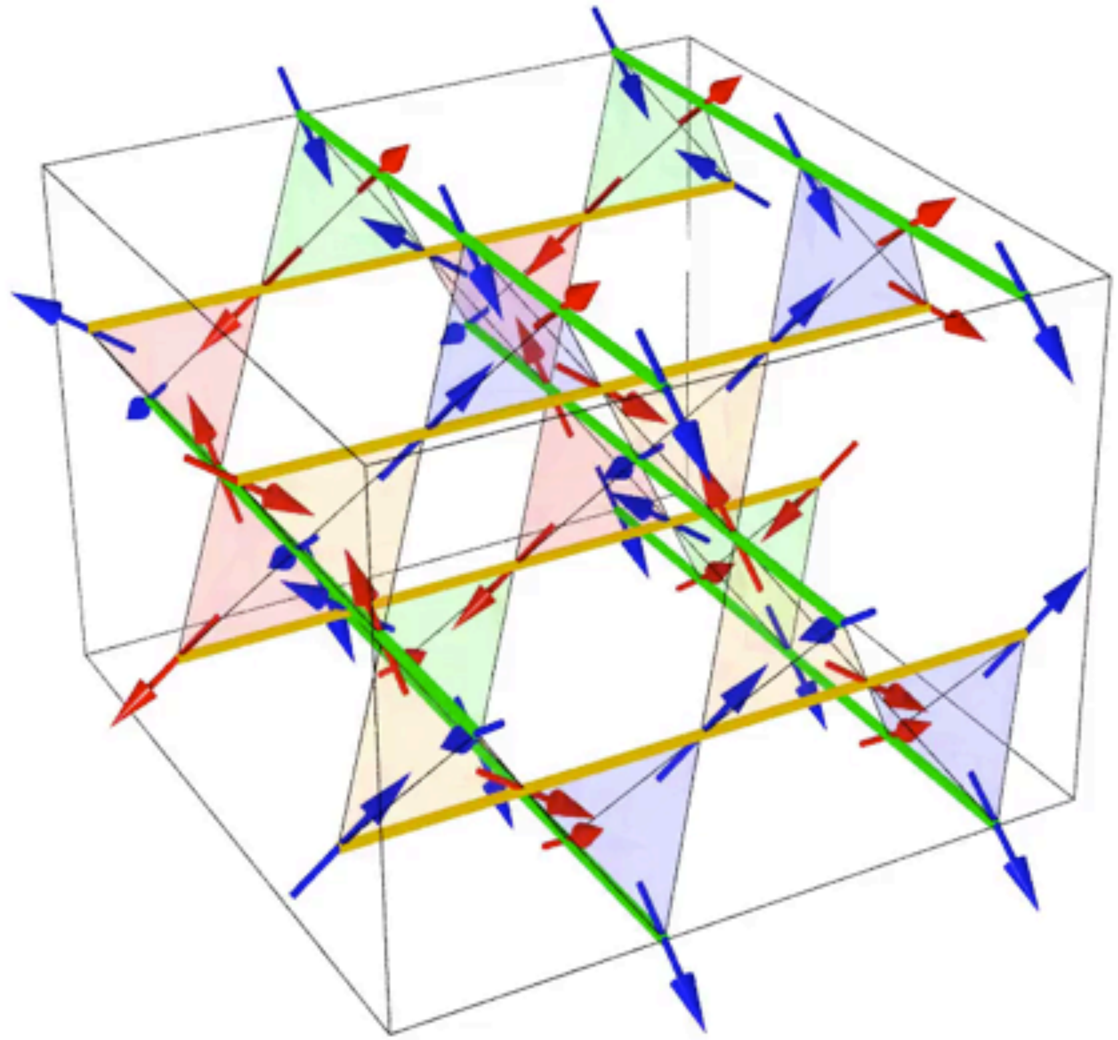


quantum spin liquid with $1/r^4$ correlations ✓

only a very small tunnelling g ~ 0.1 D is needed to achieve a QSL !

P. McClarty *et al.*, arXiv.1410.0451v1

orthorhombic zig-zag (OZZ)



spin-ice configuration composed of **ferromagnetically-polarized chains** of spins

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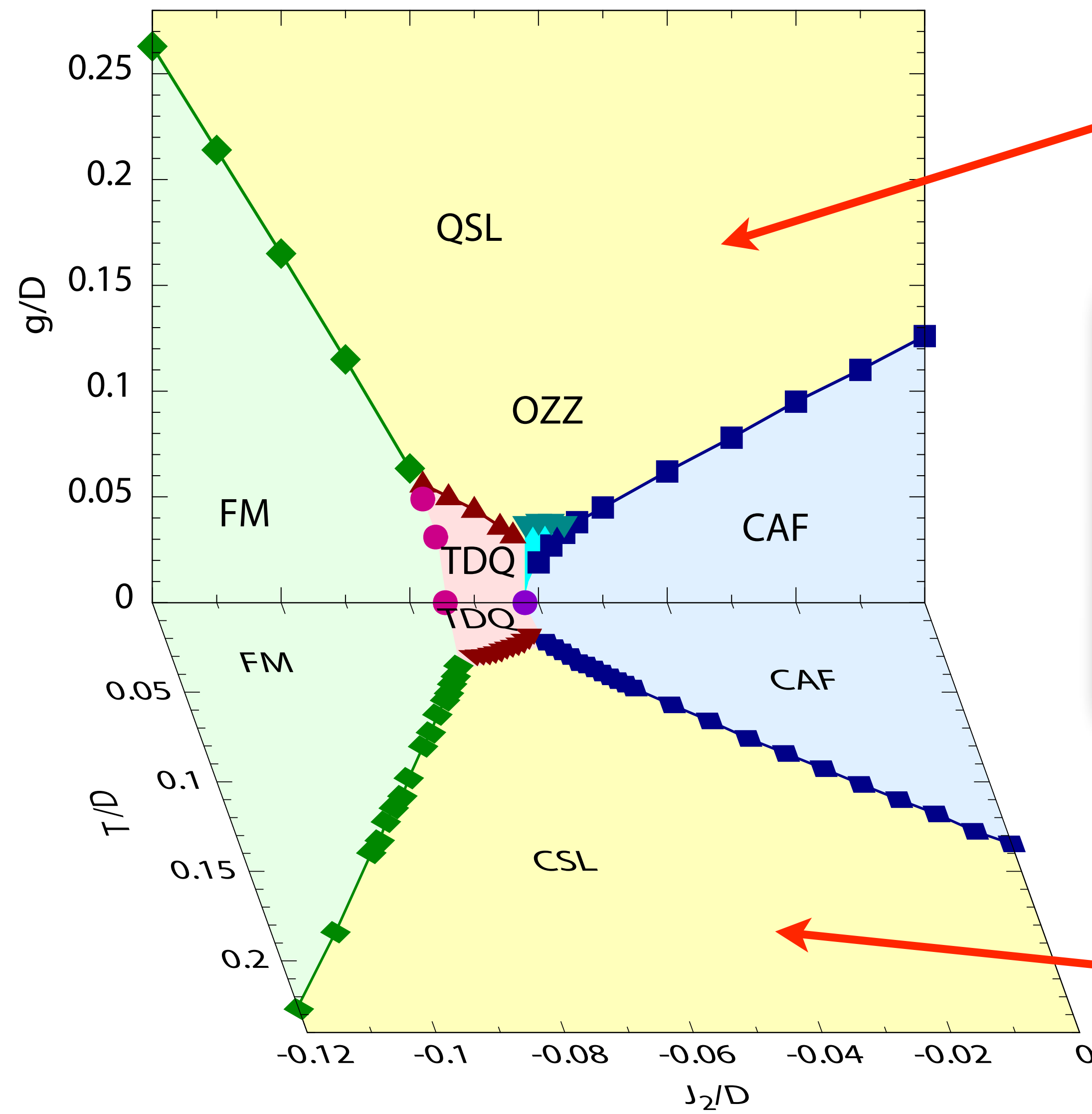
putting it all together…

