Tensor network algorithms and quantum frustrated magnetism

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Collaborators

Theorists

S. Miyahara (Fukuoka), F. Becca (Trieste)
K. Schmidt (Dortmund), J. Dorier (Lausanne)
S. Manmana, A. Honecker (Göttingen)
P. Corboz (Amsterdam)

Experimentalists

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C. Berthier, M. Horvatic (Grenoble)

Scope

- Introduction:
  - → Numerical simulations in 2D
  - → Tensor network algorithms
  - → Models of 2D frustrated quantum magnetism
- Shastry-Sutherland model:
  - → Zero-field phase diagram
  - → Magnetization plateaux
- Conclusions

Numerical simulations in 2D

- Exact diagonalizations → small clusters
- Quantum Monte Carlo → minus sign
- Degenerate pertubation theory

  → effective model still to be solved
- Series expansion → choice of initial state
- Variational Monte Carlo with Gutzwiller projected wave functions → not general
- DMRG → breaks lattice rotational symmetry

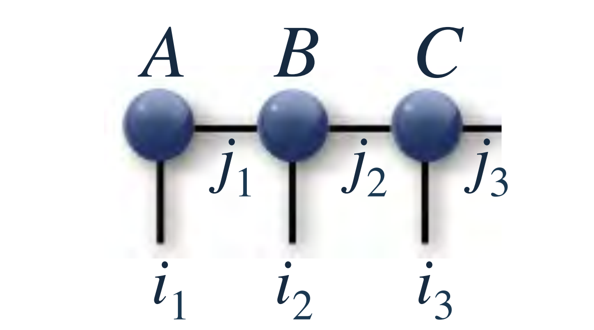
Tensor network ansatz

$$|\psi\rangle = \sum_{i_1 \dots i_N} c_{i_1 \dots i_N} |i_1\rangle \otimes \cdots \otimes |i_N\rangle$$

$$c_{i_1 \dots i_N} \simeq \text{trace over a product of tensors}$$

Example: Matrix product state in 1D

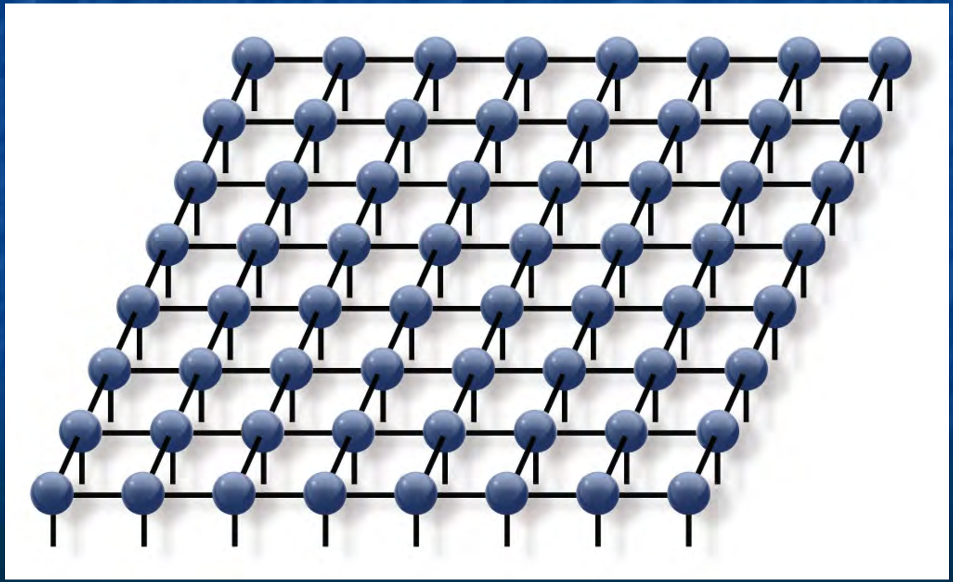
$$c_{i_1 i_2 i_3 \dots} \simeq \sum_{j_1 j_2 \dots} A_{i_1}^{j_1} B_{i_2}^{j_1 j_2} C_{i_3}^{j_2 j_3} \cdots$$



Generalization to 2D

PEPS = product of entangled pair states

Verstraete and Cirac, 2004



$A_i^{j_1 j_2 j_3 j_4}$ = rank-5 tensor

$$j_1, j_2, j_3, j_4 = 1, \ldots, D$$

Variational approach

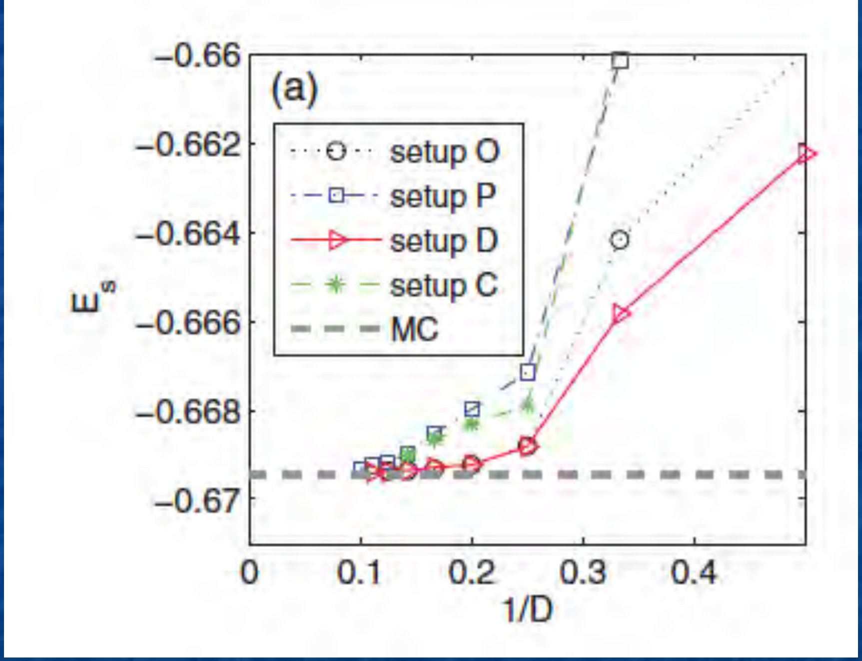
- PEPS: minimize the energy w.r.t. tensor elements
- Other schemes: renormalization (MERA,…)
- Advantage: dim=pol(D,N), not exp(N)
- Why can it work?

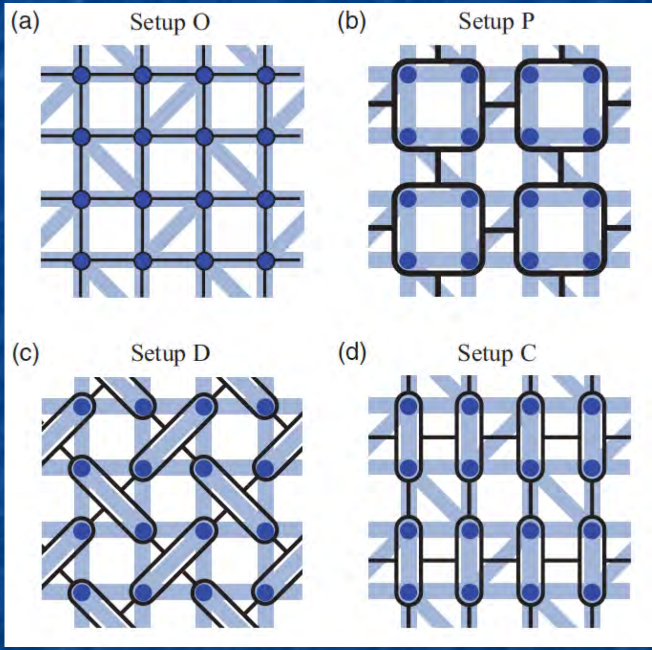
→ reproduces the 'area law' for the entanglement entropy in the GS of a local Hamiltonian

$$S = -\mathrm{tr}\left(\rho_A \log \rho_A\right) \sim \partial A$$

- How large should D be? It depends…

Spin-1/2 Heisenberg model on square lattice





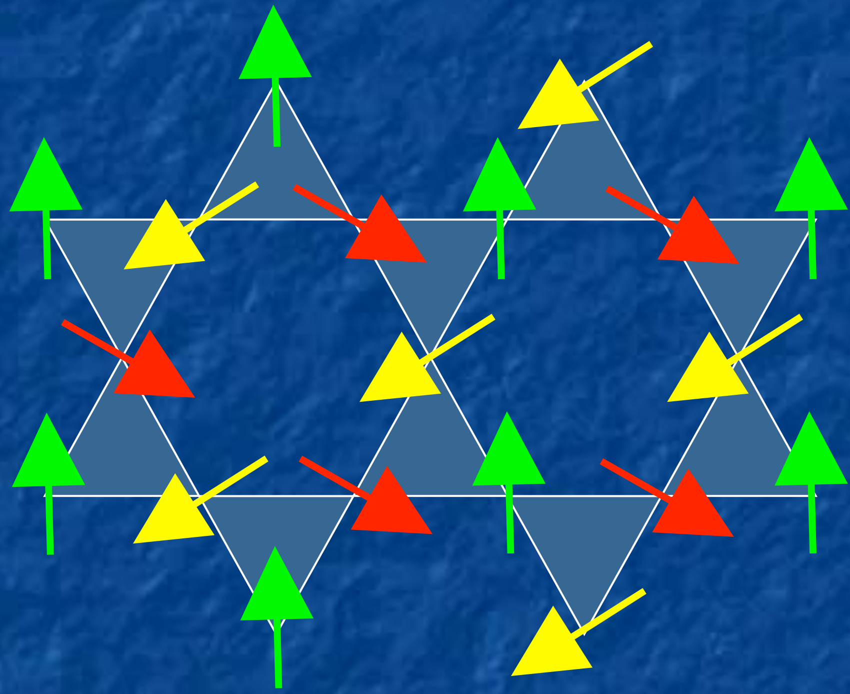
Excellent energy with D=10

Frustrated quantum magnetism

$$\mathcal{H} = \sum_{(i,j)} J_{ij}\ \vec{S}_i \cdot \vec{S}_j$$

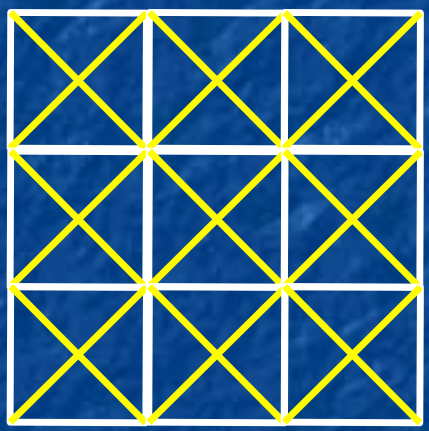
Infinite degeneracy of classical GS

Kagome lattice

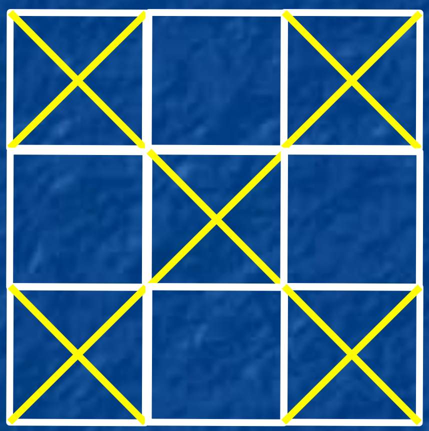


Spin liquid? Gapped? Algebraic? Valence-bond crystal?

