Thermal properties of frustrated quantum magnets

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Theorists



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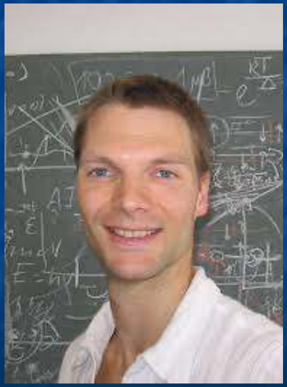
Olivier Gauthé (Lausanne)


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
- J_1-J_2 model:

  → Ising transition revealed by iPEPS
- Conclusions

AF Heisenberg model

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

- Odd loops with AF exchange integrals ($J_{ij}>0$)
  → Frustration (minimal definition)
  → Examples: triangular lattice, kagome,…
  → Minus sign for Quantum Monte Carlo

Quantum Monte Carlo

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

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

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

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

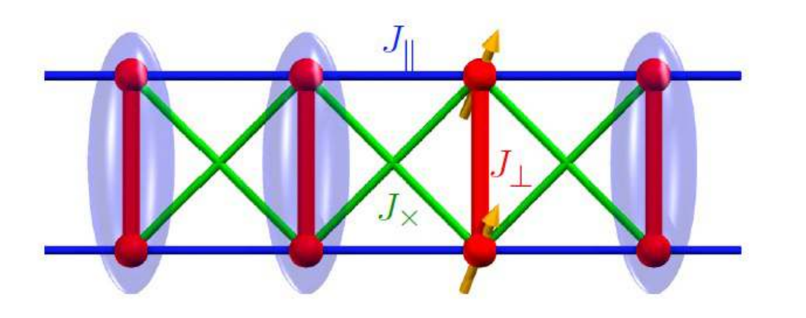
Hamiltonian in configuration basis

- For the AF Heisenberg model, 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



$$J_{\times} = J_{\parallel}$$

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

$$\vec{T}_i = \vec{S}_i^1 + \vec{S}_i^2$$

Hamiltonian in dimer basis

- In general, involves both the sum and the difference of spins on a dimer
- Full frustration: all exchange integrals between the spins of coupled dimers are equal

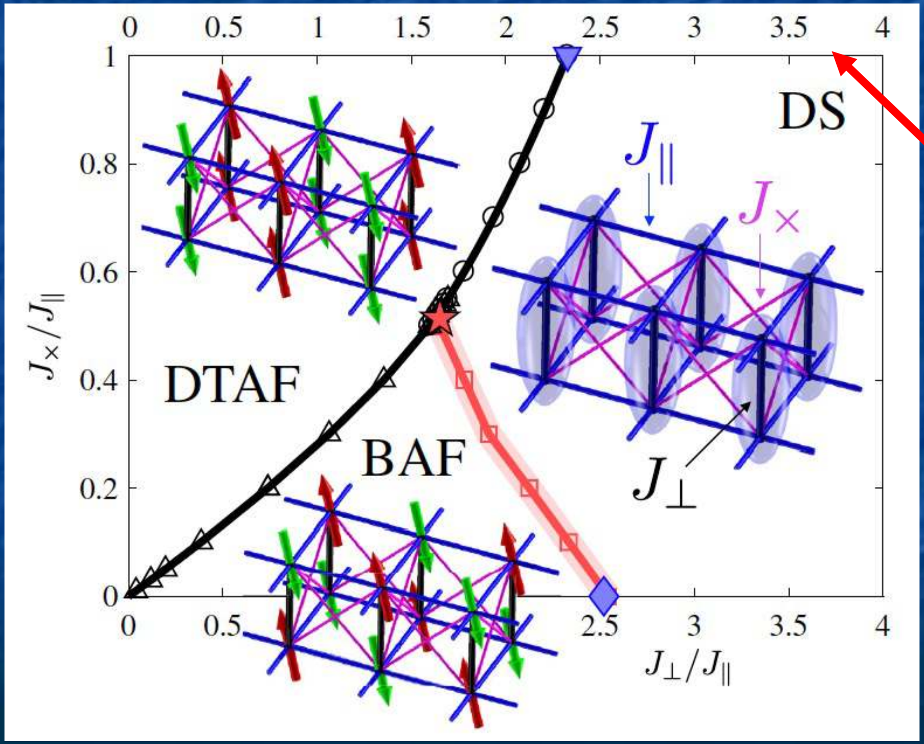
→ the Hamiltonian can be written in terms of the sum only

→ QMC possible if bipartite lattice of dimers

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

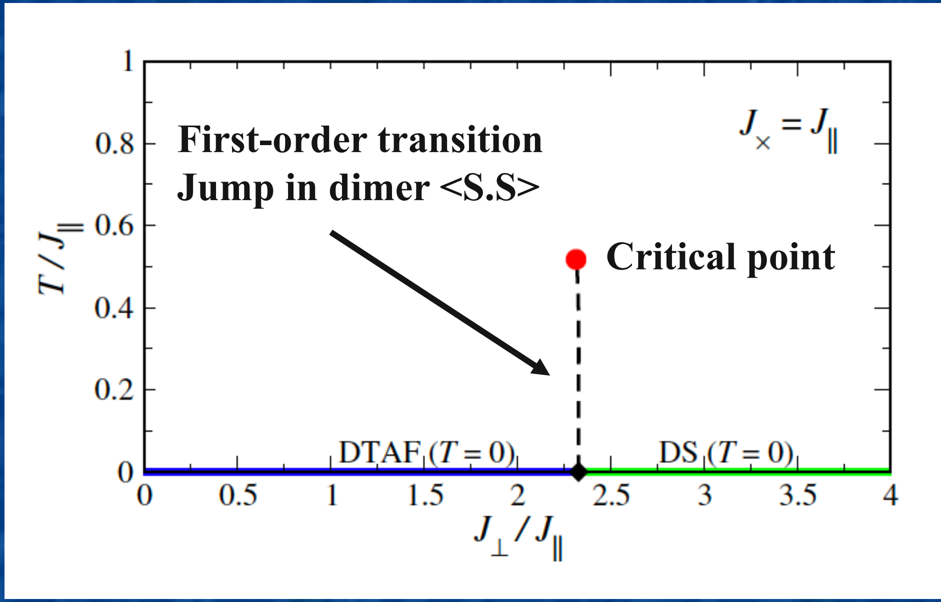
Thermal Critical Points and Quantum Critical End Point in the Frustrated Bilayer Heisenberg Antiferromagnet