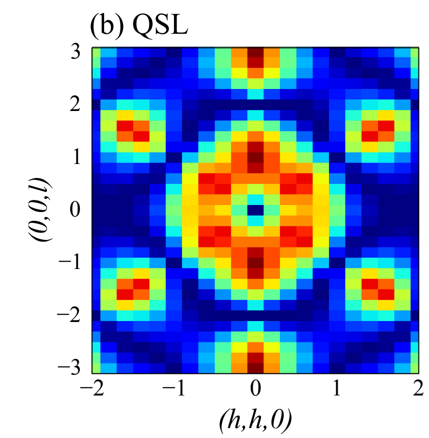
$$\mathcal{H}_{\mathrm{QDSI}} = \mathcal{H}_{\mathrm{dipolar}} + \mathcal{H}_{\mathrm{exchange}} + \mathcal{H}_{\mathrm{tunnelling}}$$

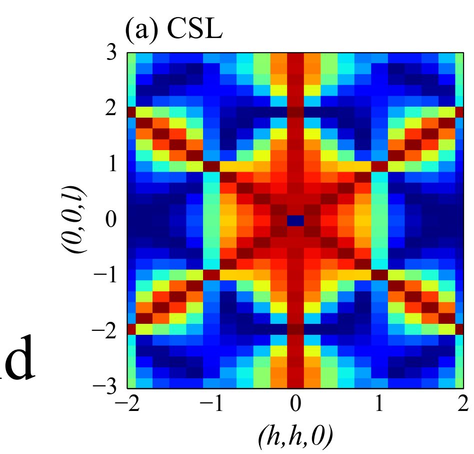


quantum spin liquid

ordered phases composed of ferromagnetically-polarised chains of spins

classical spin liquid

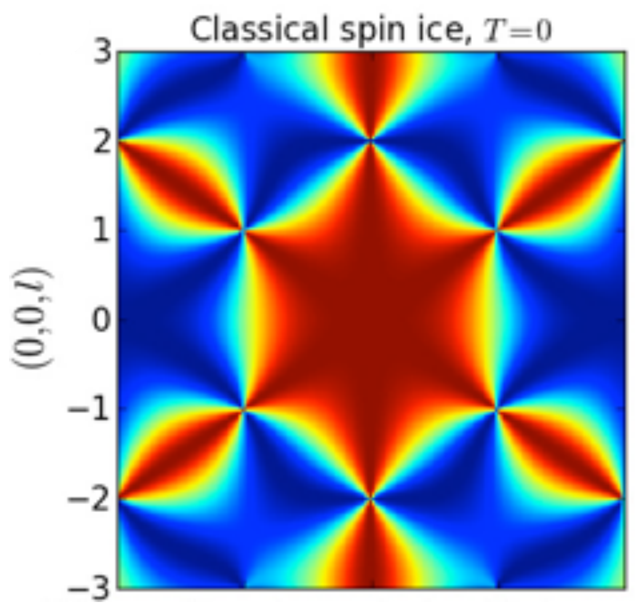




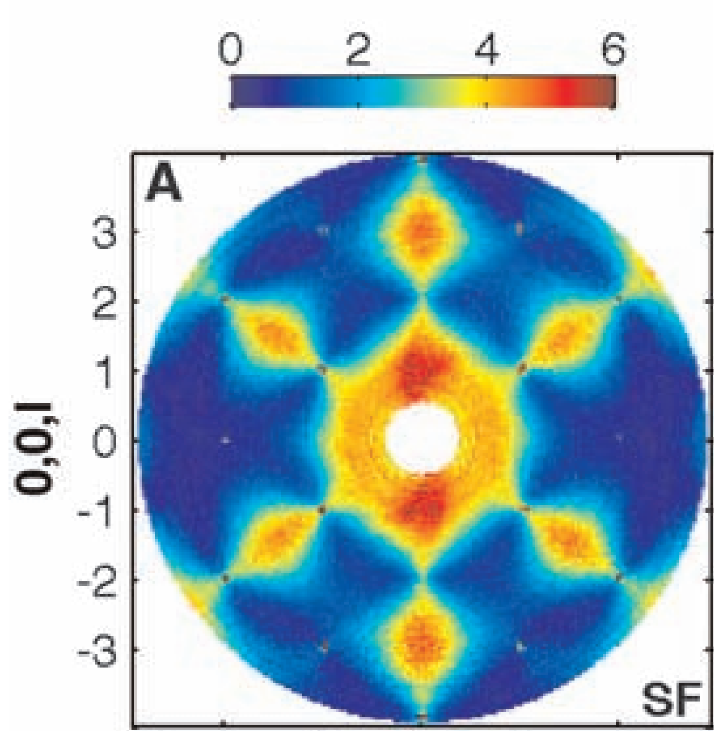
P. McClarty *et al.*, arXiv.1410.0451v1

a provocative comparison !

prediction for
classical spin ice

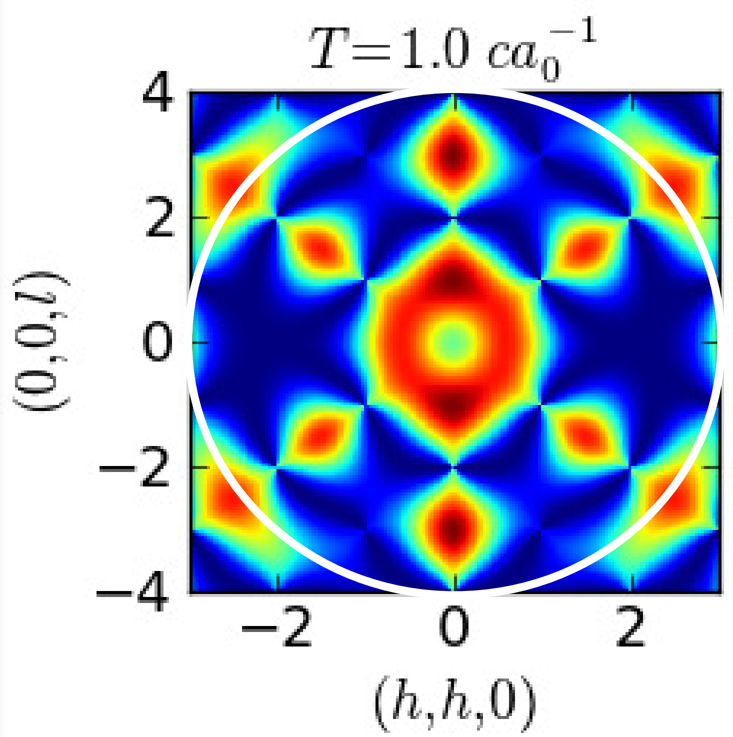


neutron scattering
on $Ho_2Ti_2O_7$



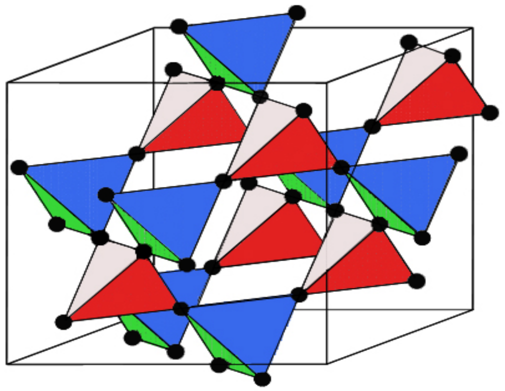
T. Fennell et al,
Science **326**, 415 (2009).