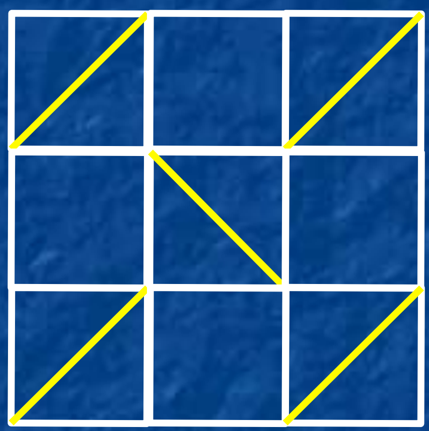
Square lattice



J_1-J_2



Checkerboard



Shastry-Sutherland

Results on frustrated magnets

- Kagome: single site does not work. Needs 3 sites.
- J_1-J_2 on square lattice: intermediate phase around $J_2/J_1=1/2$, but no consensus on its nature

  → Plaquette?

  Yu and Kao, PRB 2012

  → Topological spin liquid?

  Mezzacapo, PRB 2012; Wang, Gu, Verstraete, Wen 2012
- Checkerboard: intermediate plaquette phase, in agreement with previous results

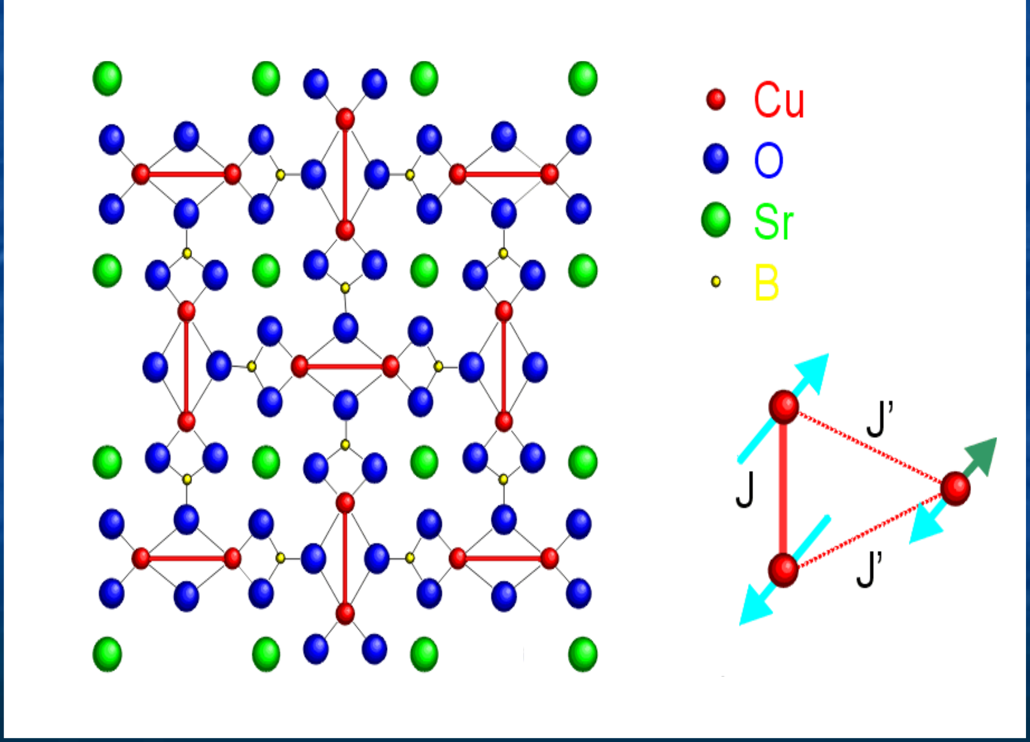
  Chan, Han, Duan, PRB 2011

Shastry-Sutherland

- Isacsson and Syljuasen, PRE 2006
  → D=2, no intermediate phase in zero field
- Lou, Suzuki, Harada, Kawashima, arxiv 2012
  → MERA
  → intermediate plaquette phase
  → plateaux and supersolid phases in a field
- P. Corboz and FM, PRB 2013, PRL 2013 and 2014
  → plateau sequence of $SrCu_2(BO_3)_2$