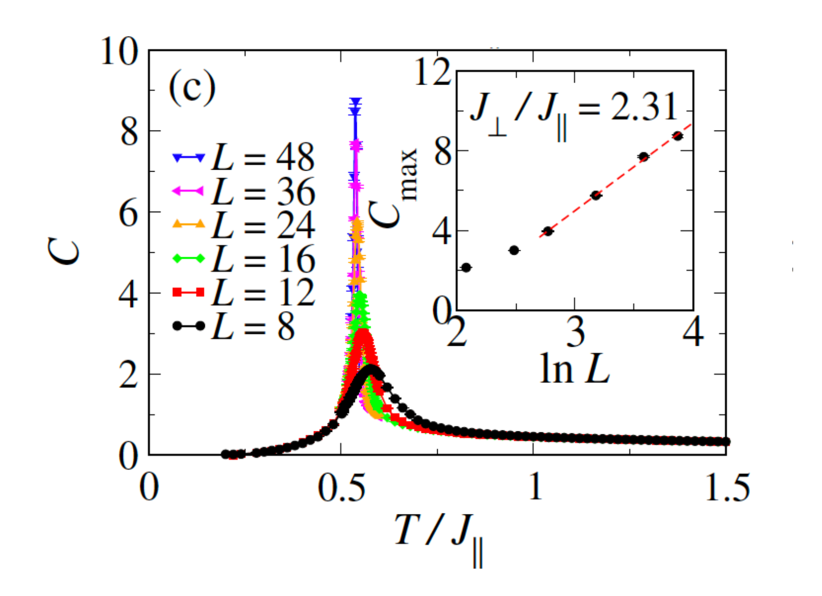
J. Stapmanns,[1] P. Corboz,[2] F. Mila,[3] A. Honecker,[4] B. Normand,[5] and S. Wessel[1]



Fully frustrated bilayer

Ising critical point



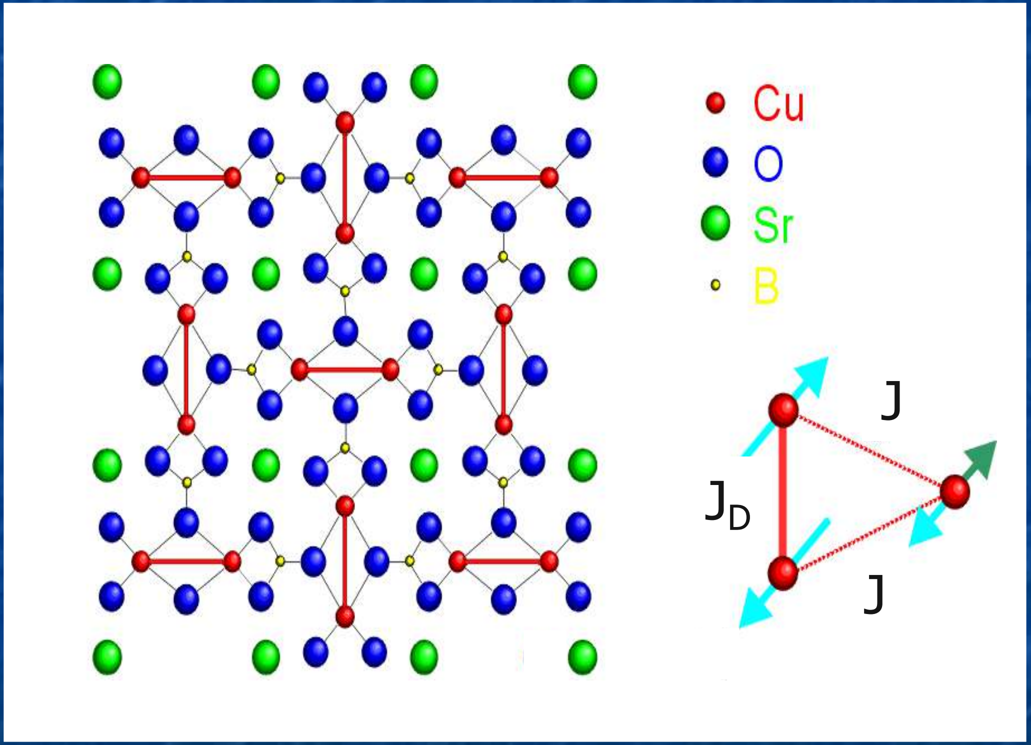


Ising 2D: $\alpha = 0$ C α ln L

- As for Mott transition (DMFT)
- Physical realization in quantum magnets?

