K-theory: Kitaev, Kagome, and Kapellasite

Leon Balents, **K**ITP

Frumag 2016, **K**loster Nimbschen

K-theory

From Wikipedia, the free encyclopedia

In mathematics, **K-theory** is, roughly speaking, the study of certain kinds of invariants of large matrices.[1] It originated as the study of a ring generated by vector bundles over a topological space or scheme. In algebraic topology, it is an extraordinary cohomology theory known as topological K-theory. In algebra and algebraic geometry, it is referred to as algebraic K-theory. It is also a fundamental tool in the field of operator algebras.

K-theory involves the construction of families of *K*-functors that map from topological spaces or schemes to associated rings; these rings reflect some aspects of the structure of the original spaces or schemes. As with functors to groups in algebraic topology, the reason for this functorial mapping is that it is easier to compute some topological properties from the mapped rings than from the original spaces or schemes. Examples of results gleaned from the K-theory approach include Bott periodicity, the Atiyah-Singer index theorem and the Adams operations.

In high energy physics, K-theory and in particular twisted K-theory have appeared in Type II string theory where it has been conjectured that they classify D-branes, Ramond–Ramond field strengths and also certain spinors on generalized complex manifolds. In condensed matter physics K-theory has been used to classify topological insulators, superconductors and stable Fermi surfaces. For more details, see K-theory (physics).

Quantum Spin Liquids

Quantum spin liquids are ground states that possess long-distance entanglement and are robust to perturbations

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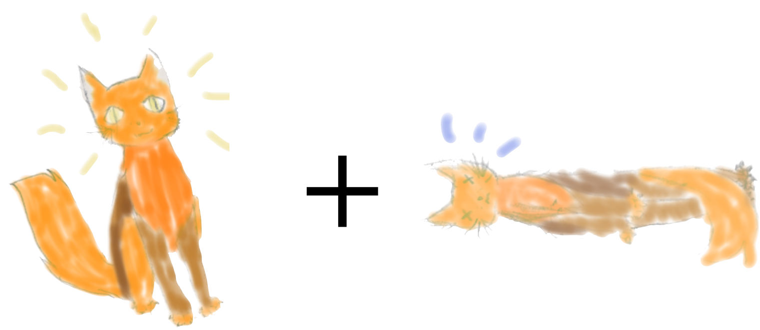
Quantum spin liquids are ground states that possess long-distance entanglement and are robust to perturbations



Schrödingers **K**atze

I decided to tell you about **K**itaev spin liquids, the **K**agomé lattice, and **K**apellasite

Here we are in **K**loster Nimbschen

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For an internationale **K**onferenz

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For an internationale **K**onferenz

at the home of Torsten **K**racht

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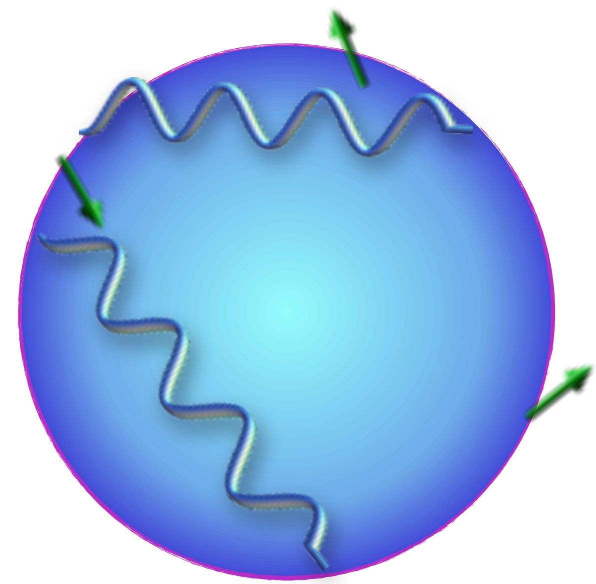
to discuss **k**wantum spin liquids



Here we are in **K**loster Nimbschen

For an internationale **K**onferenz

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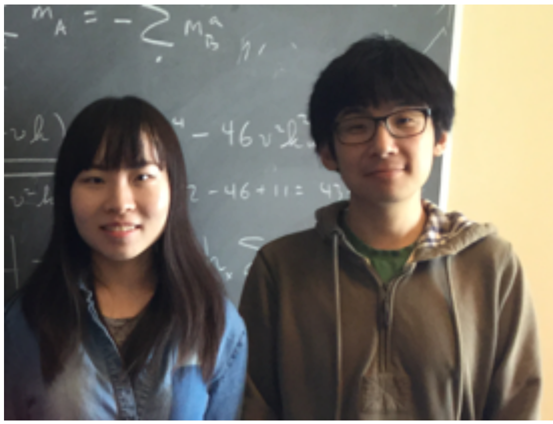
to discuss **k**wantum spin liquids

This can't be a **k**oincidence

Kollaborators



Xueyang Song

Yi-Zhuang You

Shoushu Gong

Donna Sheng

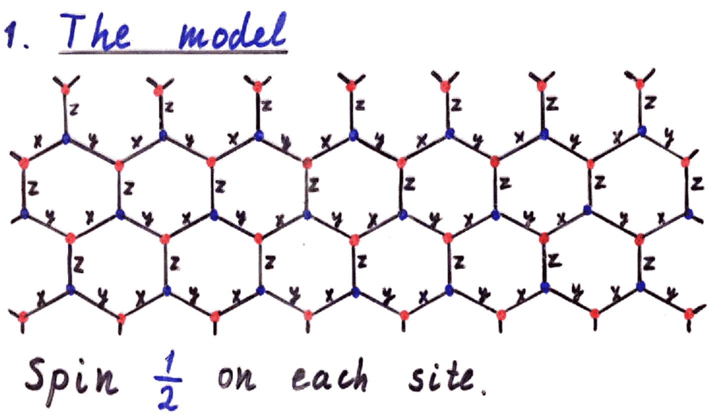
Oleg Stary**K**h

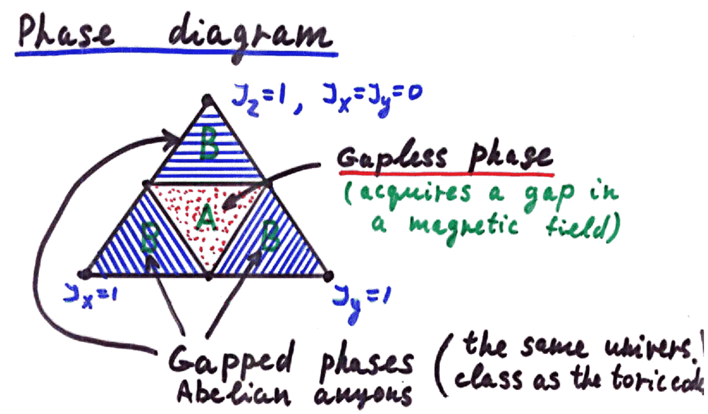
c.f. Motome, Nasu, Nagler

Kitaev model

Kitaev's honeycomb model $$H = \sum_{i,\mu} K_\mu \sigma_i^\mu \sigma_{i+\mu}^\mu$$

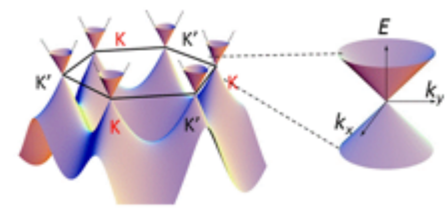
KITP, 2003





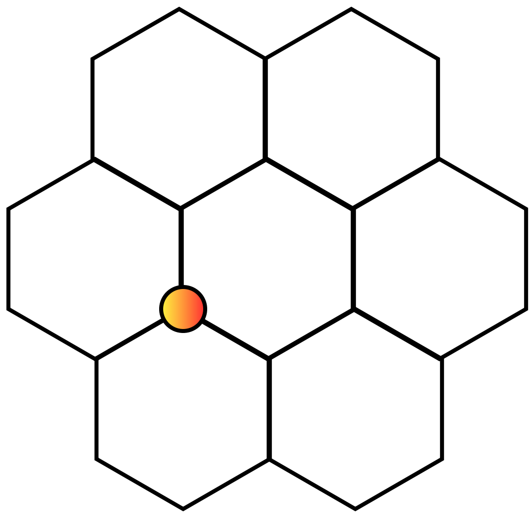
exact parton construction $\sigma_i^\mu = i c_i c_i^\mu \qquad c_i c_i^x c_i^y c_i^z = 1$

physical Majoranas $H_{\mathrm{m}} = K \sum_{\langle ij \rangle} i c_i c_j$

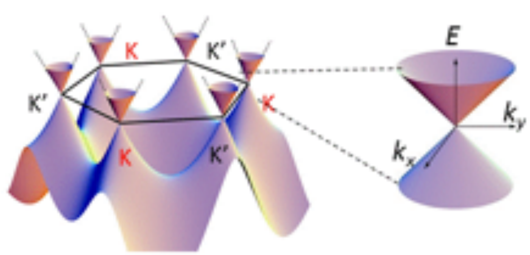


note: **K**, **K′** points!

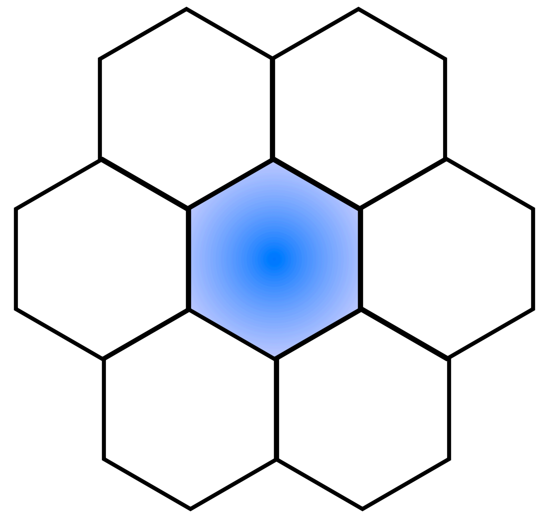
Non-local excitations



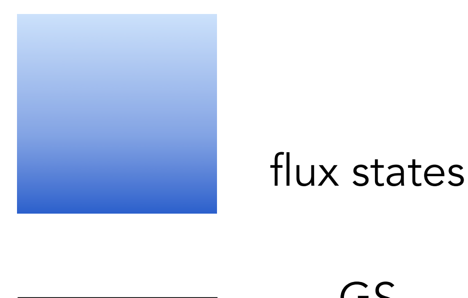
Majorana ε



gapless Dirac



Flux e, m

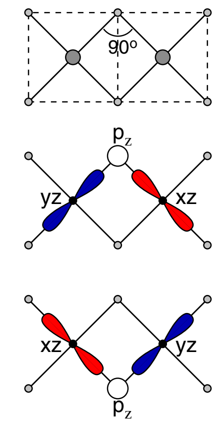


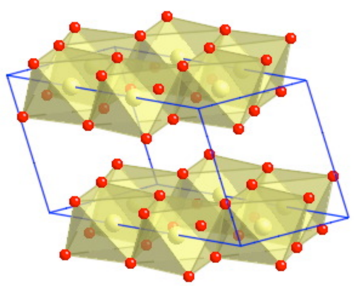
gapped

Kitaev Materials

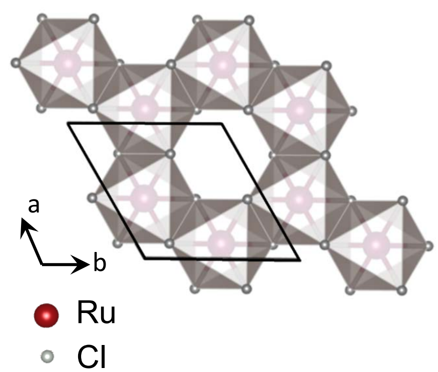
Jac**K**eli, **K**haliullin

Showed that Kitaev interaction can be large in edge-sharing octahedra with large spin-orbit-coupling