prediction for
quantum spin ice
at finite T

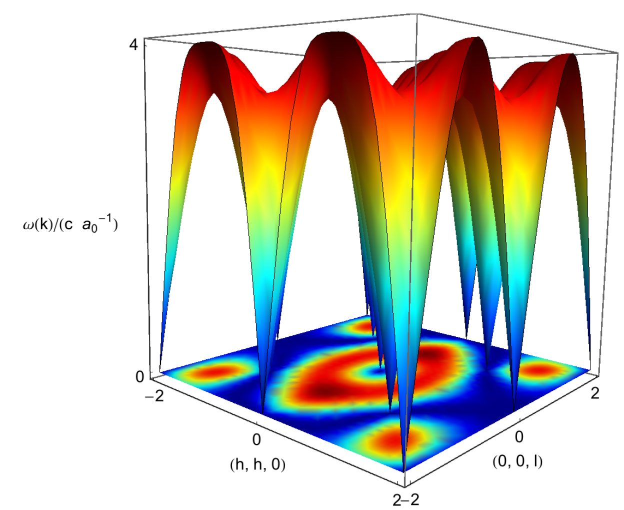


O. Benton *et al.*,
Phys. Rev. B. **83**,
075174 (2012) ❦

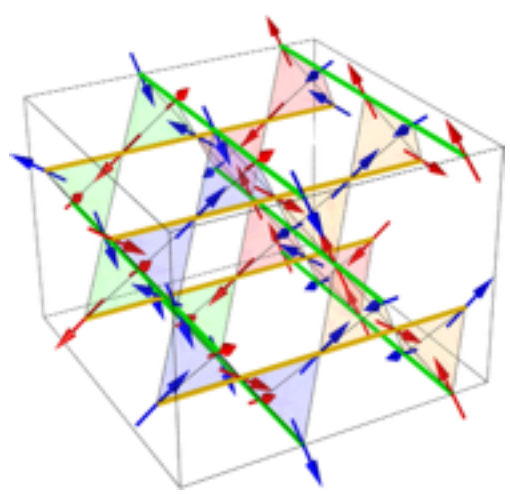
…in conclusion



the effect of quantum fluctuations on spin-ice is an interesting theoretical question, motivated by experiment **wide range of different pyrochlore oxides**



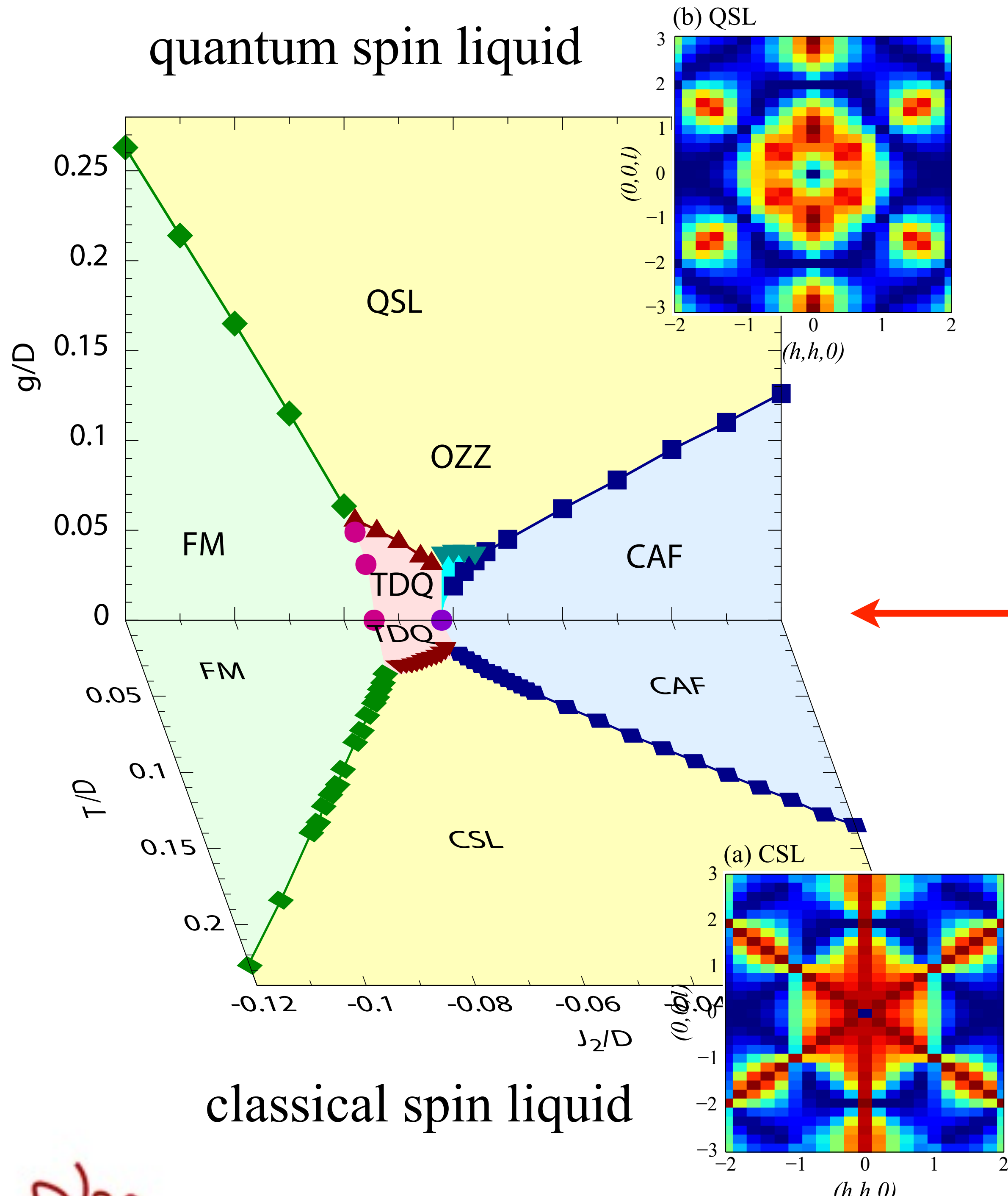
realistic models of spin-ice materials, with long-range dipolar interactions, can support a **3D quantum spin-liquid** ground state



competing ordered phases are composed of **ferromagnetic chains of alternating spins**, within which dipolar interactions are exponentially screened !

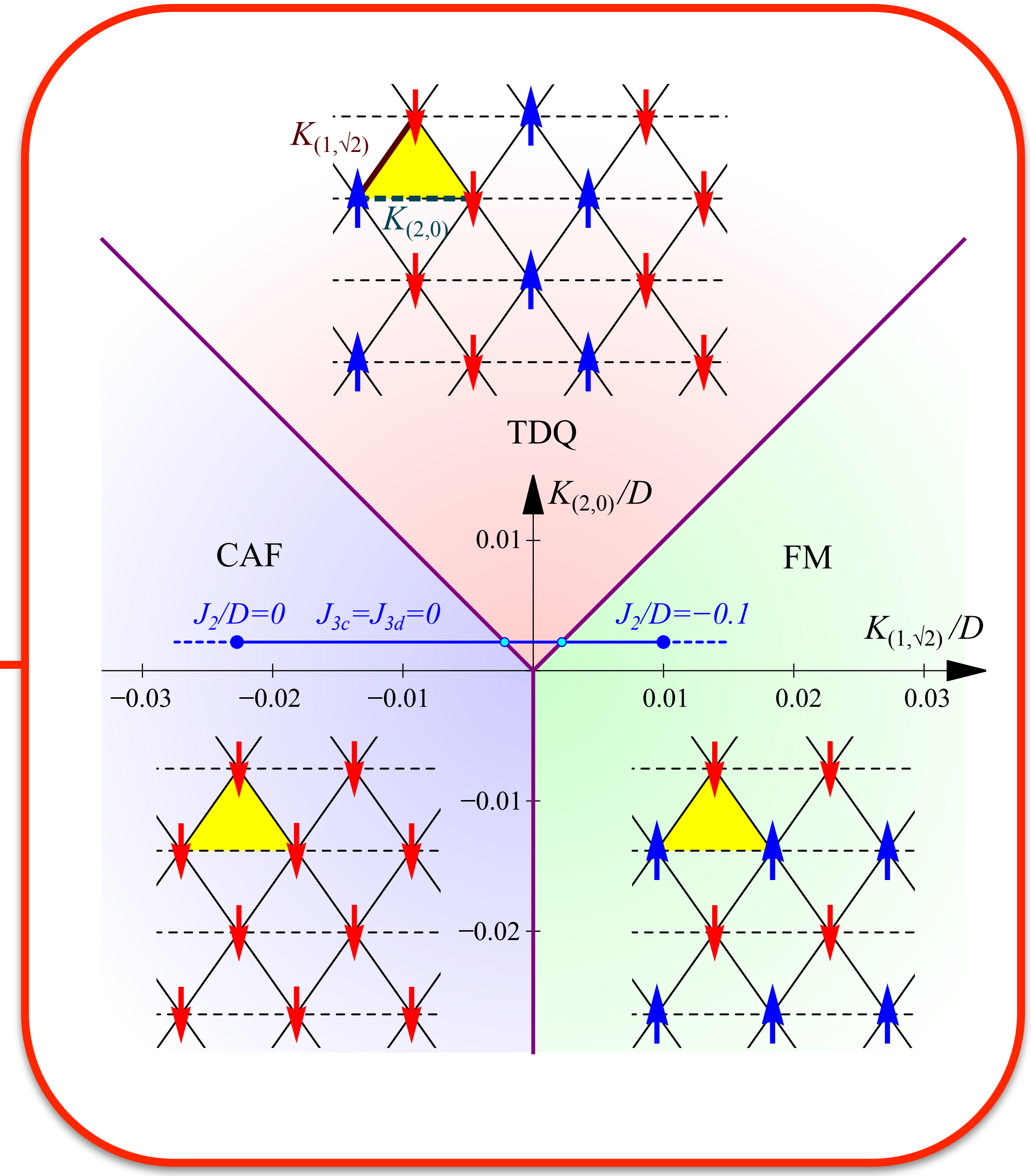
“spin ice can do it all”