$SrCu_2(BO_3)_2$

Smith and Keszler, JSSC 1991

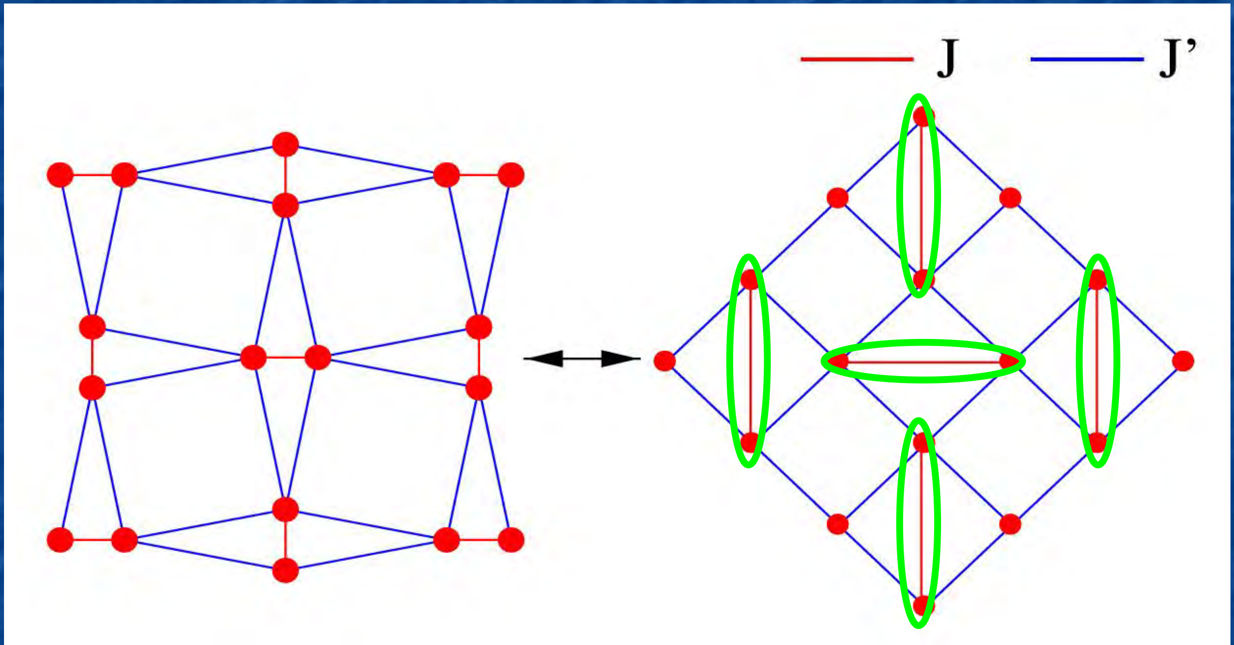


Cu^{2+} -> Spin 1/2

$J \approx 85$ K

$J'/J \approx 0.65$

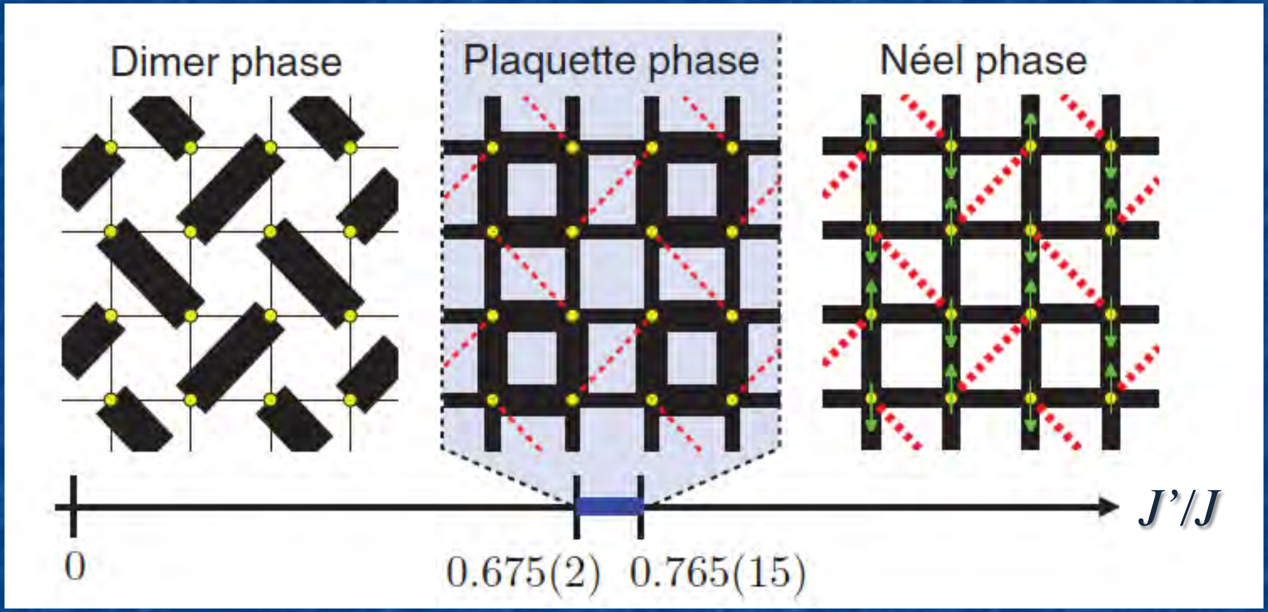
Shastry-Sutherland model



Ground-state = Product of singlets on J-bonds if J'/J not too large

Shastry and Sutherland, '81

iPEPS zero-field phase diagram



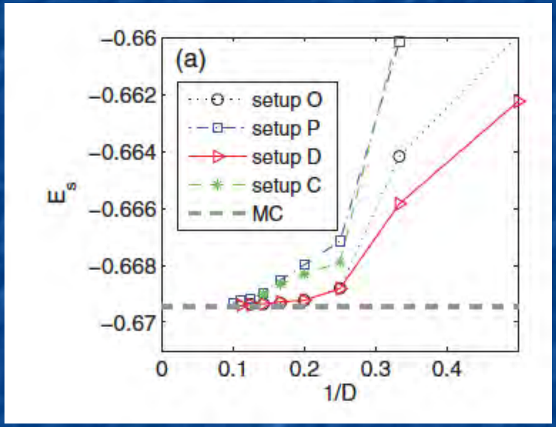
P. Corboz and FM, PRB 2013

Agrees qualitatively with former studies

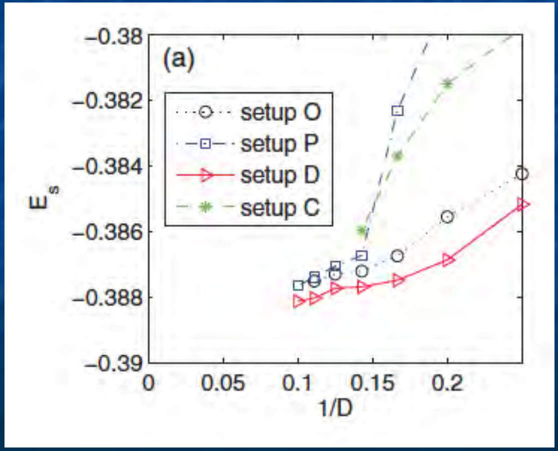
Koga-Kawakami 2000, Läuchli-Wessel-Sigrist 2002, etc.

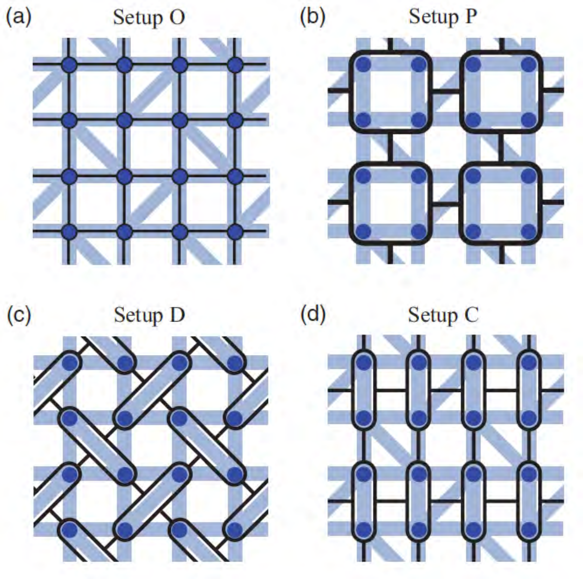
Convergence with D

Neel (J=0)



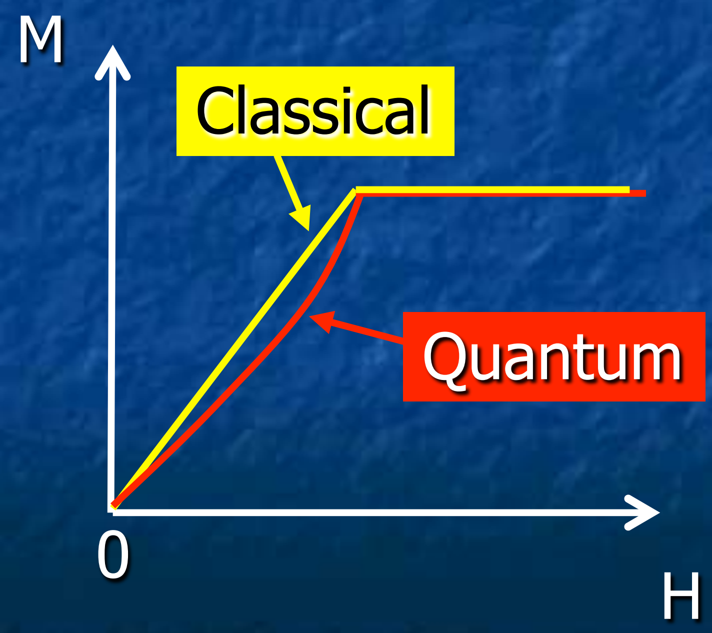
Plaquette phase

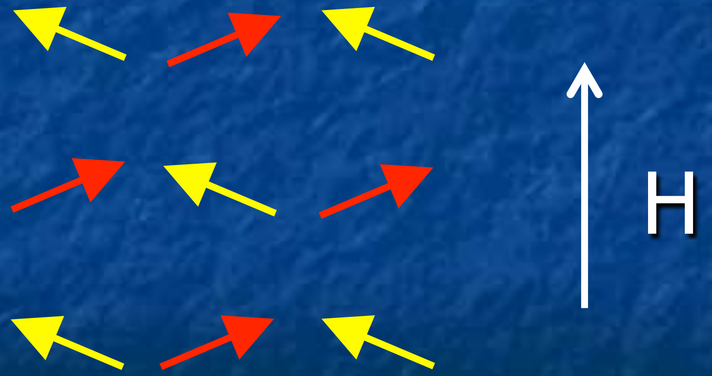




Magnetization of Néel AF

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j - g\mu_B H \sum_i S_i^z$$

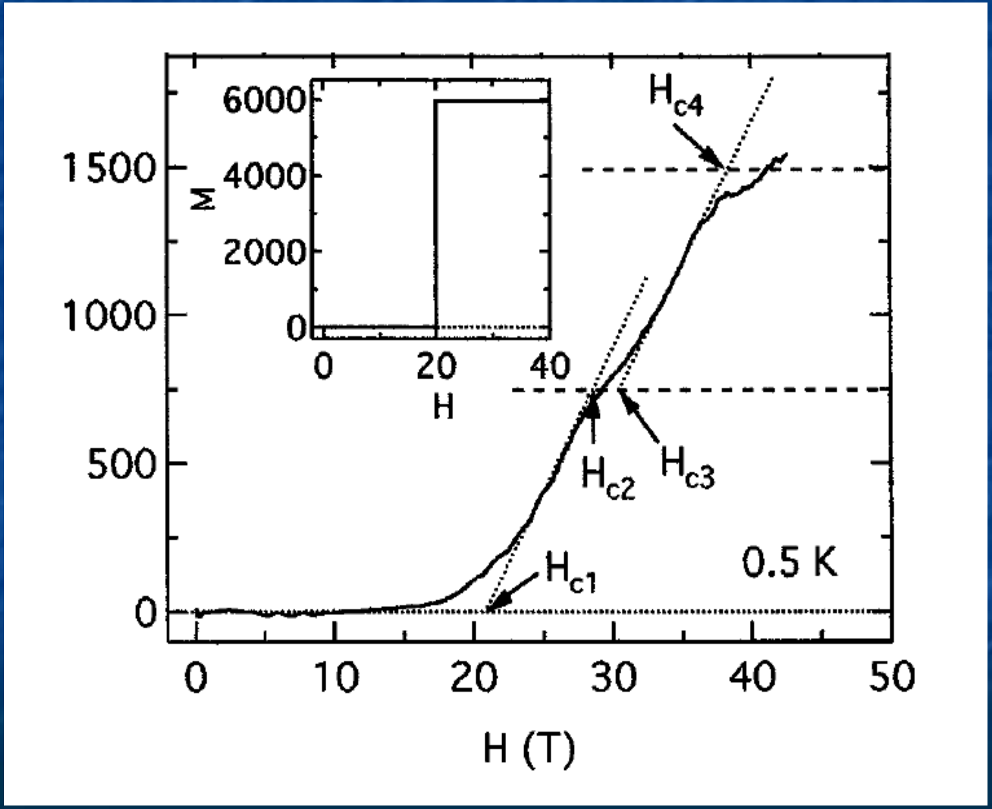




VOLUME 82, NUMBER 15 PHYSICAL REVIEW LETTERS 12 APRIL 1999

Exact Dimer Ground State and Quantized Magnetization Plateaus in the Two-Dimensional Spin System $SrCu_2(BO_3)_2$

H. Kageyama,[1,2,*] K. Yoshimura,[1,3,†] R. Stern,[3] N. V. Mushnikov,[2] K. Onizuka,[2] M. Kato,[1] K. Kosuge,[1] C.P. Slichter,[3] T. Goto,[2] and Y. Ueda[2]



Anomalies

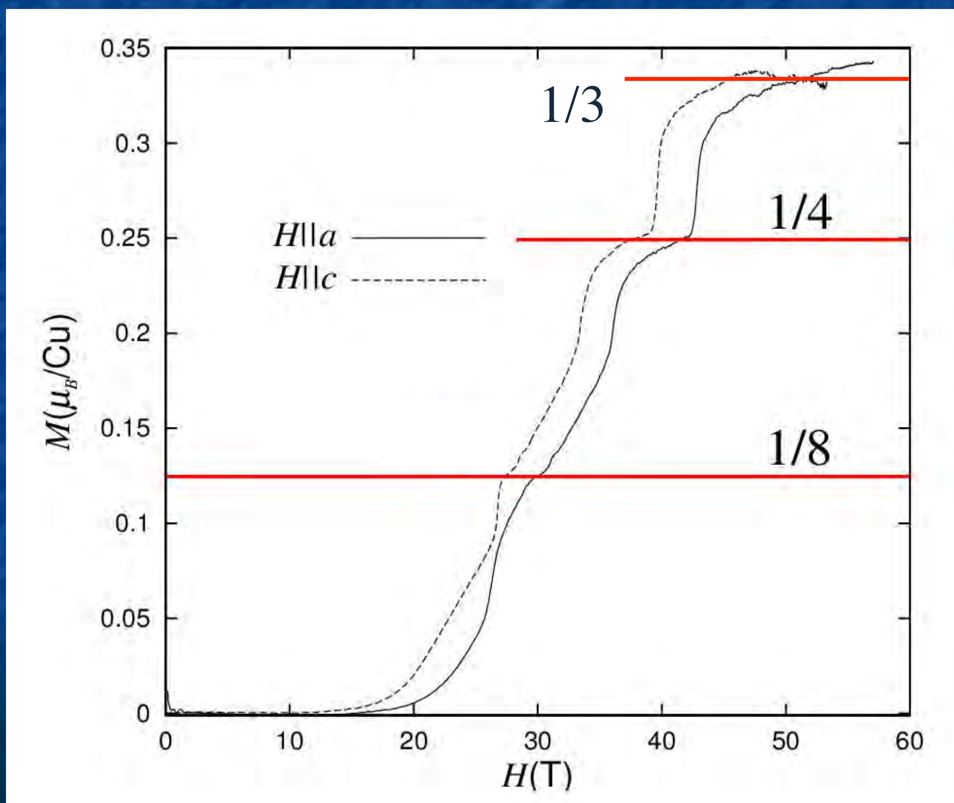
- M=0
- M=1/8
- M=1/4

Journal of the Physical Society of Japan
Vol. 69, No. 4, April, 2000, pp. 1016-1018