$SrCu_2(BO_3)_2$

Smith and Keszler, JSSC 1991



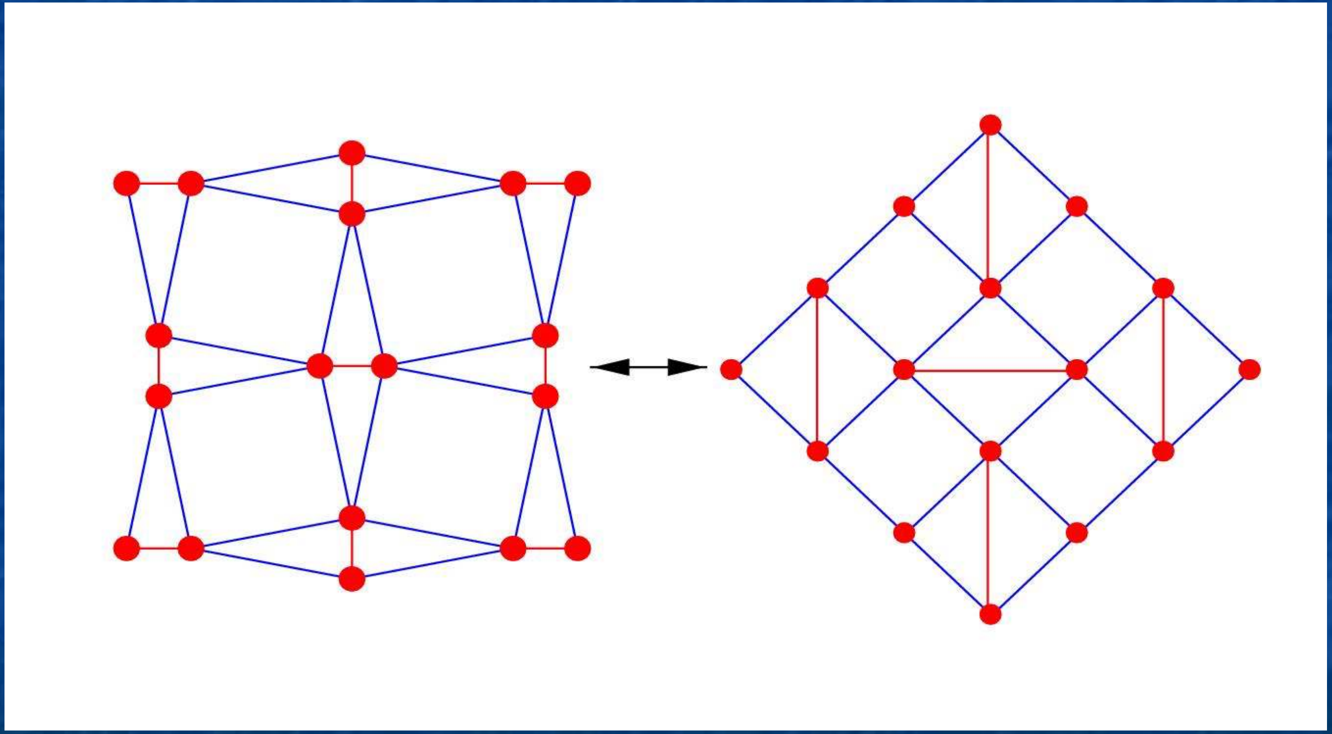
Cu^{2+} -> Spin 1/2

$J_D \approx 85$ K

$J/J_D \approx 0.63$

Famous for its magnetization plateaus

From orthogonal dimer to Shastry-Sutherland model



Shastry and Sutherland, 1981

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

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

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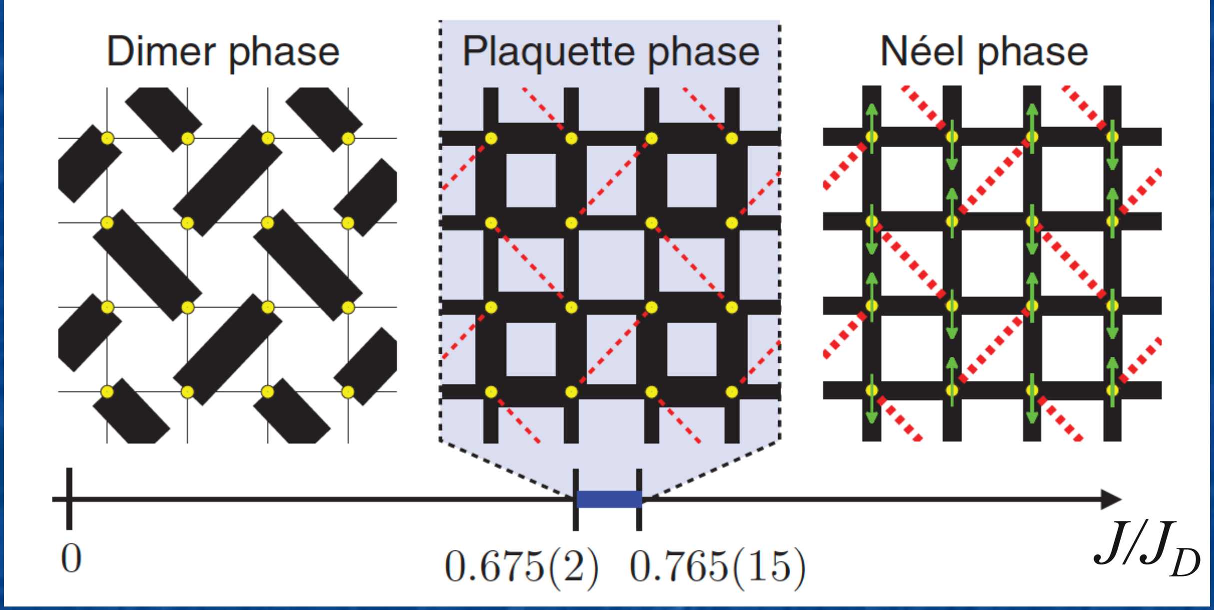


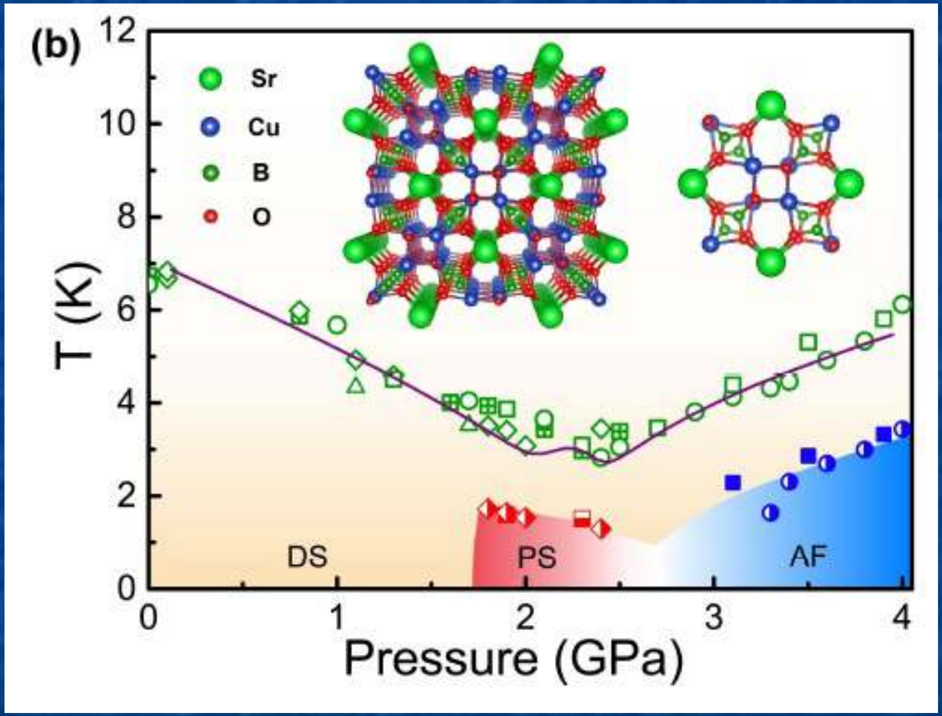
iPEPS with various setups and bond dimension up to 10