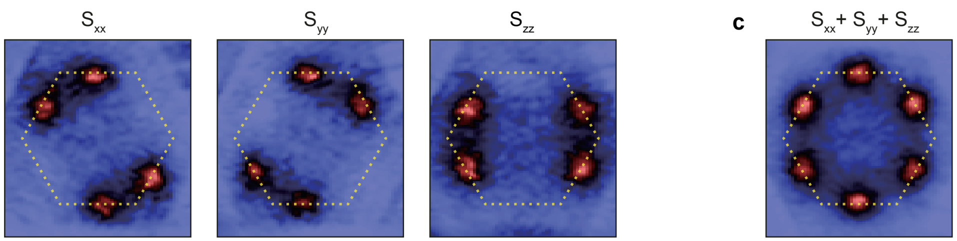
Na_2IrO_3, (α,β,γ)-Li_2IrO_3



α-$RuCl_3$

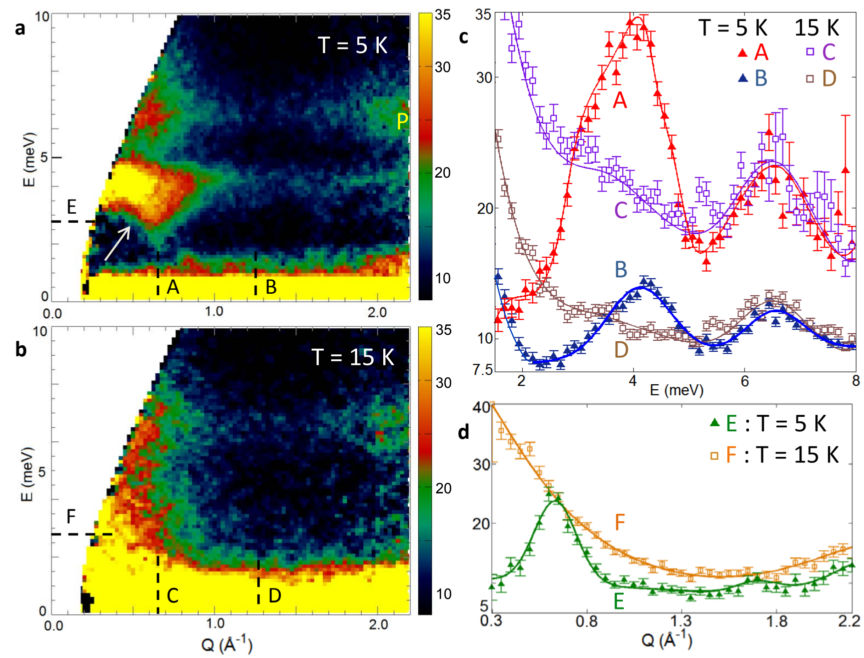
Honeycomb and hyper-honeycomb structures

Kitaev Materials



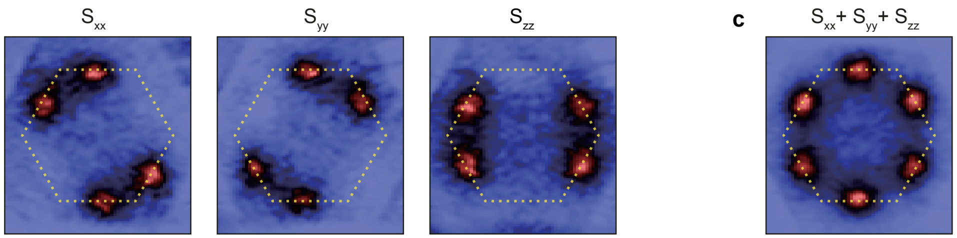
direct evidence for direction-dependent anisotropic exchange from diffuse magnetic x-ray scattering in Na_2IrO_3 (BJ Kim group)

there is pretty strong evidence of substantial Kitaev exchange in quite a few materials



Observation of gapped continuum mode persisting above T_N in α-$RuCl_3$ consistent with Majoranas (A. Banerjee *et al)*

Kitaev Materials



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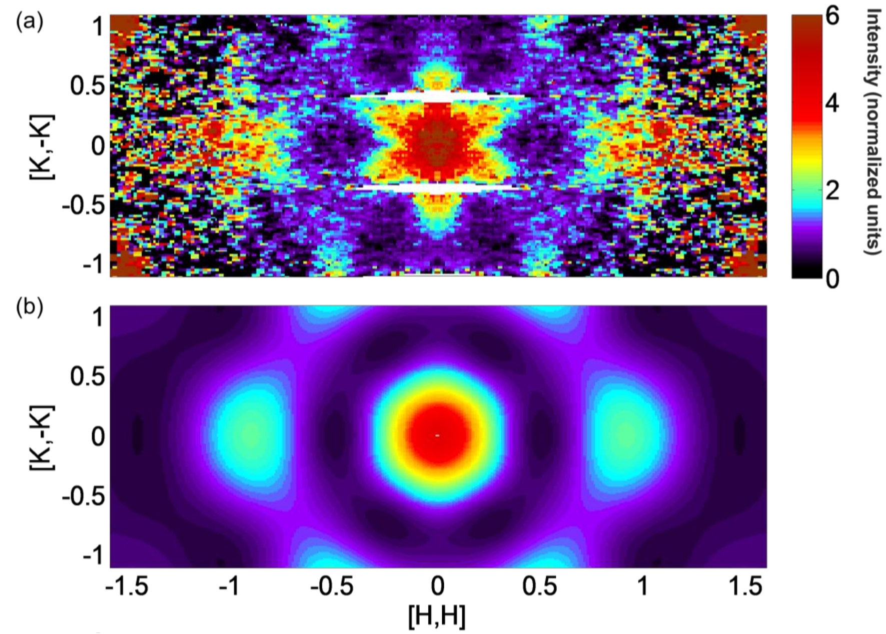
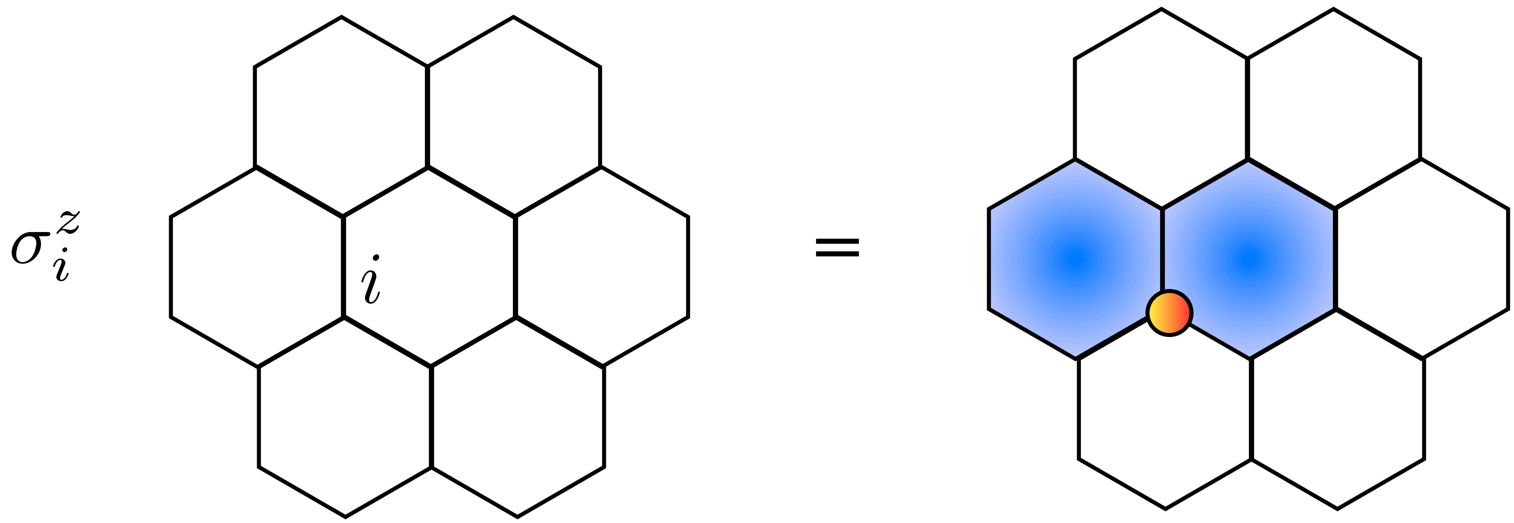


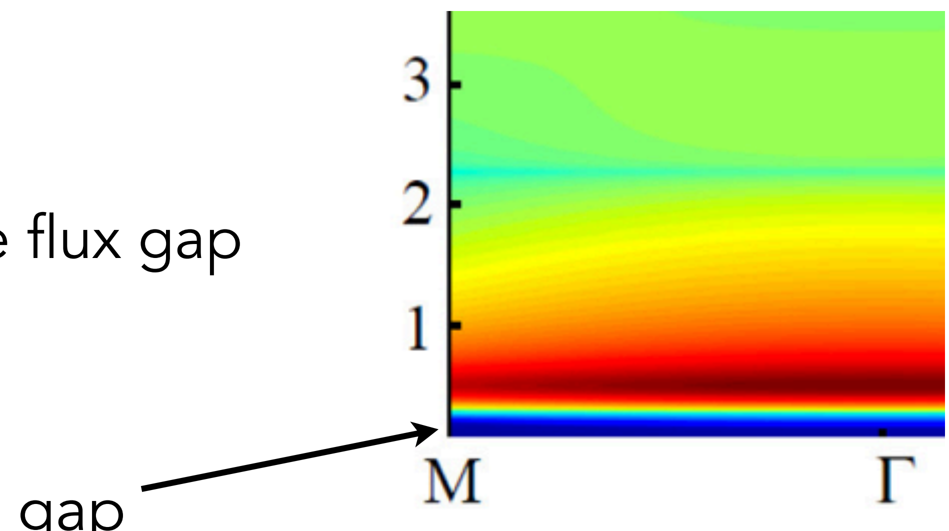
single-crystal datain α-$RuCl_3$ compared to Kitaev's soluble model (A. Banerjee *et al)*

Exact spin correlations



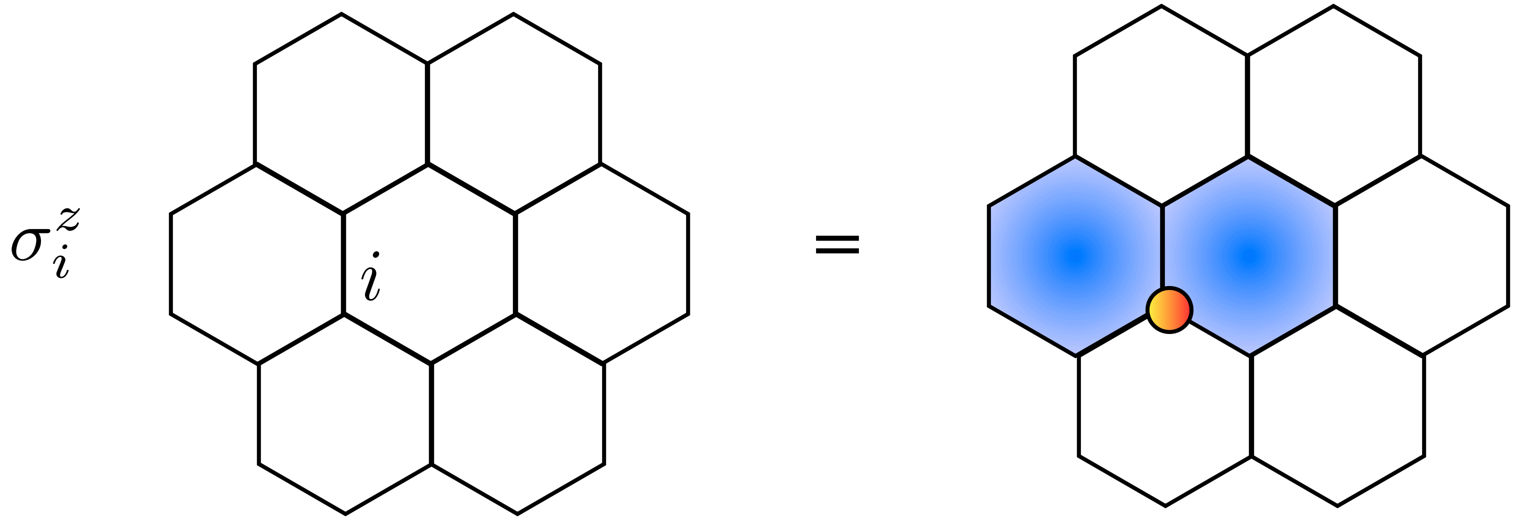
In the soluble model:

- The spin creates two fluxes
- Spectral weight is zero below the flux gap
- Correlations vanish beyond NNs



J. Knolle *et al*, 2014

Exact spin correlations

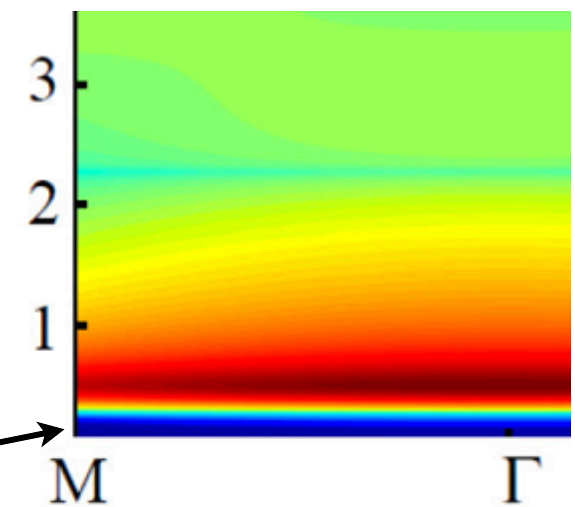


In the soluble model:

- The spin creates two f … es
- Spectral weight is … the flux gap
- Correlations vanish … NNs

But is it generic?