LETTERS

1/3 Magnetization Plateau in $SrCu_2(BO_3)_2$ - Stripe Order of Excited Triplets -

Kenzo ONIZUKA, Hiroshi KAGEYAMA*, Yasuo NARUMI[1,2], Koichi KINDO[2,1], Yutaka UEDA and Tsuneaki GOTO



Plateaus

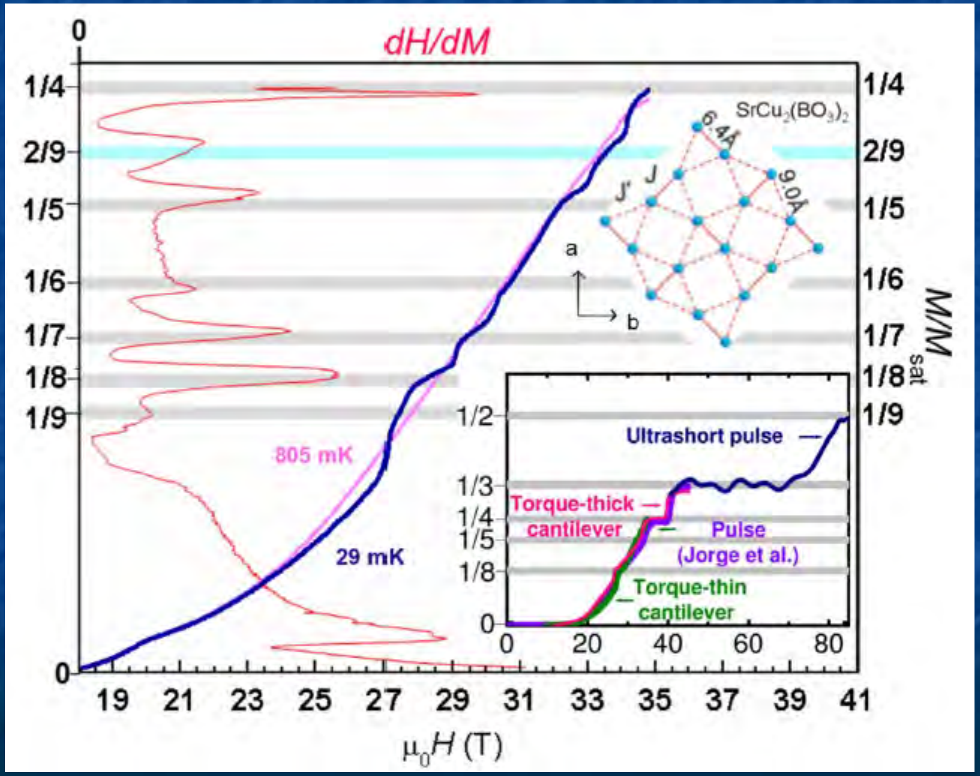
- M=0
- M=1/8
- M=1/4
- M=1/3

Fractalization drives crystalline states in a frustrated spin system

Suchitra E. Sebastian[a,1], N. Harrison[b], P. Sengupta[c], C. D. Batista[c], S. Francoual[b], E. Palm[d], T. Murphy[d], N. Marcano[a], H. A. Dabkowska[e], and B. D. Gaulin[e]

www.pnas.org/cgi/doi/10.1073/pnas.0804320105

PNAS | December 23, 2008 | vol. 105 | no. 51 | 20157–20160

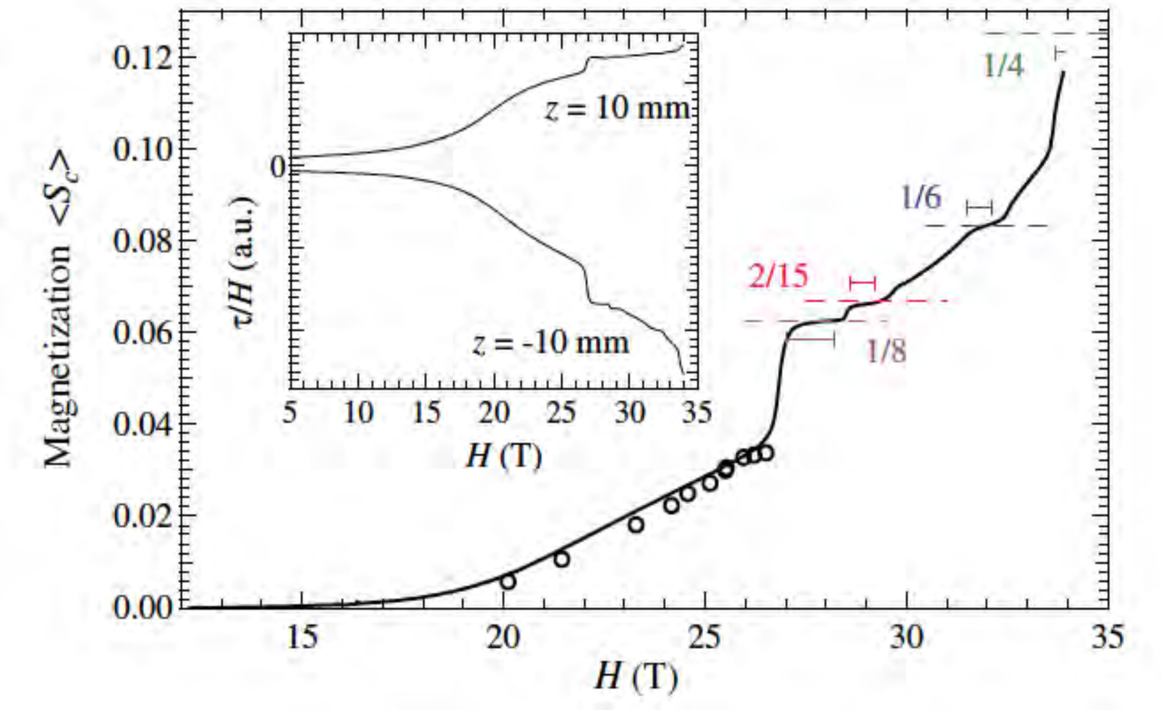


1/9, 1/8, 1/7, 1/6, 1/5, 2/9, 1/4

PRL 110, 067210 (2013) PHYSICAL REVIEW LETTERS week ending 8 FEBRUARY 2013

Incomplete Devil's Staircase in the Magnetization Curve of $SrCu_2(BO_3)_2$

M. Takigawa,[1,*] M. Horvatić,[2] T. Waki,[3] S. Krämer,[2] C. Berthier,[2] F. Lévy-Bertrand,[2,†] I. Sheikin,[2] H. Kageyama,[4] Y. Ueda,[1] and F. Mila[5]



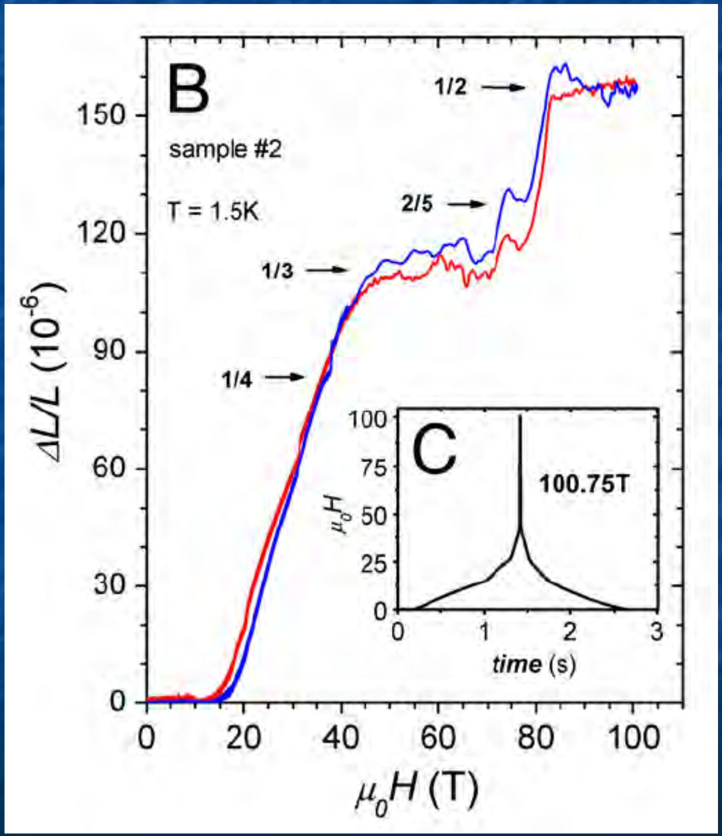
1/8, 2/15, 1/6, 1/4,…

Magnetostriction and magnetic texture to 100.75 Tesla in frustrated $SrCu_2(BO_3)_2$

Marcelo Jaime[a,b,1], Ramzy Daou[c,d], Scott A. Crooker[a,b], Franziska Weickert[b], Atsuko Uchida[a,b], Adrian E. Feiguin[e], Cristian D. Batista[f], Hanna A. Dabkowska[g], and Bruce D. Gaulin[g,h]