quantum spin liquid



classical spin liquid

ordered ground states



T=0, g=0

P. McClarty *et al.*, arXiv.1410.0451v1


thanks for listening !

how good is the lattice gauge theory ?

how well does this work…?

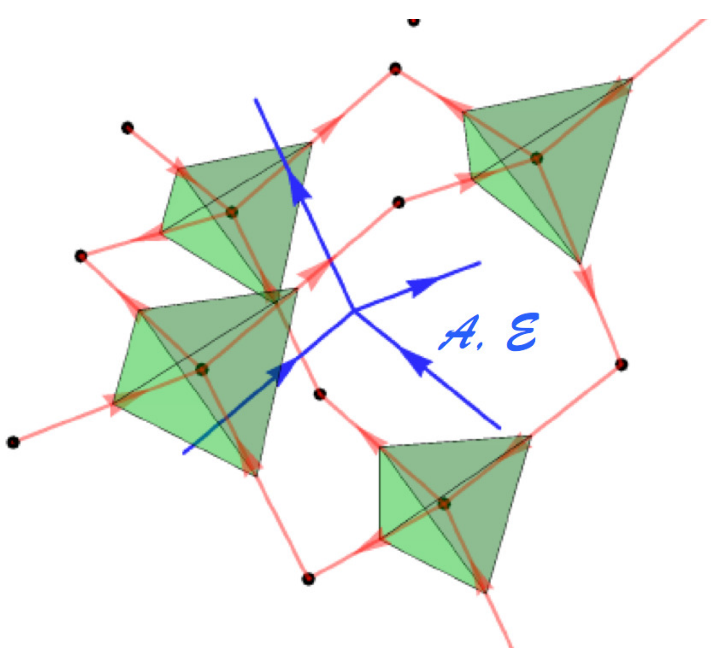
compact U(1) lattice gauge theory...

$$\mathcal{H}'_{\mathsf{U}(1)} = \frac{\mathcal{U}}{2} \sum_{\mathbf{r} \in A, n} \left[(\nabla_{\hexagon} \times \mathcal{A})_{(\mathbf{r},n)} \right]^2 + \frac{1}{2\mathcal{K}} \sum_{\mathbf{s} \in A', m} \left[\frac{\partial \mathcal{A}_{(\mathbf{s},m)}}{\partial t} \right]^2 + \frac{\mathcal{W}}{2} \sum_{\mathbf{s} \in A', m} \left[(\nabla_{\hexagon} \times \nabla_{\hexagon} \times \mathcal{A})_{(\mathbf{s},m)} \right]^2$$

"ice" term

tunnelling term

"μ" term (relevant at RK point)



...theory is quadratic in gauge field

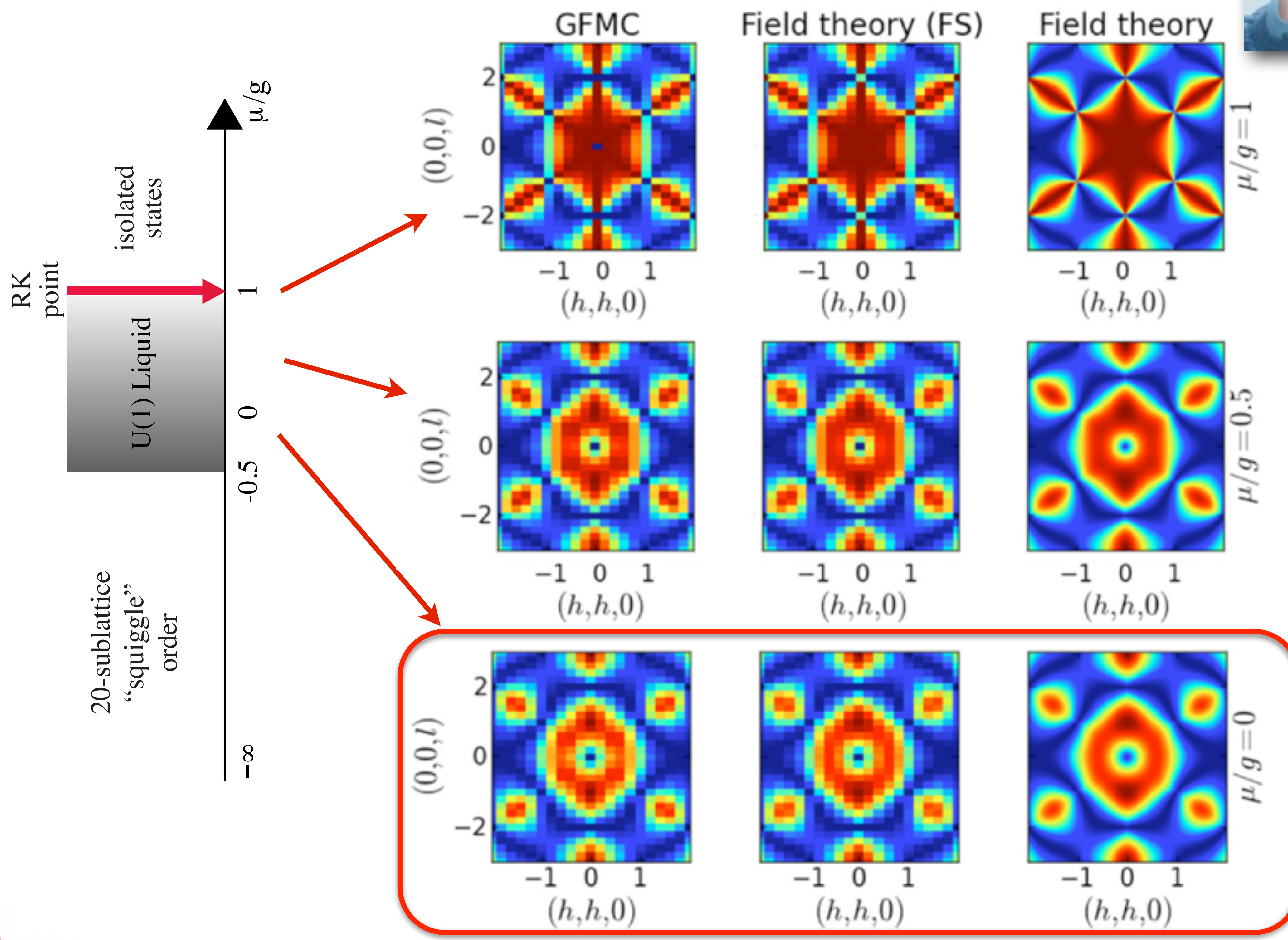
can diagonalise problem by introducing suitable photon basis :