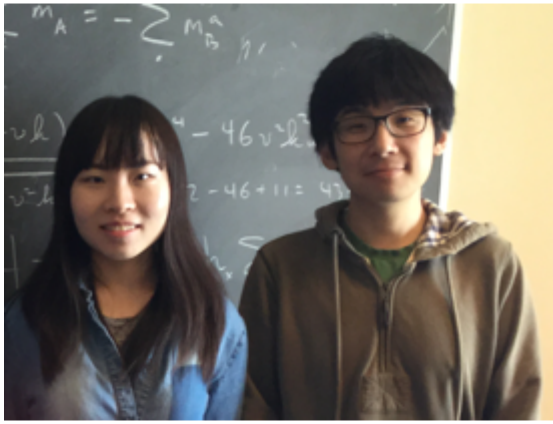
gap



J. Knolle *et al*, 2014

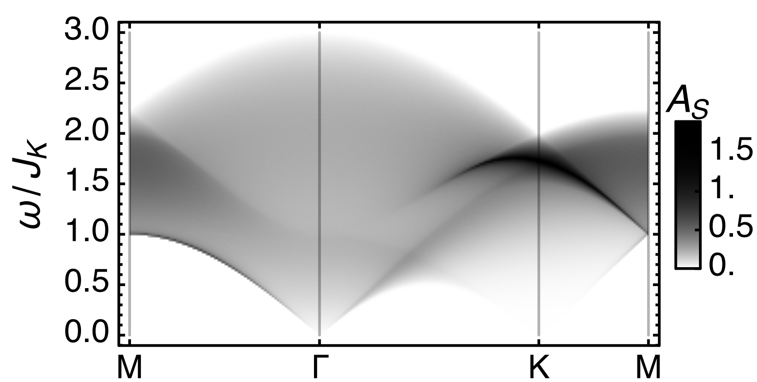
Universality

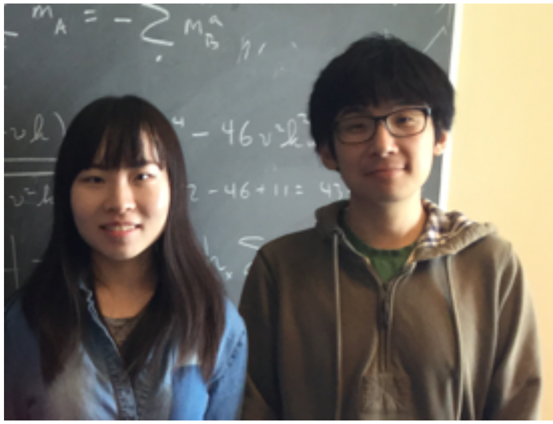
- We know the gapless QSL is locally stable provided time-reversal is maintained, *but* is this the generic behavior?
  - NN correlations? Obviously extended by perturbations.
  - Gap? This is less obvious. Is there a selection rule?



Answer

- Generically, there is *not* a gap in the structure factor
- Instead, power-law weight appears within two Dirac cones centered around k=0 and k=K





Answer

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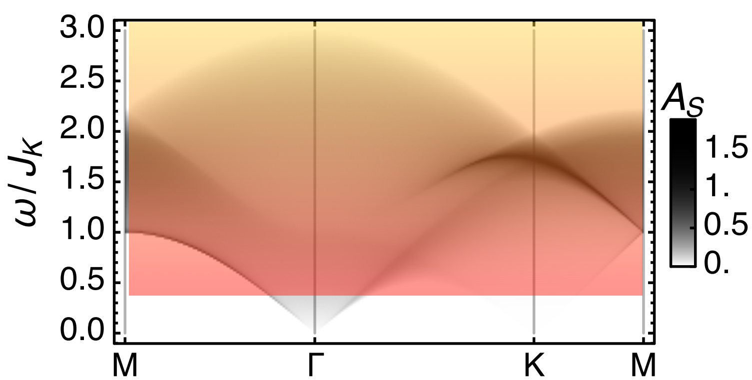
- Instead, power-law weight appears within two Dirac cones centered around k=0 and k=K

this should be added to the gapped intensity



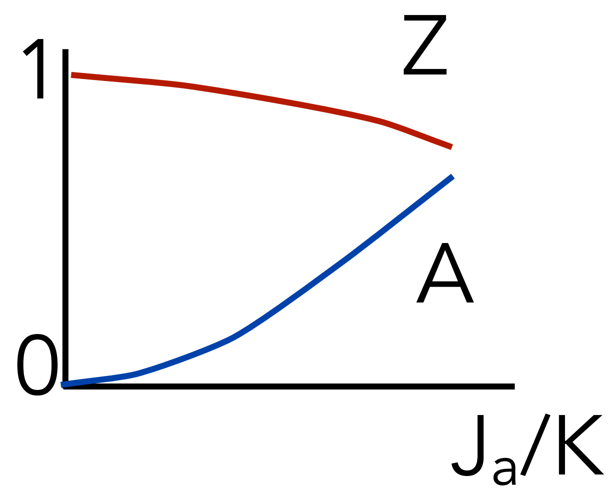
Why?

- **K**wasiparticles
  - A lattice operator can be expanded in a series of *quasiparticle* operators, which create *exact* eigenstates

$$\sigma_i^\mu = Z\, i c_i c_i^\mu + A\, i\epsilon^{\mu\nu\lambda} c_{i+\hat{\nu}} c_{i+\hat{\lambda}} + \cdots$$

above the gap   below the gap

$$\sigma \sim \varepsilon\text{em} + \varepsilon\varepsilon + \cdots$$



Microscopic origin

- A simple view: perturbations to Kitaev mix virtual excitations into ground state, which can cancel the flux introduced by naive spin operator
- Surprisingly, this *does not* occur for the Heisenberg-Kitaev model due to "dihedral" symmetry

$$X, Y, Z = \prod_i \sigma_i^\mu$$

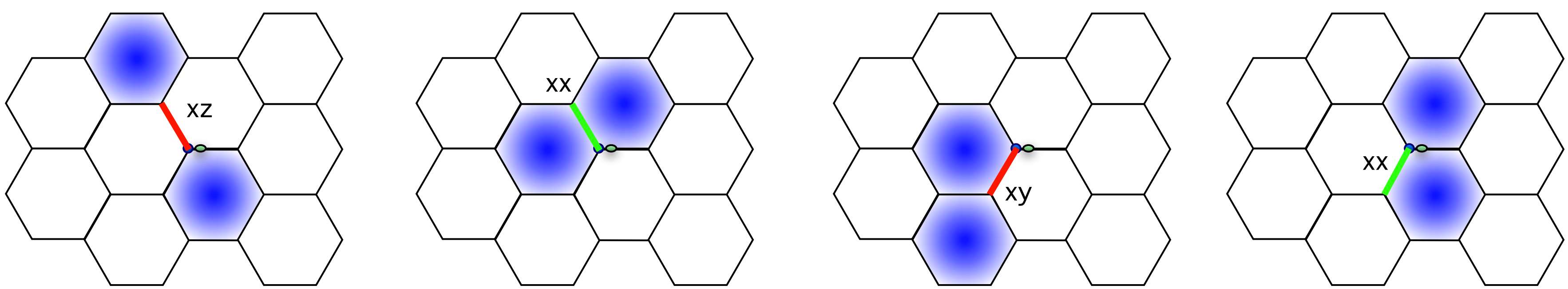
every spin is odd under 2 of these generators

Microscopic origin

- A simple view: perturbations to Kitaev mix virtual excitations into ground state, which can cancel the flux introduced by naive spin operator

$$H = \sum_{\langle ij\rangle \in \alpha\beta(\gamma)} [J\vec{S}_i \cdot \vec{S}_j + KS_i^\gamma S_j^\gamma + \Gamma(S_i^\alpha S_j^\beta + S_i^\beta S_j^\alpha)]$$

Rau, Lee, **K**ee



$$A \sim J^2\Gamma^2$$

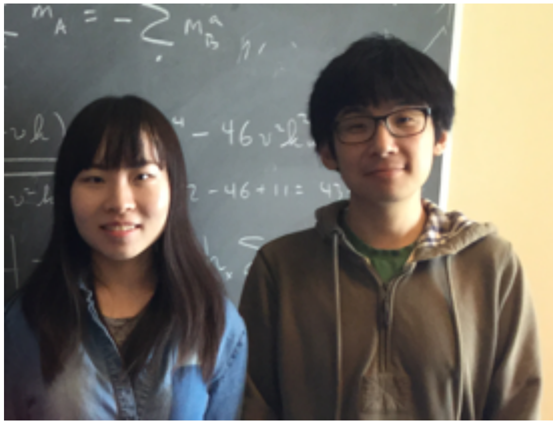
Field theory

- Highbrow picture: effective field theory
  - A lattice operator can be expanded at low energy in a series of “primary fields”. The coefficient are constrained by symmetry and depend on microscopics

$$\sigma_i^\mu \sim M^\mu_{s(i)}(\boldsymbol{x}_i) + \mathrm{Re}\left[N^\mu_{s(i)}(\boldsymbol{x}_i)e^{i\boldsymbol{K}\cdot\boldsymbol{x}_i}\right]$$

$$M^\mu_{s(i)} \sim \psi^\dagger\psi \qquad\qquad N^\mu_{s(i)} \sim \psi\partial\psi$$

- Amusing similarity to 1d Heisenberg chain

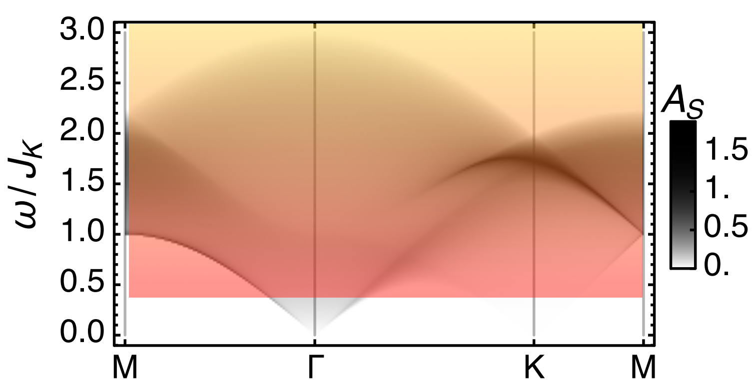


Answer

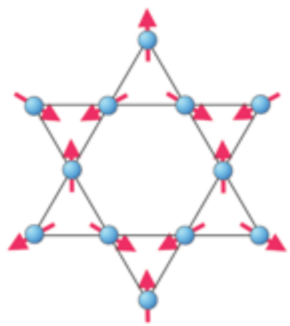
Xueyang Song, Yi-Zhuang You + LB, PRL 2016

- Generically, there is *not* a gap in the structure factor
- Instead, power-law weight appears within two Dirac cones centered around k=0 and k=2K

This is what we should expect if the Kitaev QSL is ever stabilized

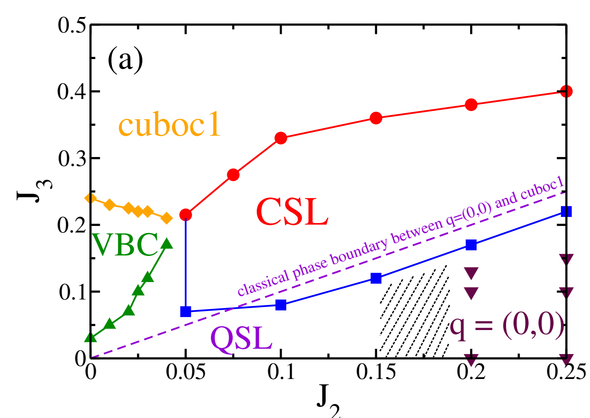


Kagomé



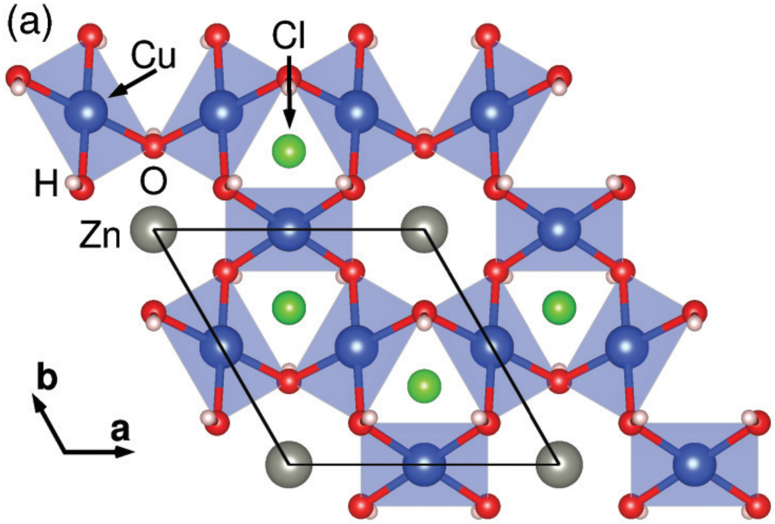
$$H = J \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