12404–12407 | PNAS | July 31, 2012 | vol. 109 | no. 31

www.pnas.org/cgi/doi/10.1073/pnas.1200743109

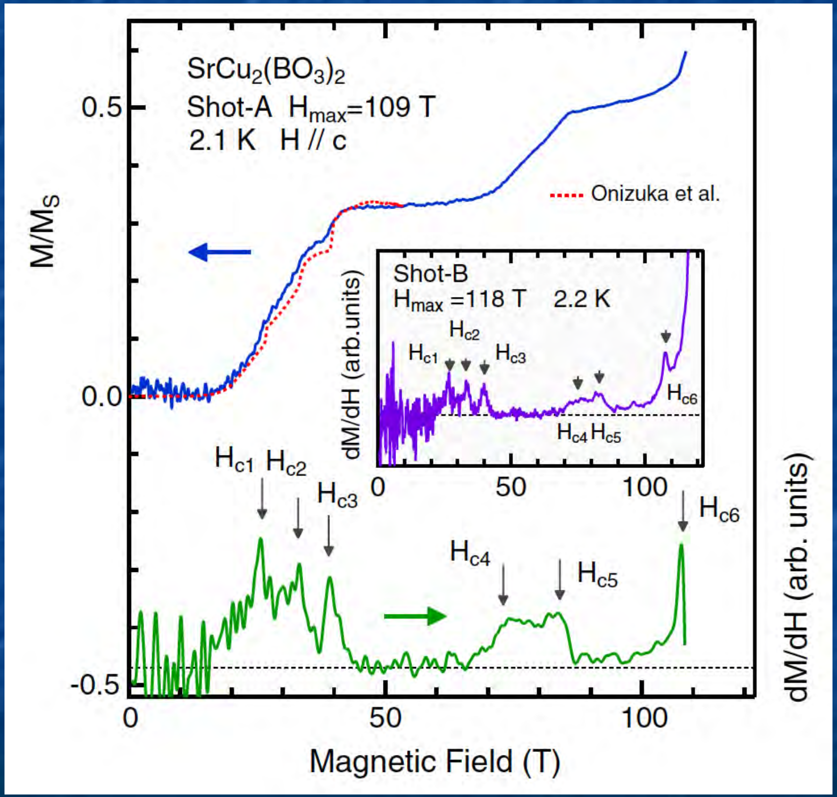


…,1/4, 1/3, 2/5, 1/2

PRL 111, 137204 (2013) PHYSICAL REVIEW LETTERS week ending 27 SEPTEMBER 2013

Magnetization of $SrCu_2(BO_3)_2$ in Ultrahigh Magnetic Fields up to 118 T

Y. H. Matsuda,[1,*] N. Abe,[1] S. Takeyama,[1] H. Kageyama,[2] P. Corboz,[3] A. Honecker,[4,5] S. R. Manmana,[4] G. R. Foltin,[6] K. P. Schmidt,[6] and F. Mila[7]



...1/3, 1/2

Critical summary I

0, 1/9, 1/8, 2/15, 1/7, 1/6, 1/5, 2/9, 1/4, 1/3, 2/5, 1/2

Too many suspects!

Critical summary II

Only pulsed field   Only magnetostriction

0, 1/9, 1/8, 2/15, 1/7, 1/6, 1/5, 2/9, 1/4, 1/3, 2/5, 1/2

0, 1/8, 2/15, 1/6, 1/4, 1/3, 1/2

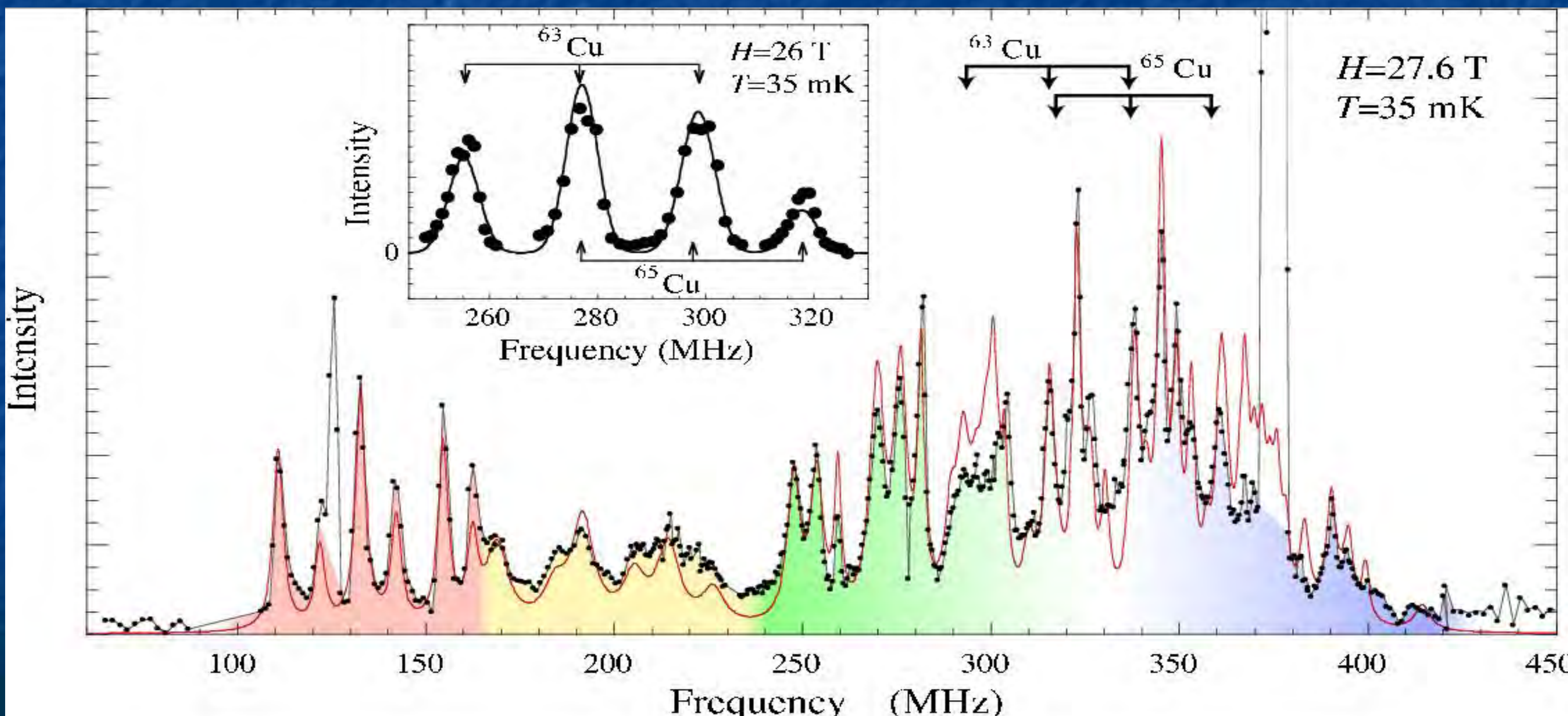
Quantum Hall Effect or broken spatial symmetry?

Magnetic Superstructure in the Two-Dimensional Quantum Antiferromagnet $SrCu_2(BO_3)_2$

K. Kodama,[1] M. Takigawa,[1*] M. Horvatić,[2] C. Berthier,[2,3]
H. Kageyama,[1] Y. Ueda,[1] S. Miyahara,[1,4] F. Becca,[4] F. Mila[4]

www.sciencemag.org SCIENCE VOL 298 11 OCTOBER 2002

Broken symmetry in 1/8 plateau



PRL 110, 067210 (2013) PHYSICAL REVIEW LETTERS week ending 8 FEBRUARY 2013

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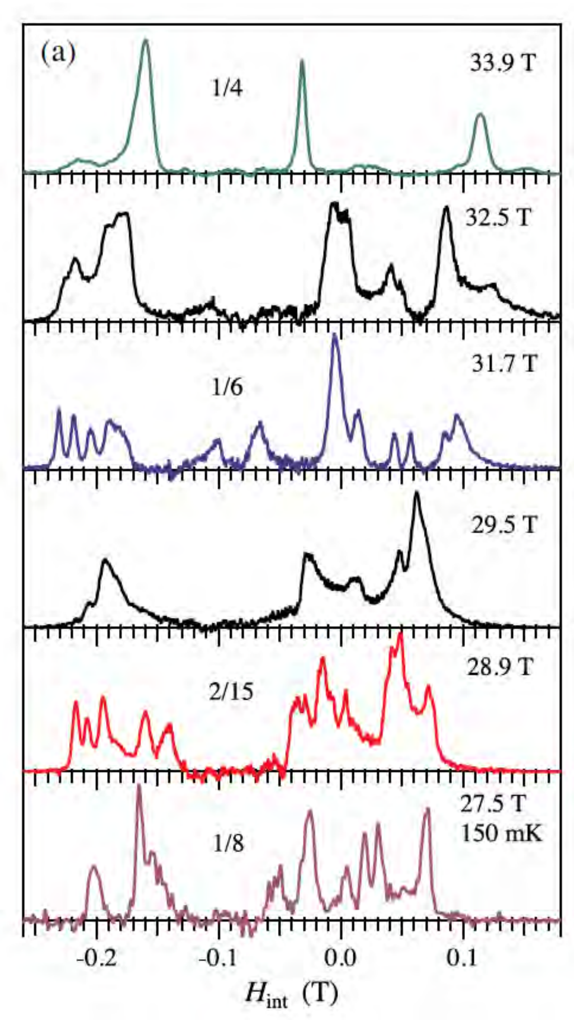
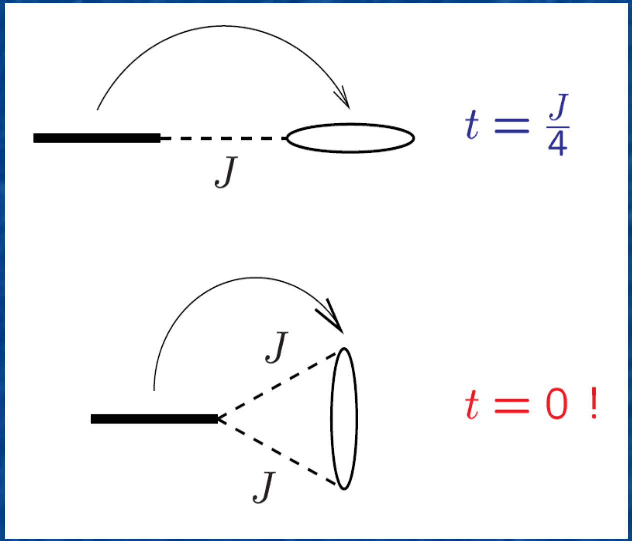