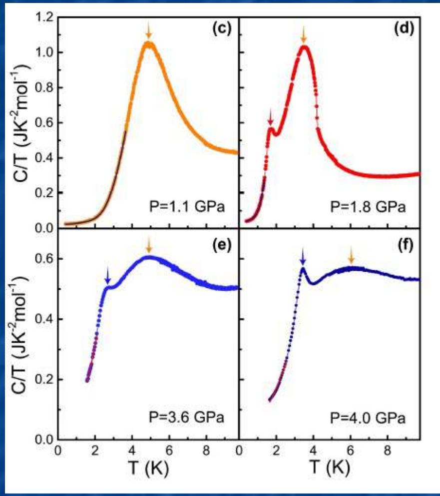
$SrCu_2(BO_3)_2$ under pressure

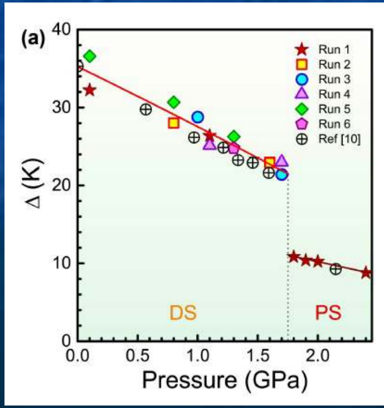
- Pressure: expected to change J/J_D and found to increase it
- NMR (Waki et al 2007): intermediate phase around 24 kbar
- Intermediate phase confirmed by neutron scattering (Zayed et al, 2017), ESR (Sakurai et al, 2018), and specific heat (Guo et al, 2020)

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

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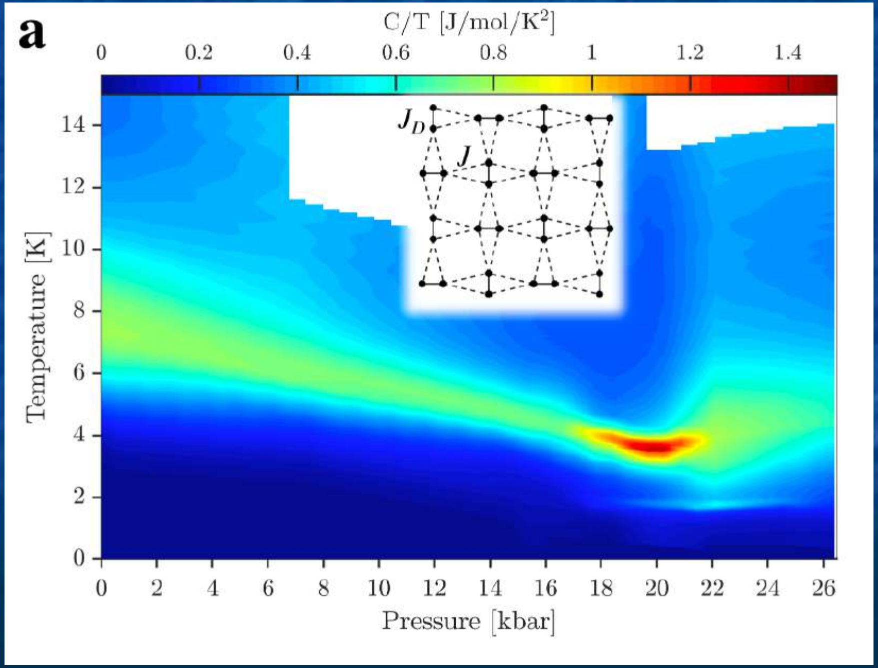
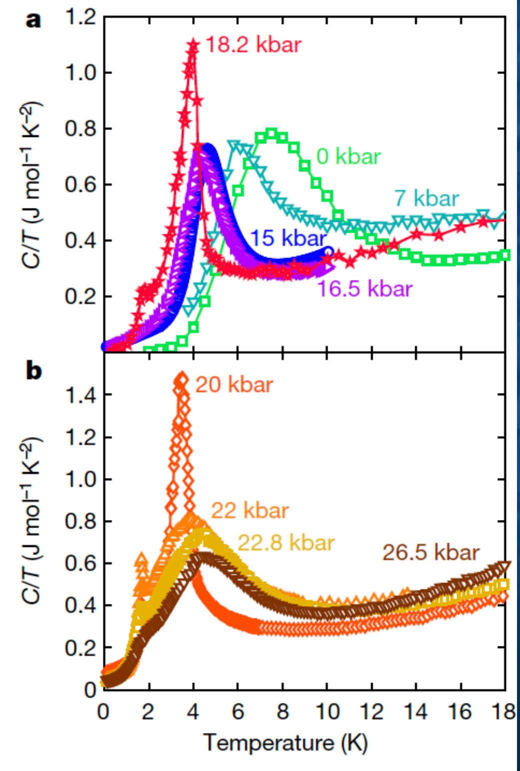
J. Larrea Jiménez[1,2], S. P. G. Crone[3,4], E. Fogh[2], M. E. Zayed[5], R. Lortz[6], E. Pomjakushina[7], K. Conder[7], A. M. Läuchli[8], L. Weber[9], S. Wessel[9], A. Honecker[10], B. Normand[2,11], Ch. Rüegg[2,11,12,13], P. Corboz[3,4], H. M. Rønnow[2]✉ & F. Mila[2]





Thermal properties of Shastry-Sutherland model

Hamiltonian : cannot be written in terms of sum of spins of dimers → minus sign problem