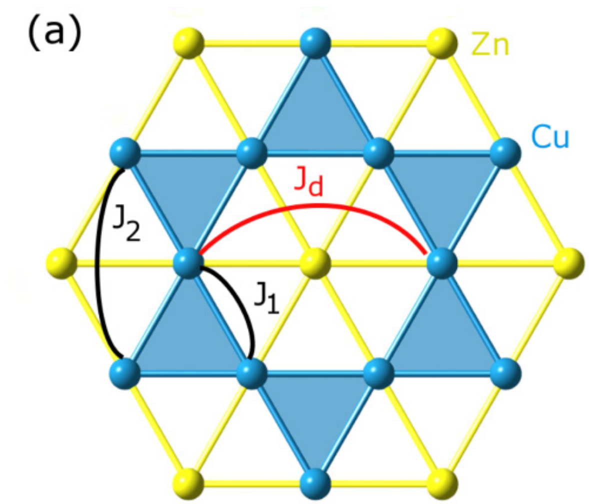
- Probably most-studied problem in frustrated magnetism
- Controversial! Most agree on non-magnetic ground state, but... Elser V 1989
  - Many gapless singlets? — Lechemninant *et al*, 1997
  - Dimer solid state? — Singh and Huse, 2007
  - Gapless Dirac QSL? — Ran *et al*, 2007
  - Gapped Z_2 QSL? — Yan, Huse, White 2011



SS Gong *et al*, 2015

Kapellasite α-$Cu_3Zn(OH)_6Cl_2$





Modified Kagome Physics in the Natural Spin-1/2 Kagome Lattice Systems: Kapellasite $Cu_3Zn(OH)_6Cl_2$ and Haydeeite $Cu_3Mg(OH)_6Cl_2$

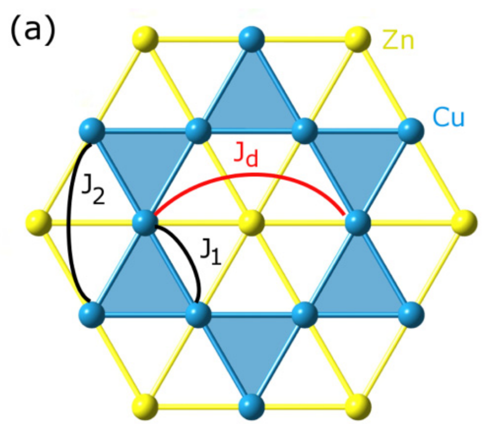
O. Janson,[1] J. Richter,[2] and H. Rosner[1,*]
[1]*Max-Planck-Institut für Chemische Physik fester Stoffe, D-01187 Dresden, Germany*
[2]*Institut für Theoretische Physik, Universität Magdeburg, D-39016 Magdeburg, Germany*
(Received 26 May 2008; published 3 September 2008)

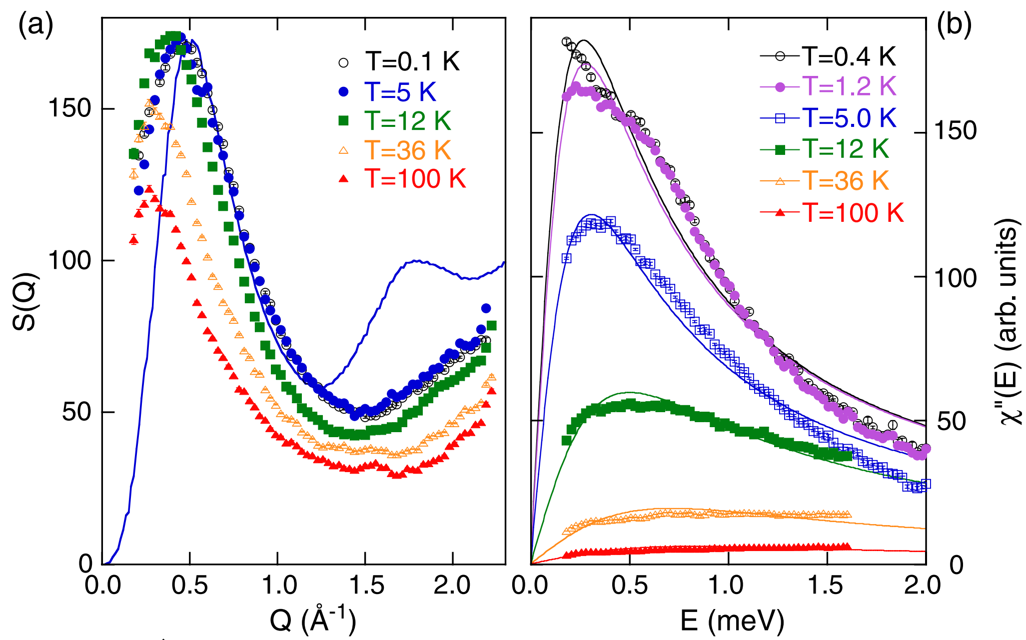
The recently discovered natural minerals $Cu_3Zn(OH)_6Cl_2$ and $Cu_3Mg(OH)_6Cl_2$ are spin 1/2 systems with an ideal kagome geometry. Based on electronic structure calculations, we develop a realistic model which includes couplings across the kagome hexagons beyond the original kagome model that are intrinsic in real kagome materials. Exact diagonalization studies for the derived model reveal a strong impact of these couplings on the magnetic ground state. Our predictions could be compared to and supplied with neutron scattering, thermodynamic data, and NMR data.

J_1 FM

J_d ~ $-J_1$ AFM

Kapellasite

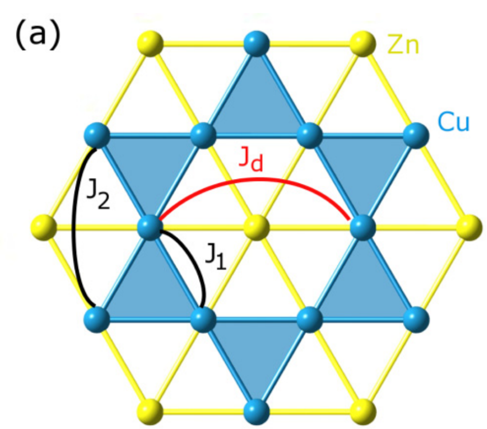


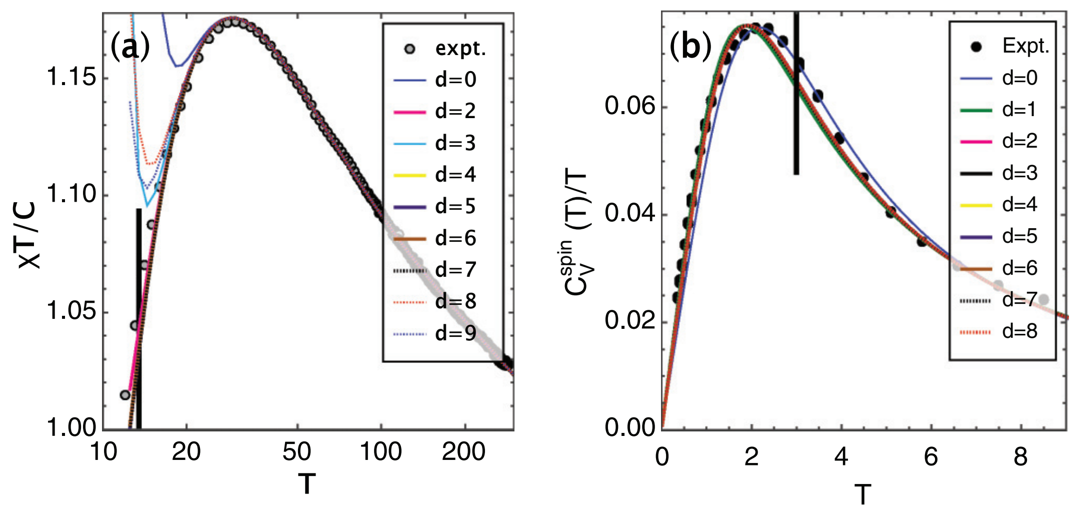


B. Fåk *et al*, 2012

Wavevector suggests short-range order with large unit cell

Kapellasite



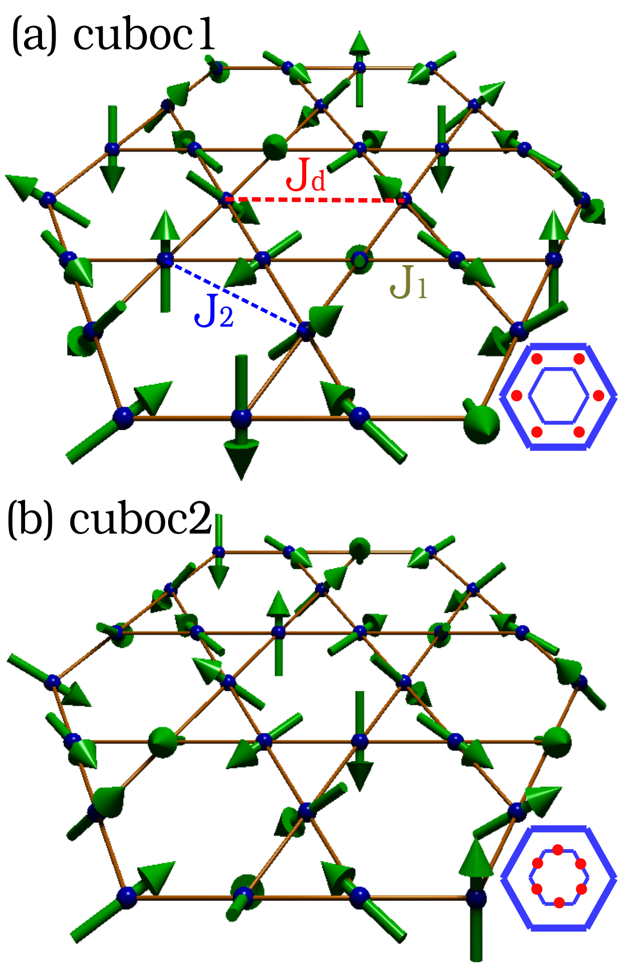


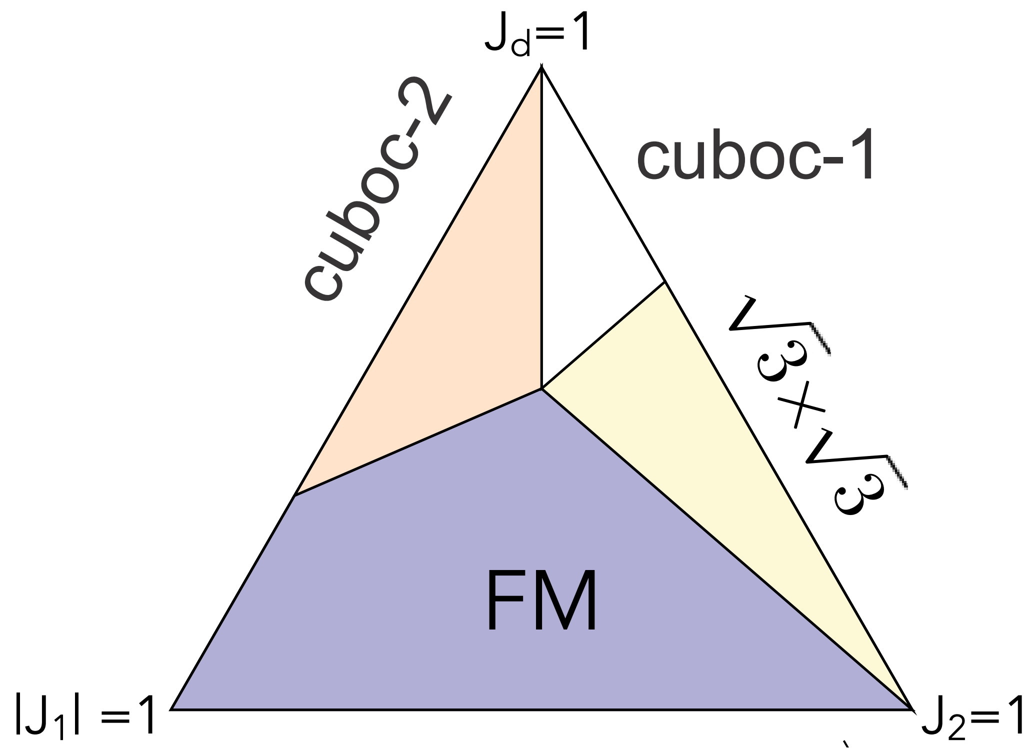
B. Bernu *et al*, 2013

$$J_1 = -12,\ J_2 = -4, \text{ and } J_d = 15.6 \text{ K},$$

What are the ground states for large J_d?