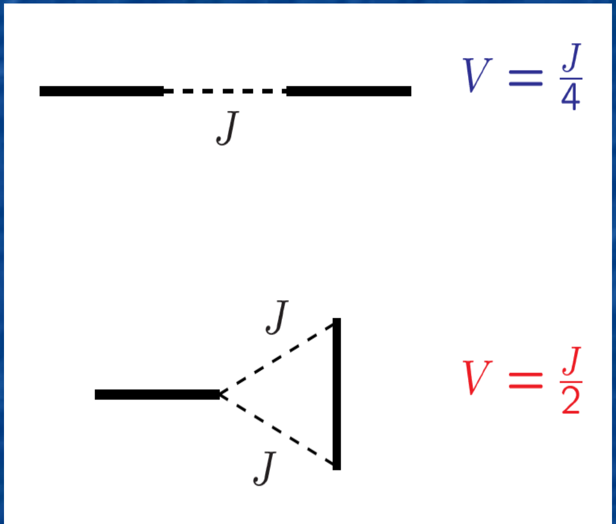
Broken symmetry in
1/8, 2/15, 1/6 and 1/4 plateaus

Effect of frustration

Triplet Hopping



Triplet Repulsion



- Kinetic energy << potential energy
- Long-range repulsion

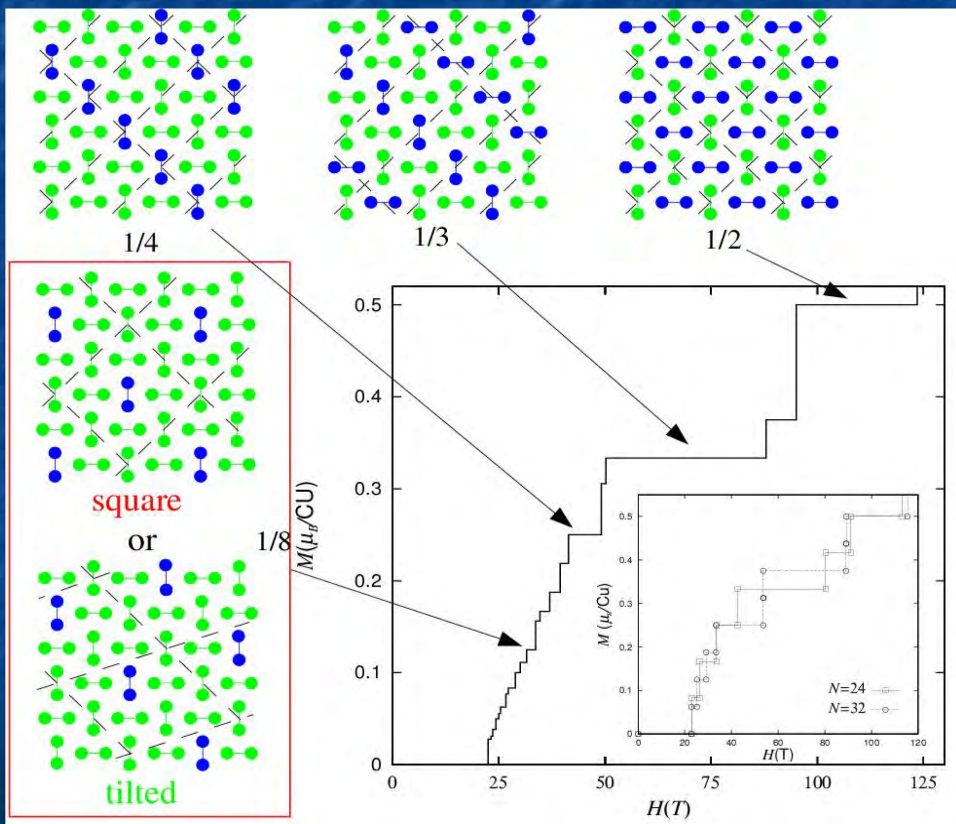
  → Crystals of triplets with high commensurability

  → Magnetization plateaux

PHYSICAL REVIEW B VOLUME 61, NUMBER 5 1 FEBRUARY 2000-I

Superstructures at magnetization plateaus in $SrCu_2(BO_3)_2$

Shin Miyahara and Kazuo Ueda



- Simple ansatz for long-range triplet-triplet interaction
- Many plateaus

PHYSICAL REVIEW B VOLUME 62, NUMBER 22 1 DECEMBER 2000-II

Magnetization plateaus of the Shastry-Sutherland model for $SrCu_2(BO_3)_2$: Spin-density wave, supersolid, and bound states

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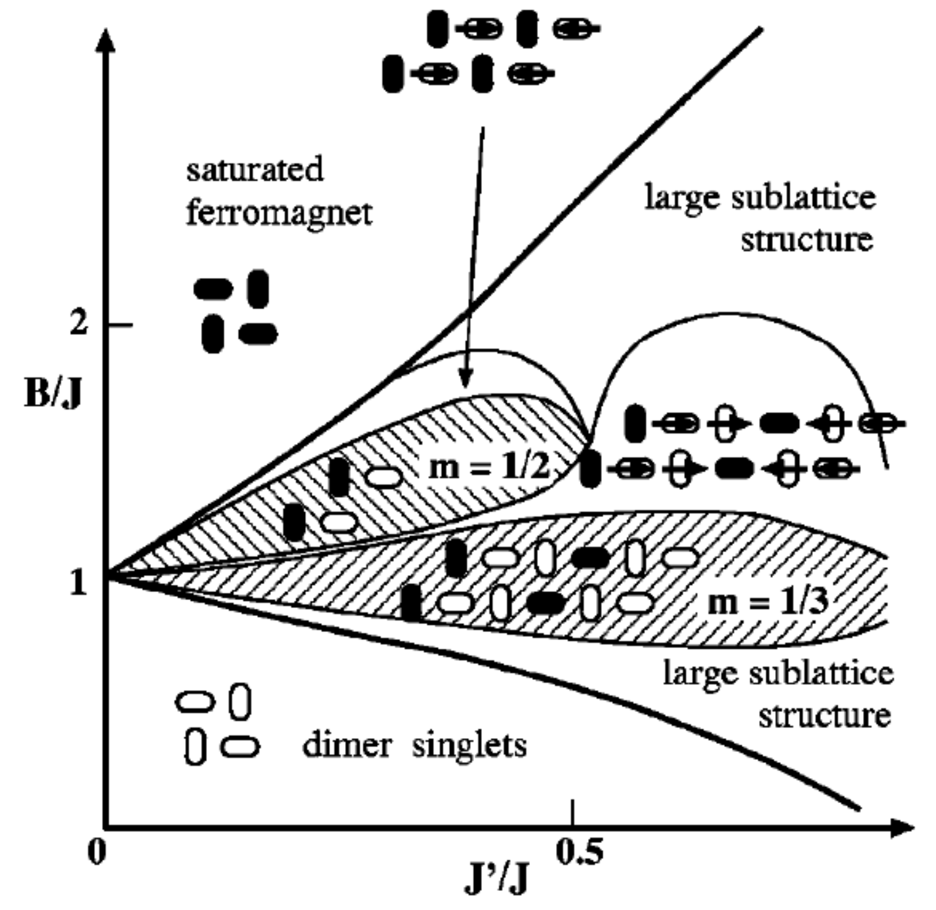
Department of Physics, Kyushu University, Hakozaki, Higashi-ku, Fukuoka-shi 812-8581, Japan

(Received 1 June 2000)



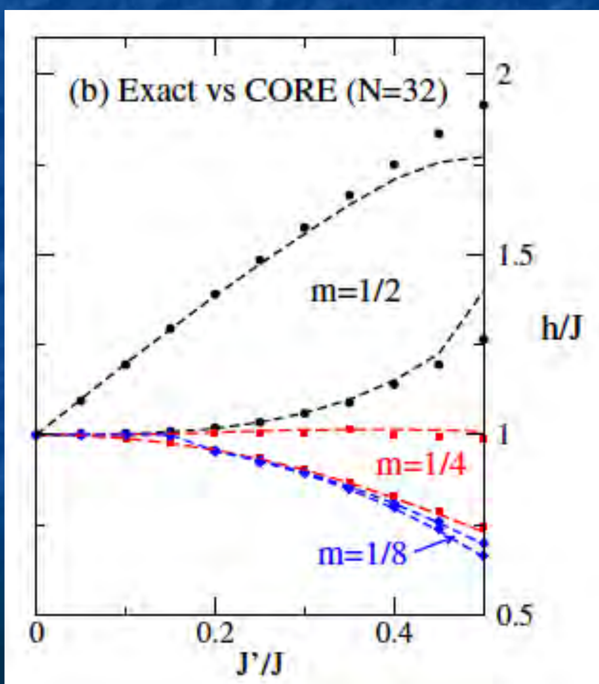
- Effective model to third order in $(J'/J)^3$
- Only short-range triplet-triplet interaction
- Only 1/3 and 1/2 plateaus
- Spin-supersolids

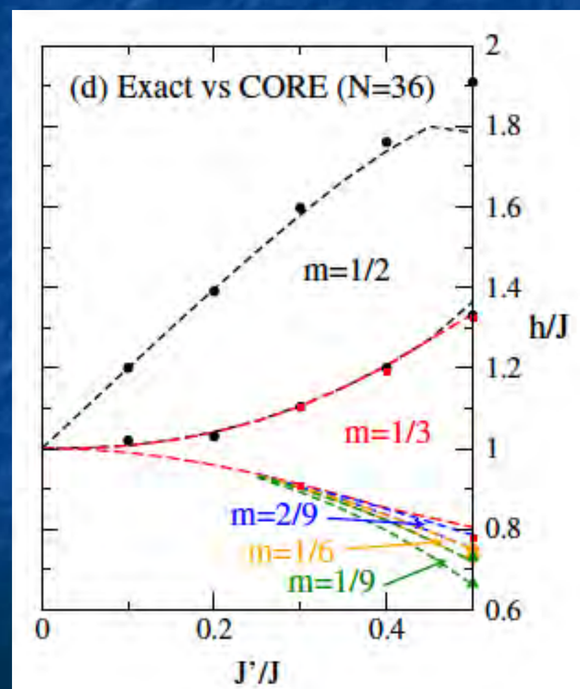
PRL 101, 227201 (2008) PHYSICAL REVIEW LETTERS week ending 28 NOVEMBER 2008

Effective Theory of Magnetization Plateaux in the Shastry-Sutherland Lattice

A. Abendschein[1,2] and S. Capponi[1,2,*]

Effective model with CORE (Contractor Renormalization) Exact diagonalization on small clusters