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

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

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

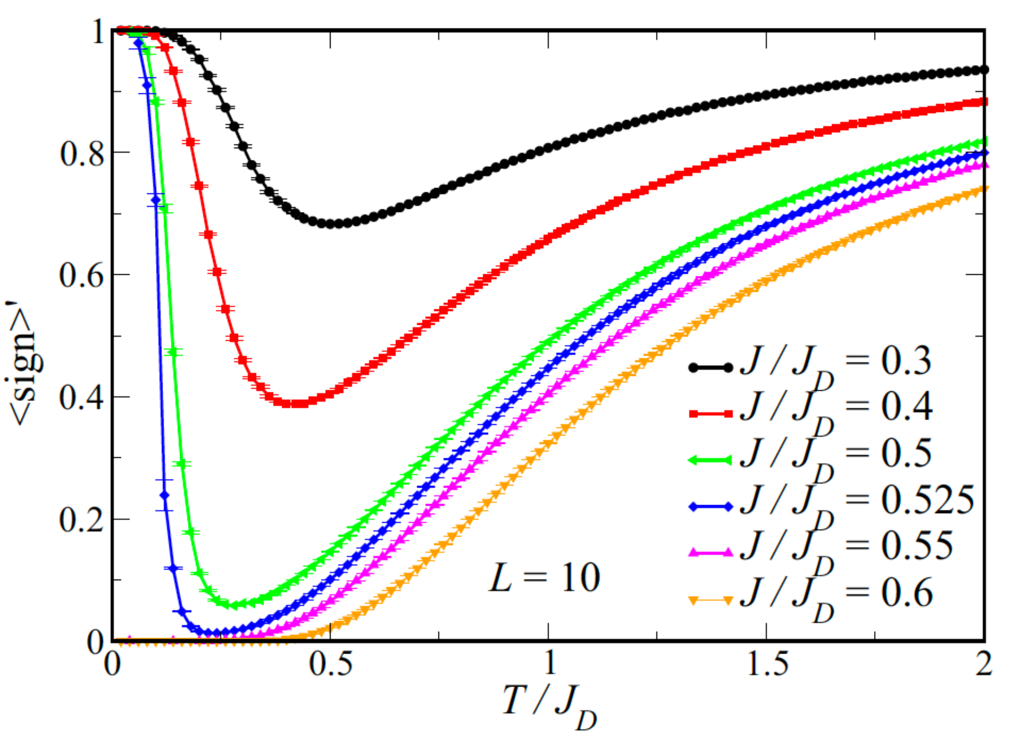
→ $\langle \mathrm{sign}\rangle' \to 1$ as $T \to 0$

→ 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]



And above $J/J_D = 0.526$?

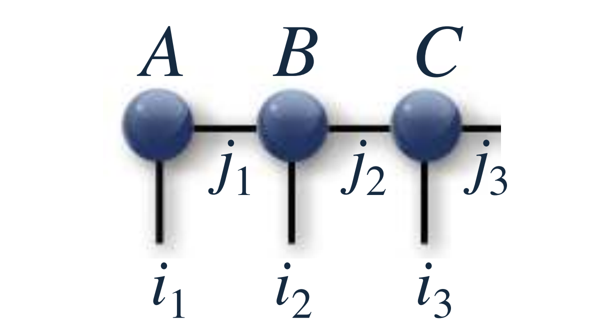
Tensor networks

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

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

Example: Matrix product state in 1D (DMRG)

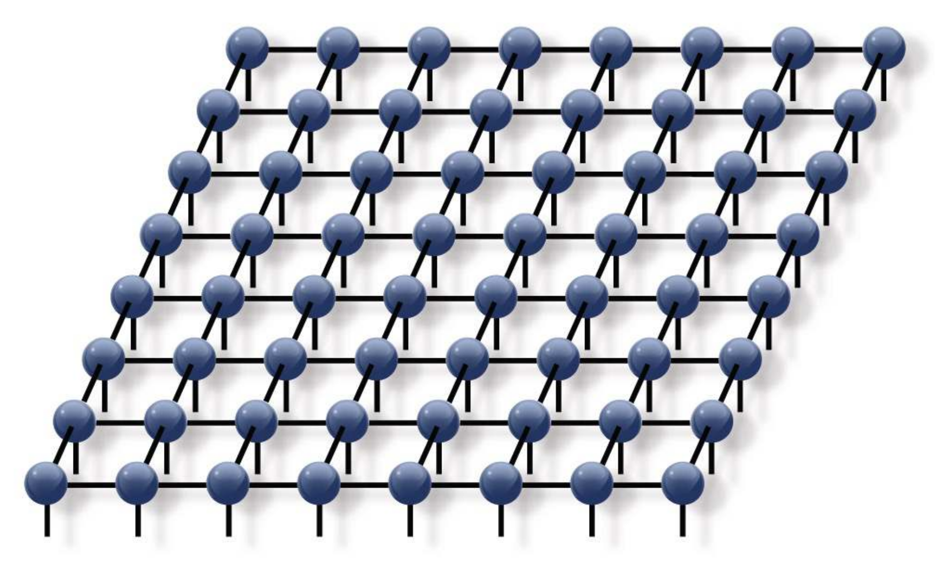
$$c_{i_1 i_2 i_3 \ldots} \simeq \sum_{j_1 j_2 \ldots} A_{i_1}^{j_1} B_{i_2}^{j_1 j_2} C_{i_3}^{j_2 j_3} \cdots$$



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
- 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)