$$\mathcal{A}_{(\mathbf{s},m)} = \sqrt{\frac{2}{N}} \sum_{\mathbf{k}} \sum_{\lambda=1}^{4} \sqrt{\frac{\mathcal{K}}{\omega_\lambda(\mathbf{k})}} \times \Big(\exp\left[-i\mathbf{k} \cdot (\mathbf{s} + \mathbf{e}_m/2)\right] \eta_{m\lambda}(\mathbf{k}) a_\lambda(\mathbf{k}) + \exp\left[i\mathbf{k} \cdot (\mathbf{s} + \mathbf{e}_m/2)\right] \eta^*_{\lambda m}(\mathbf{k}) a^\dagger_\lambda(\mathbf{k}) \Big)$$

use quantum Monte Carlo simulation to validate - and parameterise - theory

how well does this work…?

$$\mathcal{H}_\mu = -g \sum_{\hexagon} |\circlearrowright\rangle\langle\circlearrowleft| + |\circlearrowleft\rangle\langle\circlearrowright| + \mu \sum_{\hexagon} |\circlearrowright\rangle\langle\circlearrowright| + |\circlearrowleft\rangle\langle\circlearrowleft|$$



O. Benton *et al.*, Phys. Rev. B. **86**, 075174 (2012)

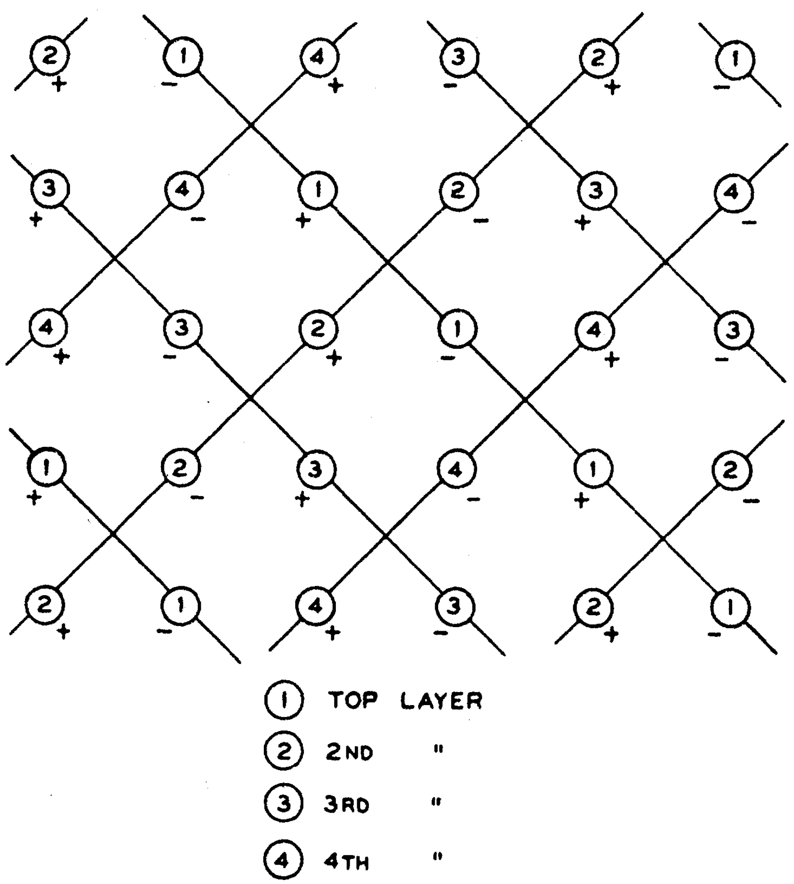
why all these chain states ?

PHYSICAL REVIEW VOLUME 102, NUMBER 4 MAY 15, 1956

Ordering and Antiferromagnetism in Ferrites

P. W. ANDERSON
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received January 9, 1956)

Verway proposal for charge-order in Fe_3O_4 :
ice-like state state composed of alternating lines of charge

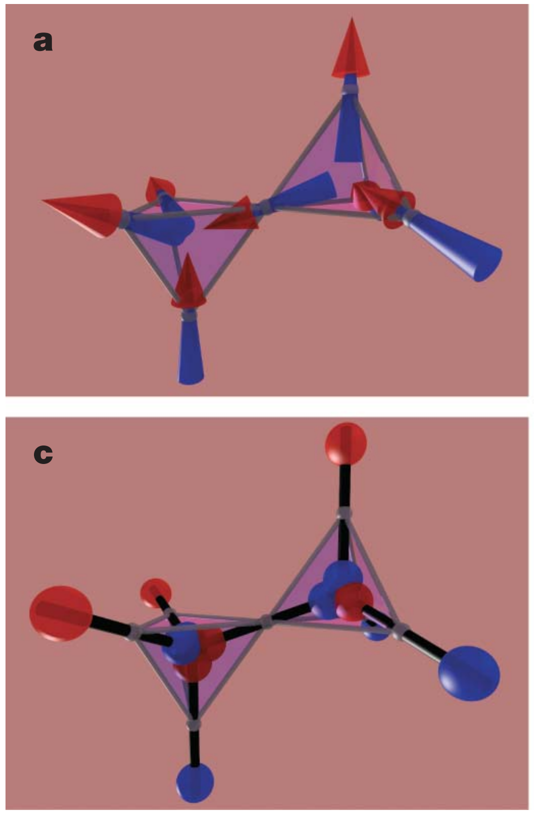


"In the Madelung method, one divides the lattice into neutral lines of atoms […]
In the present case… only next-nearest neighbouring lines interact".

i.e. charge-ice states with composed of alternating chains have the lowest Coulomb energy….

what’s the connection ?

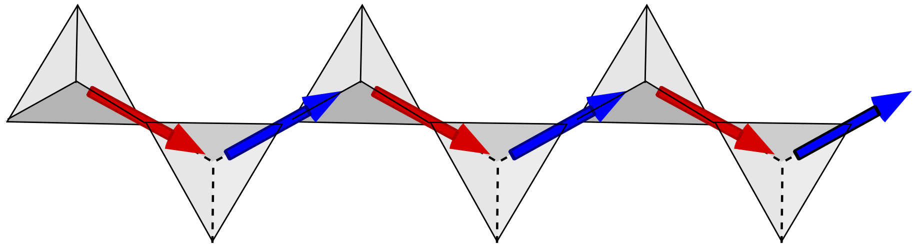
“dumbbell” picture of spin ice…



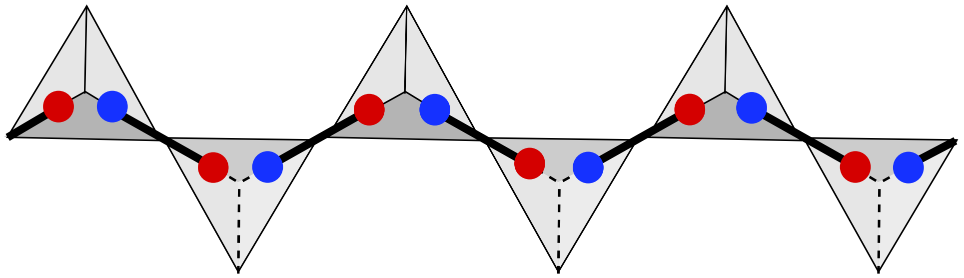
…magnetic dipoles (spins)
expressed in terms of magnetic charge