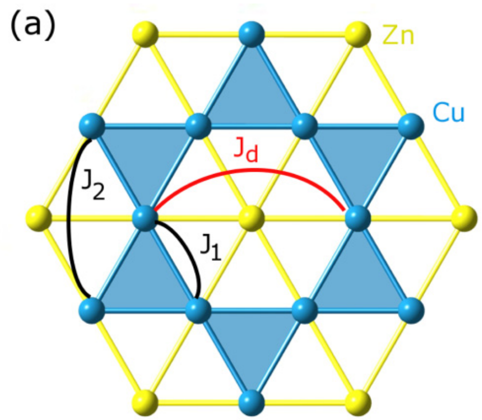
Kapellasite

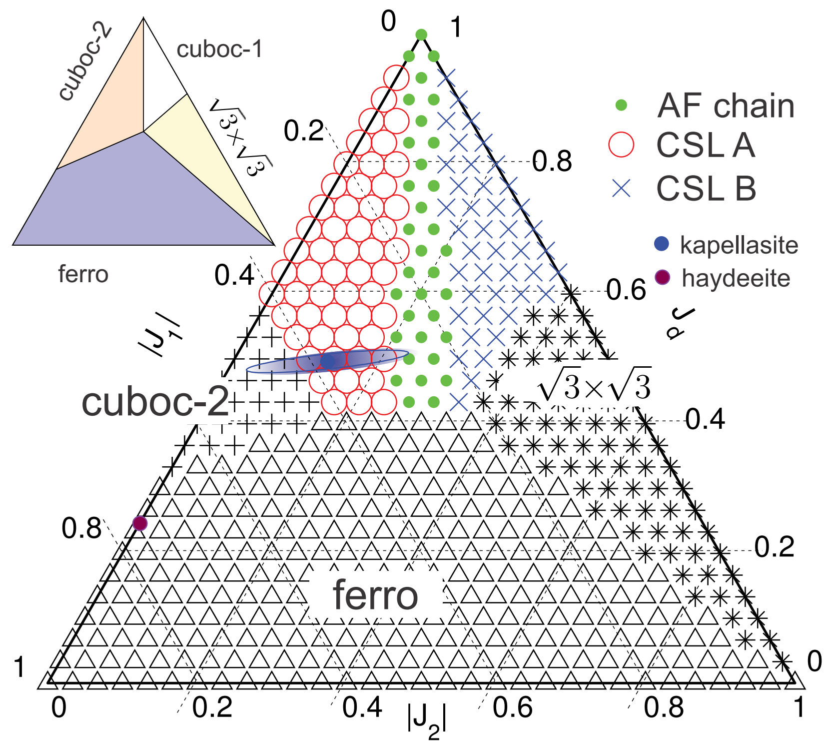




classical phase diagram

Kapellasite

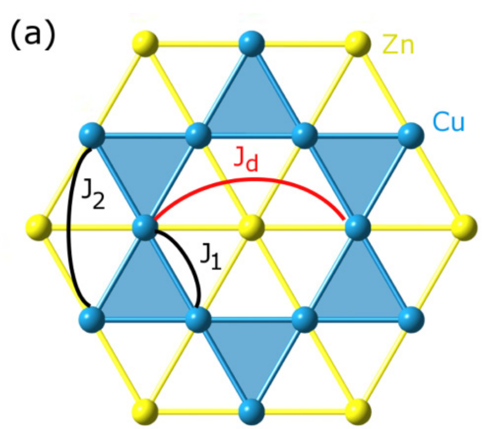




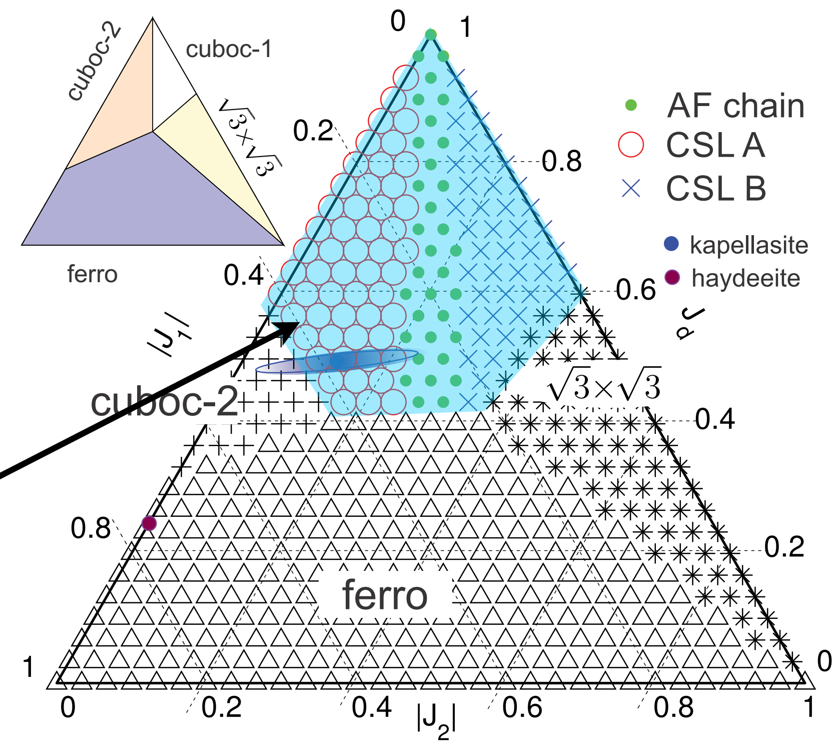
phase diagram from
variational wavefunctions

S. Bieri *et al*, 2015

Kapellasite



spin liquids?