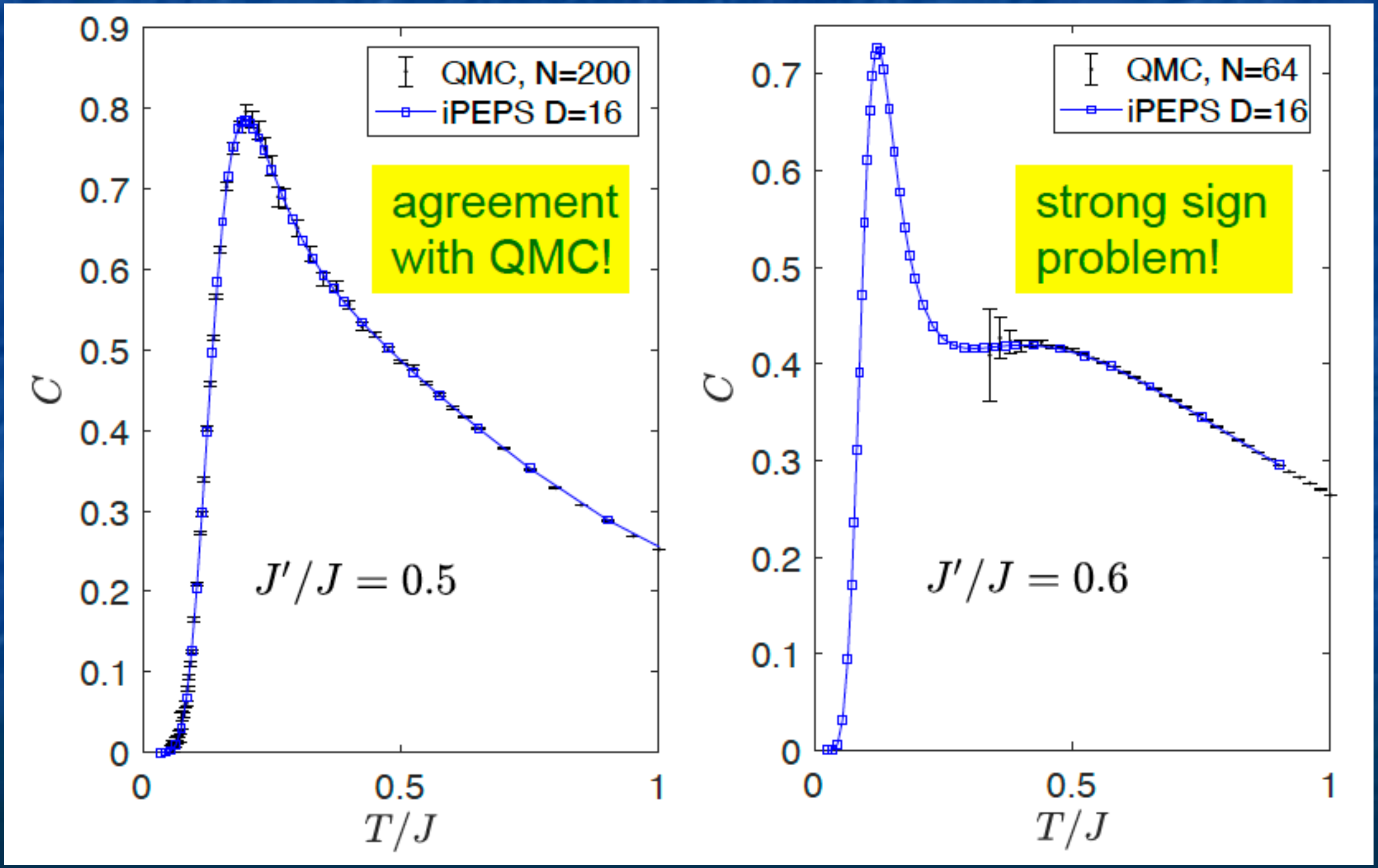
Tensor network study of the $m = \frac{1}{2}$ magnetization plateau in the Shastry-Sutherland model at finite temperature

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

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

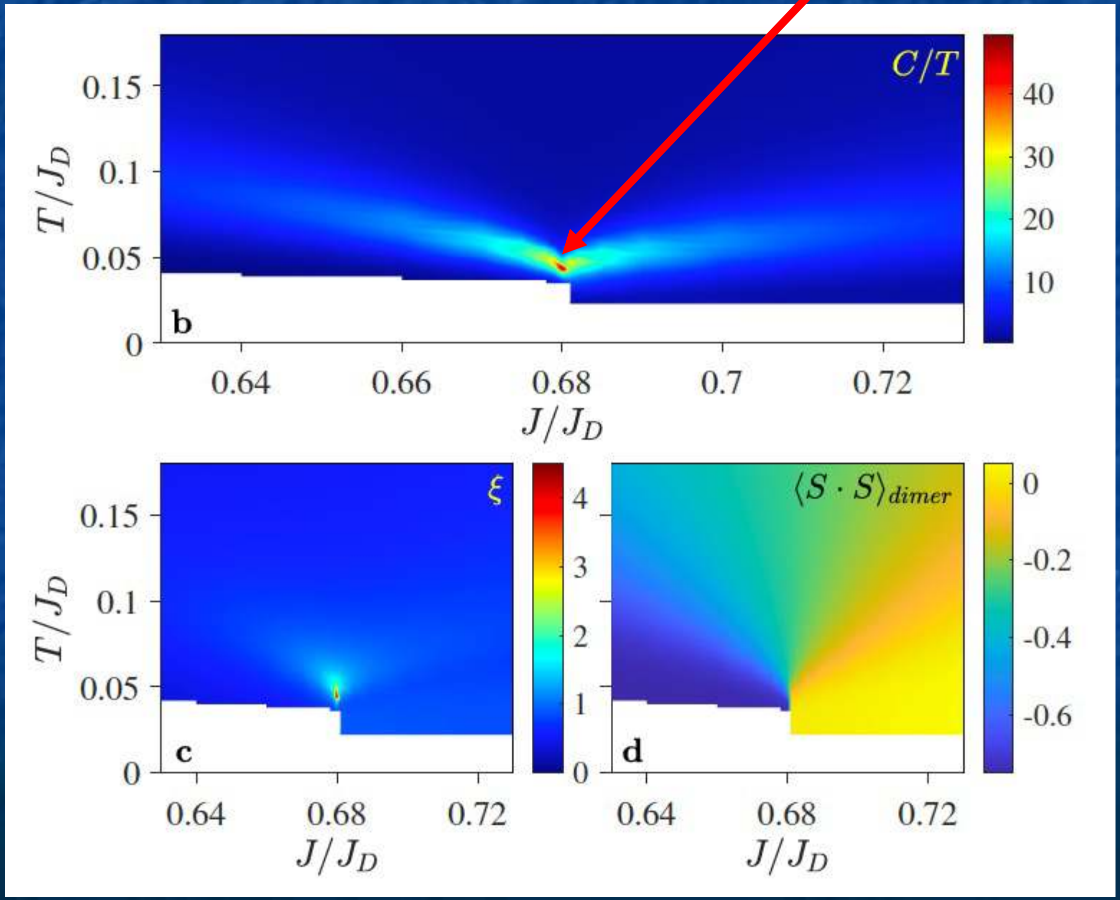
Thermodynamic properties of the Shastry-Sutherland model throughout the dimer-product phase