C. Castelnovo *et al*., Nature **451**, 42 (2007)

within the “dumbbell” picture, an alternating chain of spins…

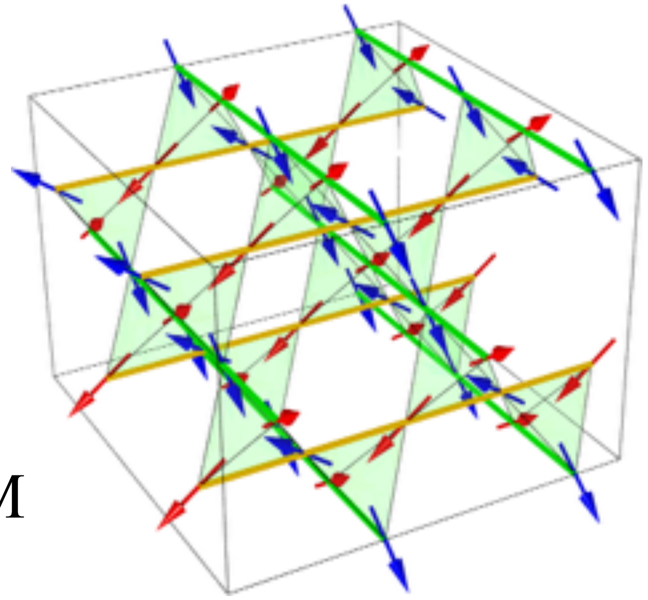


…becomes an
alternating chain of (magnetic) charges :



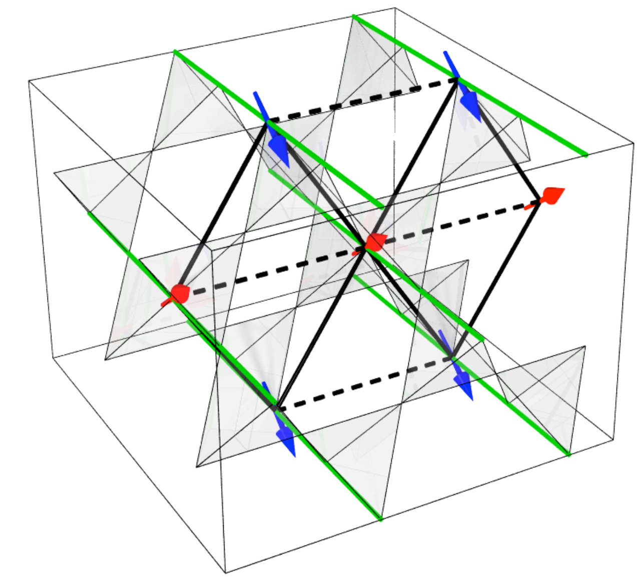
same strategy works here !

how does this work ?



FM

two sets of chains // [110]



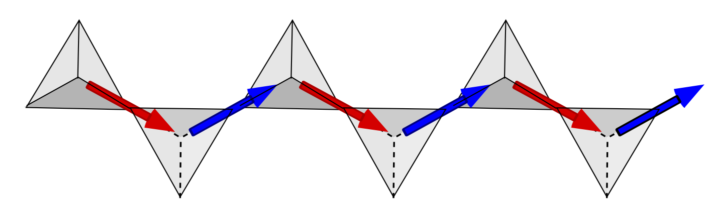
each chain acts like an Ising degree of freedom

$$\mathcal{H}_{\text{DSI}} = \mathcal{H}_{\text{dipolar}} + \mathcal{H}_{\text{exchange}}$$

$$\mathcal{H}_{\text{dipolar}} = 4D \sum_{i<j} \left(\frac{r_1}{r_{ij}}\right)^3 \left[\hat{\mathbf{z}}_i \cdot \hat{\mathbf{z}}_j - 3\left(\hat{\mathbf{z}}_i \cdot \hat{\mathbf{r}}_{ij}\right)\left(\hat{\mathbf{z}}_j \cdot \hat{\mathbf{r}}_{ij}\right)\right] \mathsf{S}_i^z \mathsf{S}_j^z$$

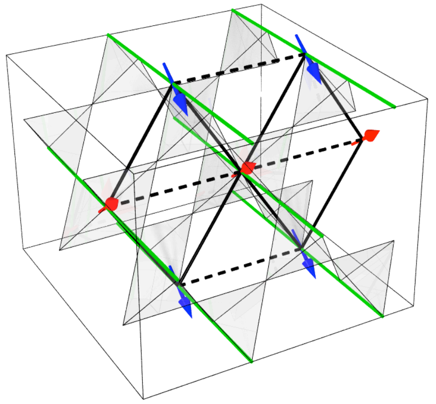
$$\mathcal{H}_{\text{exchange}} = \sum_k 4J_k \sum_{\langle ij\rangle_k} \left(\hat{\mathbf{z}}_i \cdot \hat{\mathbf{z}}_j\right) \mathsf{S}_i^z \mathsf{S}_j^z$$

$$\mathcal{H}^{\text{2D}}_{\text{Ising}} = \frac{1}{2} \sum_{\boldsymbol{r},\boldsymbol{\delta}} K_{\boldsymbol{\delta}}\, \sigma_{\boldsymbol{r}}\, \sigma_{\boldsymbol{r}+\boldsymbol{\delta}}$$



P. McClarty *et al.*, arXiv.1410.0451v1

how does this work ?



dipolar interaction between FM chains of spins separated by distance $\delta = |(\delta_1, \delta_2)|$

$$K_{\boldsymbol{\delta}} = \sqrt{2}^3 D \sum_{l=-\infty}^{\infty} \left[(-1)^l \frac{2}{3} \frac{(\delta_1^2 - 2\delta_2^2 + l^2)}{2^{5/2} (\delta_1^2 + \delta_2^2 + l^2)^{5/2}} + (-1)^{\delta_1} \frac{4}{3} \frac{(\delta_1^2 + \delta_2^2 - 2l^2)}{2^{5/2} (\delta_1^2 + \delta_2^2 + l^2)^{5/2}} \right]$$

sum over infinitely-long chain

$$K_{\boldsymbol{\delta}}/D \approx \frac{4\pi}{3\delta} K_1(\pi\delta) - \frac{4\pi^2 \delta_2^2}{3\delta^2} K_2(\pi\delta) \approx -\frac{2\sqrt{2}}{3} \left[\pi^2 \left(\frac{\delta_2}{\delta} \right)^2 \delta^{-1/2} - \pi \delta^{-3/2} + \cdots \right] e^{-\pi\delta}$$