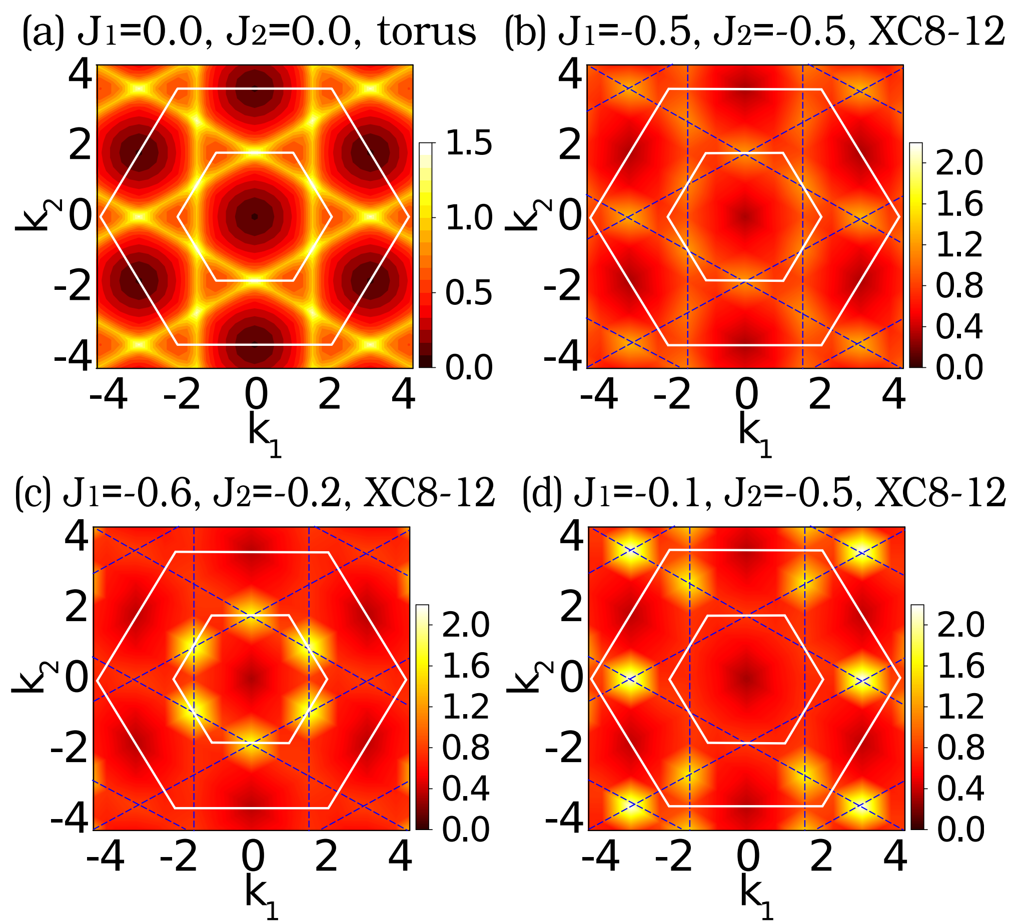


phase diagram from
variational wavefunctions

S. Bieri *et al*, 2015

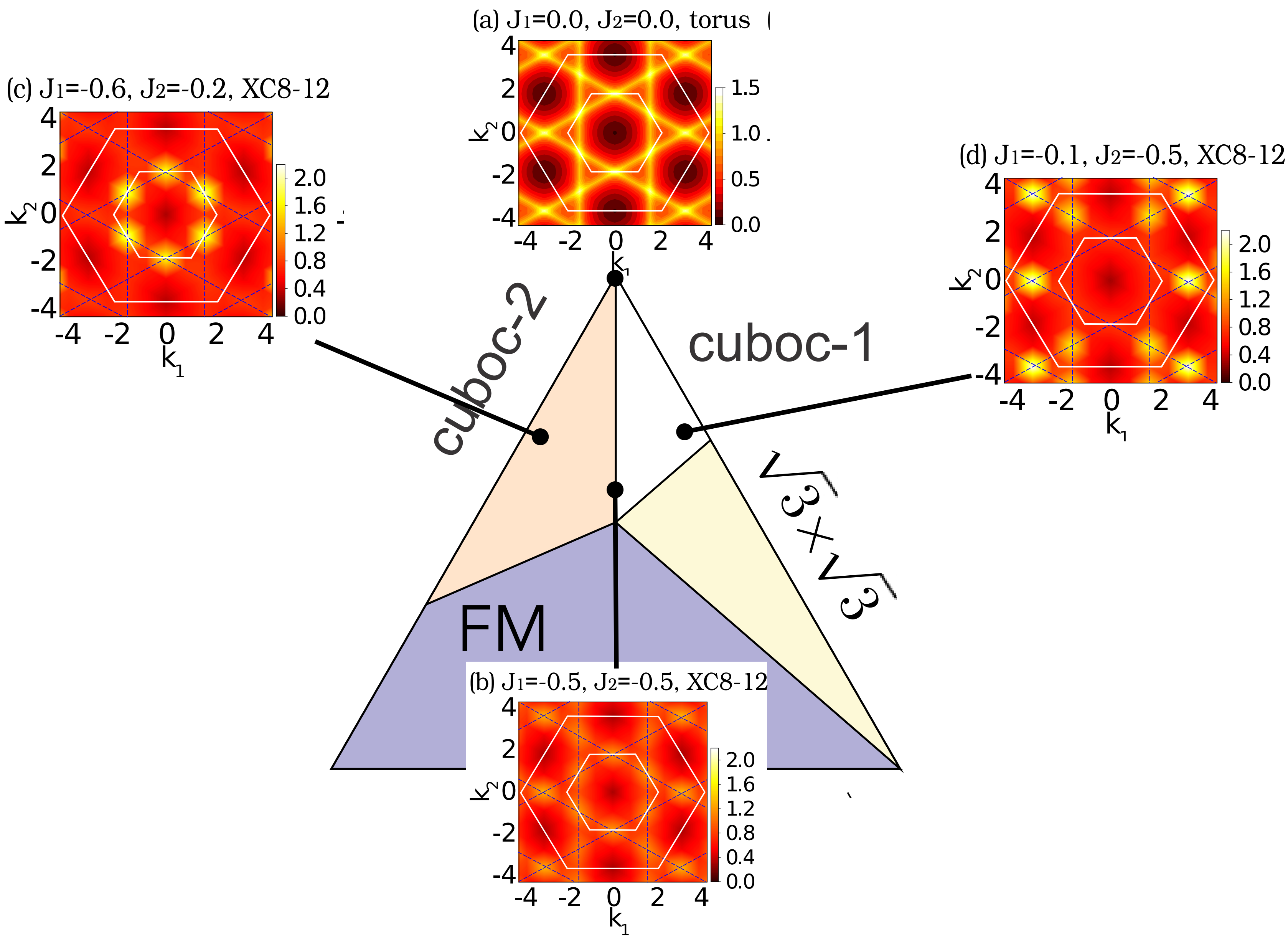
DMRG

numerically exact results
on long cylinders



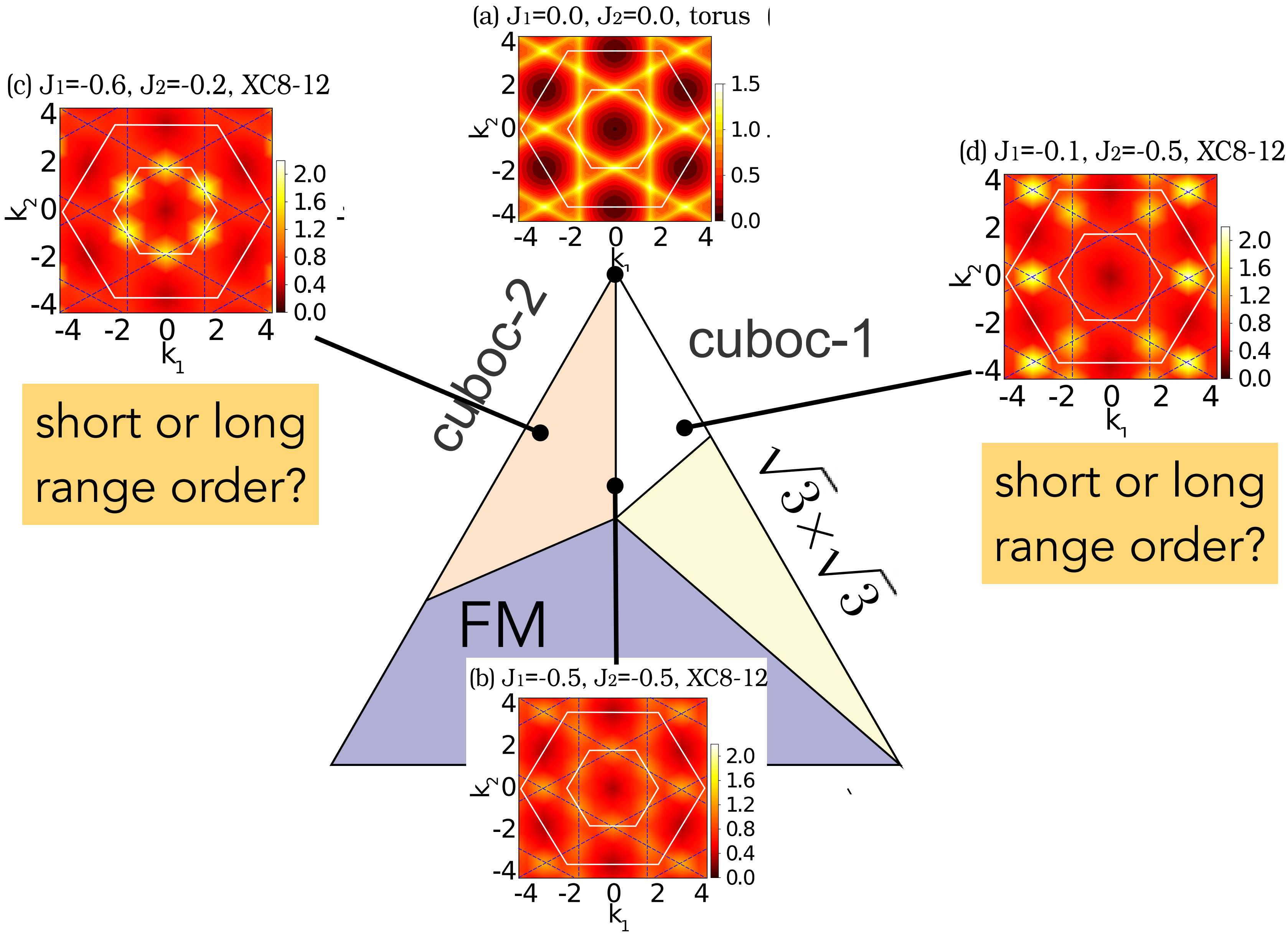
$S(k,\omega)$

DMRG



(a) J1=0.0, J2=0.0, torus
(c) J1=-0.6, J2=-0.2, XC8-12
(d) J1=-0.1, J2=-0.5, XC8-12
(b) J1=-0.5, J2=-0.5, XC8-12
cuboc-2
cuboc-1
FM
$\sqrt{3}\times\sqrt{3}$
k1
k2

DMRG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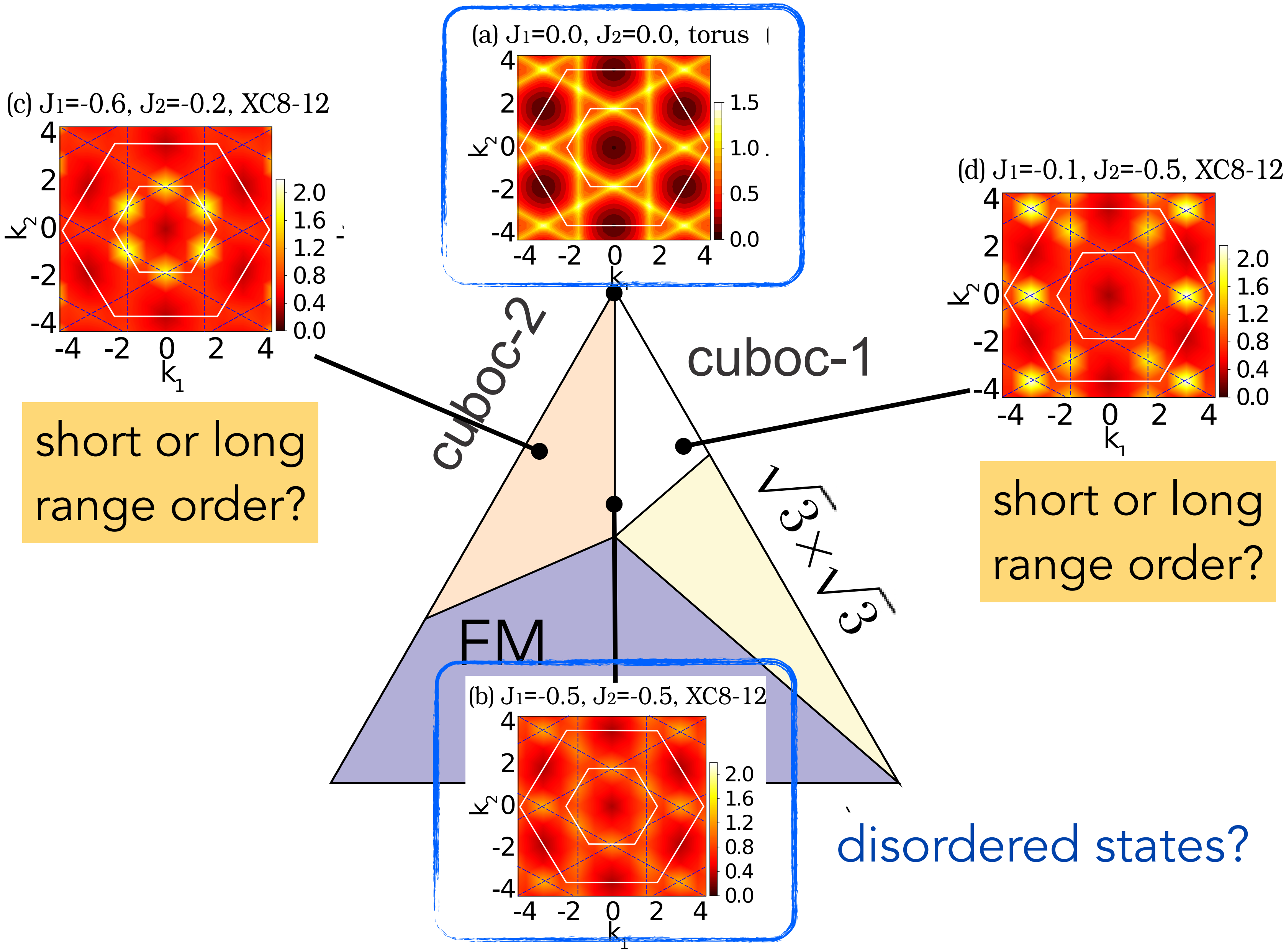
cuboc-2
cuboc-1
$\sqrt{3}\times\sqrt{3}$
FM
short or long range order?
short or long range order?

DMRG



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cuboc-2
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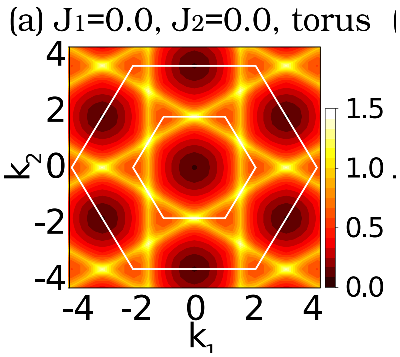
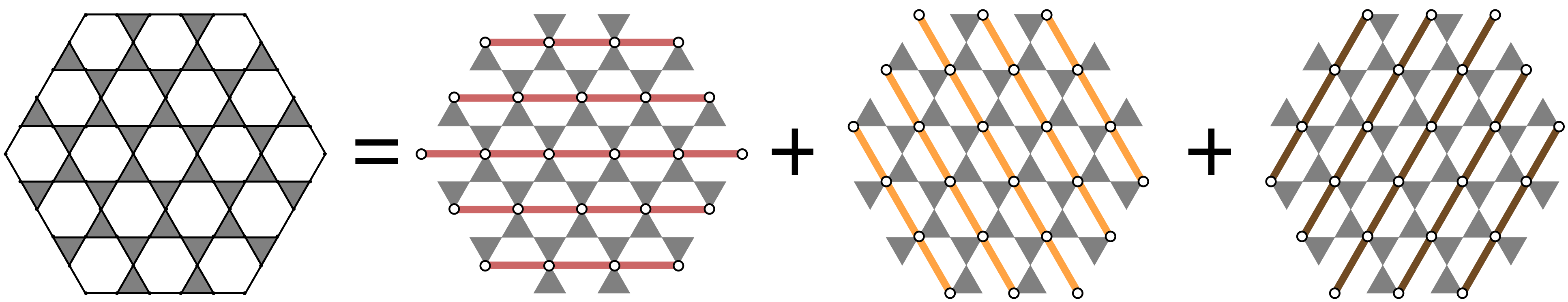
$\sqrt{3}\times\sqrt{3}$
short or long range order?
short or long range order?
disordered states?