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



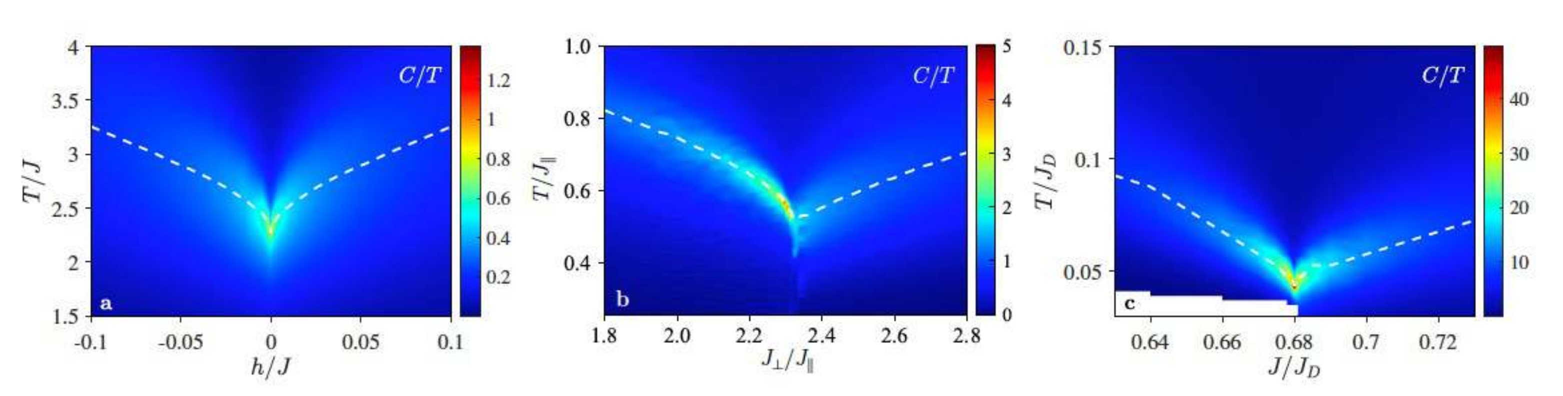
iPEPS for Shastry-Sutherland

Critical point

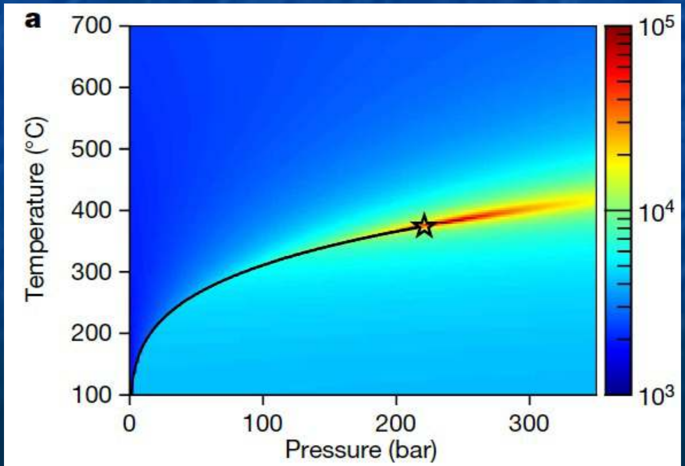


Critical point in various models…

Ising in a field FFB Shastry-Sutherland



… and in water

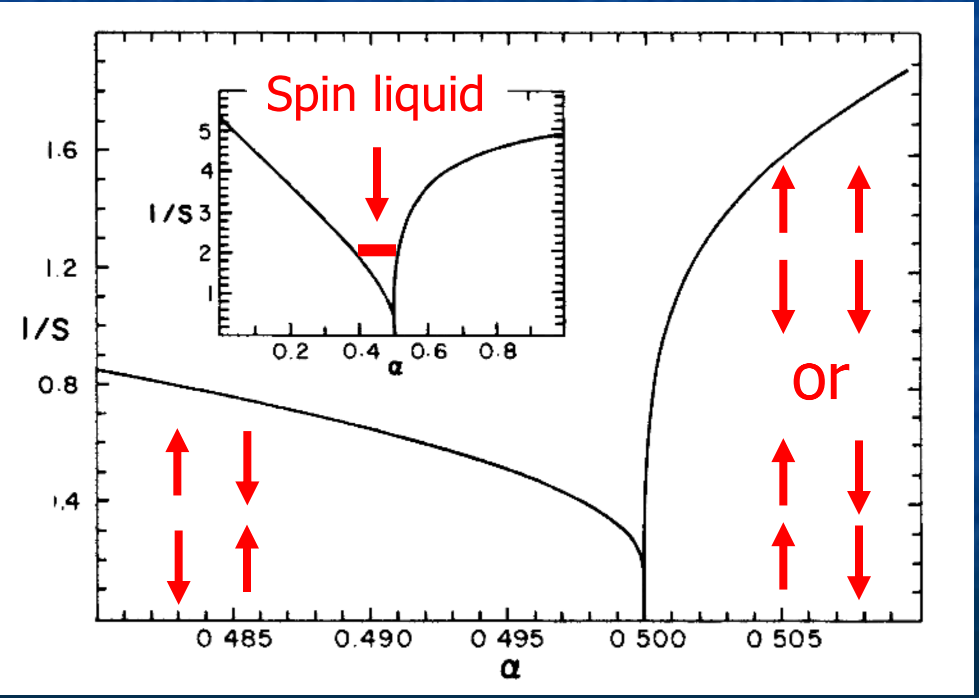


T_c=374° C
P_c=218 bar

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?