modified Bessel functions

exponential decay

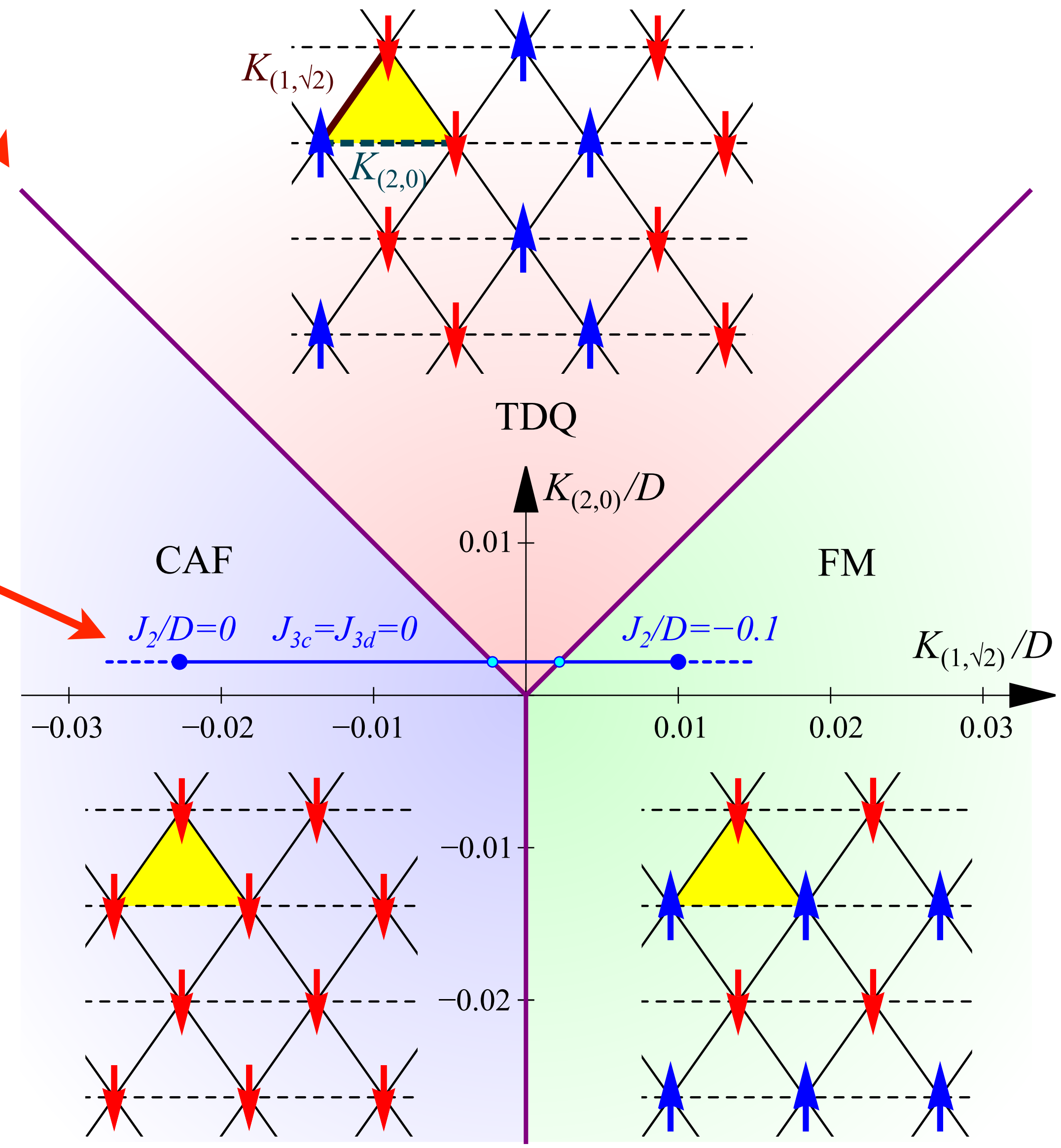
chains described by 2D Ising model with only short-range interactions !

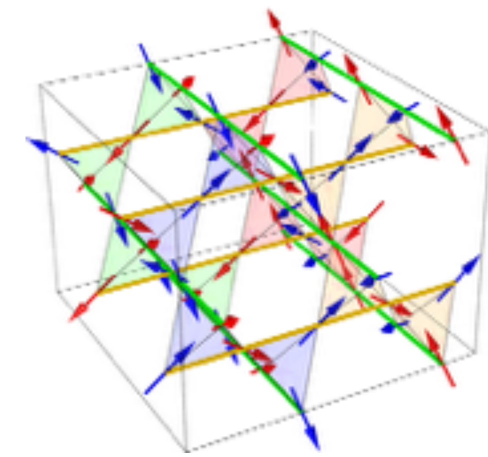
P. McClarty *et al.*, arXiv.1410.0451v1

what states do we find ?

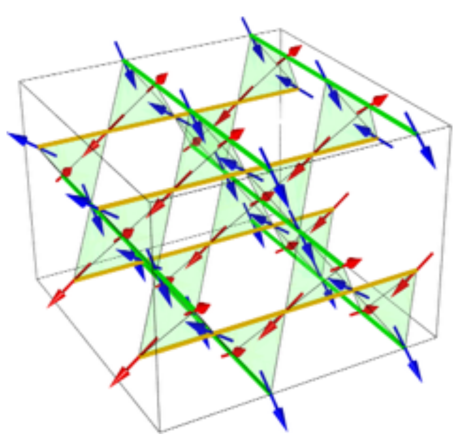
additional degeneracy
on phase boundary
cf. ANNNI model

parameters used
in simulations

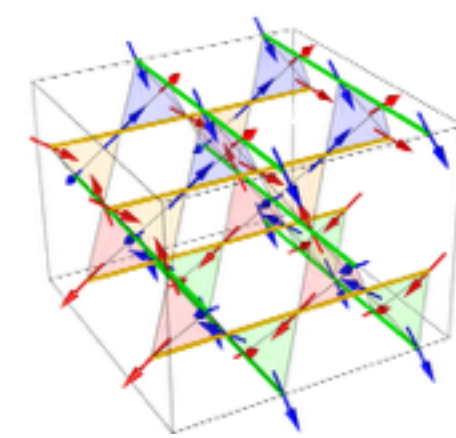




TDQ



CAF



FM

P. McClarty *et al.*, arXiv.1410.0451v1

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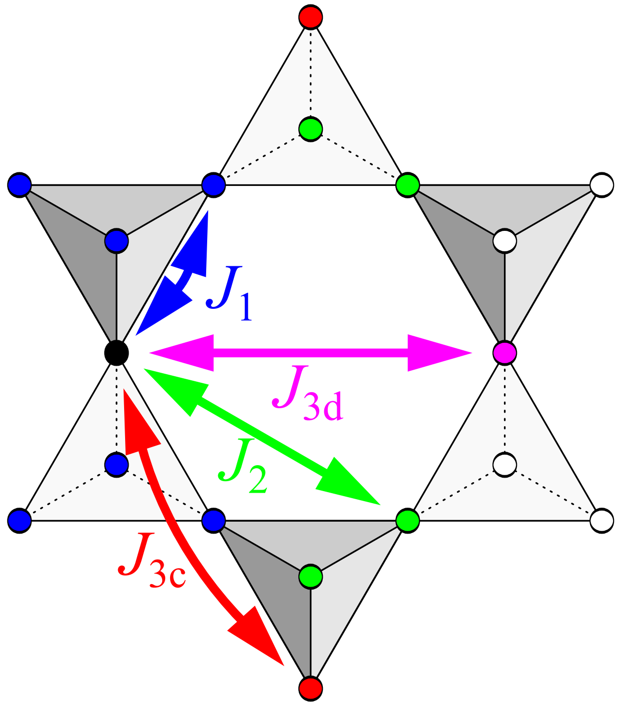
how good is the chain picture ?