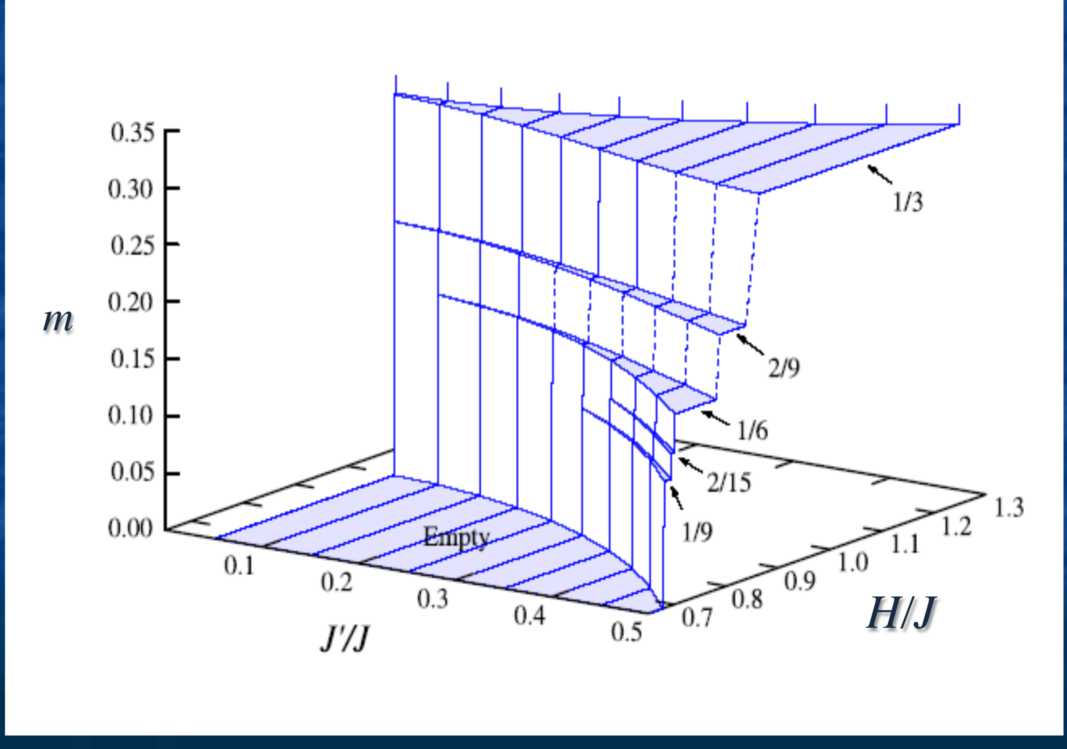
- Large finite-size effects
- No 2/15 plateau
- No information on plateau structures

PRL 101, 250402 (2008) PHYSICAL REVIEW LETTERS week ending 19 DECEMBER 2008

Theory of Magnetization Plateaux in the Shastry-Sutherland Model

J. Dorier,[1] K. P. Schmidt,[2,*] and F. Mila[1]

Long-range triplet-triplet interaction with high-order perturbation theory in J'/J

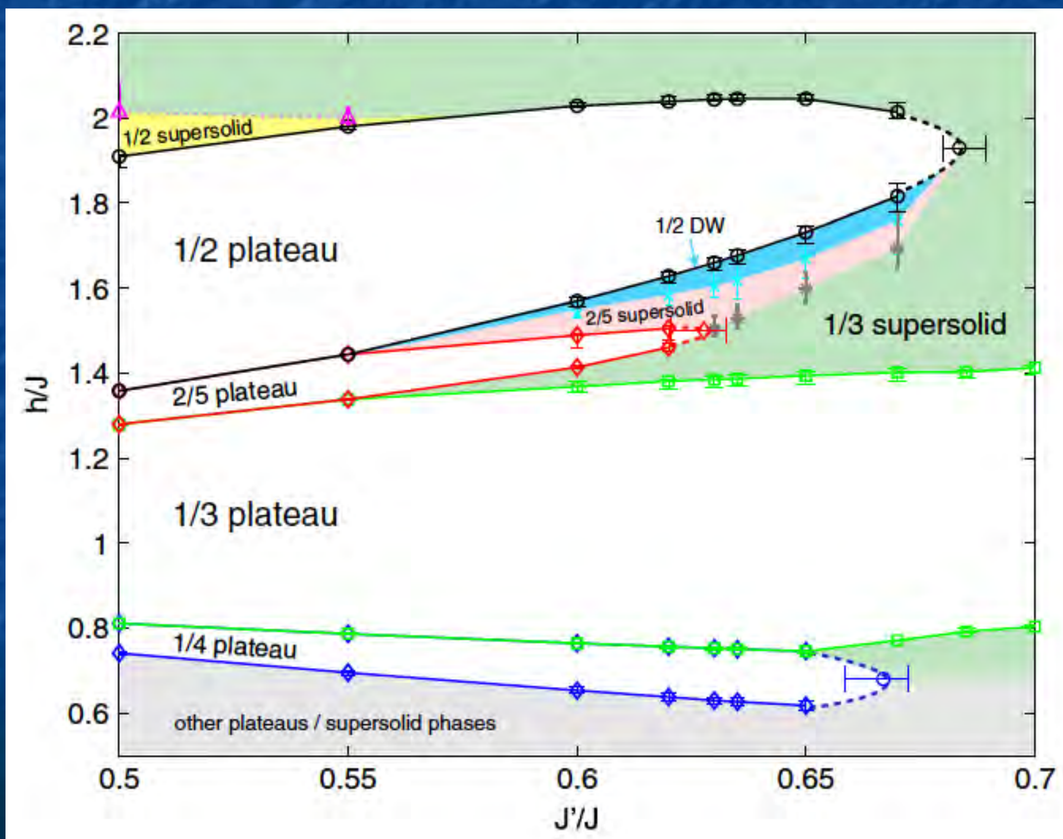


Triplet crystals:
not the right sequence
(at least up to J'/J=0.5)

PRL 111, 137204 (2013) PHYSICAL REVIEW LETTERS week ending 27 SEPTEMBER 2013

Magnetization of $SrCu_2(BO_3)_2$ in Ultrahigh Magnetic Fields up to 118 T

Y. H. Matsuda,[1,*] N. Abe,[1] S. Takeyama,[1] H. Kageyama,[2] P. Corboz,[3] A. Honecker,[4,5] S. R. Manmana,[4] G. R. Foltin,[6] K. P. Schmidt,[6] and F. Mila[7]



iPEPS

A variational approach derived from quantum information

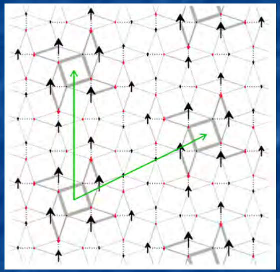
Verstraete & Cirac, 2004

PRL 112, 147203 (2014) PHYSICAL REVIEW LETTERS week ending 11 APRIL 2014

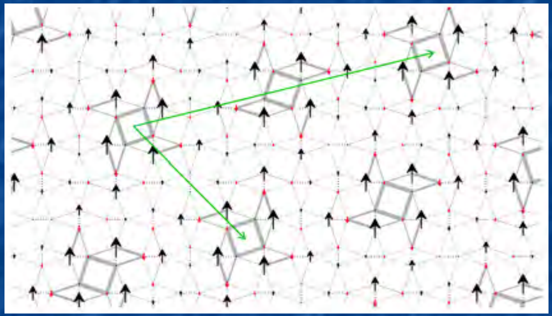
Crystals of Bound States in the Magnetization Plateaus of the Shastry-Sutherland Model

Philippe Corboz[1] and Frédéric Mila[2]

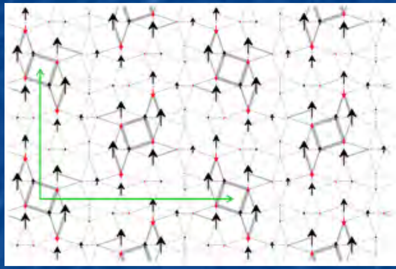
1/8

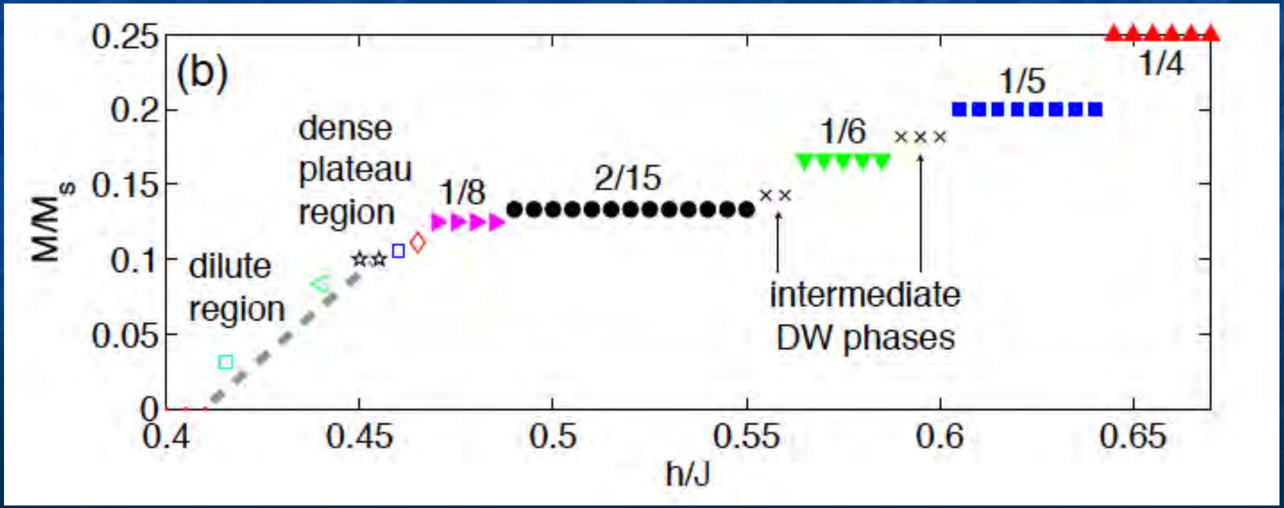


2/15



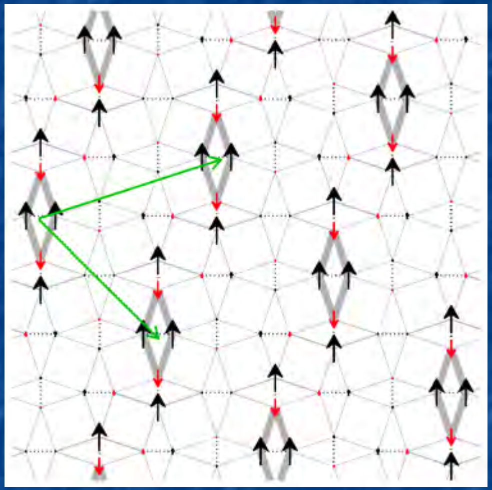
1/6



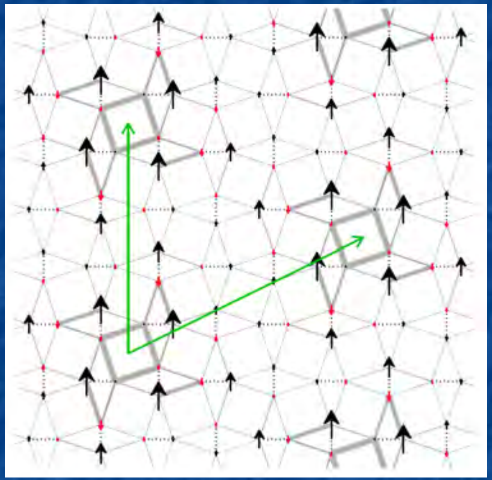


Triplets versus bound-states

Triplet crystal



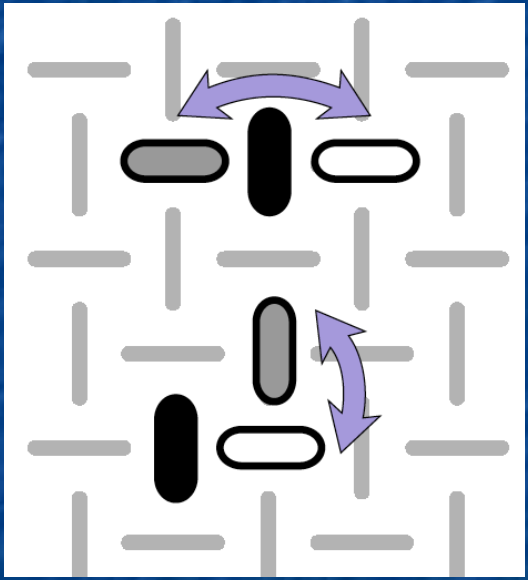
Bound state crystal



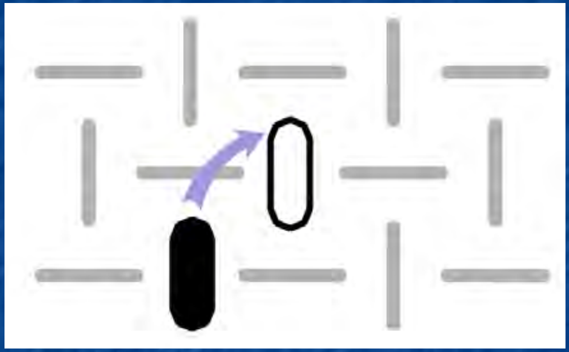
- Why are bound state crystals favoured?
- Why did it take 15 years to identify them?

Why are bound states favoured?

Correlated hopping



Single particle hopping

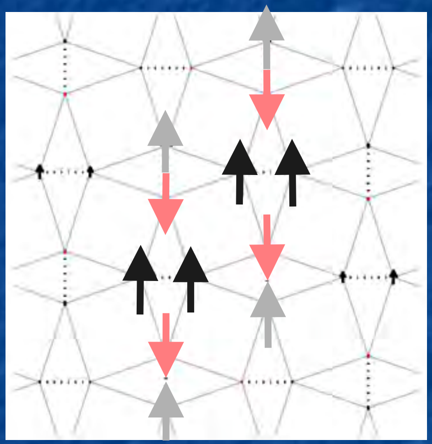


α $(J'/J)^6$

α $(J'/J)^2$ → gain in kinetic energy

Boundstates as pinwheels

Order $(J'/J)^3$



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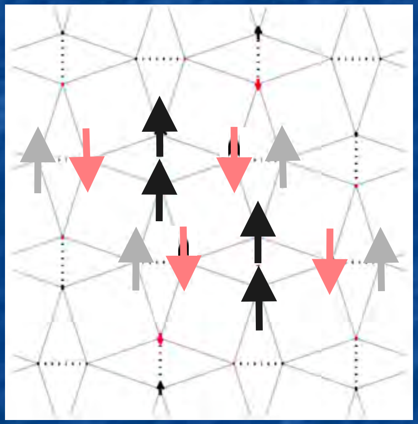

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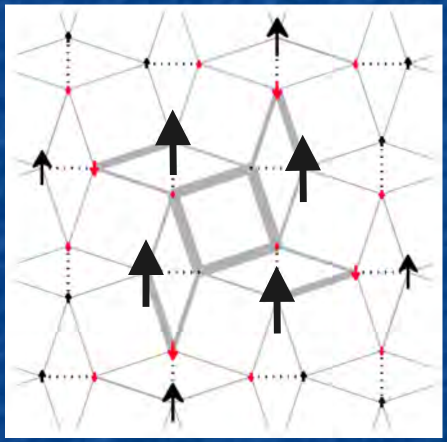

Higher order

PHYSICAL REVIEW B VOLUME 62, NUMBER 22 1 DECEMBER 2000-II

Magnetization plateaus of the Shastry-Sutherland model for $SrCu_2(BO_3)_2$: Spin-density wave, supersolid, and bound states

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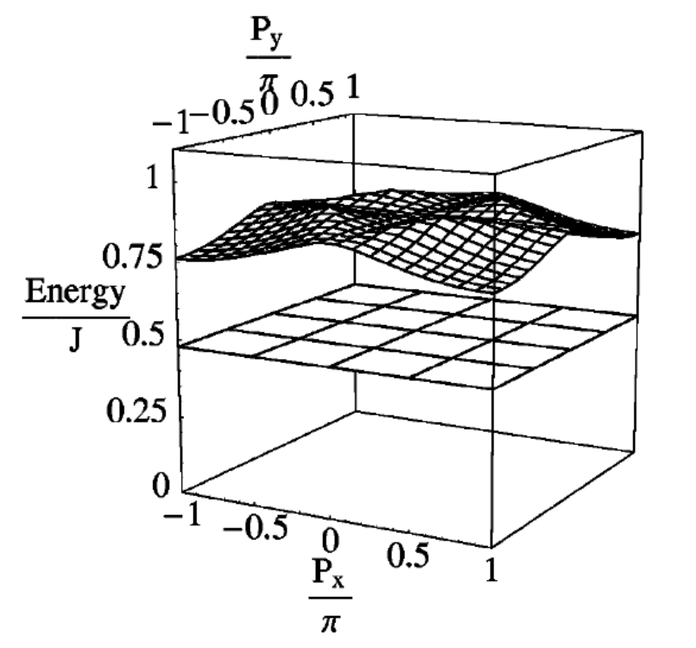
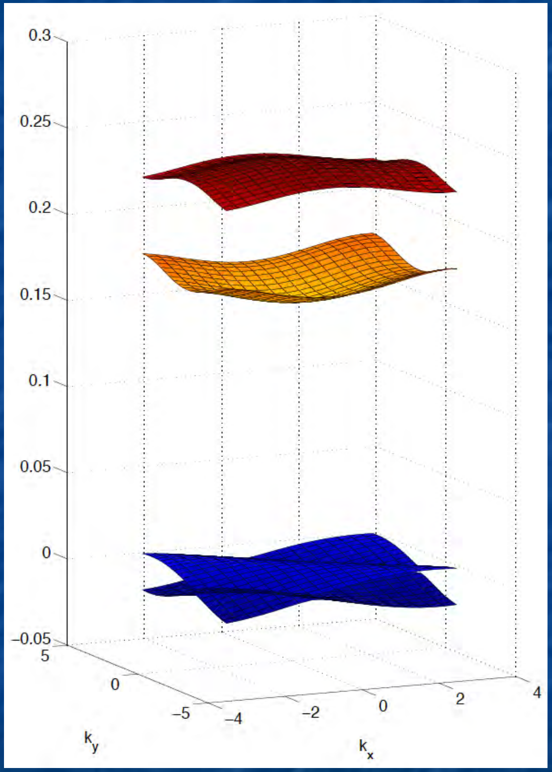
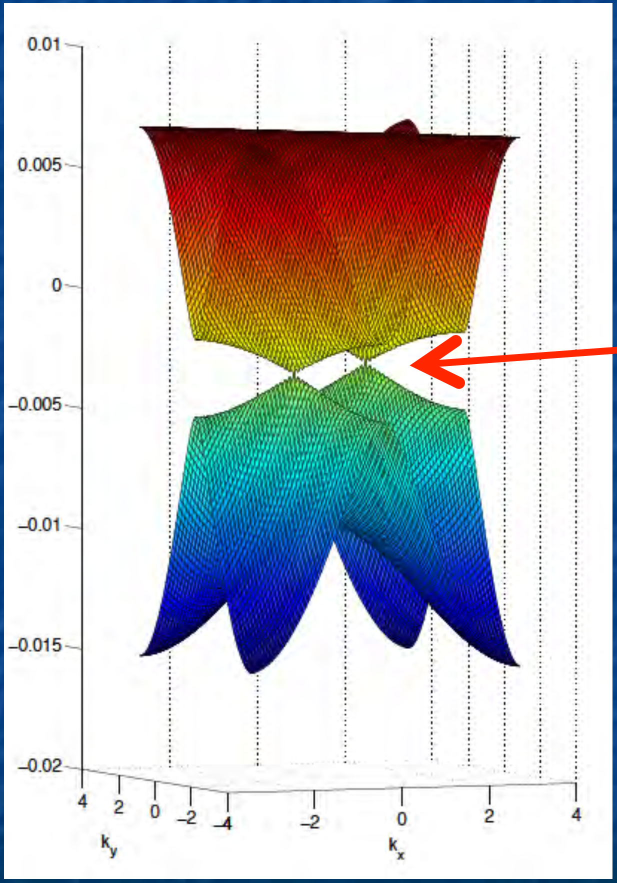


Bound state dispersion: minimum at the zone corner

Localized bound state





Negative reference energy!

P. Corboz, FM, PRL 2014

Conclusions on $SrCu_2(BO_3)_2$

- Natural plateau sequence
  → 1/8, 2/15, 1/6: crystals of bound states
  → new predictions for their symmetry
- To be done next
  → revisit effective triplet model
  → compare predictions with NMR
  → X-ray or neutron in high field (>27 T)?

Conclusions

- Tensor network algorithms

→ very promising new method in 2D

→ encouraging results on various frustrated models

→ solved the 15-year old puzzle of magnetization plateaux in $SrCu_2(BO_3)_2$