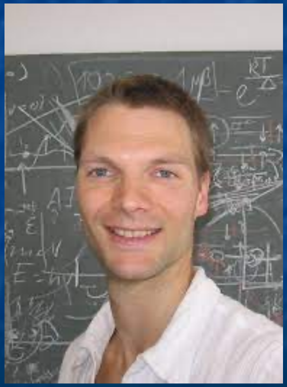
Thermal properties of frustrated quantum magnets

F. Mila
Ecole Polytechnique Fédérale de Lausanne
Switzerland

Theorists



Stefan Wessel (Aachen)
Andreas Honecker (Cergy)
Bruce Normand (PSI)
Philippe Corboz (Amsterdam)
Olivier Gauthé (Lausanne)


Experimentalists

Henrik Ronnow (Lausanne)
Christian Rüegg (Villigen)

and many more...

Scope

- Thermal properties: quantum Monte Carlo and minus sign
- Fully frustrated bilayer:
  → Minus sign free QMC in dimer basis
  → Ising critical point
- Shastry-Sutherland model:
  → From QMC to iPEPS (tensor network)
  → $SrCu_2(BO_3)_2$ under pressure: Critical point
- J1-J2 model:
  → Ising transition revealed by iPEPS
- Conclusions

Quantum Monte Carlo I

- Partition function as a path integral
- Starting point:

$$Z = \mathrm{Tr}(e^{-\beta\mathcal{H}}) = \sum_{\alpha} \langle \alpha | e^{-\beta\mathcal{H}} | \alpha \rangle$$

- Problem: to calculate the exponential of $\mathcal{H}$, one needs to diagonalize it!

Quantum Monte Carlo II

$$Z = \sum_{\alpha} \langle \alpha | \prod_{l=1}^{L} e^{-\Delta\tau\mathcal{H}} | \alpha \rangle, \;\; \Delta\tau = \frac{\beta}{L}$$

$$Z = \sum_{\alpha_1,\ldots,\alpha_L} \langle \alpha_1 | e^{-\Delta\tau\mathcal{H}} | \alpha_2 \rangle \langle \alpha_2 | e^{-\Delta\tau\mathcal{H}} | \alpha_3 \rangle \ldots \langle \alpha_L | e^{-\Delta\tau\mathcal{H}} | \alpha_1 \rangle$$

$$Z \simeq \sum_{\alpha_1,\ldots,\alpha_L} \langle \alpha_1 | 1 - \Delta\tau\mathcal{H} | \alpha_2 \rangle \langle \alpha_2 | 1 - \Delta\tau\mathcal{H} | \alpha_3 \rangle \ldots \langle \alpha_L | 1 - \Delta\tau\mathcal{H} | \alpha_1 \rangle$$

$$\langle \alpha_i | 1 - \Delta\tau\mathcal{H} | \alpha_{i+1} \rangle > 0 \text{ iff } \langle \alpha_i | \mathcal{H} | \alpha_{i+1} \rangle < 0 \text{ when } \langle \alpha_i | \alpha_{i+1} \rangle = 0$$

Quantum Monte Carlo III

Then $Z \simeq \sum_{\{\alpha\}} W(\{\alpha\})$ with $W(\{\alpha\}) > 0$

No minus sign!

$$\langle A \rangle = \frac{1}{Z} \sum_{\alpha_1,\ldots,\alpha_L} \langle \alpha_1 | 1 - \Delta\tau\mathcal{H} | \alpha_2 \rangle \ldots \langle \alpha_L | (1 - \Delta\tau\mathcal{H}) A | \alpha_1 \rangle$$

$$\langle A \rangle = \frac{\sum_{\{\alpha\}} A(\{\alpha\}) W(\{\alpha\})}{\sum_{\{\alpha\}} W(\{\alpha\})}$$

Monte Carlo sampling

where $A(\{\alpha\}) = A(\alpha_1)$ if A is diagonal

Quantum Monte Carlo IV

- Heisenberg AF in configuration basis:

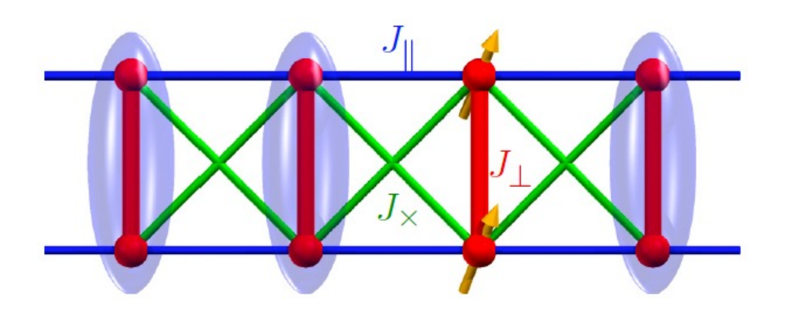
  → All off-diagonal matrix elements are positive!

  → Bipartite lattice: rotation by π on one sublattice to change the signs of all off-diagonal matrix elements

  → Non-bipartite lattice: no way out in configuration basis

Fully frustrated dimer models

- Example: fully-frustrated ladder



$$J_\times = J_\parallel$$

$$H = J_\parallel \sum_{i=1}^{L} \vec{T}_i \cdot \vec{T}_{i+1} + J_\perp \sum_{i=1}^{L} \left(\frac{1}{2} \vec{T}_i^2 - S(S+1) \right)$$

$\vec{T}_i = \vec{S}_i^1 + \vec{S}_i^2$ Total spin on a rung is a good quantum number

Hamiltonian in dimer basis

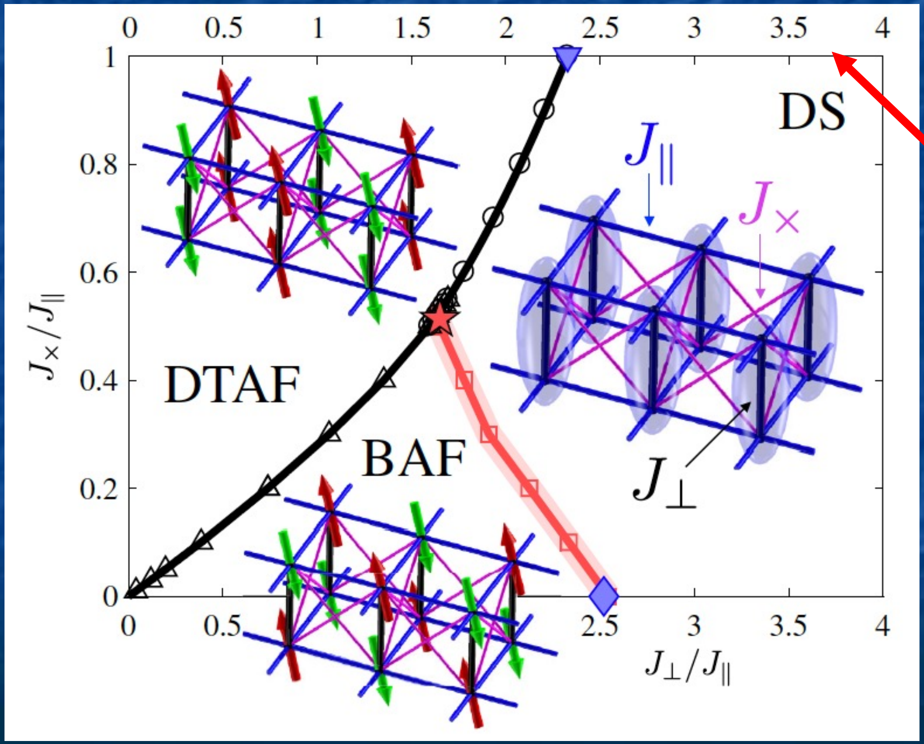
- In general, involves both the sum and the difference of spins on a dimer
- If all exchange integrals between the spins of coupled dimers are equal (maximal frustration), the Hamiltonian can be written in terms of the sum only

→ QMC possible if bipartite lattice of dimers

PHYSICAL REVIEW LETTERS **121**, 127201 (2018)

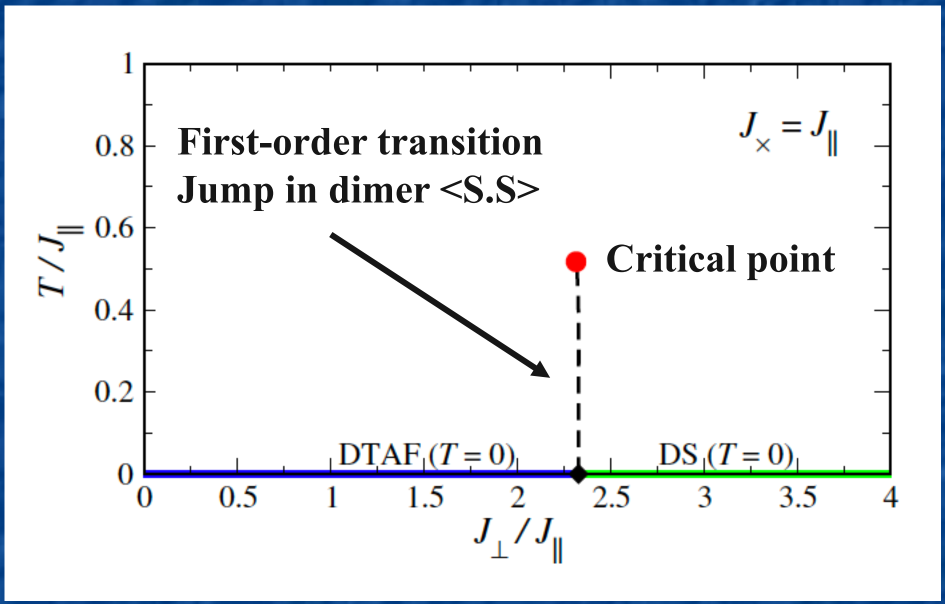
Thermal Critical Points and Quantum Critical End Point in the Frustrated Bilayer Heisenberg Antiferromagnet

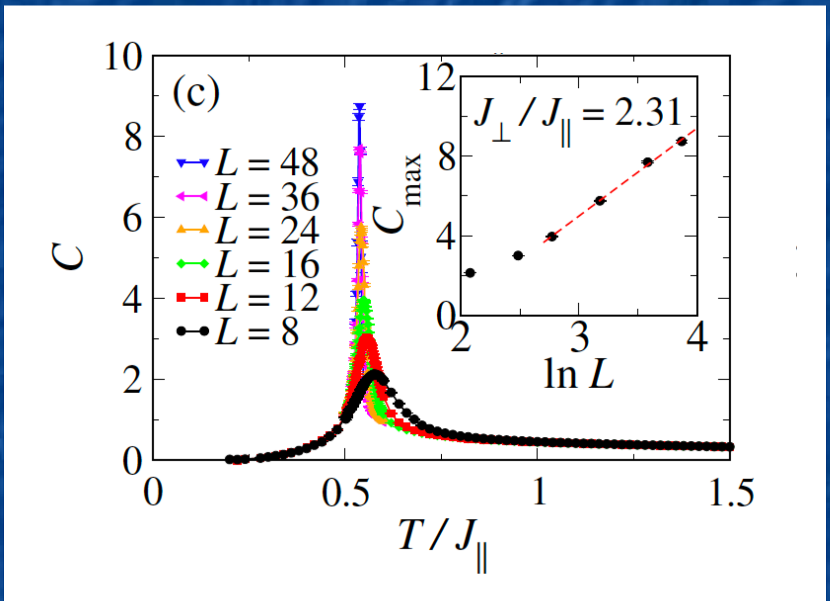
J. Stapmanns,[1] P. Corboz,[2] F. Mila,[3] A. Honecker,[4] B. Normand,[5] and S. Wessel[1]



Fully frustrated bilayer

Ising critical point





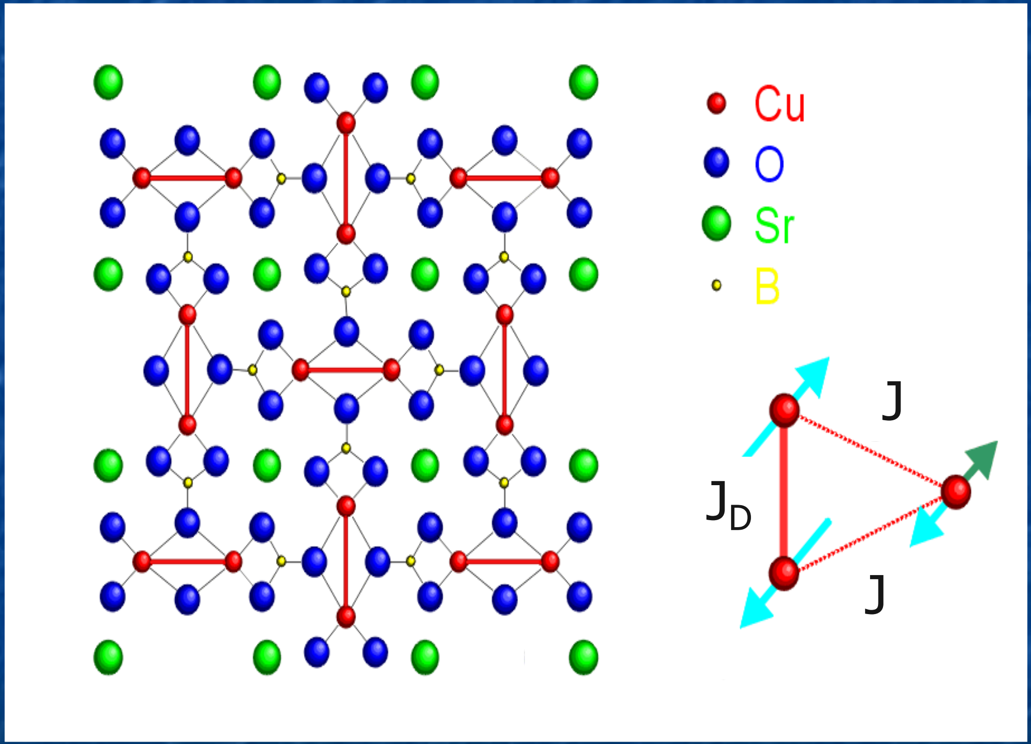
Ising 2D: $\alpha = 0$

C α ln L

Physical realization?

$SrCu_2(BO_3)_2$

Smith and Keszler, JSSC 1991



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

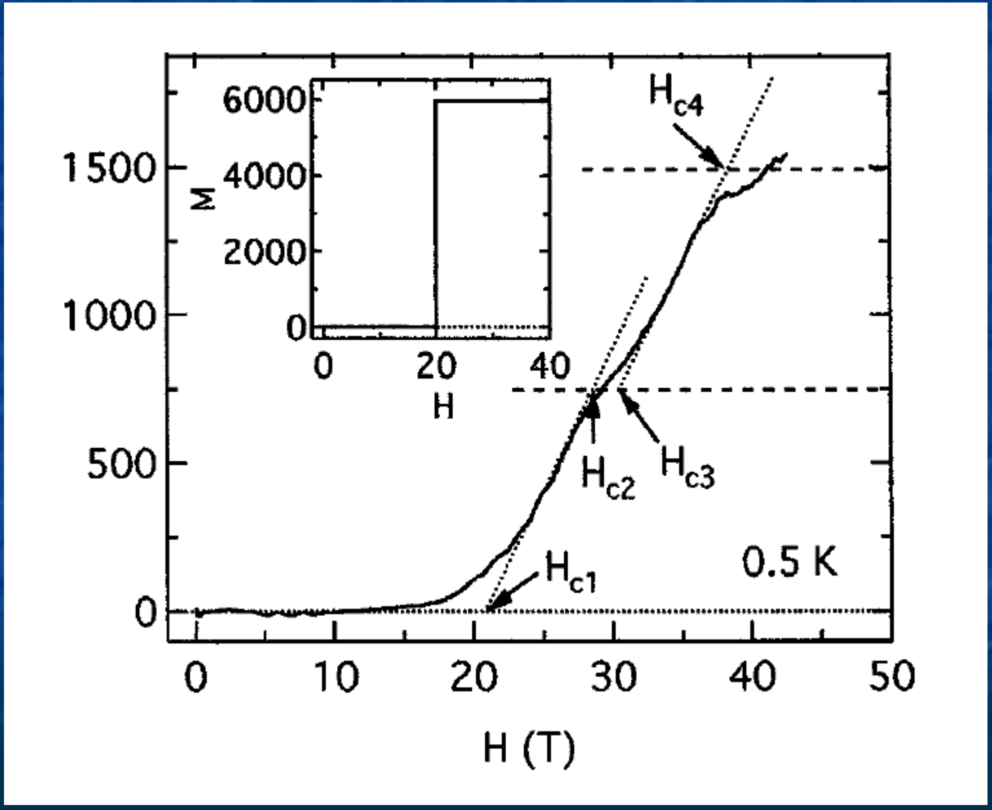
$J_D \approx 85$ K

$J/J_D \approx 0.63$

Orthogonal dimer model

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

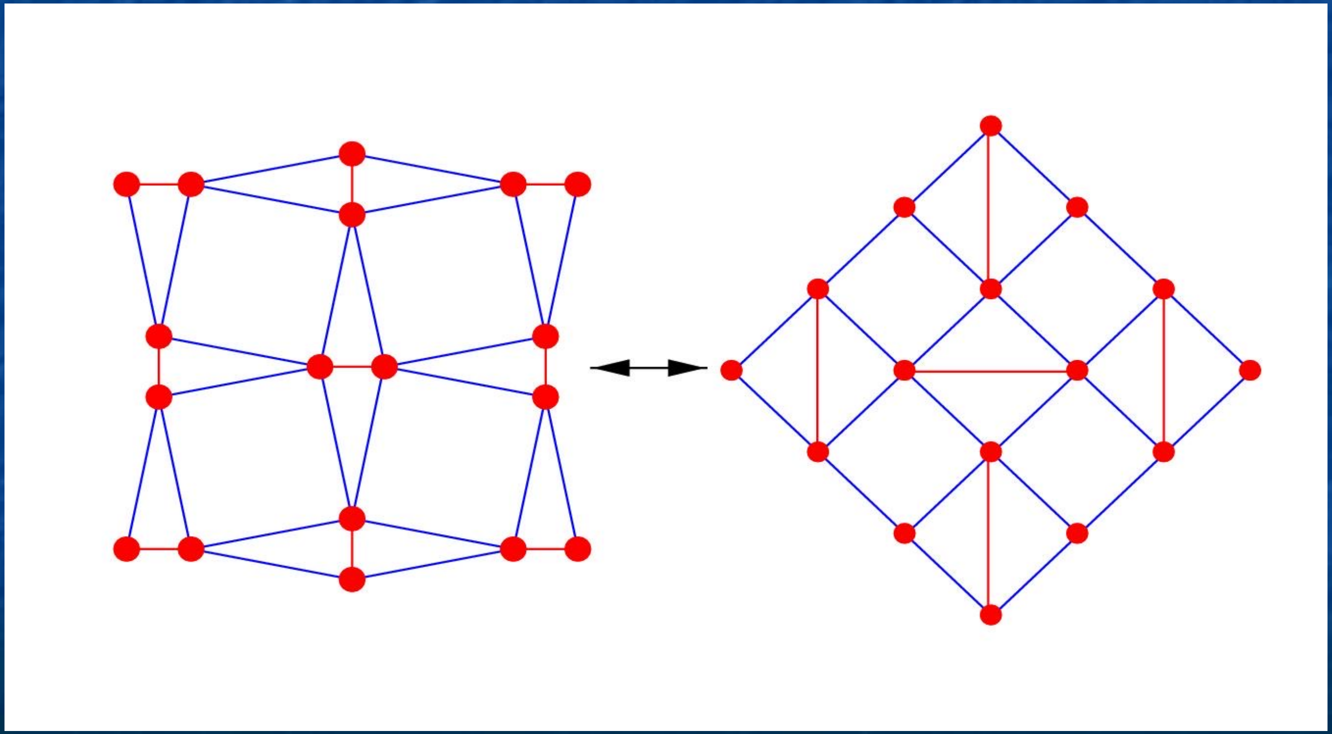
H. Kageyama,[1,2,*] K. Yoshimura,[1,3,†] R. Stern,[3] N. V. Mushnikov,[2] K. Onizuka,[2] M. Kato,[1] K. Kosuge,[1] C. P. Slichter,[3] T. Goto,[2] and Y. Ueda[2]



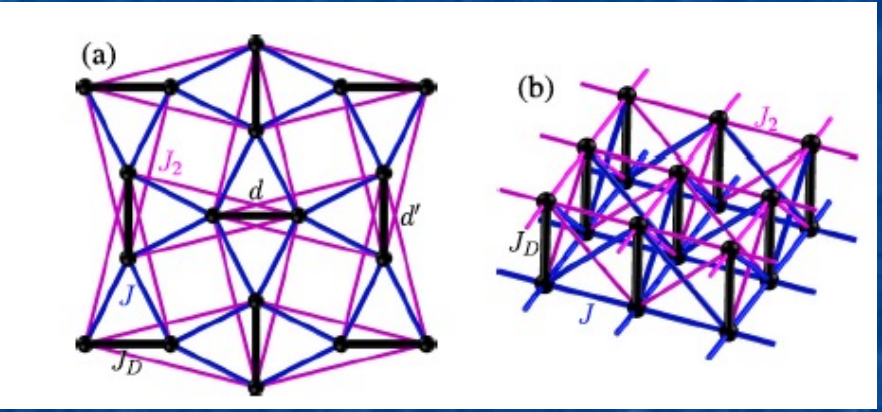
Anomalies
- M=0
- M=1/8
- M=1/4

and many more

From orthogonal dimer to Shastry-Sutherland model



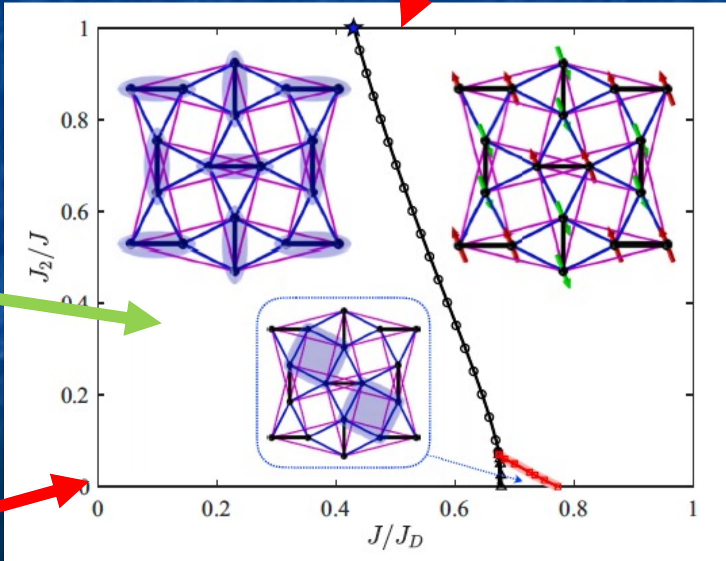
From FFB to Shastry-Sutherland



Fully-frustrated bilayer

GS = product of dimers

Shastry-Sutherland model



Thermal properties of Shastry-Sutherland model

Hamiltonian : cannot be written
in terms of sum of spins of dimers

$$\langle A \rangle = \frac{\sum_c W_c A_c}{\sum_c W_c} = \frac{\sum_c \mathrm{sign}(W_c)|W_c|A_c}{\sum_c \mathrm{sign}(W_c)|W_c|} = \frac{\langle \mathrm{sign} A \rangle'}{\langle \mathrm{sign} \rangle'}$$

- Up to $J/J_D = 0.526\ldots$

→ The model with all off-diagonal matrix elements put arbitrarily negative has the same GS

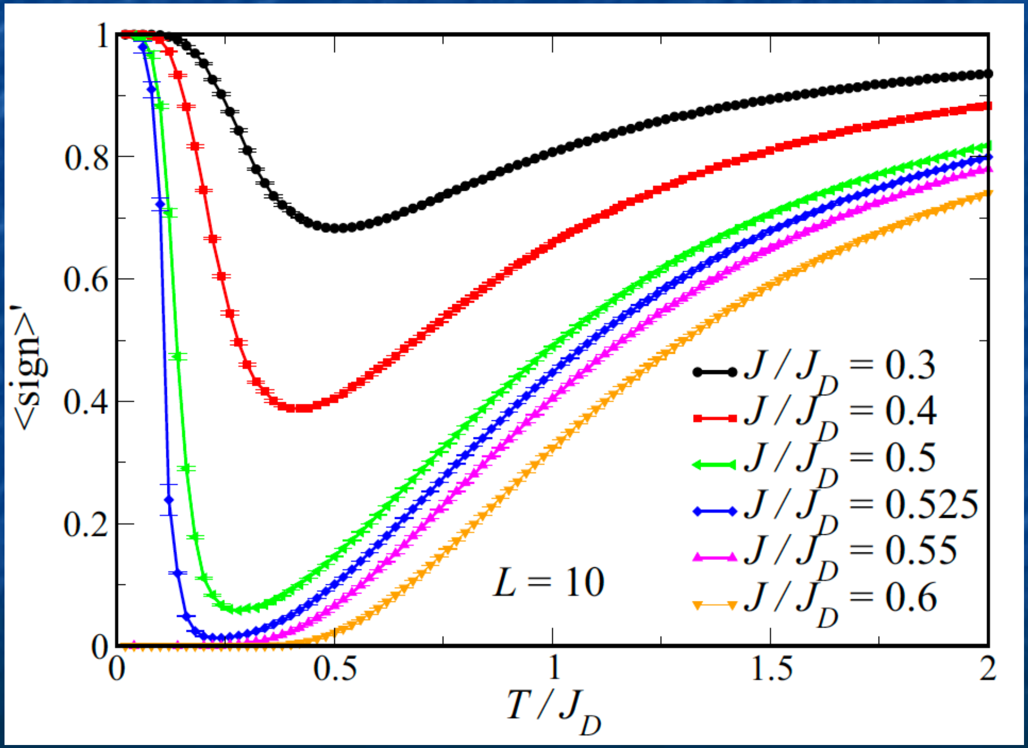
→ <sign>' → 1 as T → 0

→ QMC possible!

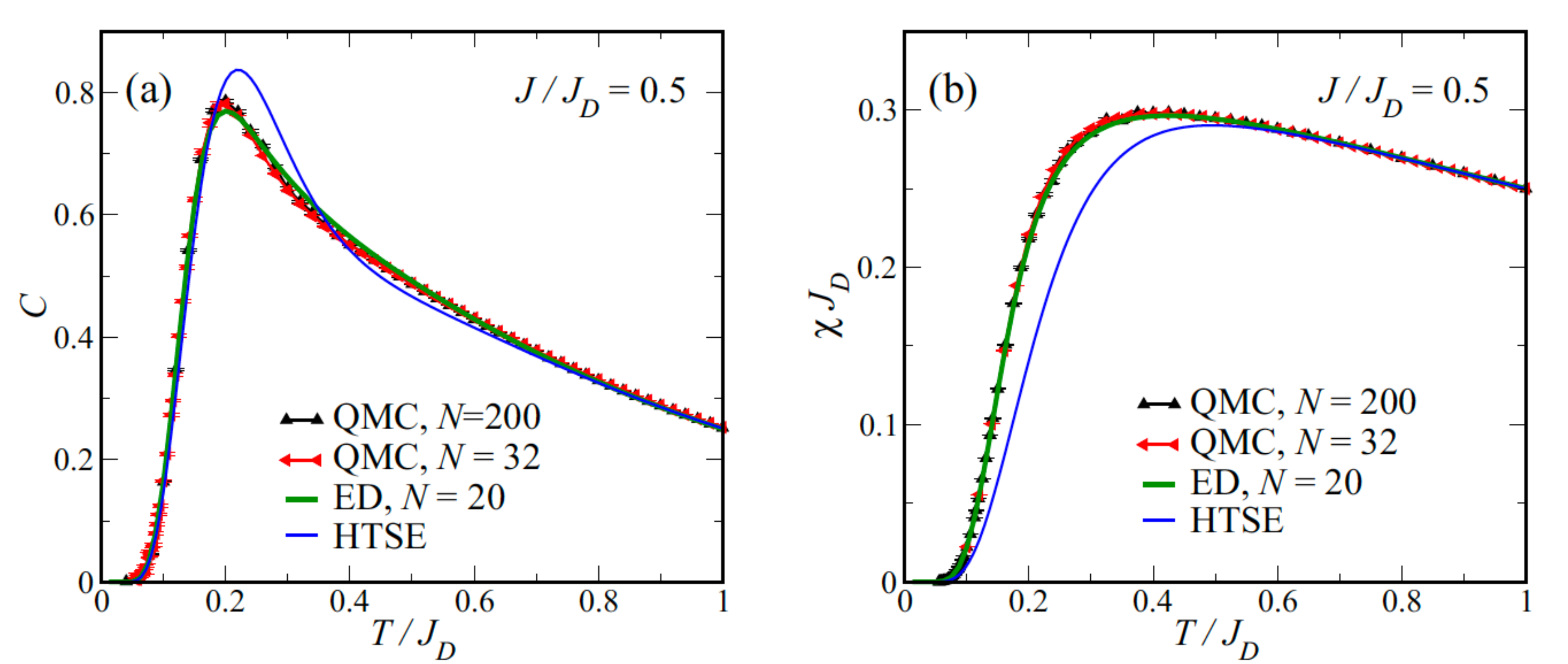
PHYSICAL REVIEW B **98**, 174432 (2018)

Thermodynamic properties of the Shastry-Sutherland model from quantum Monte Carlo simulations

Stefan Wessel,[1] Ido Niesen,[2] Jonas Stapmanns,[1] B. Normand,[3] Frédéric Mila,[4] Philippe Corboz,[2] and Andreas Honecker[5]



Specific heat and susceptibility



And above J/J_D =0.526?

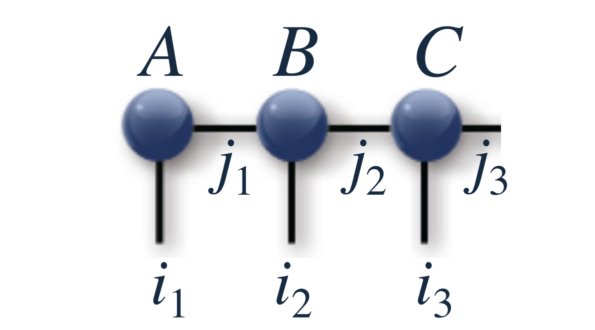
Tensor networks

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

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

Example: Matrix product state in 1D (DMRG)

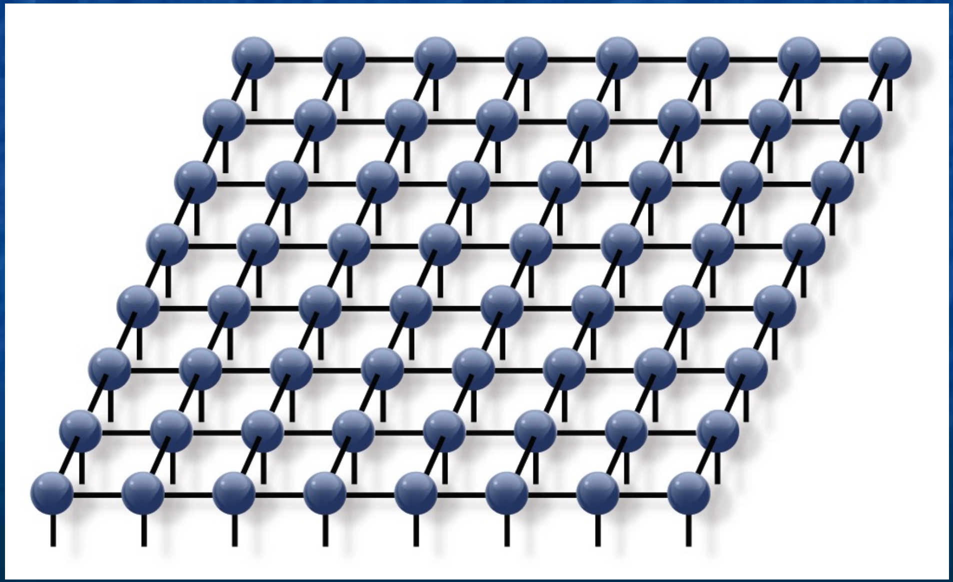
$$c_{i_1 i_2 i_3 \dots} \simeq \sum_{j_1 j_2 \dots} A_{i_1}^{j_1} B_{i_2}^{j_1 j_2} C_{i_3}^{j_2 j_3} \cdots$$



Generalization to 2D

PEPS = product of entangled pair states

Verstraete and Cirac, 2004



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

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

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...

Tensor network for T>0

- Purified state: density matrix can be written as the partial trace of a quantum state in an enlarged Hilbert space (with extra “ancilla” degrees of freedom)
- T infinite: Singlets between physical and ancilla degrees of freedom
- Finite T: imaginary-time evolution from T infinite

F. Verstraete, J. J. Garcia-Ripoll, and J. I. Cirac, PRL 2004

PHYSICAL REVIEW B **86**, 245101 (2012)

Projected entangled pair states at finite temperature: Imaginary time evolution with ancillas

Piotr Czarnik,[1] Lukasz Cincio,[2] and Jacek Dziarmaga[1]

PHYSICAL REVIEW B **92**, 035120 (2015)

Projected entangled pair states at finite temperature: Iterative self-consistent bond renormalization for exact imaginary time evolution

Piotr Czarnik and Jacek Dziarmaga

PHYSICAL REVIEW B **99**, 245107 (2019)

Finite correlation length scaling with infinite projected entangled pair states at finite temperature

Piotr Czarnik[1] and Philippe Corboz[2]

PHYSICAL REVIEW B **103**, 075113 (2021)

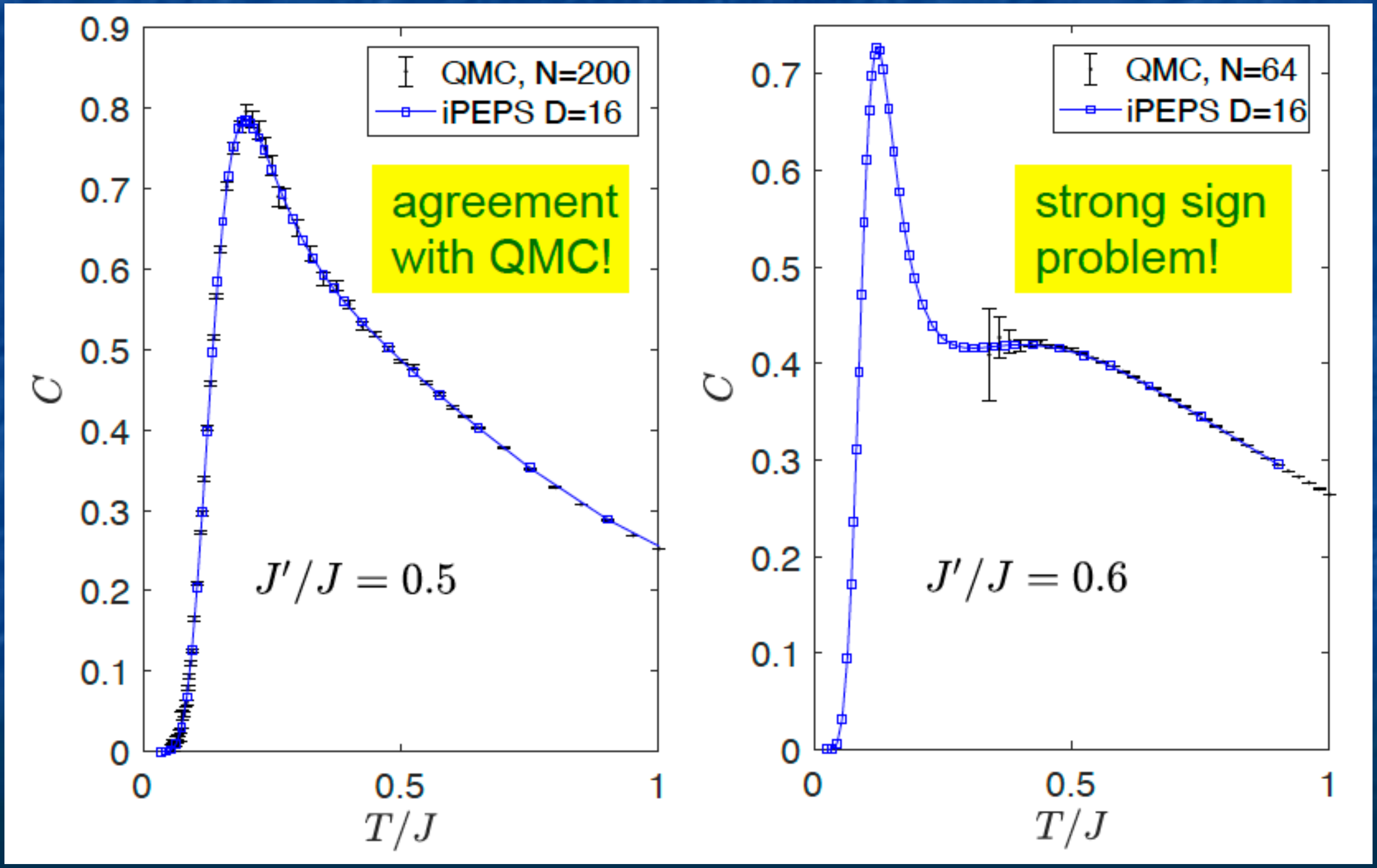
Tensor network study of the $m = \frac{1}{2}$ magnetization plateau in the Shastry-Sutherland model at finite temperature

Piotr Czarnik,[1] Marek M. Rams,[2] Philippe Corboz,[3] and Jacek Dziarmaga[2]

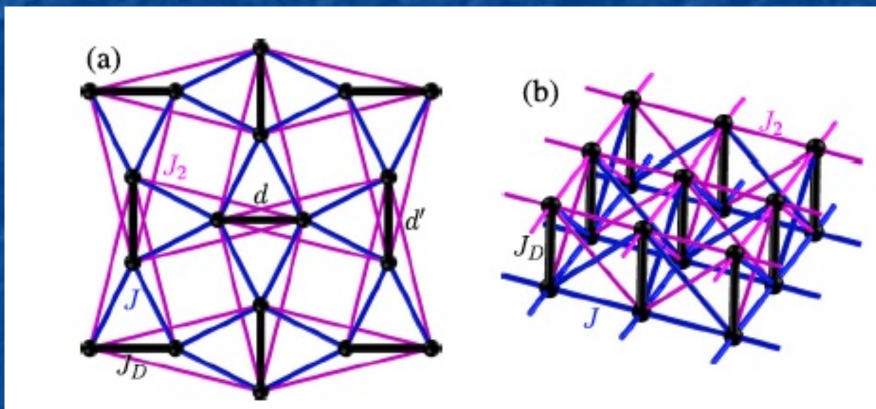
PHYSICAL REVIEW RESEARCH **1**, 033038 (2019)

Thermodynamic properties of the Shastry-Sutherland model throughout the dimer-product phase

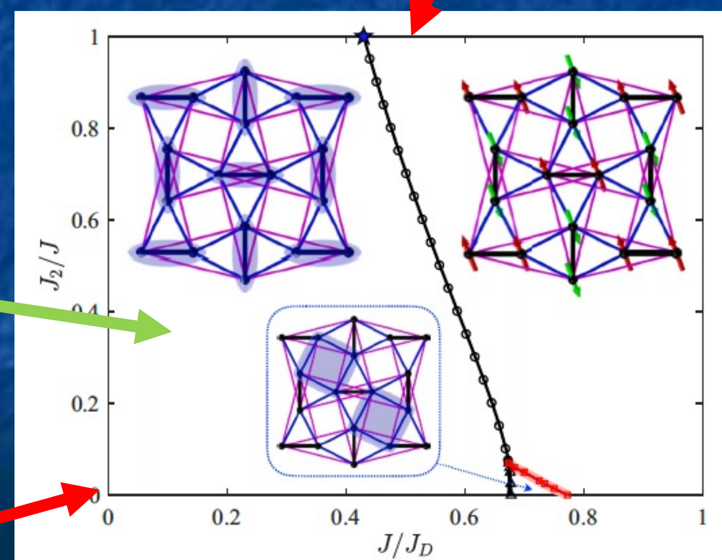
Alexander Wietek,[1,2,*] Philippe Corboz,[3] Stefan Wessel,[4] B. Normand,[5] Frédéric Mila,[6] and Andreas Honecker[7]



From FFB to Shastry-Sutherland



Fully-frustrated bilayer



GS = product of dimers

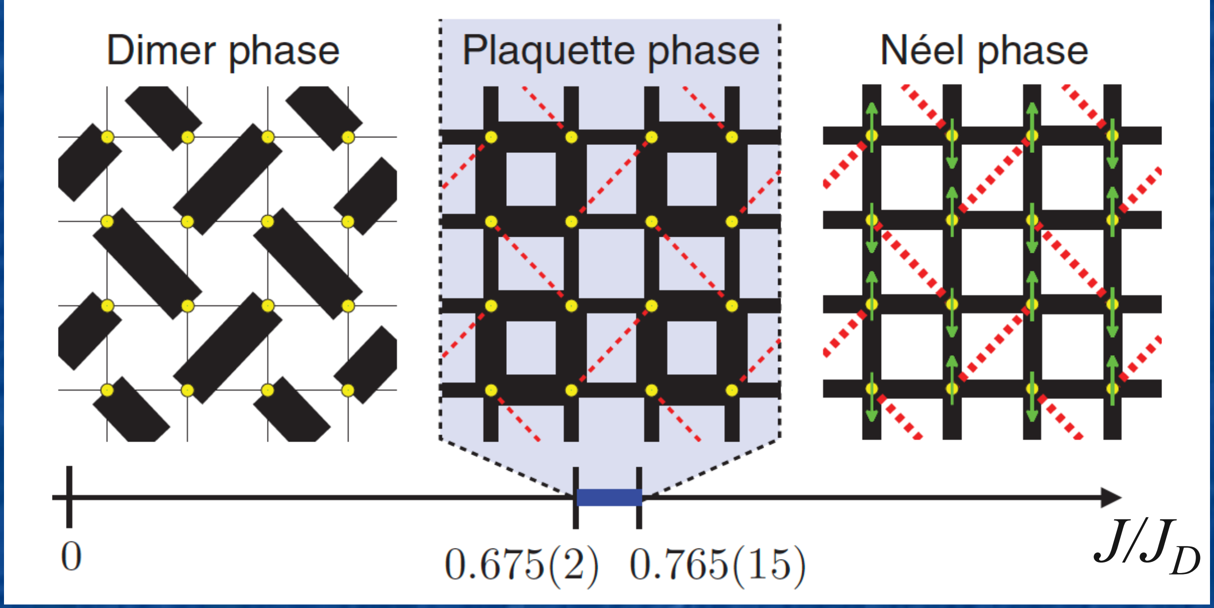
Shastry-Sutherland model

PHYSICAL REVIEW B **87**, 115144 (2013)

Tensor network study of the Shastry-Sutherland model in zero magnetic field

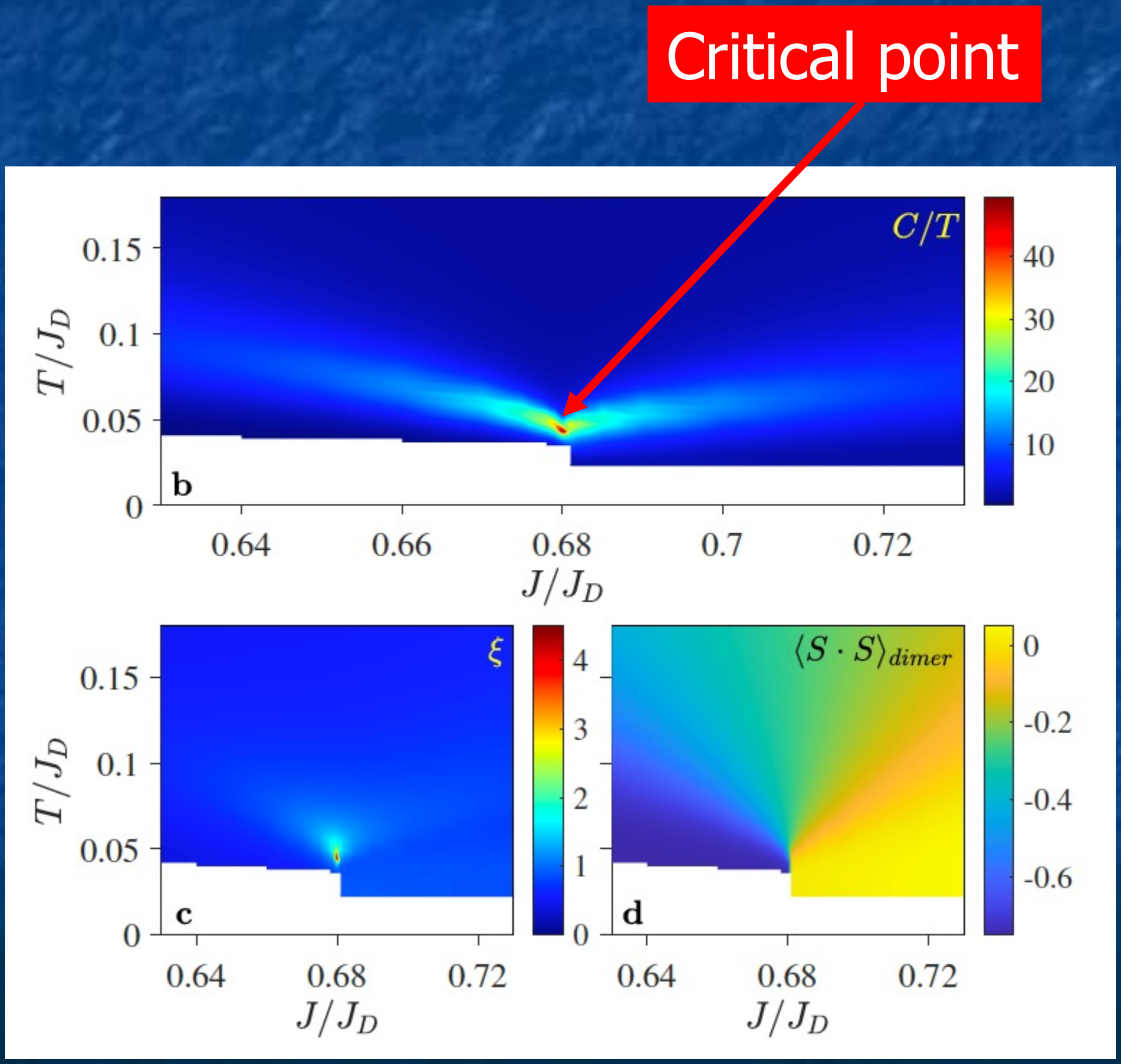
Philippe Corboz[1] and Frédéric Mila[2]
[1]*Theoretische Physik, ETH Zürich, CH-8093 Zürich, Switzerland*
[2]*Institut de théorie des phénomènes physiques, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland*

(Received 13 December 2012; revised manuscript received 27 February 2013; published 27 March 2013)



iPEPS with various setups and bond dimension up to 10

iPEPS for Shastry-Sutherland



$SrCu_2(BO_3)_2$ under pressure

- Pressure: expected to change J/J_D and found to increase it
- NMR (Waki et al 2007): intermediate phase around 24 kbar, but 2 Cu sites

  → NOT the expected plaquette phase!
- Intermediate phase confirmed by neutron scattering (Zayed et a, 2017), ESR (Sakurai et al, 2018), and specific heat (Guo et al, 2020)

Journal of the Physical Society of Japan
Vol. 76, No. 7, July, 2007, 073710

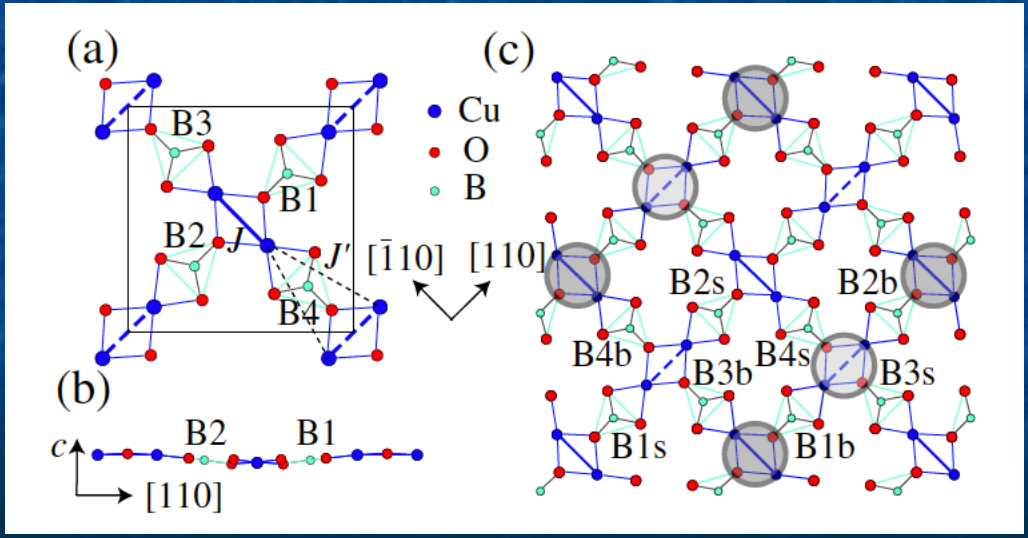
LETTERS

A Novel Ordered Phase in $SrCu_2(BO_3)_2$ under High Pressure

Takeshi WAKI[1*], Koichi ARAI[1†], Masashi TAKIGAWA[1‡], Yuta SAIGA[1,2], Yoshiya UWATOKO[1], Hiroshi KAGEYAMA[3], and Yutaka UEDA[1]

[1]*Institute for Solid State Physics, The University of Tokyo, Kashiwa, Chiba 277-8581*
[2]*Graduate School of Science and Engineering, Saitama University, Saitama 338-8570*
[3]*Department of Chemistry, Graduate School of Science, Kyoto University, Kyoto 606-8502*

(Received May 2, 2007; accepted May 31, 2007; published July 10, 2007)



Intermediate phase under pressure, but two types of Cu sites

↓

NOT the empty plaquette phase

nature COMMUNICATIONS

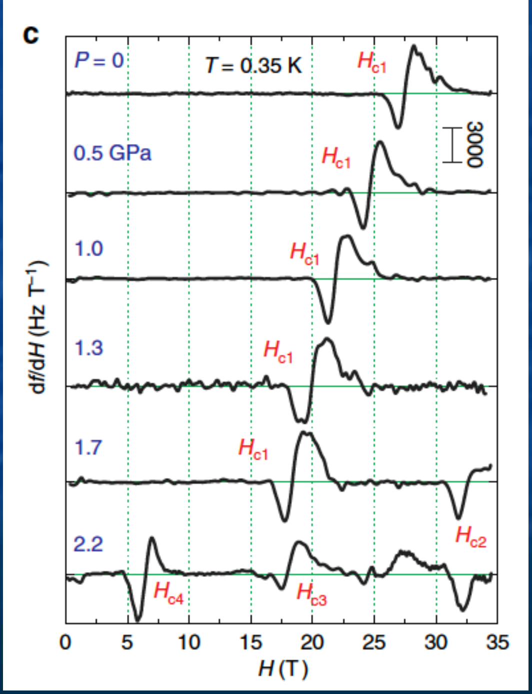
ARTICLE

Received 17 Jun 2015 | Accepted 16 May 2016 | Published 20 Jun 2016 DOI: 10.1038/ncomms11956 OPEN

Crystallization of spin superlattices with pressure and field in the layered magnet $SrCu_2(BO_3)_2$

S. Haravifard[1,2,3], D. Graf[4], A.E. Feiguin[5], C.D. Batista[6,7,8], J.C. Lang[3], D.M. Silevitch[2,9], G. Srajer[3], B.D. Gaulin[10], H.A. Dabkowska[10] & T.F. Rosenbaum[2,9]

Second derivative of magnetization



Magnetic field response under pressure

↓

Confirmation of a phase transition around 2GPa

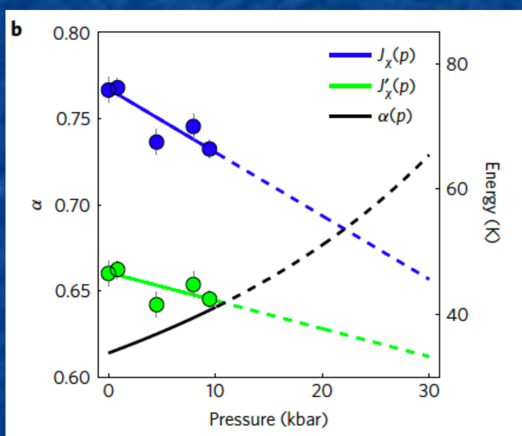
LETTERS
PUBLISHED ONLINE: 17 JULY 2017 | DOI: 10.1038/NPHYS4190
nature physics

4-spin plaquette singlet state in the Shastry–Sutherland compound $SrCu_2(BO_3)_2$

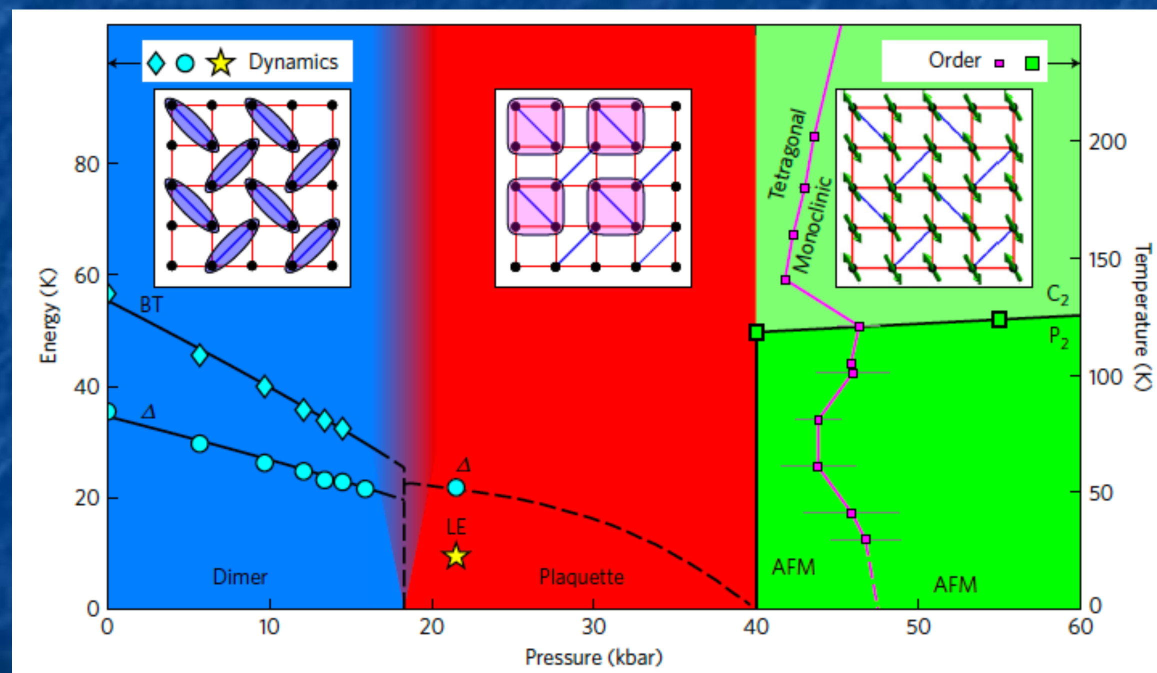
M. E. Zayed[1,2,3]*, Ch. Rüegg[2,4,5], J. Larrea J.[1,6], A. M. Läuchli[7], C. Panagopoulos[8,9], S. S. Saxena[8], M. Ellerby[5], D. F. McMorrow[5], Th. Strässle[2], S. Klotz[10], G. Hamel[10], R. A. Sadykov[11,12], V. Pomjakushin[2], M. Boehm[13], M. Jiménez-Ruiz[13], A. Schneidewind[14], E. Pomjakushina[15], M. Stingaciu[15], K. Conder[15] and H. M. Rønnow[1]

Neutron scattering

Susceptibility



J/J_D increases



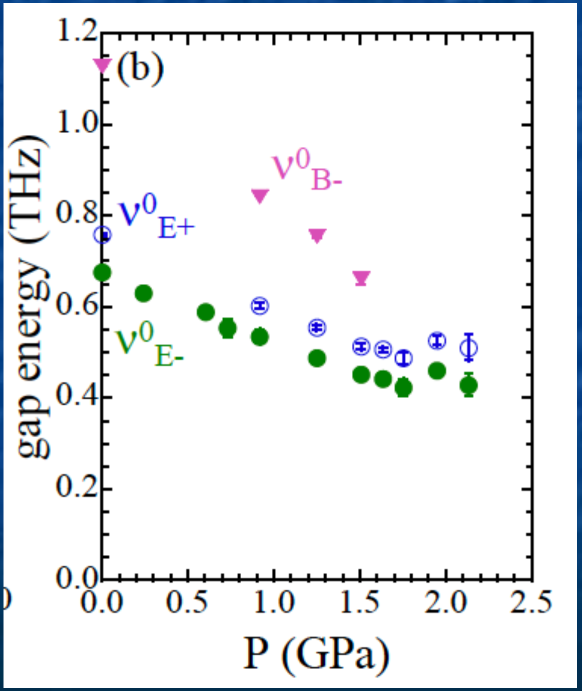
Full plaquette intermediate phase

Journal of the Physical Society of Japan 87, 033701 (2018) Letters
https://doi.org/10.7566/JPSJ.87.033701

Direct Observation of the Quantum Phase Transition of $SrCu_2(BO_3)_2$ by High-Pressure and Terahertz Electron Spin Resonance

Takahiro Sakurai[1*], Yuki Hirao[2], Keigo Hijii[3], Susumu Okubo[3], Hitoshi Ohta[3],
Yoshiya Uwatoko[4], Kazutaka Kudo[5], and Yoji Koike[6]

ESR



The gap levels off around 1.8 GPa

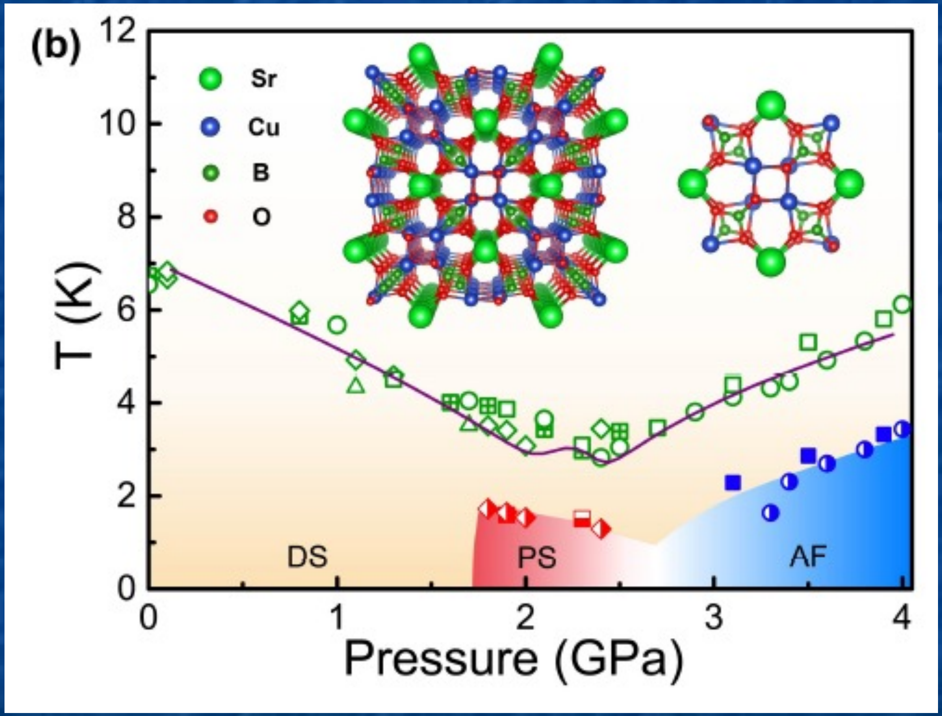
↓

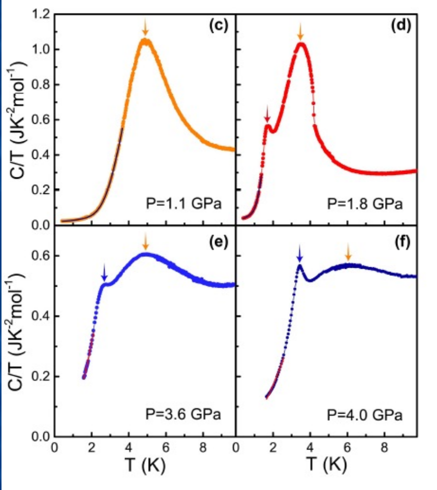
Confirmation of a phase transition around 1.8 GPa

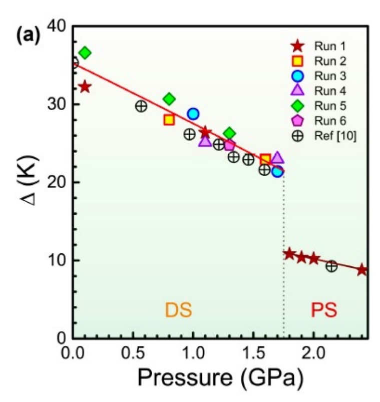
PHYSICAL REVIEW LETTERS **124**, 206602 (2020)

Quantum Phases of $SrCu_2(BO_3)_2$ from High-Pressure Thermodynamics

Jing Guo,[1] Guangyu Sun,[1,2] Bowen Zhao,[3] Ling Wang,[4,5] Wenshan Hong,[1,2] Vladimir A. Sidorov,[6] Nvsen Ma,[1] Qi Wu,[1] Shiliang Li,[1,2,7] Zi Yang Meng,[1,8,7,*] Anders W. Sandvik,[3,1,†] and Liling Sun[1,2,7,‡]







Intermediate phase with critical temperature around 2K

Article

A quantum magnetic analogue to the critical point of water

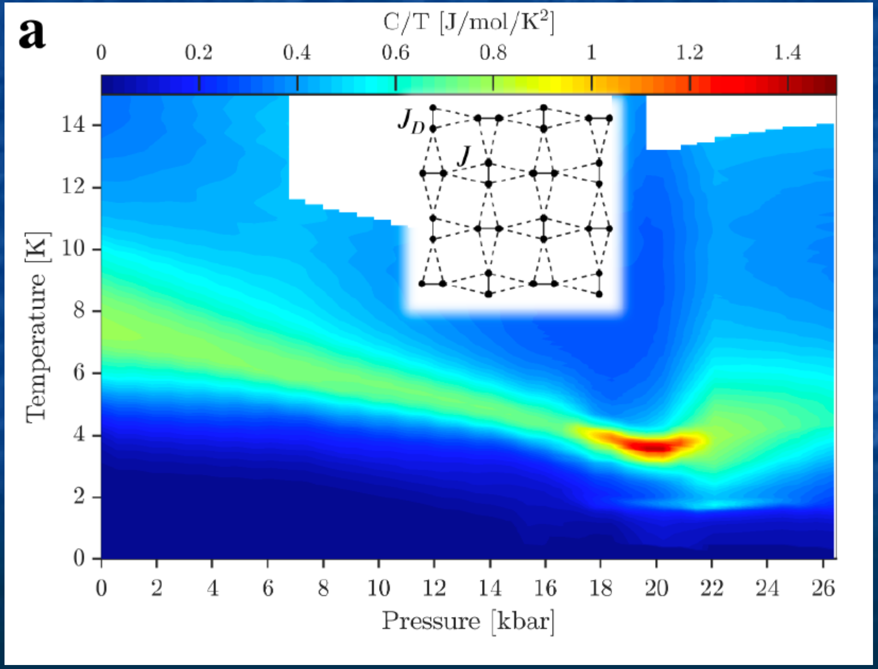
Nature | Vol 592 | 15 April 2021

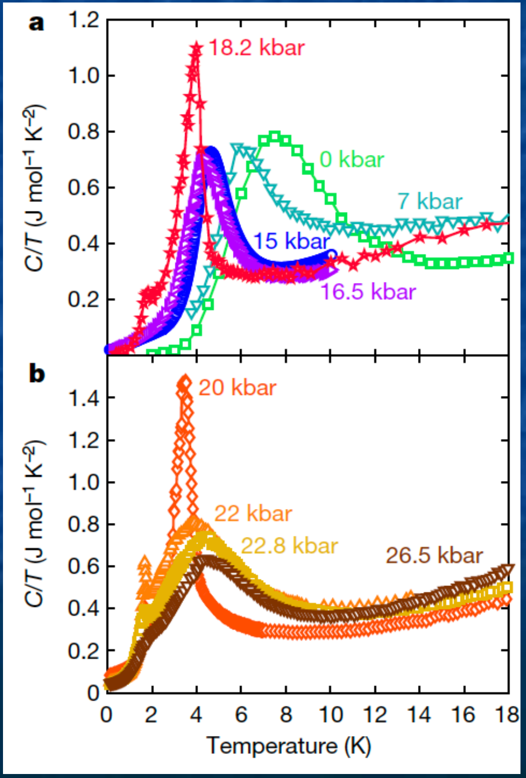
https://doi.org/10.1038/s41586-021-03411-8

Received: 30 September 2020

Accepted: 26 February 2021

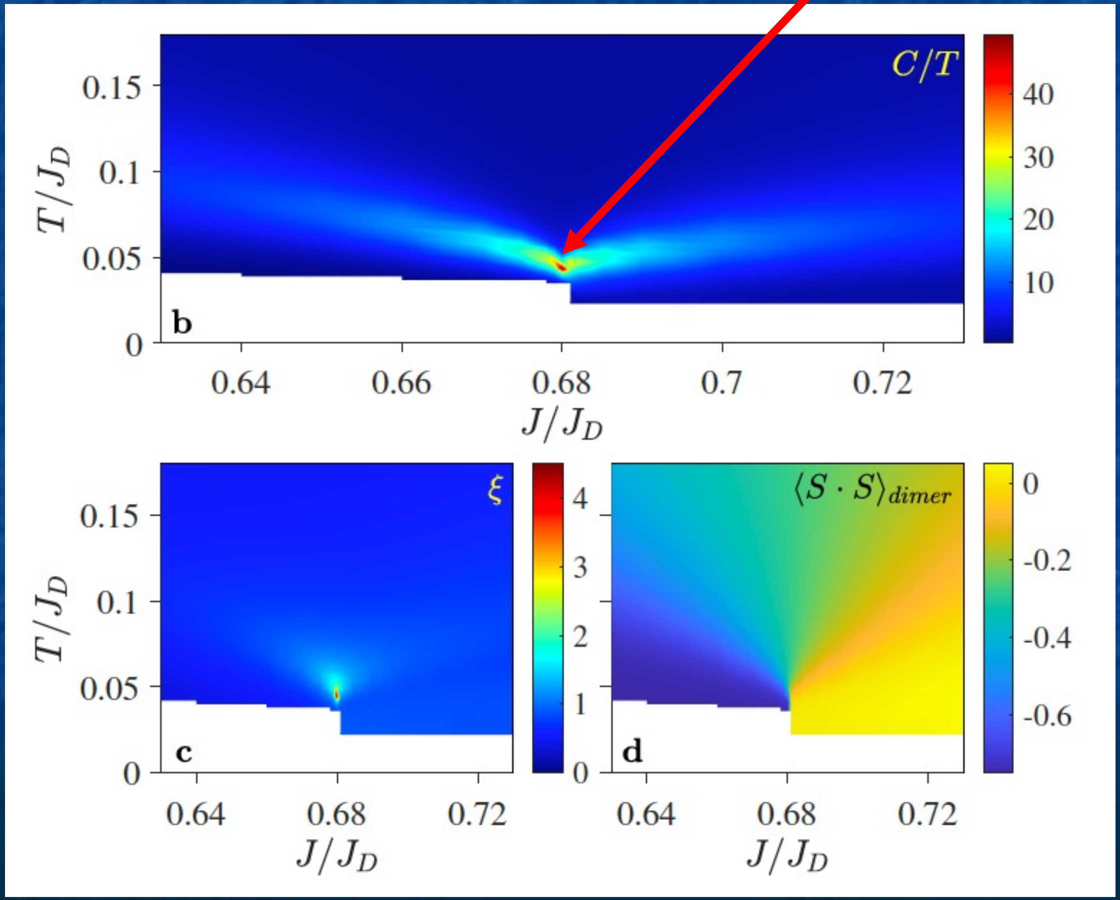
J. Larrea Jiménez[1,2], S. P. G. Crone[3,4], E. Fogh[2], M. E. Zayed[5], R. Lortz[6], E. Pomjakushina[7], K. Conder[7], A. M. Läuchli[8], L. Weber[9], S. Wessel[9], A. Honecker[10], B. Normand[2,11], Ch. Rüegg[2,11,12,13], P. Corboz[3,4], H. M. Rønnow[2]✉ & F. Mila[2]





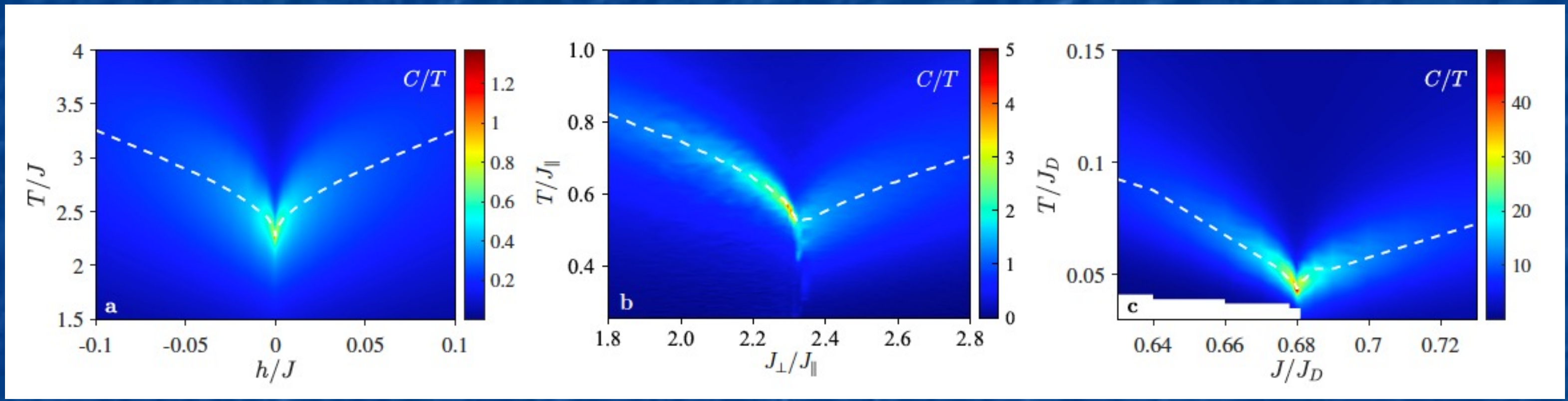
iPEPS for Shastry-Sutherland

Critical point around P=19 kbar and T=3.3K

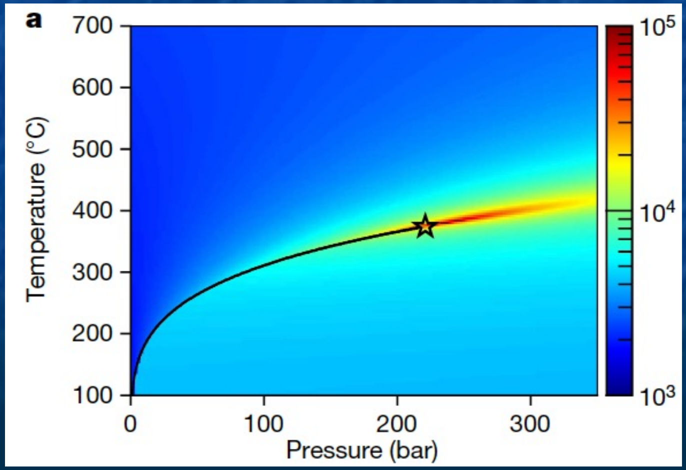


Critical point in various models…

Ising in a field FFB Shastry-Sutherland



… and in water

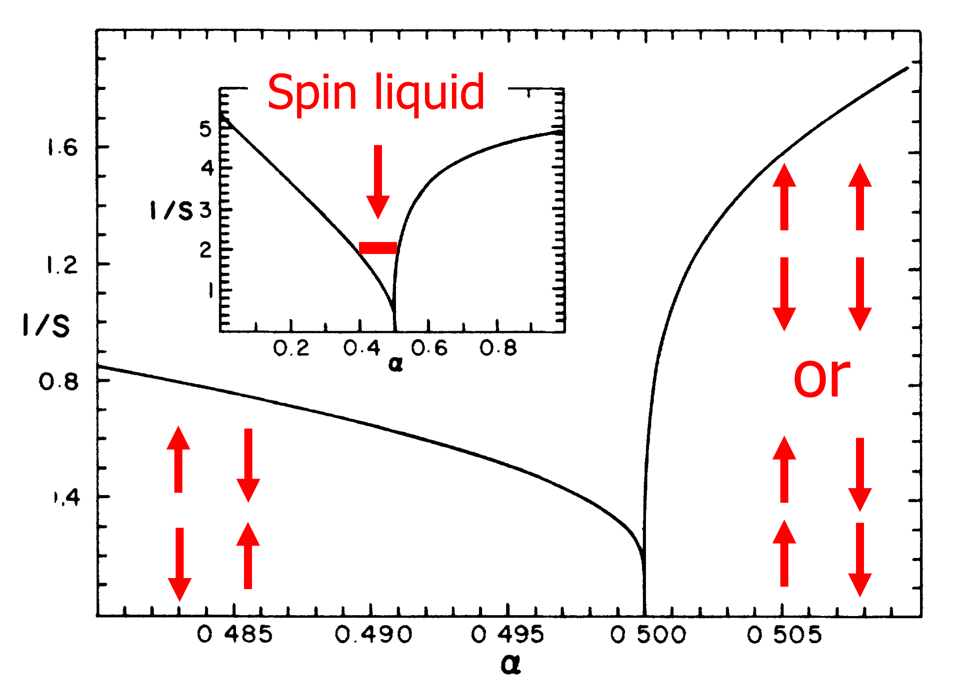


T_c=374° C
P_c=218 bar

1822: Cagniard de la Tour

J_1-J_2 model on square lattice

$$\mathcal{H} = J_1 \sum_{NN} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{NNN} \mathbf{S}_i \cdot \mathbf{S}_j$$



Chandra and Douçot, PRB 1988

$\alpha = J_2/J_1$

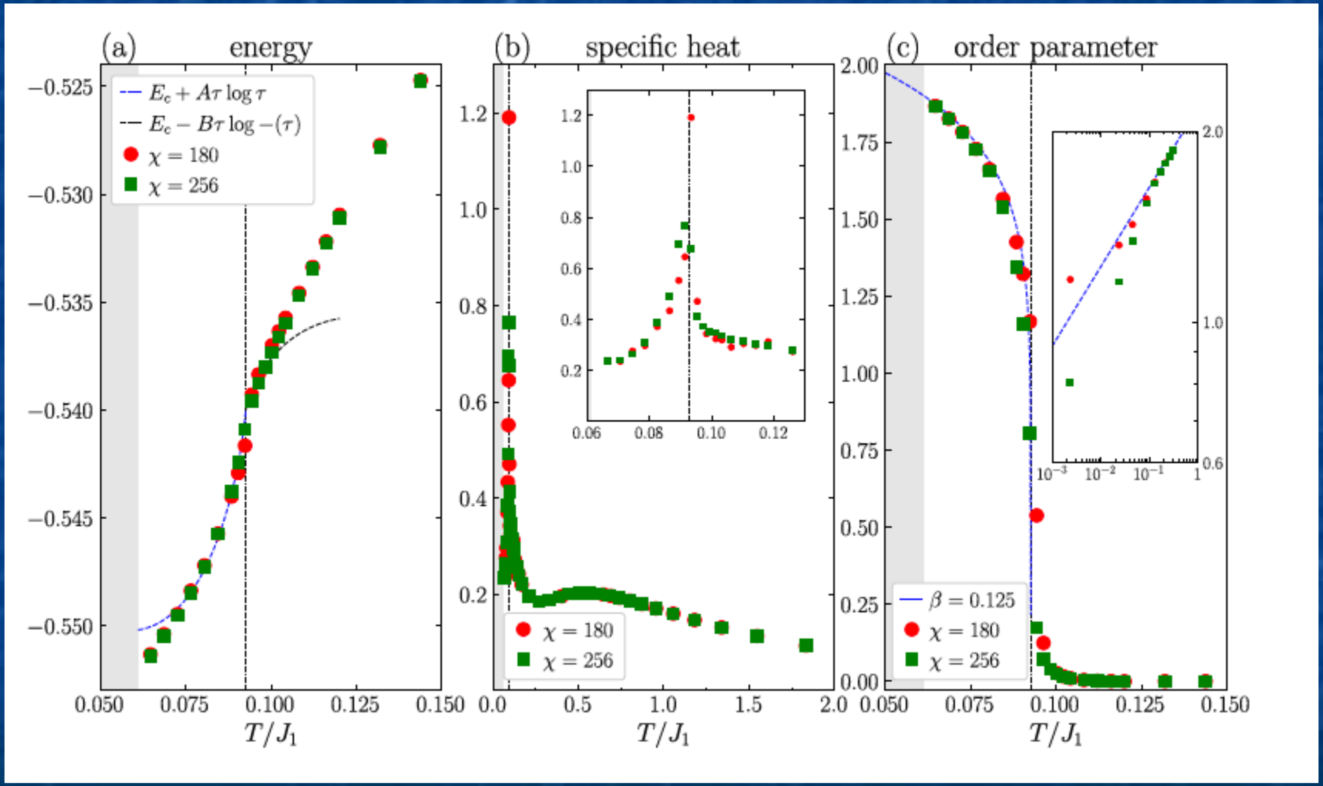
iPEPS for J_1-J_2 model

- Two helical states in collinear phase at large J_2
  → Ising transition at finite temperature
  Chandra, Coleman and Larkin, PRL 1990
- Numerical confirmation?
  → QMC: very severe minus sign problem
  → iPEPS: Yes if SU(2) symmetry strictly enforced during imaginary time evolution

PHYSICAL REVIEW LETTERS **128**, 227202 (2022)

Thermal Ising Transition in the Spin-1/2 J_1-J_2 Heisenberg Model

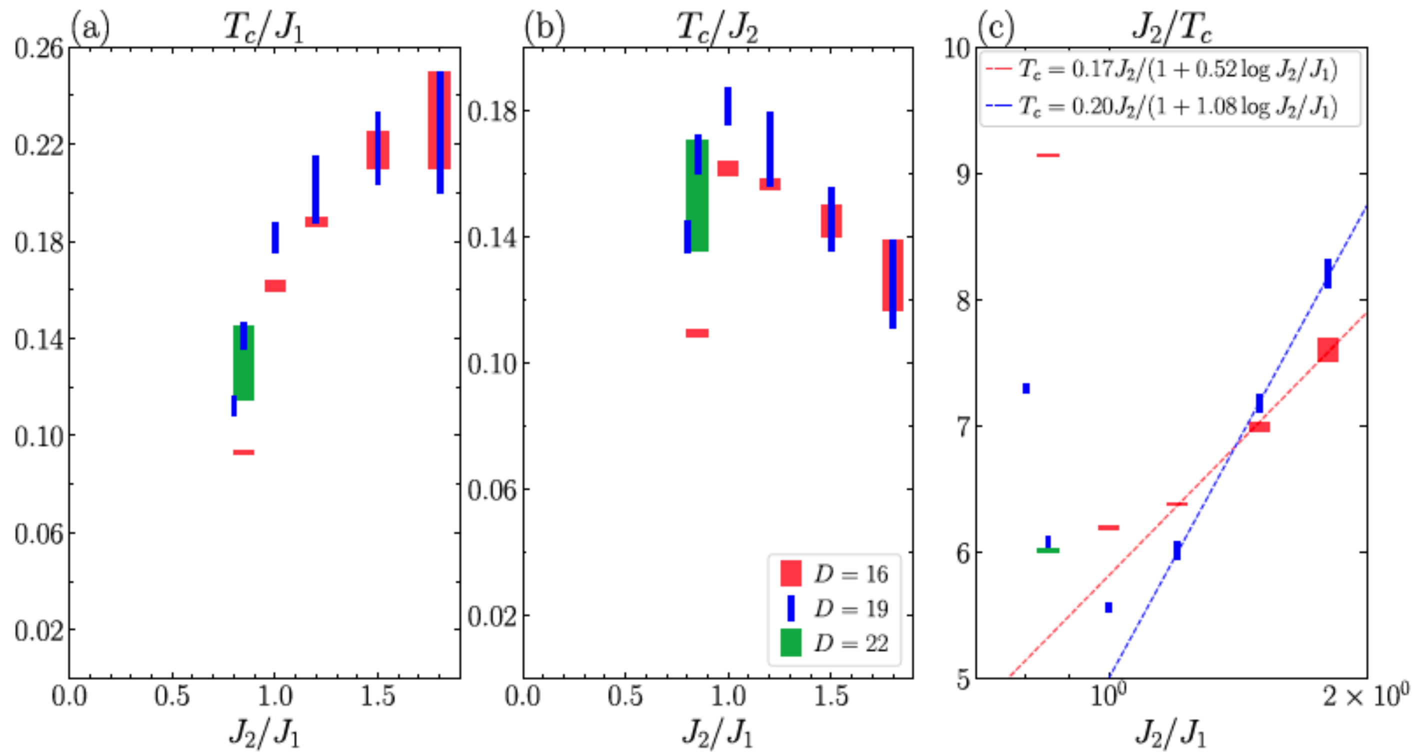
Olivier Gauthé* and Frédéric Mila



J_2/J_1=0.85

Ising transition for J_2/J_1 large enough from finite T iPEPS

Phase diagram of J_1-J_2 model



Conclusions

- Thermal properties of frustrated quantum magnets are no longer inaccessible

  → QMC: sometimes possible, e.g. in dimer basis

  → iPEPS: thermal Ising transition and critical point in J_1-J_2 and Shastry-Sutherland models
- Extensions:

  → QMC: generalize to other situations

  → iPEPS: combine with real-time evolution to access T dependence of spectral function