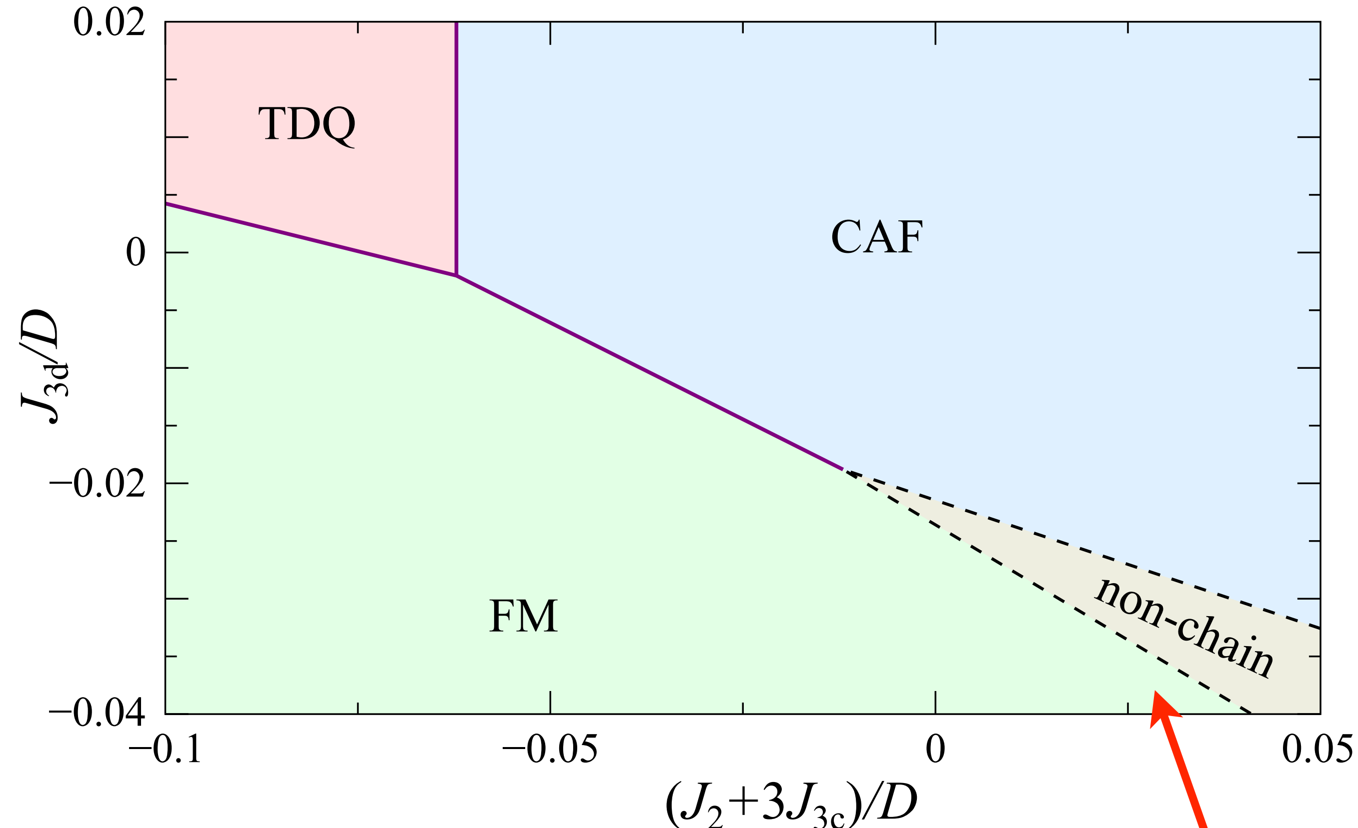
limits of the chain picture ?

$$\mathcal{H}_{\mathsf{DSI}} = \mathcal{H}_{\mathsf{dipolar}} + \mathcal{H}_{\mathsf{exchange}}$$

what happens if we include further-neighbor exchange ?



numerical search of ground states for 128-site cluster



N.B. within spin-ice states J_{3c} is equivalent to $J_2/3$

$$J_{\text{eff}} = J_2 + 3J_{3c}$$

small incursion of non-chain states for $J_{3d} < -0.02$

P. McClarty *et al.*, arXiv.1410.0451v1

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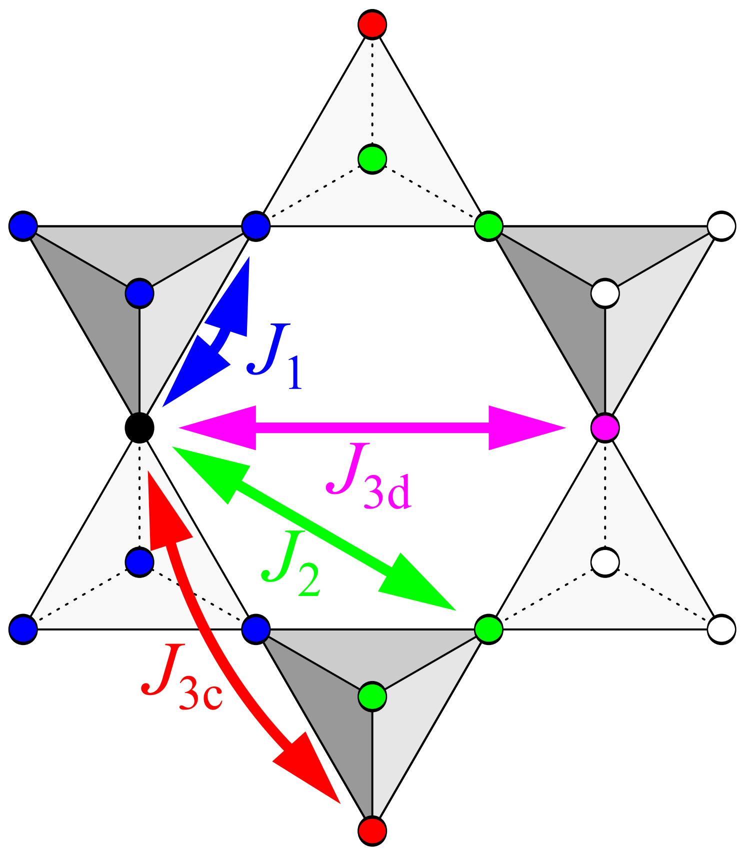
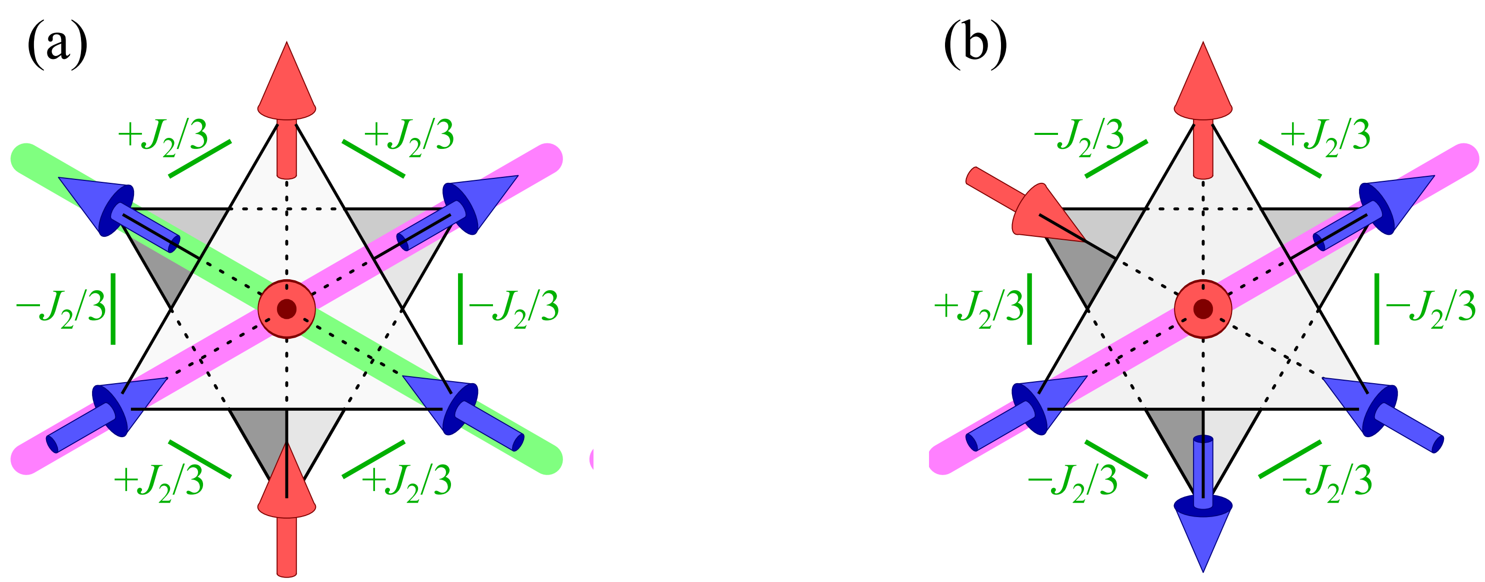
equivalence of J_2 and J_{3c}

consider a pair of tetrahedra sharing a single common spin, both with spin configurations obeying the ice rules



16 possible states, falling into two types :



$$E_a = J_{3c} + \frac{2}{3}\left(J_2 + 3J_{3c}\right) \qquad E_b = J_{3c} - \frac{2}{3}\left(J_2 + 3J_{3c}\right)$$

energy difference determined by combination of parameters : $J_{\text{eff}} = J_2 + 3J_{3c}$

P. McClarty *et al.*, arXiv.1410.0451v1