Theory

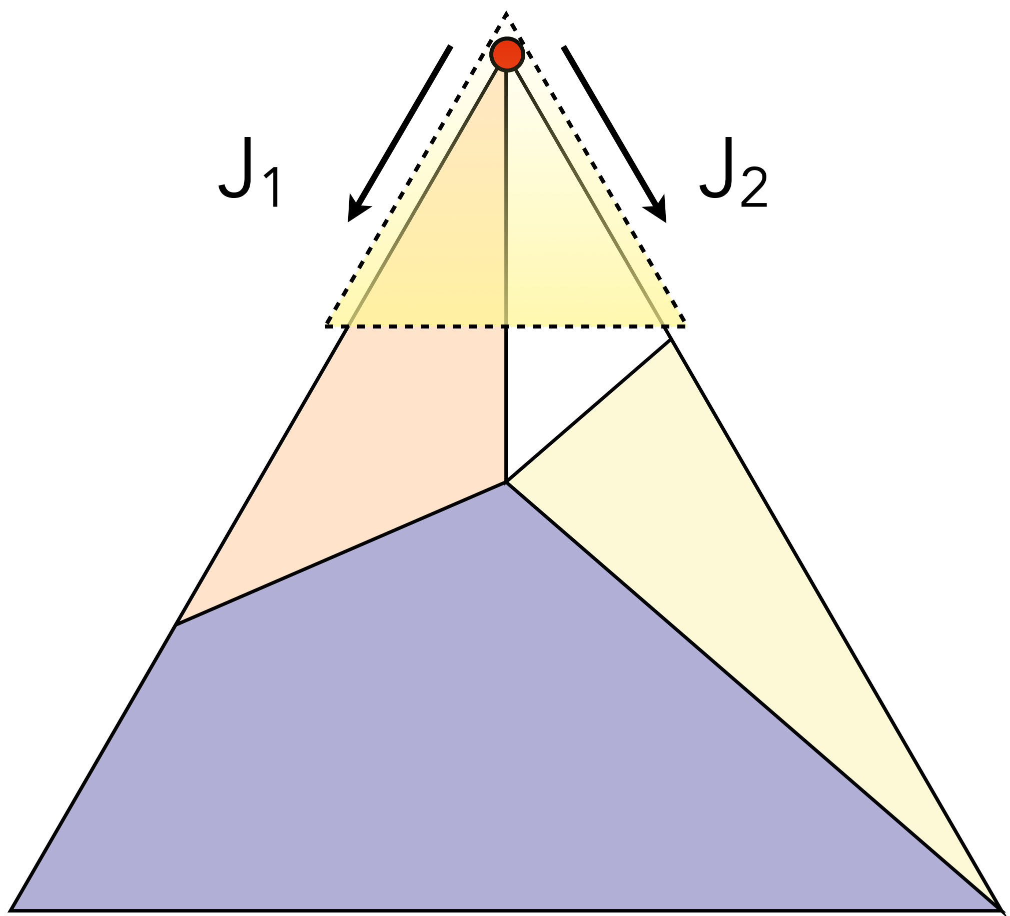


J_d only: one-dimensional chains



$$H = \sum_{a,y} H_{a,y}^{\mathrm{Heis}}$$

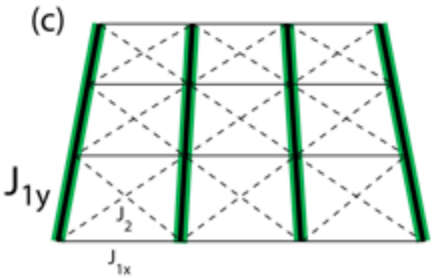
Theory

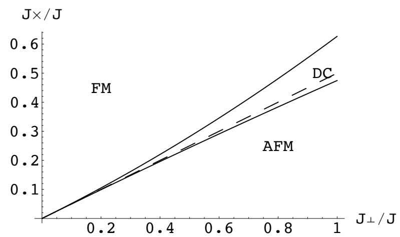


approach from
decoupled
chains

perturbative
renormalization group +
chain mean field theory

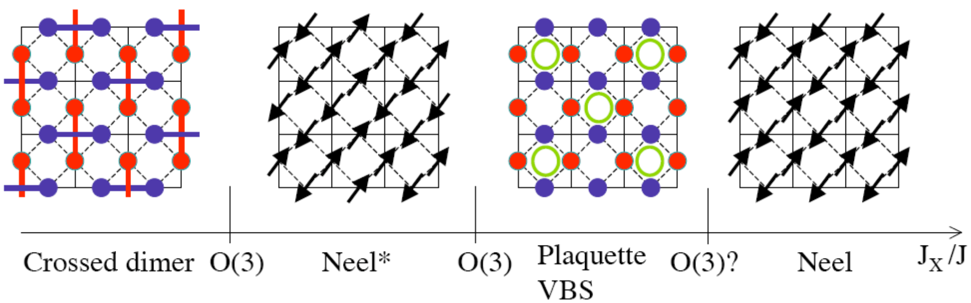
Koupled Chains





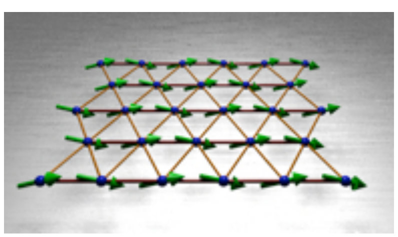
frustrated square lattice

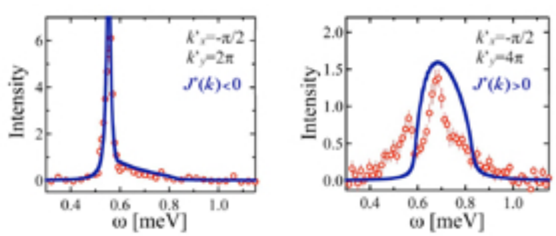
O. Starykh, L.B., *2004*



crossed chains/
planar pyrochlore

O. Starykh, A. Furusaki, L.B., *2005*





anisotropic triangular lattice

Cs_2CuCl_4

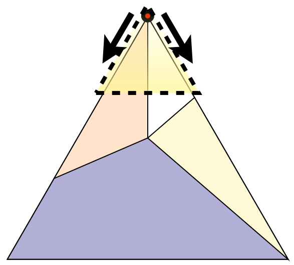
Cs_2CuBr_4

M. Kohno, O. Starykh, L.B., *2007*

O. Starykh, L.B., *2007*

O. Starykh, H. Katsura, L.B., *2010*

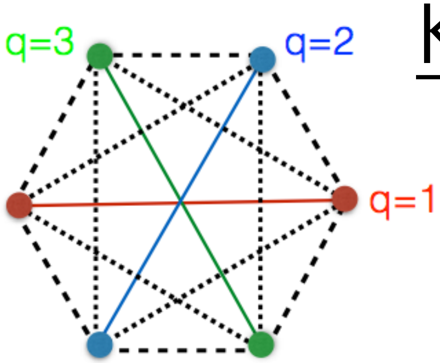
Theory



Decoupled chains:

low energy $SU(2)_1$ WZW field theory

primary fields = scaling operators $\boldsymbol{N}_{q,\mathrm{y}}, \varepsilon_{q,\mathrm{y}}$



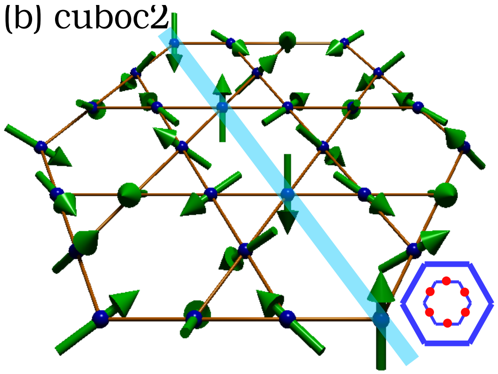
Koupling

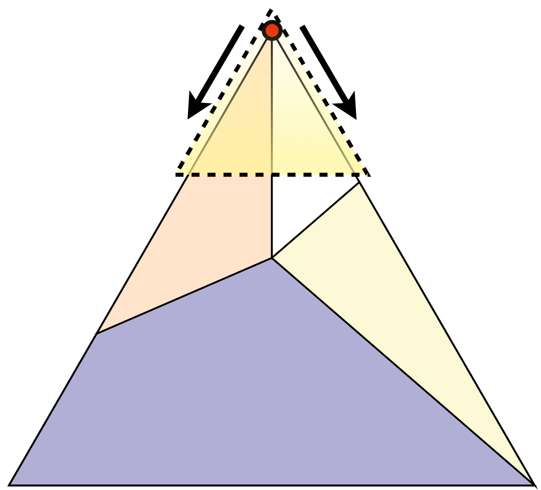
$$H'_{\mathrm{dom}} \sim 2(J_2 - J_1) \sum_{q} \sum_{\mathrm{y},\mathrm{y}'} (-1)^{\mathrm{y}} \boldsymbol{N}_{q,\mathrm{y}}(-\mathrm{y}') \cdot \boldsymbol{N}_{q+1,\mathrm{y}'}(\mathrm{y}+\mathrm{y}').$$

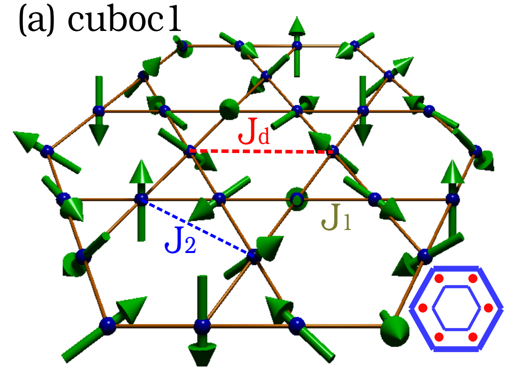
$$-c\frac{J_1^2}{J_d} \sum_{\mathrm{y},\mathrm{y}',q} (-1)^{\mathrm{y}} \varepsilon_{q,\mathrm{y}} \varepsilon_{q+1,\mathrm{y}'}$$

CMFT

$$H_{CMFT} \sim (J_2 - J_1) \sum_{q,\mathrm{y},\mathrm{y}'} (-1)^{\mathrm{y}} \langle \boldsymbol{N}_{q,\mathrm{y}} \rangle \cdot \boldsymbol{N}_{q+1,\mathrm{y}'}$$



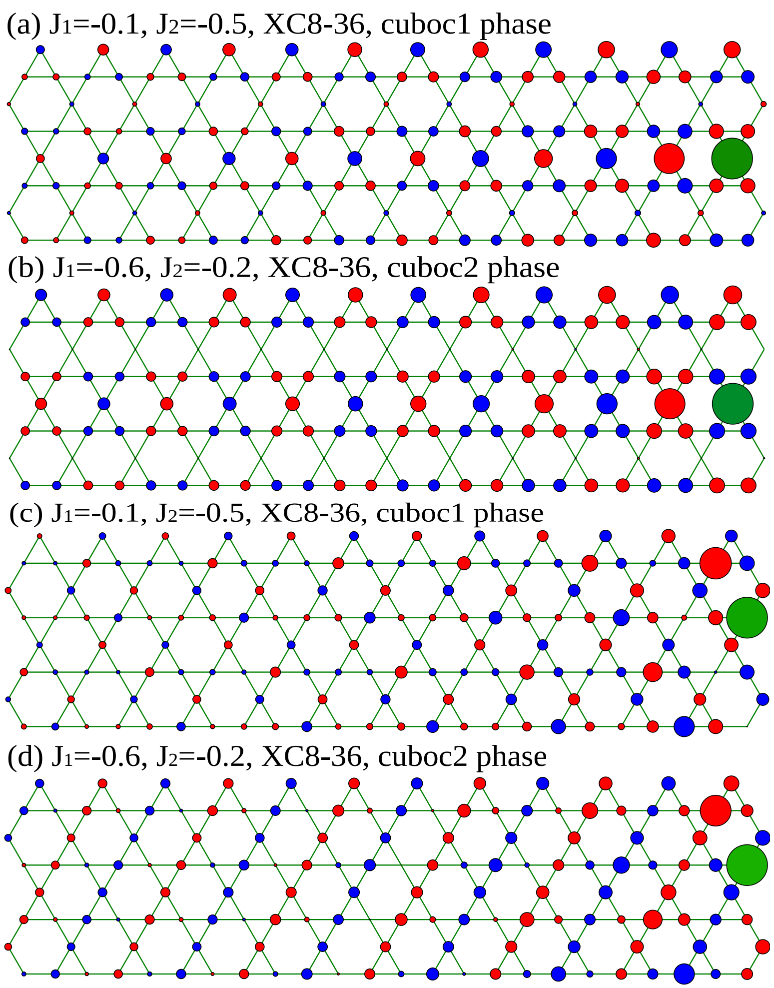




cuboc states fall out naturally from 1d chains

long range order $\quad |\langle \mathbf{S}_i \rangle| \propto \sqrt{|J_1 - J_2|/J_d}$

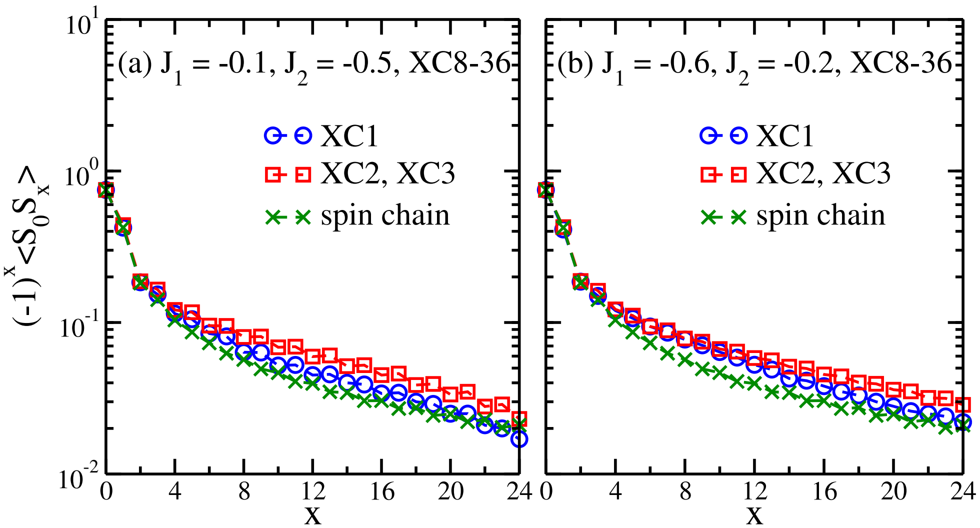
DMRG



Form of correlations are just what is expected for cuboc states

But can see underlying 1d structure

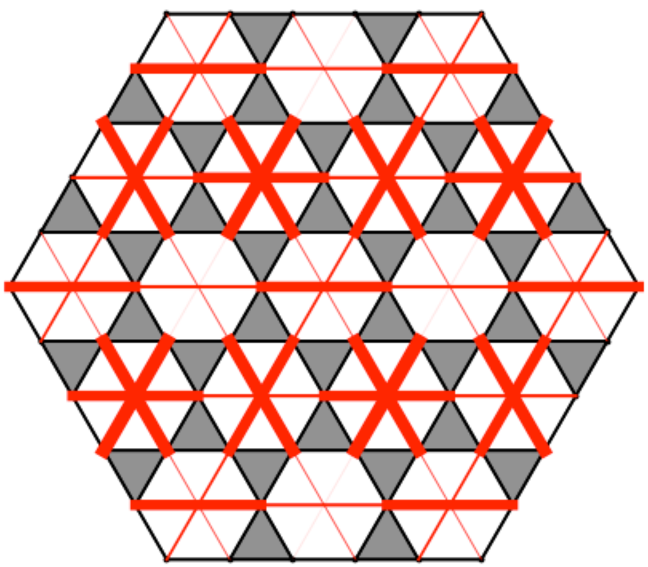
No LRO in 1d, but correlations are clearly enhanced beyond chains