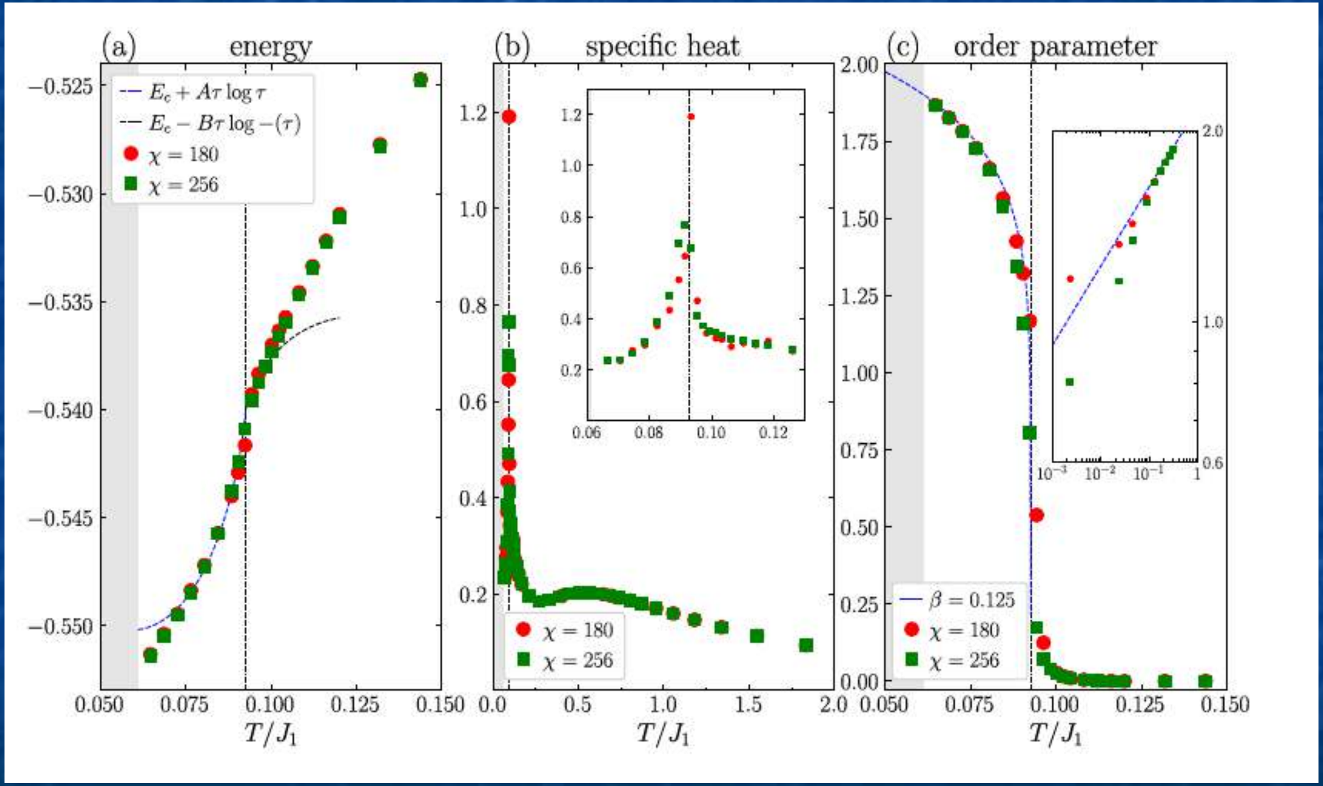
  → QMC: very severe minus sign problem

  → 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

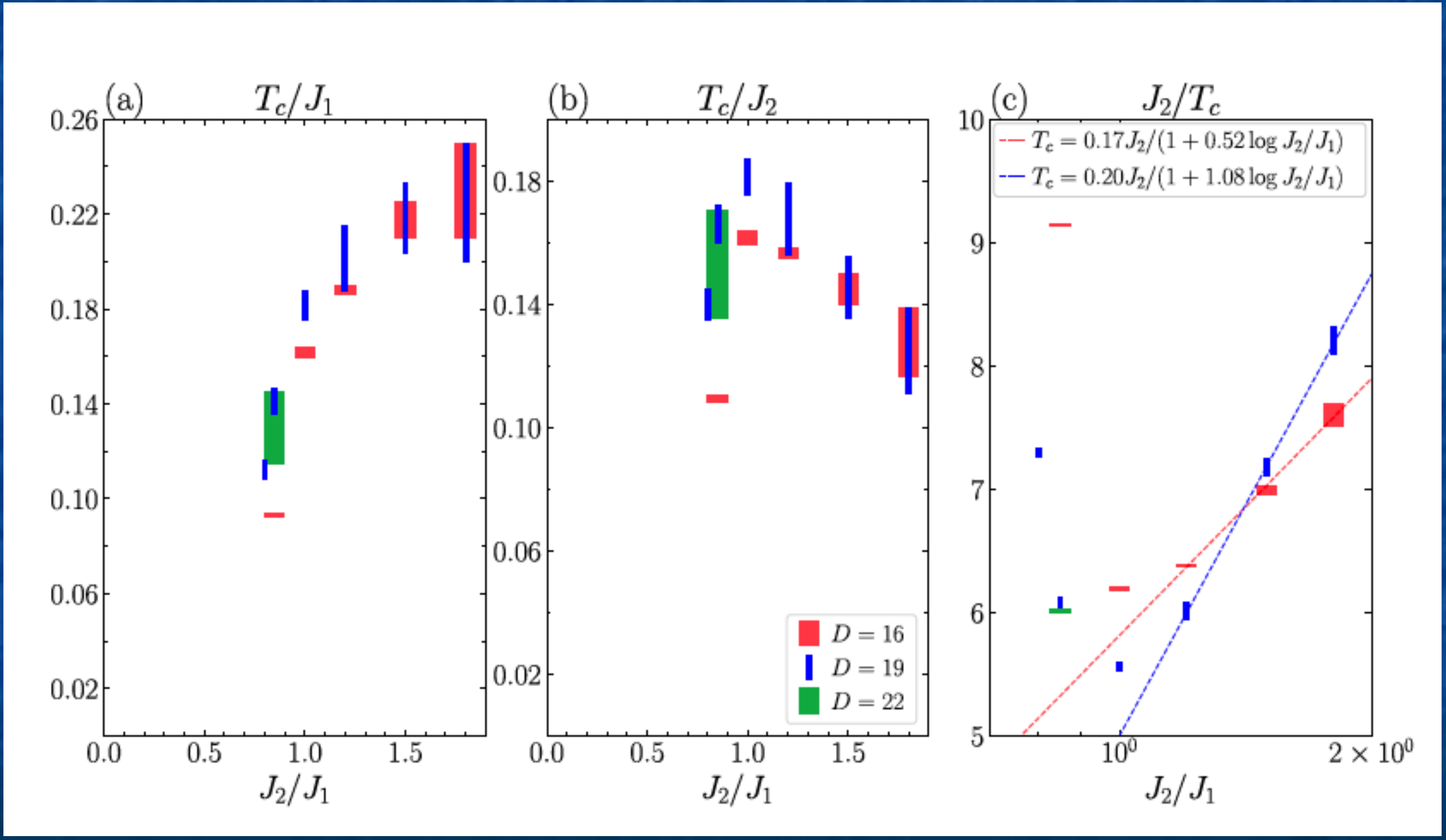
Olivier Gauthé* and Frédéric Mila



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

  → No minus sign in dimer basis for fully frustrated models on bipartite lattices

  → Can even work at low T if there is a minus sign under certain conditions
- iPEPS

  → Critical point in Shastry-Sutherland model

  → Thermal Ising transition in J_1-J_2 model

  → …