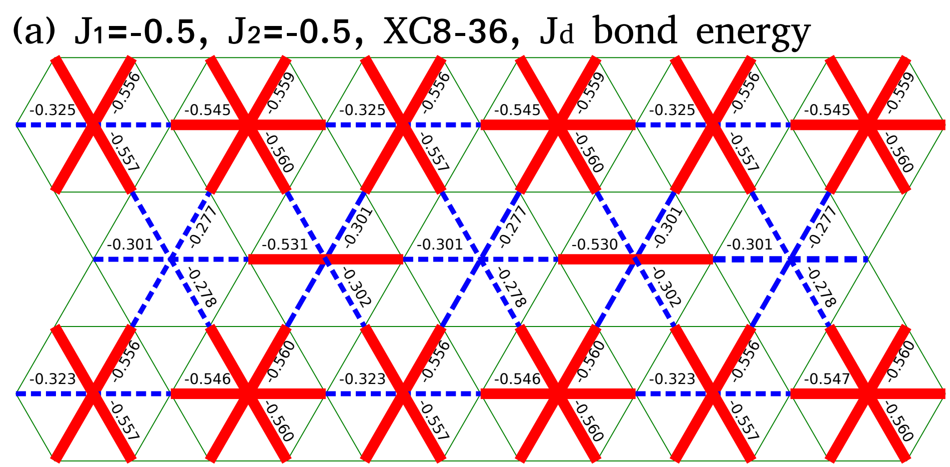
Kompensated regime

$J_1 = J_2$: leading coupling cancels

$O[(J_1)^2]$ *dimerization* coupling dominates



theoretical VBS pattern
from dimerized chains

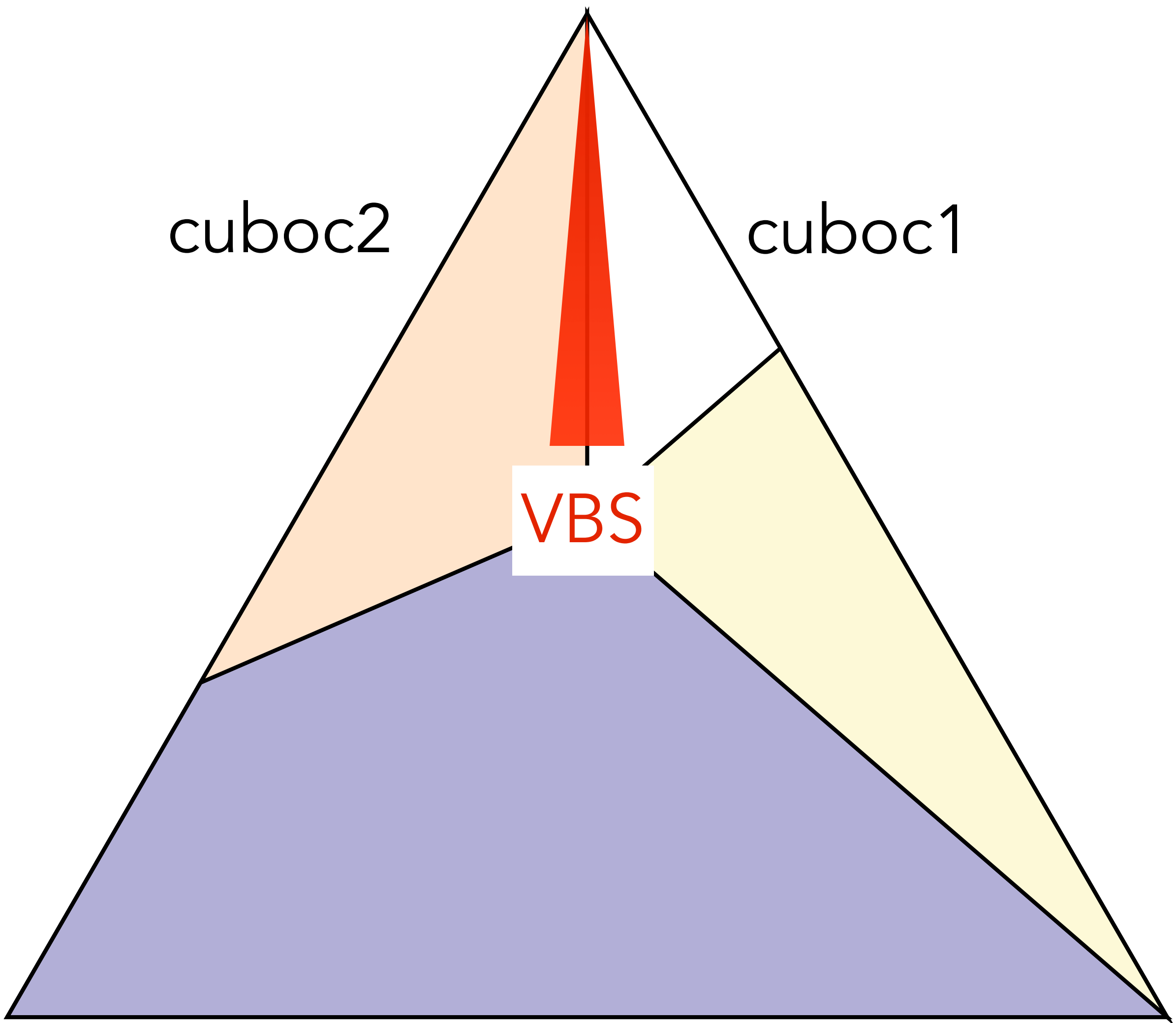


DMRG bond energies

strong confirmation of chain theory

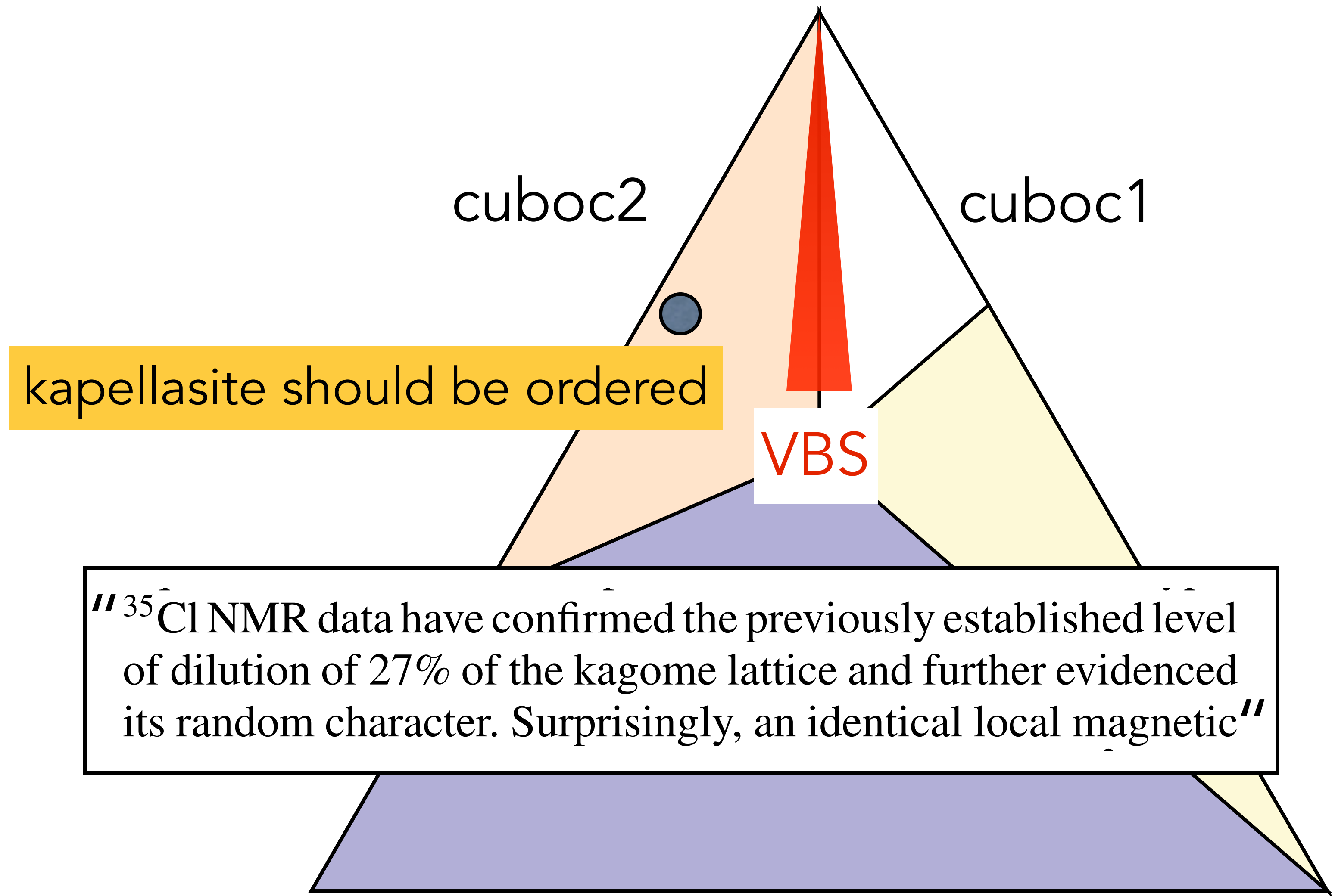
ReKapitulation

S.S. Gong *et al*, PRB 2016



ReKapitulation

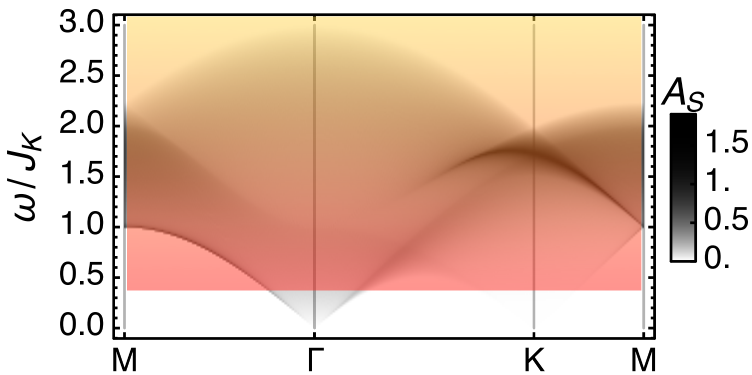
S.S. Gong *et al*, PRB 2016



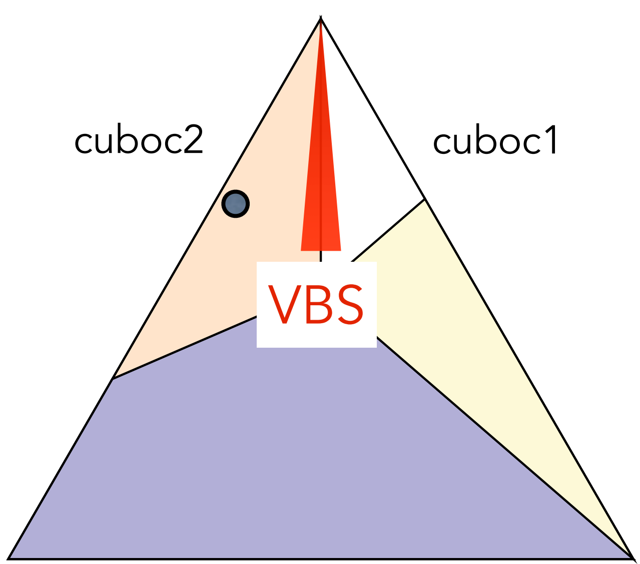
"[35]Cl NMR data have confirmed the previously established level of dilution of 27% of the kagome lattice and further evidenced its random character. Surprisingly, an identical local magnetic"

E. **K**ermarrec *et al*, 2014

Konklusion



The Kitaev spin liquid, if we ever find it, will have Dirac-like power-law spectral weight.



The J_d-J_1-J_2 model for kapellasite may *not* support any QSLs. Disorder is probably playing a role in the actual material.

$$: