Investigating thermal critical points with tensor networks

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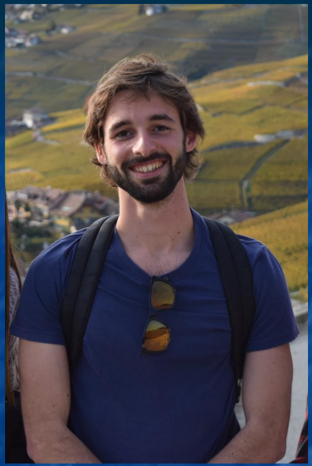

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Scope

- Tensor networks for classical thermal transitions

  → Need for an alternative to Monte Carlo?

  → CTMRG for 3-state Potts model

  → CTMRG for incommensurate melting
- Thermal properties of quantum systems

  → Quantum purification

  → Critical point of Shastry-Sutherland model and of $SrCu_2(BO_3)_2$ under pressure

  → Ising transition of J1-J2 model on square lattice
- Conclusions

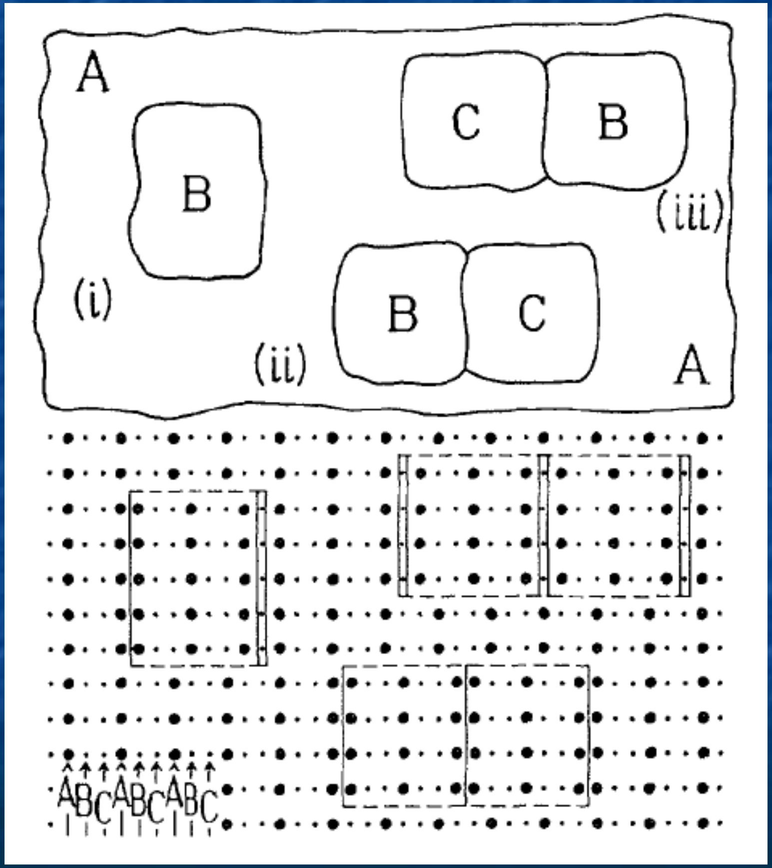
Thermal transitions in classical 2D systems

- Exact results (Onsager, Baxter,…)
- Renormalization group
- Conformal field theory

  → Minimal models, universality classes
- Monte Carlo simulations (Binder,…)

Is there a need for new approaches?

Commensurate-Incommensurate transition in adsorbed layers



3 types of domains
→ 3-state Potts?

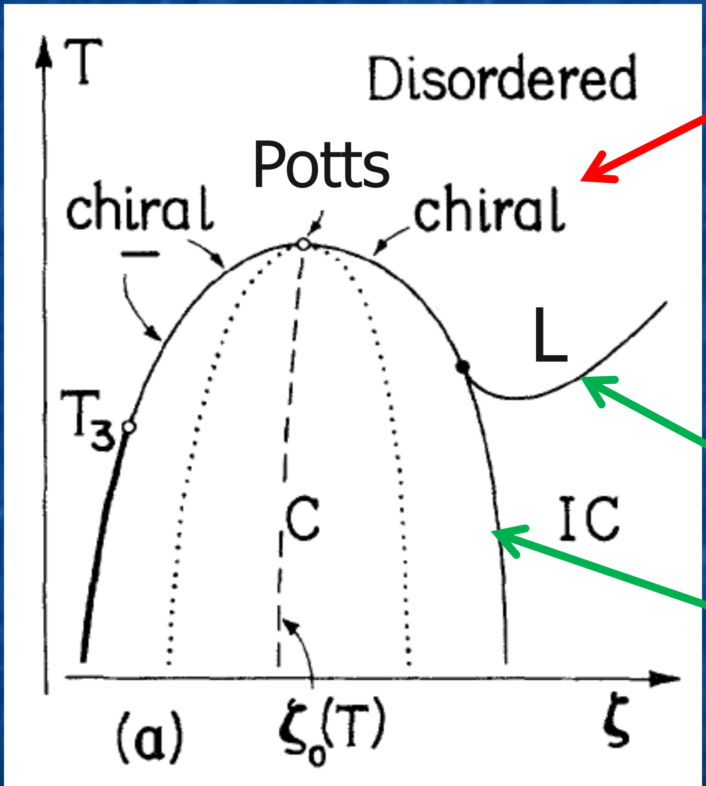
Not so simple!

A B C ≠ A C B

Chiral perturbation

Huse-Fisher, 1982

Huse-Fisher phase diagram



Chiral: Anisotropic scaling

→ $\nu_x \neq \nu_y$

→ dynamical exponent z >1

Kosterlitz-Thouless

Pokrovsky-Talapov

Huse and Fisher, 1982

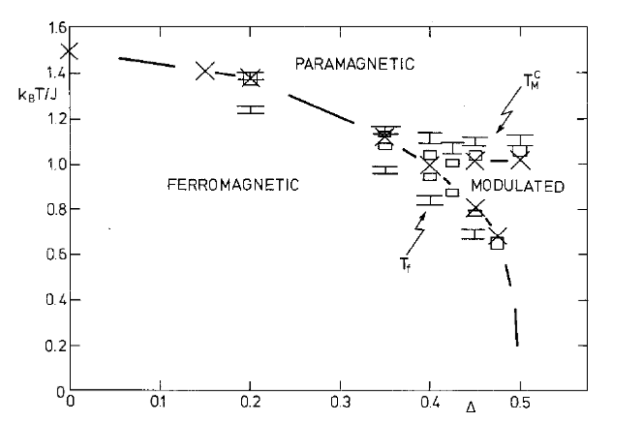
Difference between the 3 cases

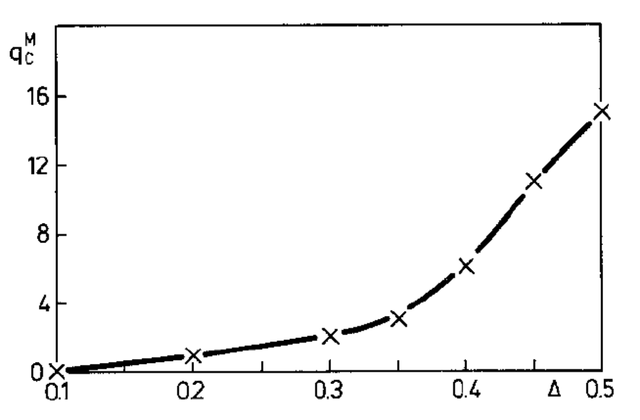
- Δq: distance to $2\pi/3$, vanishes with exponent $\overline{\beta}$
- ξ : correlation length in IC direction, diverges with exponent ν_x

- $\Delta q\, \xi$ → 0 for Potts ($\overline{\beta} > \nu_x$)
  → cst > 0 for chiral ($\overline{\beta} = \nu_x$)
  → + ∞ for KT transition
  (ξ diverges before Δq vanishes)

MC simulations of chiral Potts model

$$\mathscr{H} = -J_x \sum_{\langle ij \rangle}^{x} \cos\left[\frac{2\pi}{3}(n_i - n_j + \Delta)\right] - J_y \sum_{\langle ij \rangle}^{y} \cos\left[\frac{2\pi}{3}(n_i - n_j)\right]$$





Selke and Yeomans, 1982

→ Impossible to extract Δq with sufficient precision
→ Many other investigations in the following years
→ No consensus at the end of the eighties

Si (113) 3 x 1

D. L. Abernathy, S. Song, K. I. Blum, R. J. Birgeneau, and S. G. J. Mochrie, PRB 1994

- Single transition with anisotropic scaling

$\nu_x \simeq 0.65,\ \nu_y \simeq 1.06$

$\bar{\beta} \simeq 0.66$ (exponent of Δq)

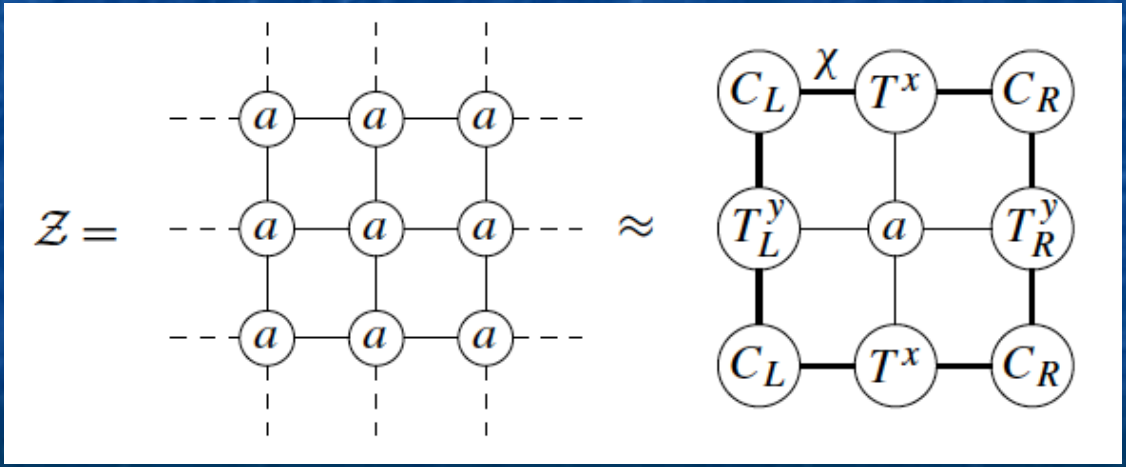
$z \simeq 1.6$

NB: $\bar{\beta} \simeq \nu_x \Longrightarrow \Delta q\ \xi \rightarrow$ Cst $\Longrightarrow$ Chiral transition

CTMRG for 2D classical systems

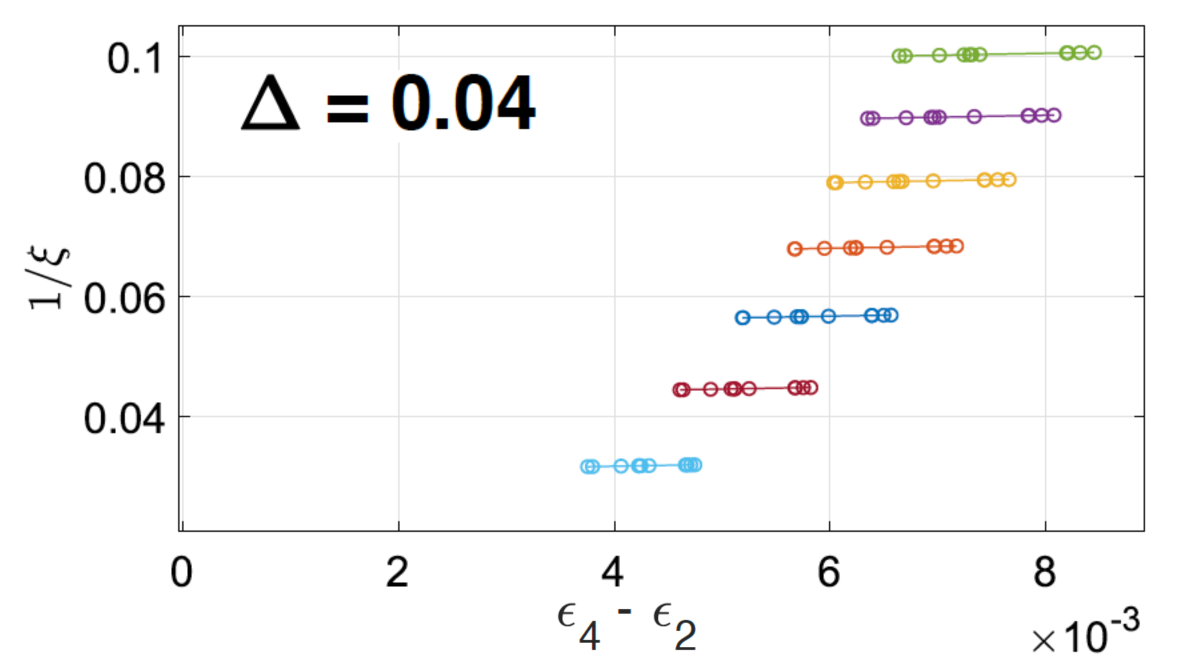
Corner Transfer Matrix Renormalization Group

Nishino, 1995; Nishino and Okunishi, 1996



Chiral 3-state Potts model

$$E = -\sum_{\vec{r}} \cos[2\pi/3(n_{\vec{r}+\vec{x}} - n_{\vec{r}} + \Delta)] - \sum_{\vec{r}} \cos[2\pi/3(n_{\vec{r}+\vec{y}} - n_{\vec{r}})]$$



$$\lambda_j = e^{-\epsilon_j - i\phi_j}$$

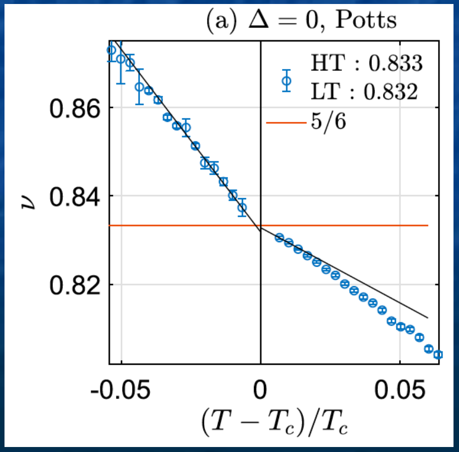
S. Nyckees, J. Colbois, FM, Nuclear Phys B 2021

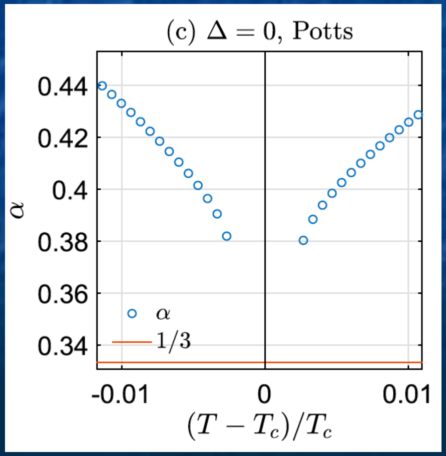
Benchmark: 3-state Potts model

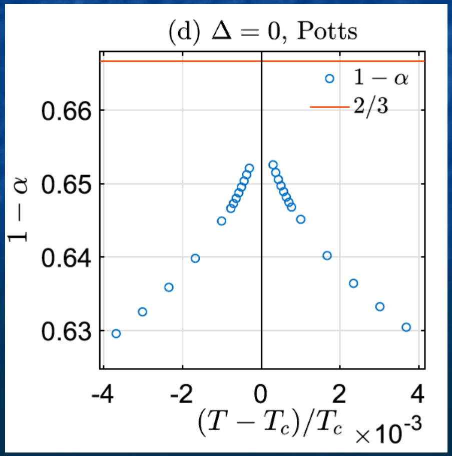
Effective exponents (instead of fit of finite window)

$$A \propto |t|^{-\theta} \qquad \theta(|t|) = -\frac{d\ln A}{d\ln|t|} \qquad \theta = \lim_{|t|\to 0} \theta(|t|)$$

Possible thanks to high precision

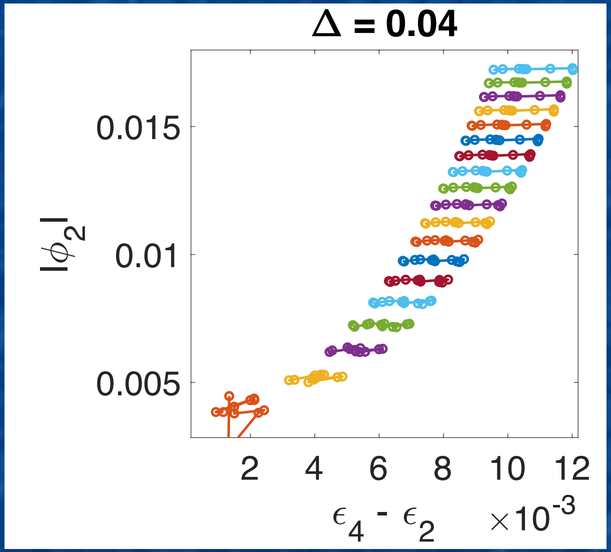


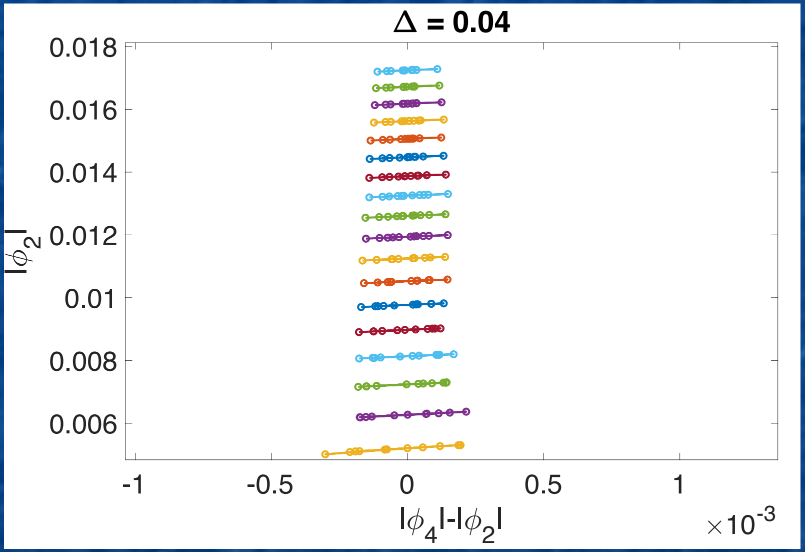




Chiral 3-state Potts model

$$E = -\sum_{\vec{r}} \cos[2\pi/3(n_{\vec{r}+\vec{x}} - n_{\vec{r}} + \Delta)] - \sum_{\vec{r}} \cos[2\pi/3(n_{\vec{r}+\vec{y}} - n_{\vec{r}})]$$

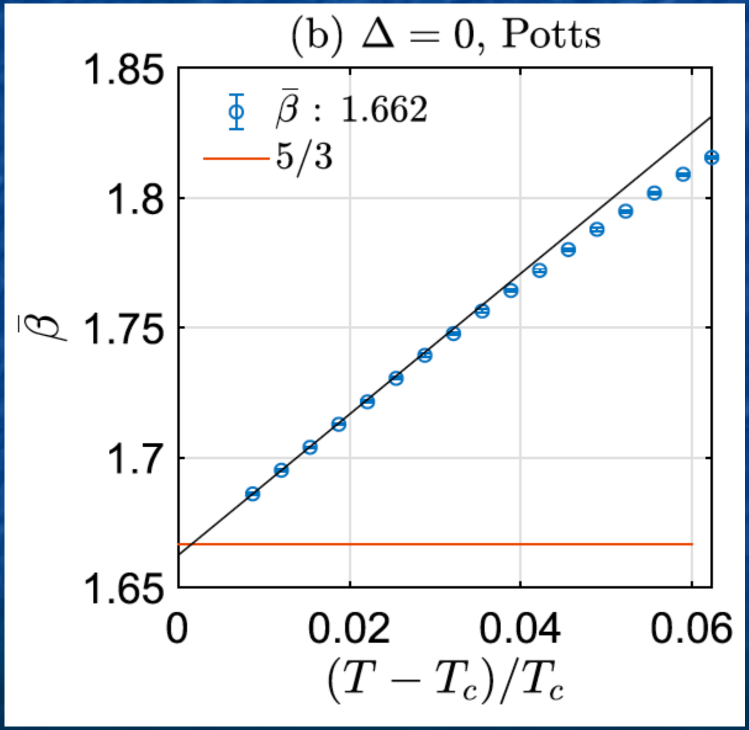


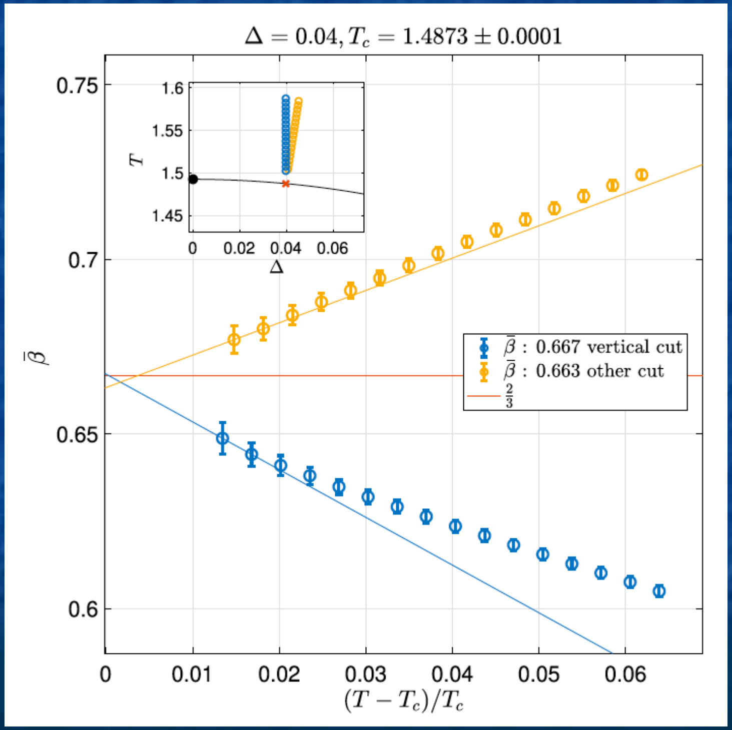


S. Nyckees, J. Colbois, FM, Nuclear Phys B 2021

Scaling of Δq

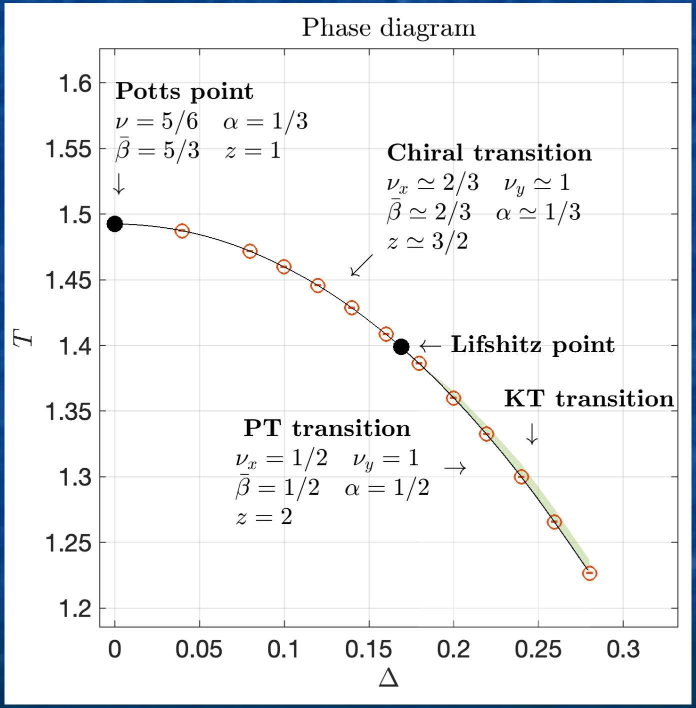
$$\Delta q \propto (T/T_c - 1)^{\bar{\beta}}$$





CTMRG phase diagram

$$E = -\sum_{\vec{r}} \cos[2\pi/3(n_{\vec{r}+\vec{x}} - n_{\vec{r}} + \Delta)] - \sum_{\vec{r}} \cos[2\pi/3(n_{\vec{r}+\vec{y}} - n_{\vec{r}})]$$



- Exponents similar to those of a self-dual version of the model with complex *Δ* (Cardy, 1993)
- Consistent with the experimental results on Si(113) 3 x 1
- Reasonable agreement with recent field theory results (Whitsitt, Samajdar, Sachdev, 2018)

S. Nyckees, J. Colbois, FM, Nuclear Phys B 2021

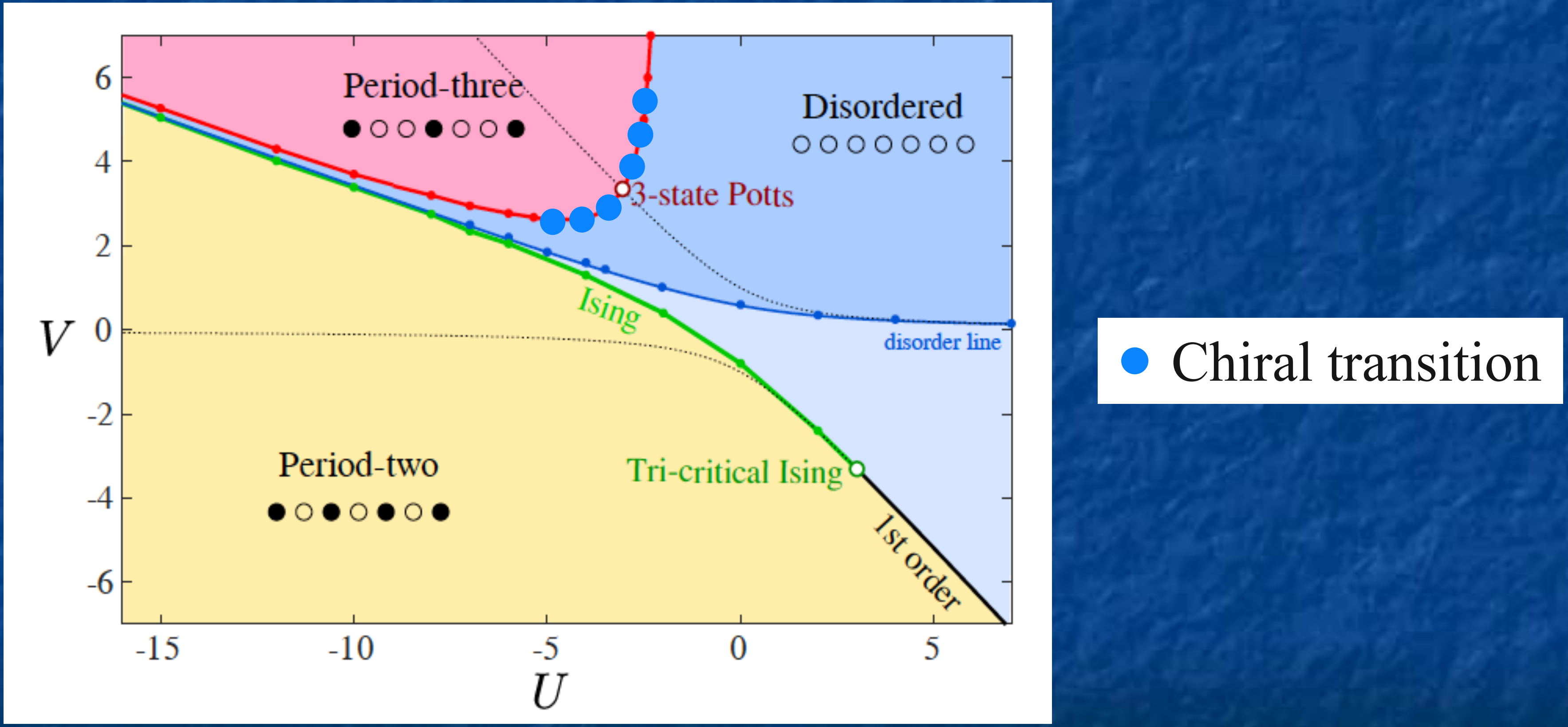
Quantum 1D version

$$H_{\mathrm{HB}} = \sum_j \left[-w(d_j^\dagger + d_j) + U n_j + V n_{j-1} n_{j+1} \right]$$

- Two constraints $n_j(n_j - 1) = 0$ $n_j n_{j+1} = 0$
- Hilbert space: grows as Fibonacci number
- Toy model for Rydberg chains

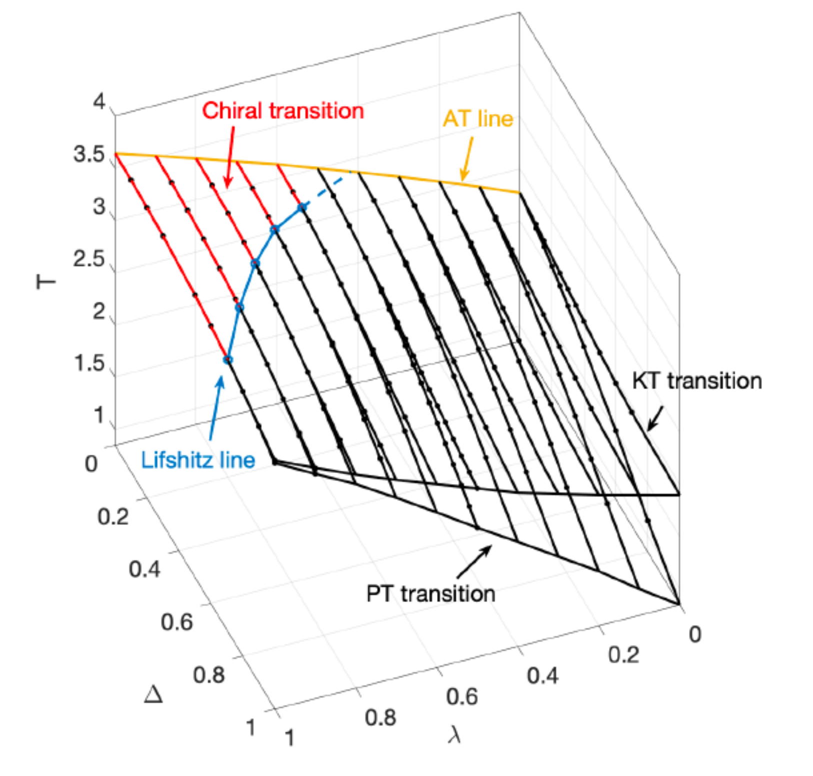
Fendley, Sengupta, Sachdev 2004

Hard-bosons: phase diagram



Chepiga and FM, PRL 2019

Period-4 case: Ashkin-Teller



$$H_0 = -\sum_{\langle i,j \rangle} \sigma_i\sigma_j + \tau_i\tau_j + \lambda\sigma_i\sigma_j\tau_i\tau_j$$

Chiral perturbation

$$\Delta \sum_{x,y} (\tau_{x+1,y}\sigma_{x,y} - \sigma_{x+1,y}\tau_{x,y})$$

S. Nyckees and FM, Phys Rev Research 2022

Thermal transitions in 2D quantum antiferromagnets

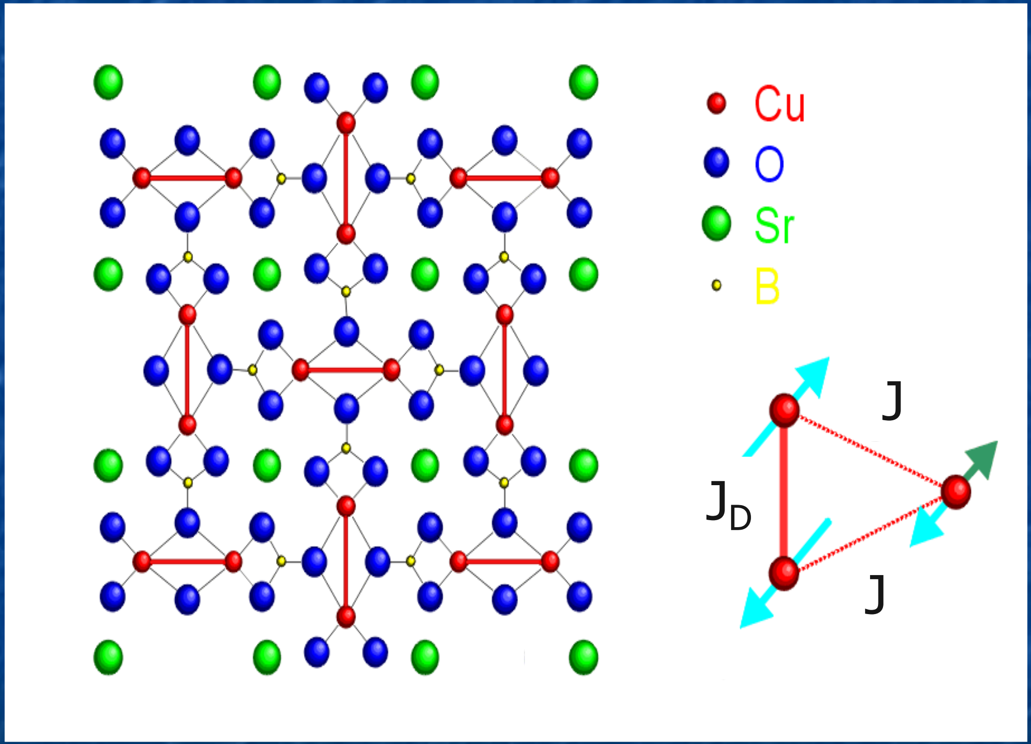
- Mermin-Wagner theorem → no long-range order at T>0 for Heisenberg

No critical point, really? Not quite!

- Frustrated quantum magnets
  - First-order transition → critical point
  - Spontaneous breaking of spatial symmetry → Ising transition

$SrCu_2(BO_3)_2$

Smith and Keszler, JSSC 1991



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

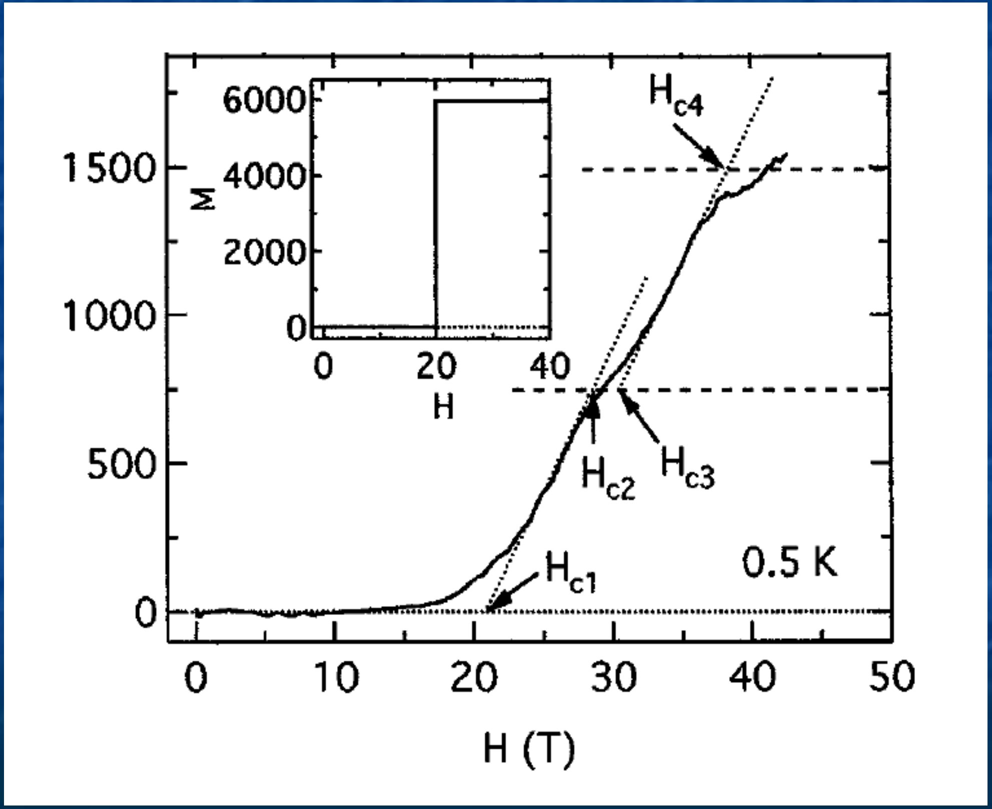
$J_D \approx 85$ K

$J/J_D \approx 0.63$

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]

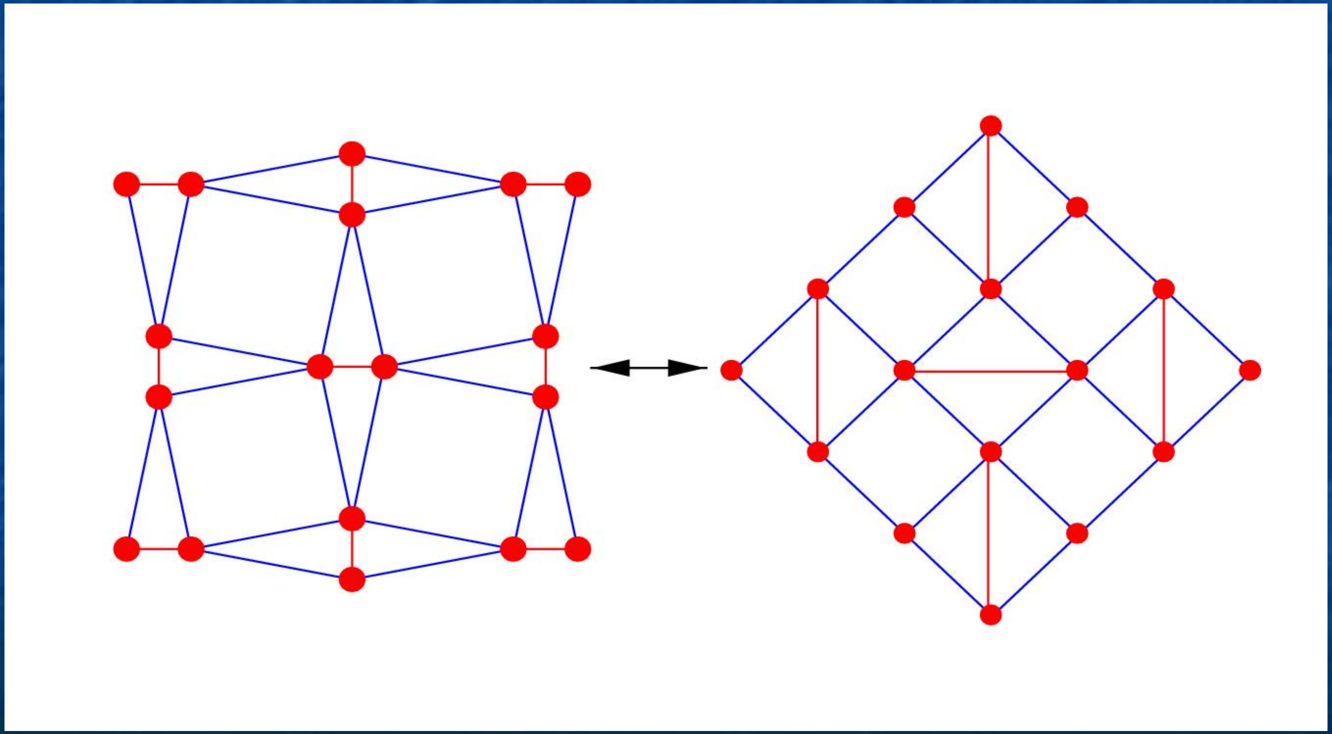


Anomalies

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

and many more

From orthogonal dimer to Shastry-Sutherland model



$SrCu_2(BO_3)_2$ 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]

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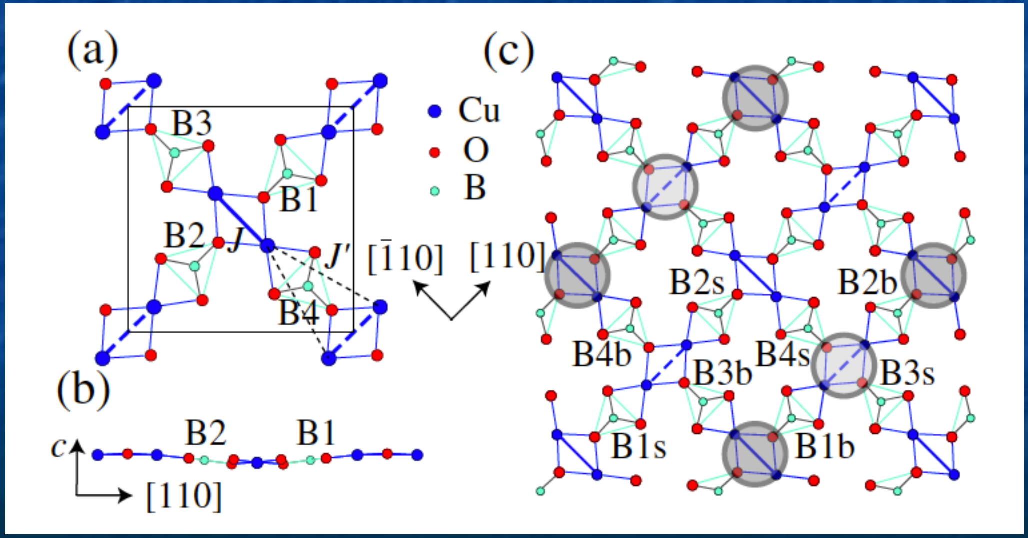


Intermediate phase under pressure, but two types of Cu sites

↓

NOT the empty plaquette phase

nature COMMUNICATIONS

ARTICLE

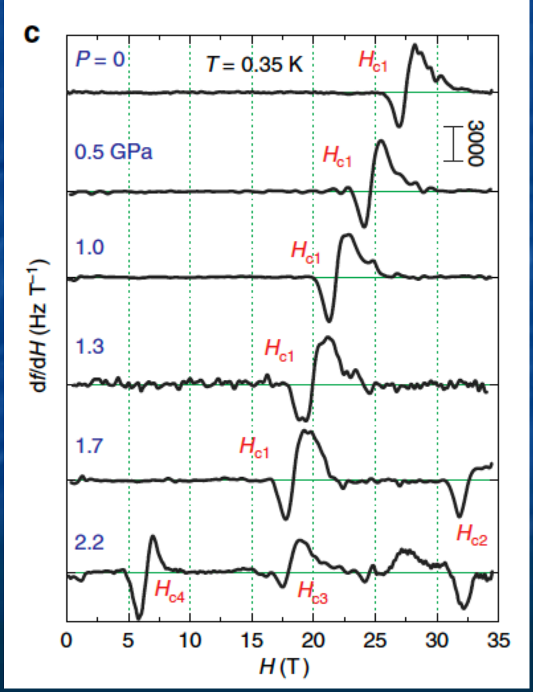
Received 17 Jun 2015 | Accepted 16 May 2016 | Published 20 Jun 2016

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

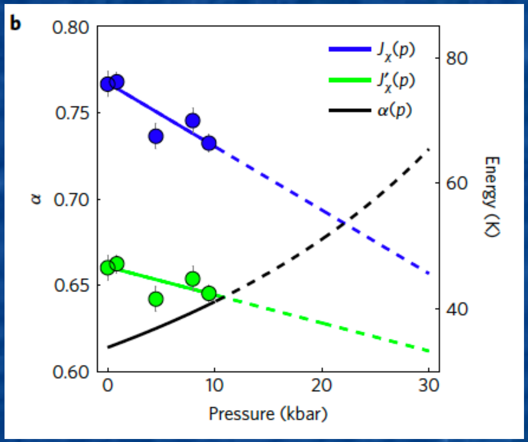
LETTERS
PUBLISHED ONLINE: 17 JULY 2017 | DOI: 10.1038/NPHYS4190
nature physics

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

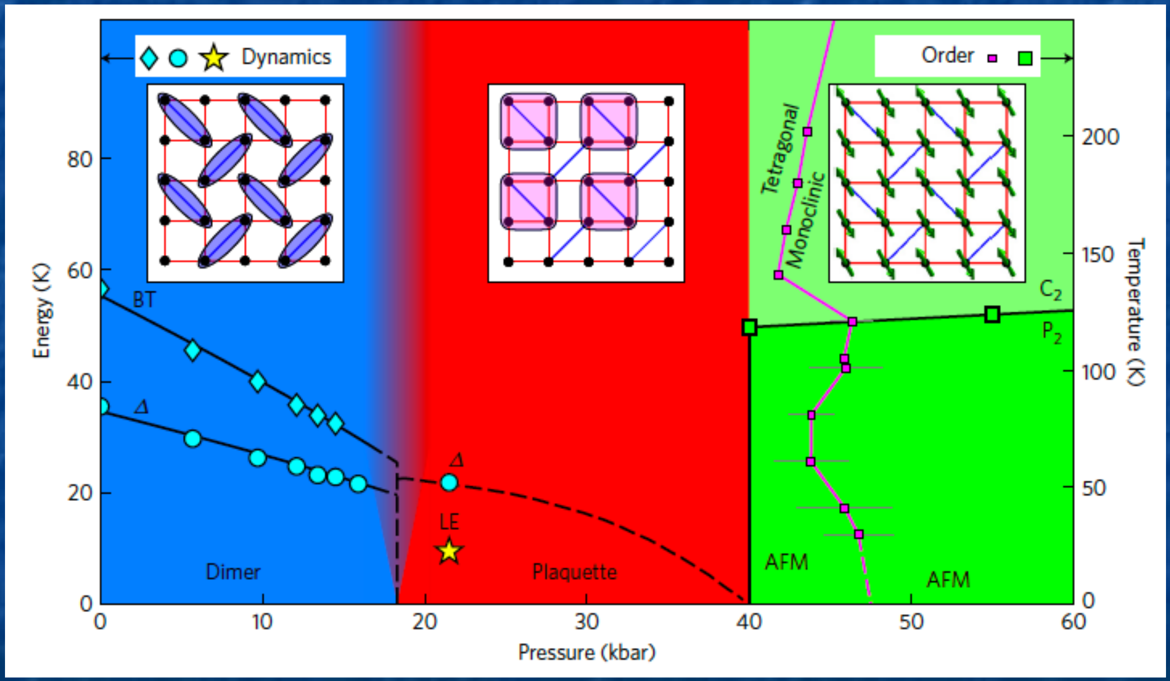
M. E. Zayed[1,2,3*], Ch. Rüegg[2,4,5], J. Larrea J.[1,6], A. M. Läuchli[7], C. Panagopoulos[8,9], S. S. Saxena[8], M. Ellerby[5], D. F. McMorrow[5], Th. Strässle[2], S. Klotz[10], G. Hamel[10], R. A. Sadykov[11,12], V. Pomjakushin[2], M. Boehm[13], M. Jiménez-Ruiz[13], A. Schneidewind[14], E. Pomjakushina[15],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

Neutron scattering

Susceptibility



J/J_D increases



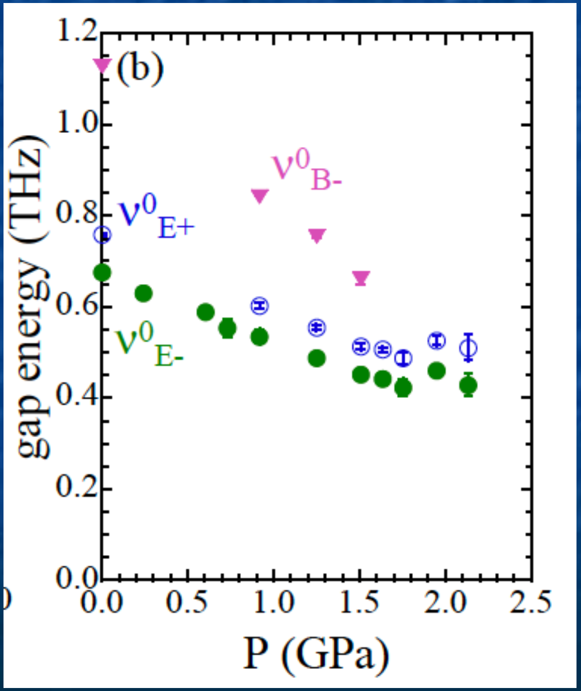
Full plaquette intermediate phase

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

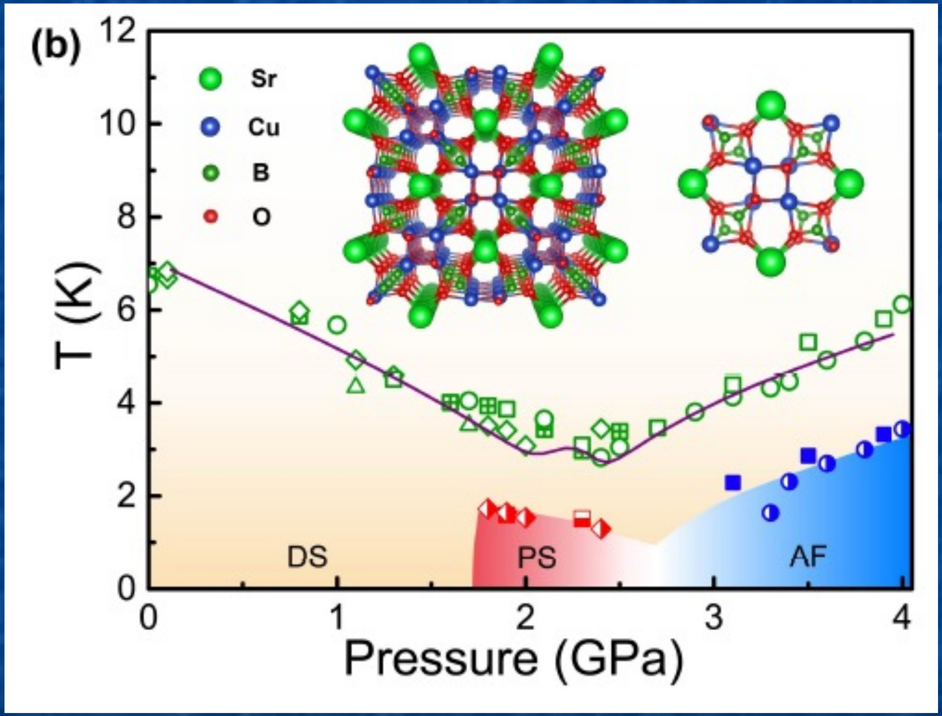
↓

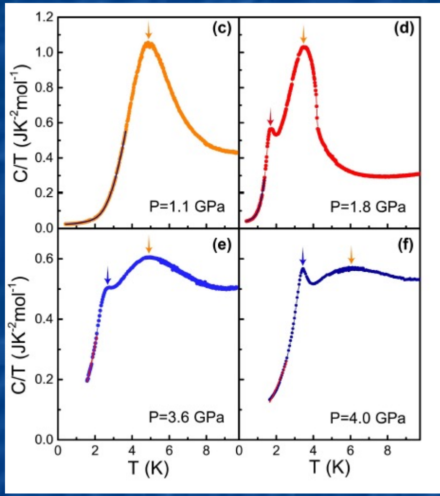
Confirmation of a phase transition around 1.8 GPa

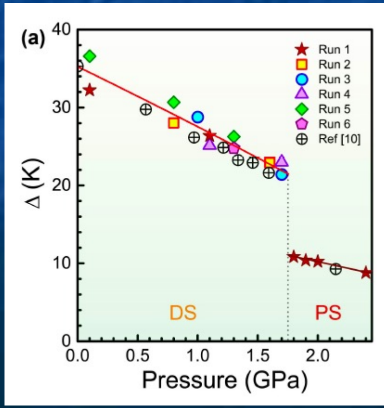
PHYSICAL REVIEW LETTERS 124, 206602 (2020)

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

A quantum magnetic analogue to the critical point of water

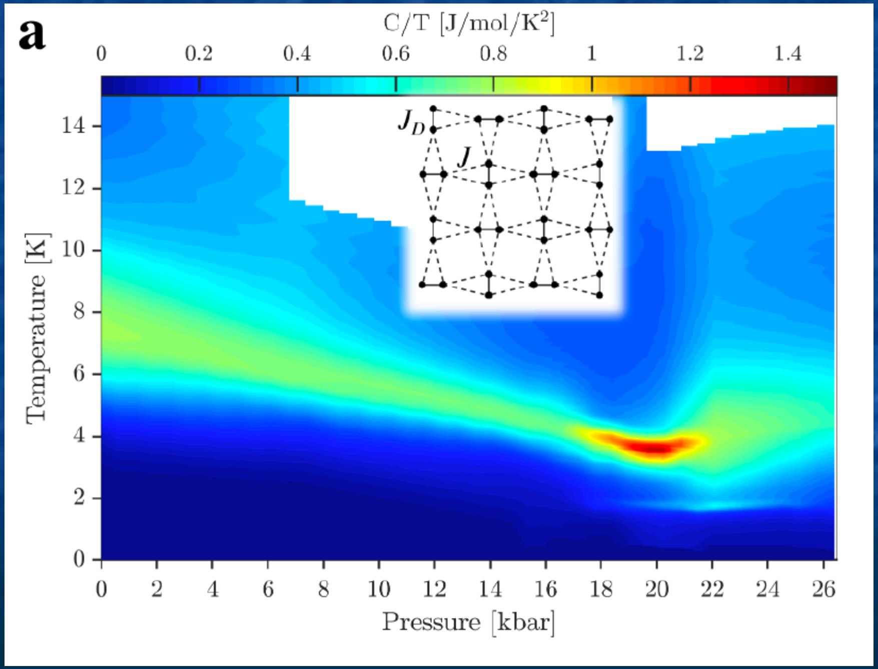
Nature | Vol 592 | 15 April 2021

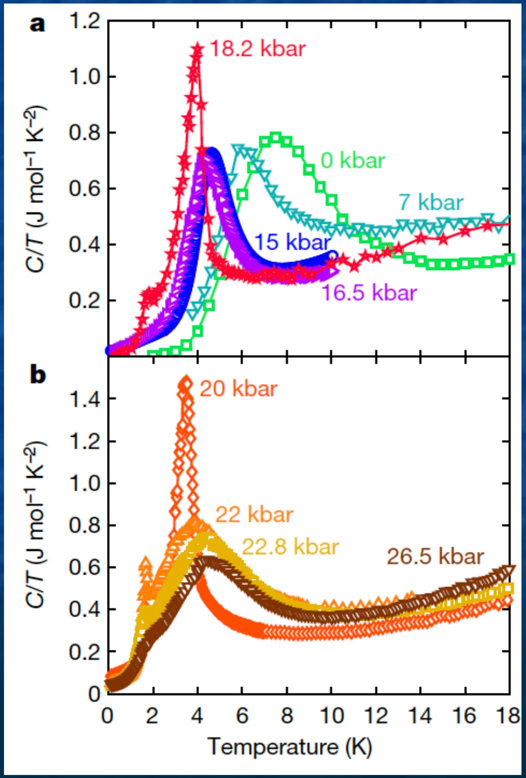
https://doi.org/10.1038/s41586-021-03411-8

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]

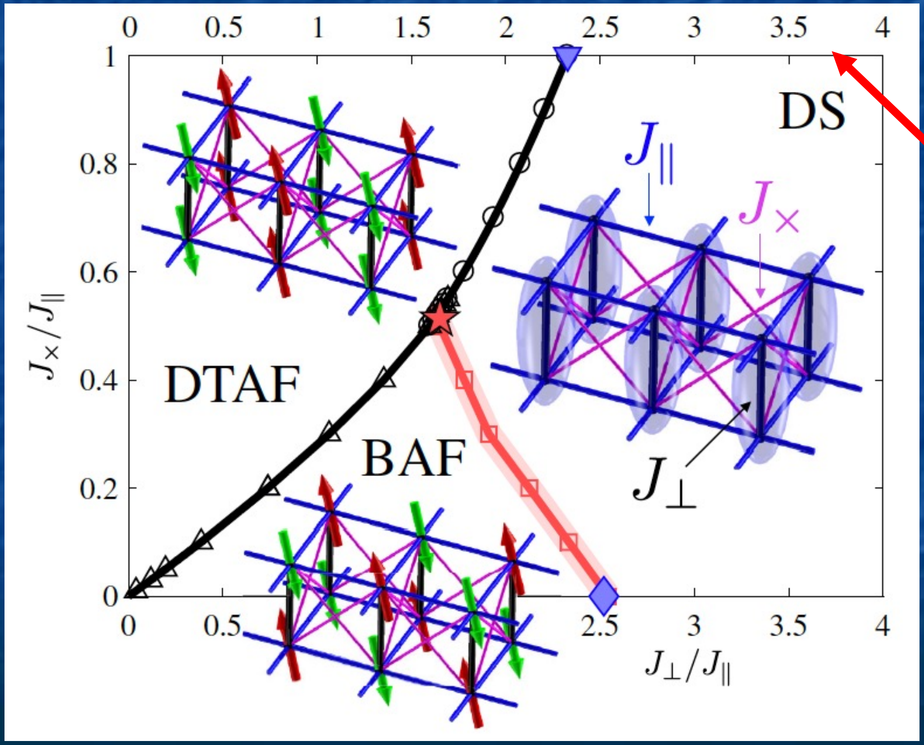




PHYSICAL REVIEW LETTERS **121**, 127201 (2018)

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

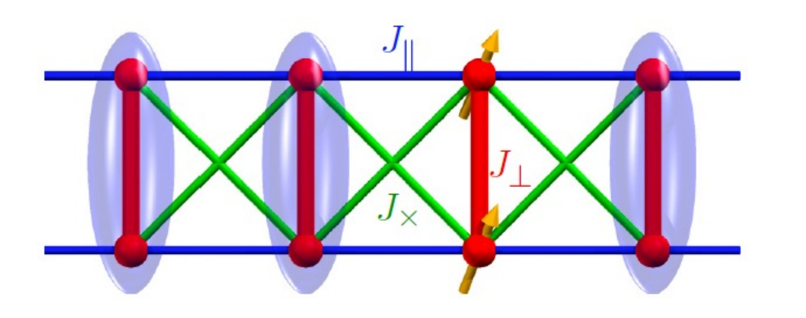
J. Stapmanns,[1] P. Corboz,[2] F. Mila,[3] A. Honecker,[4] B. Normand,[5] and S. Wessel[1]



Fully frustrated bilayer

Fully frustrated dimer models

- Example: fully-frustrated ladder



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

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

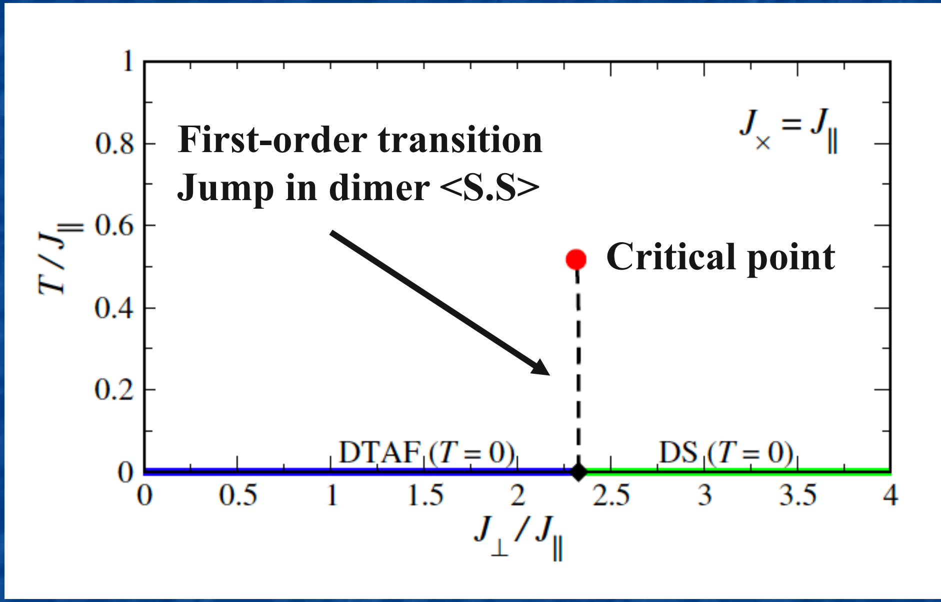
$\vec{T}_i = \vec{S}_i^1 + \vec{S}_i^2$ Total spin on a rung is a good quantum number

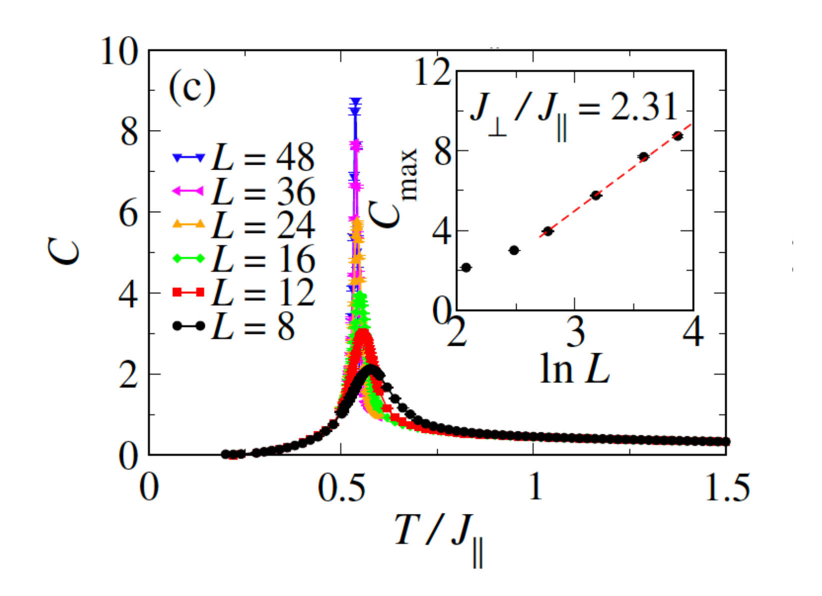
Hamiltonian in dimer basis

- 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

Ising critical point

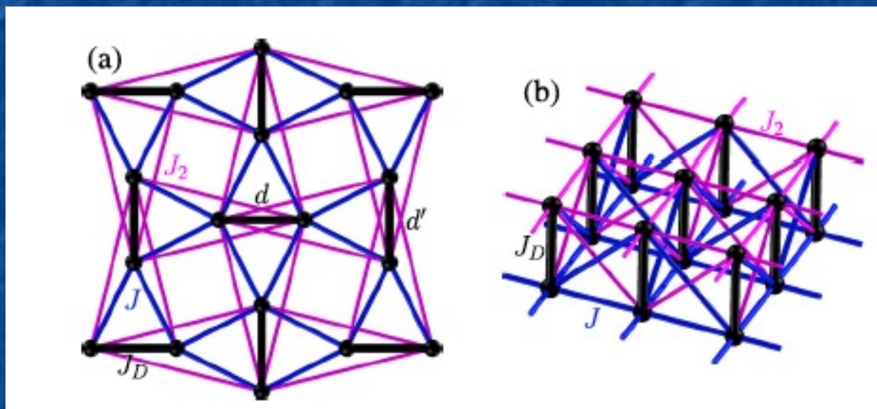




Ising 2D: $\alpha = 0$

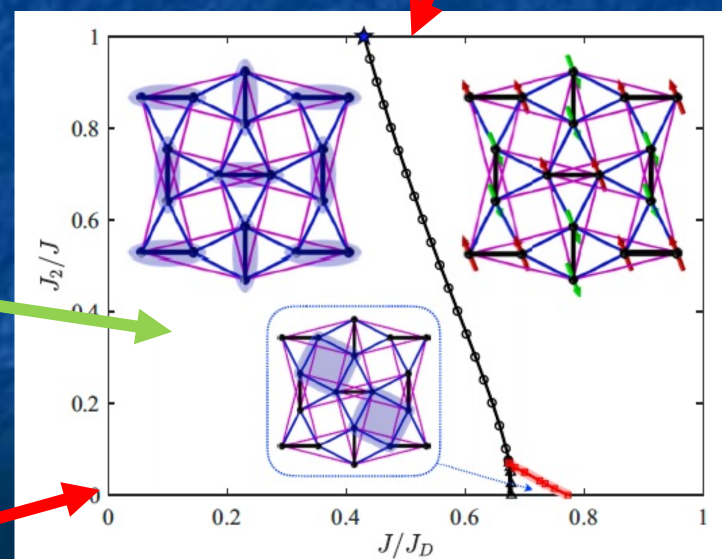
C α ln L

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

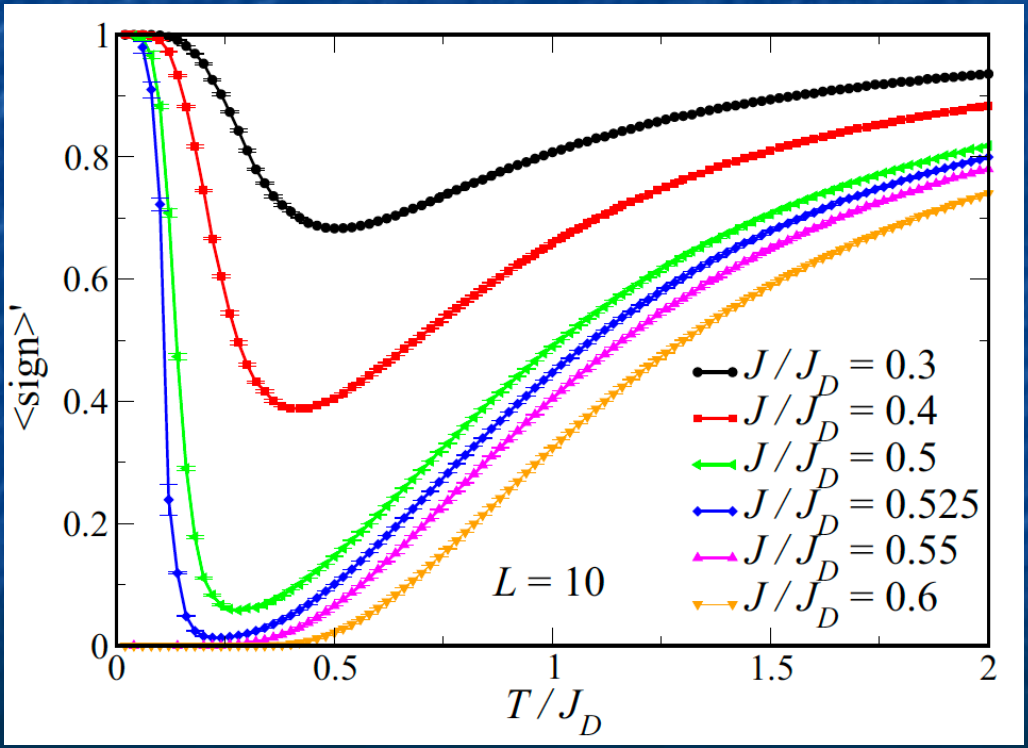
  → <sign>' → 1 as T → 0

  → QMC possible!

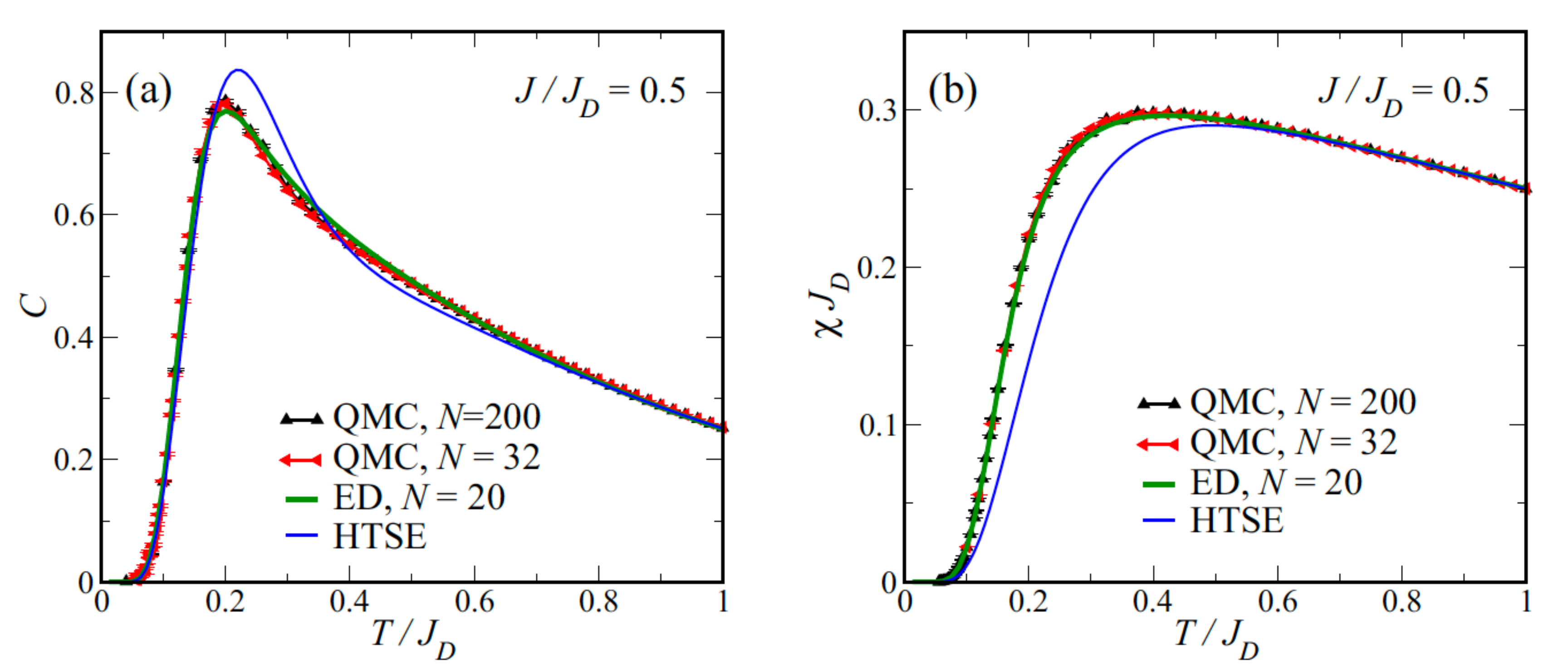
PHYSICAL REVIEW B **98**, 174432 (2018)

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 $J/J_D = 0.526$?

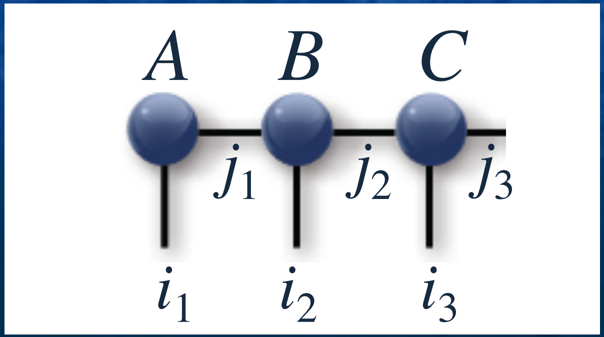
Tensor networks

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

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

Example: Matrix product state in 1D (DMRG)

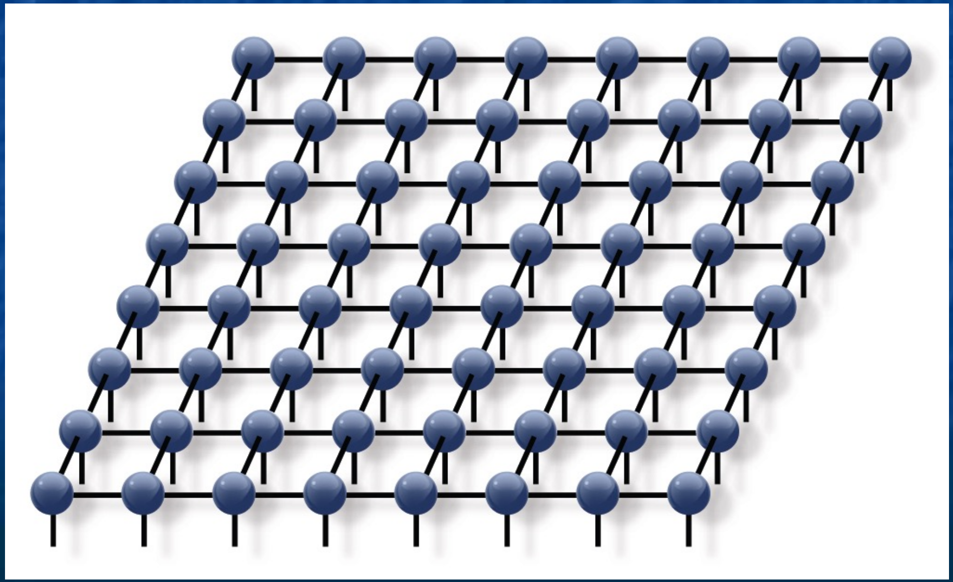
$$c_{i_1 i_2 i_3 \ldots} \simeq \sum_{j_1 j_2 \ldots} A_{i_1}^{j_1} B_{i_2}^{j_1 j_2} C_{i_3}^{j_2 j_3} \cdots$$



Generalization to 2D

PEPS = product of entangled pair states

Verstraete and Cirac, 2004



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

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

Tensor network for T>0

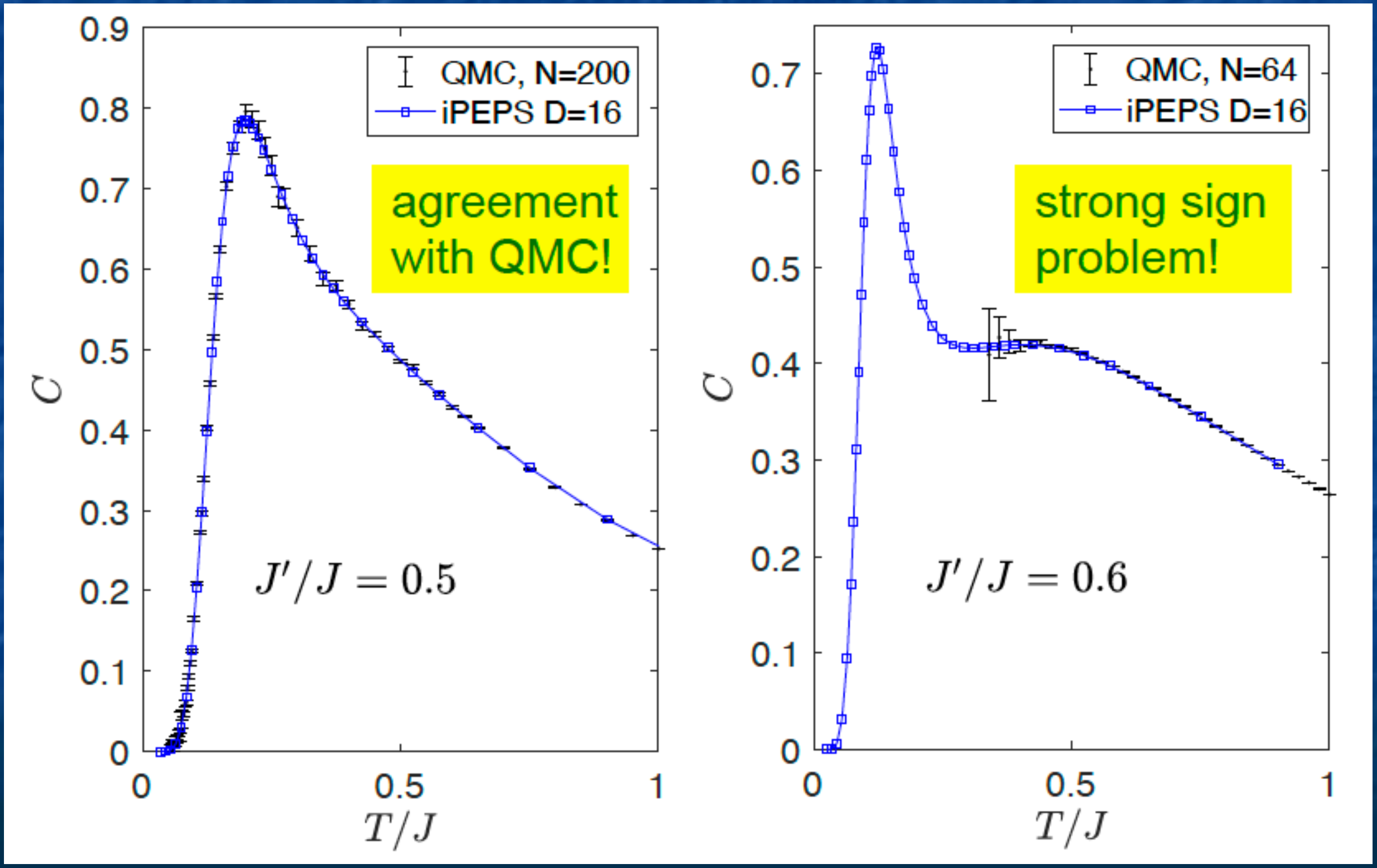
- Purified state: density matrix can be written as the partial trace of a quantum state in an enlarged Hilbert space (with extra "ancilla" degrees of freedom)
- T infinite: Singlets between physical and ancilla degrees of freedom
- Finite T: imaginary-time evolution from T infinite

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

PHYSICAL REVIEW 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]



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

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

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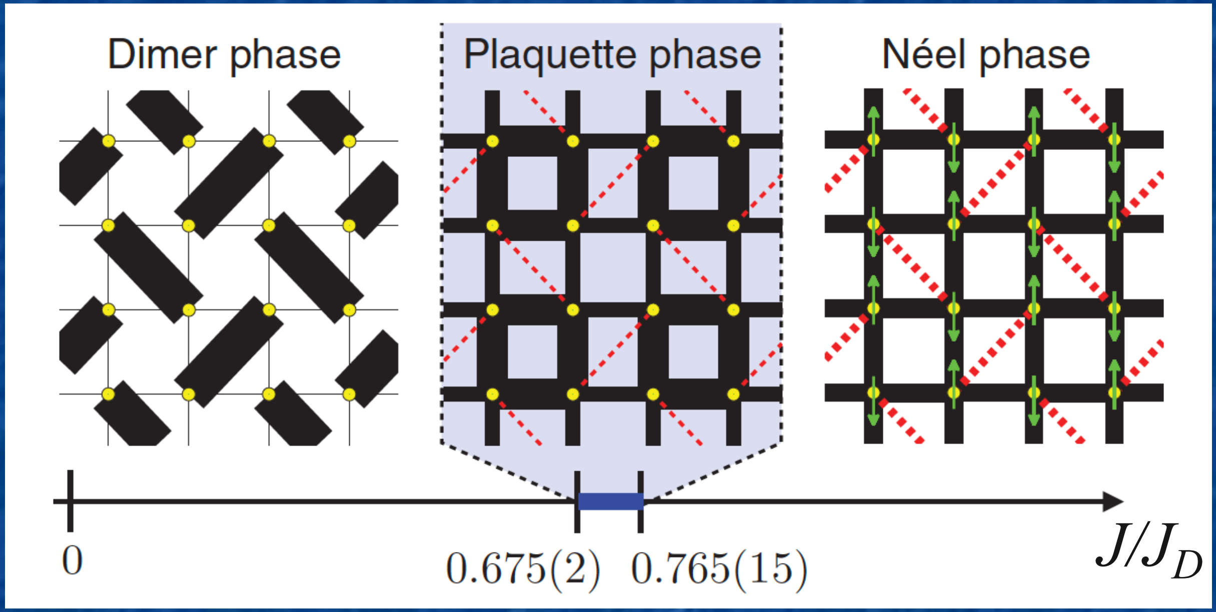
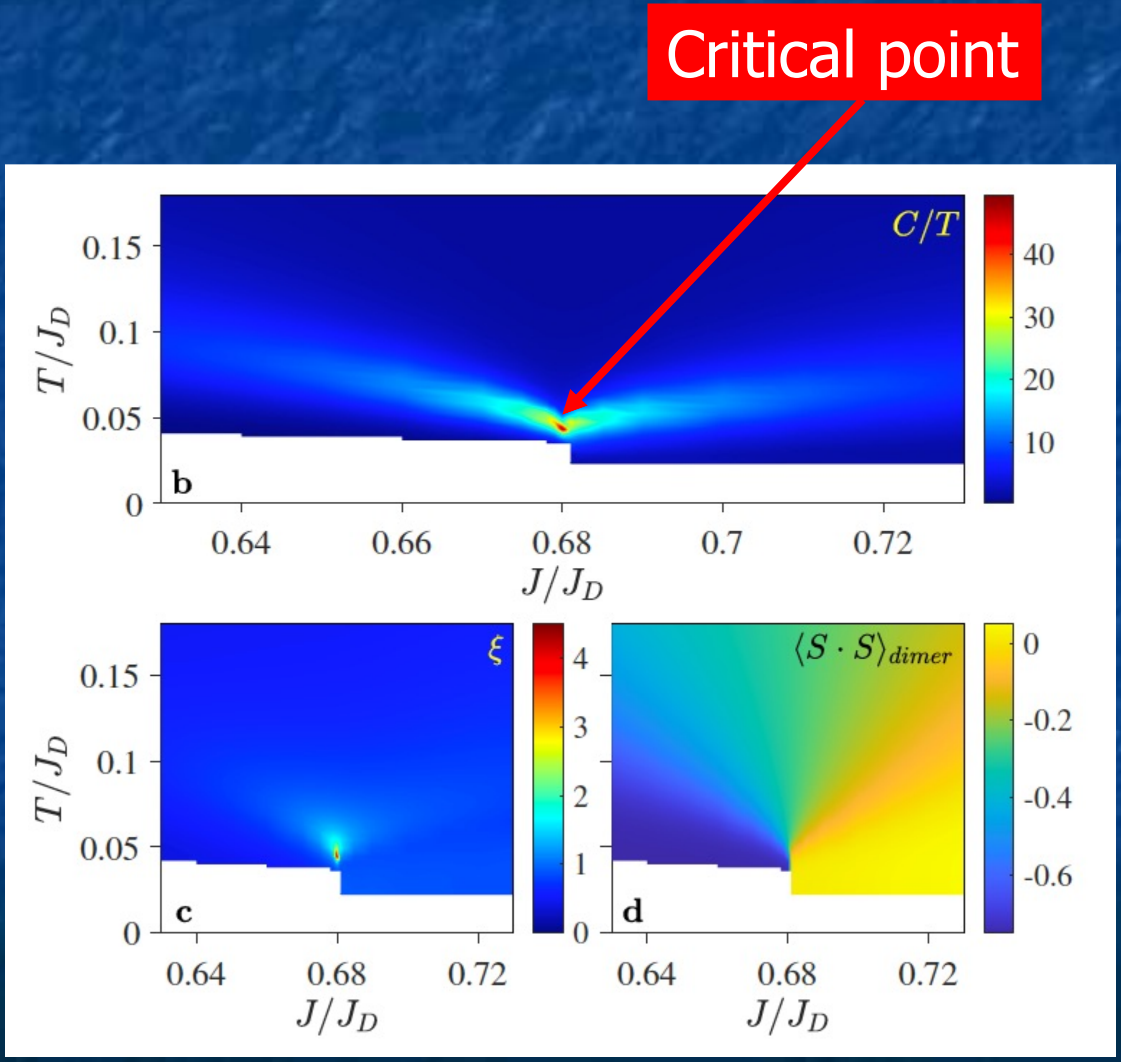
(Received 13 December 2012; revised manuscript received 27 February 2013; published 27 March 2013)



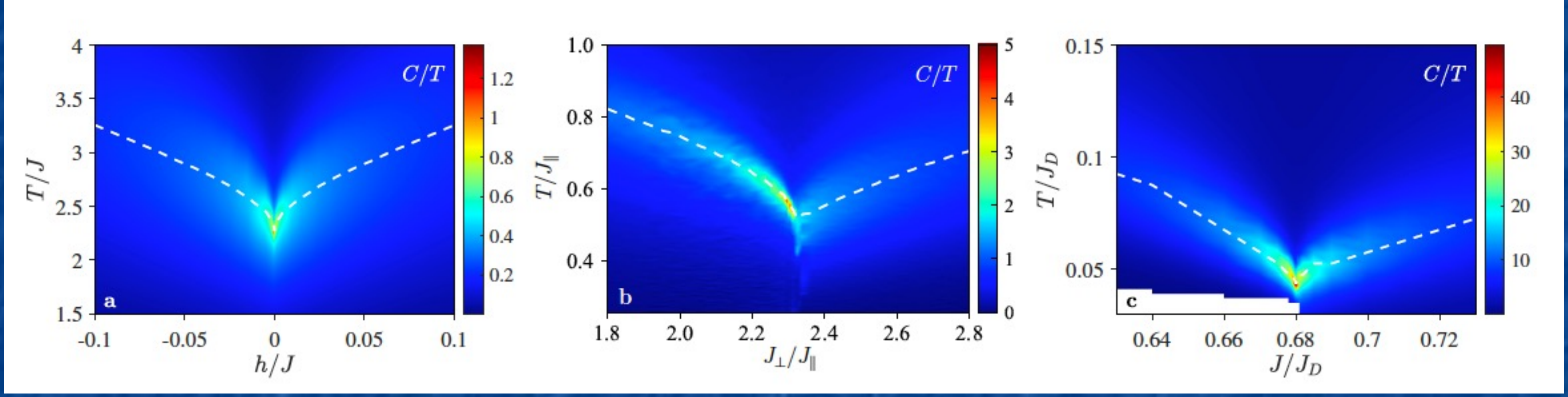
iPEPS with various setups and bond dimension up to 10

iPEPS for Shastry-Sutherland

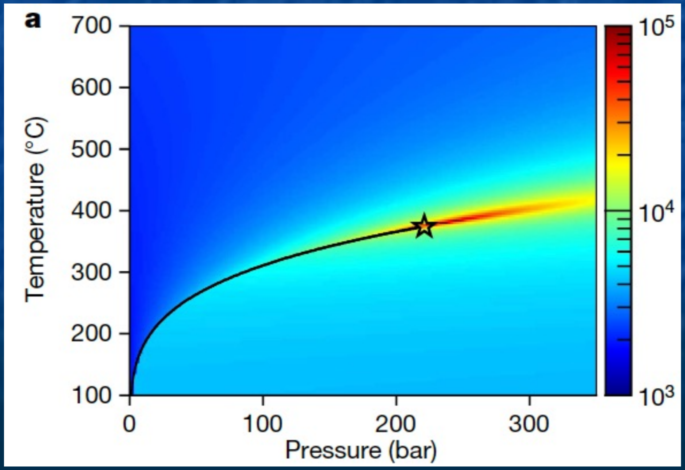


Critical point in various models…

Ising in a field FFB Shastry-Sutherland



… and in water

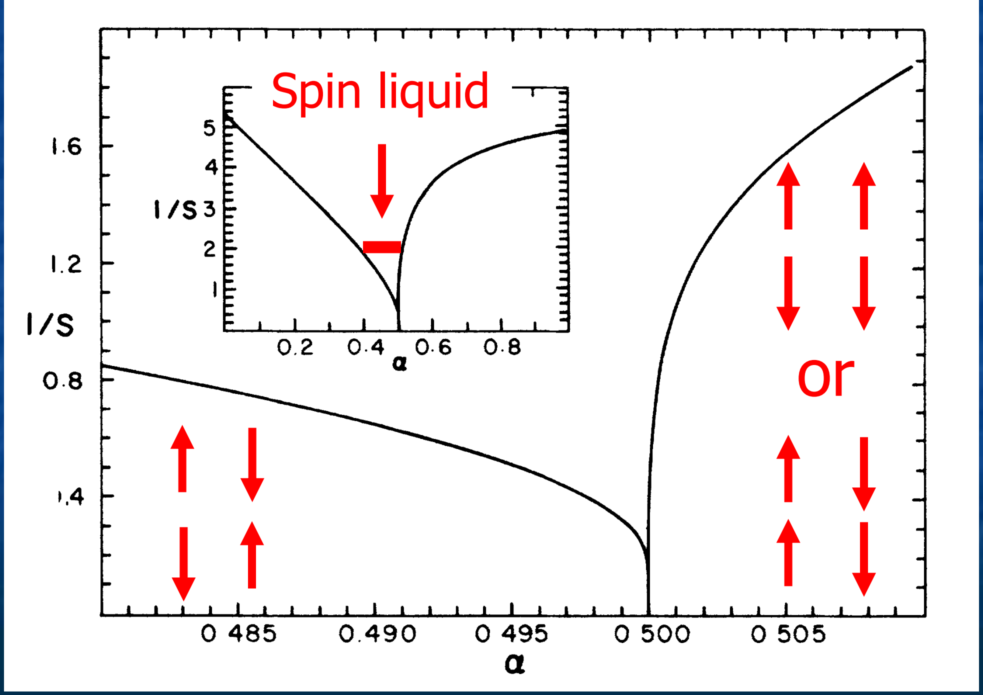


T_c=374° C
P_c=218 bar

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

$\alpha = J_2/J_1$

Ising transtion in 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?

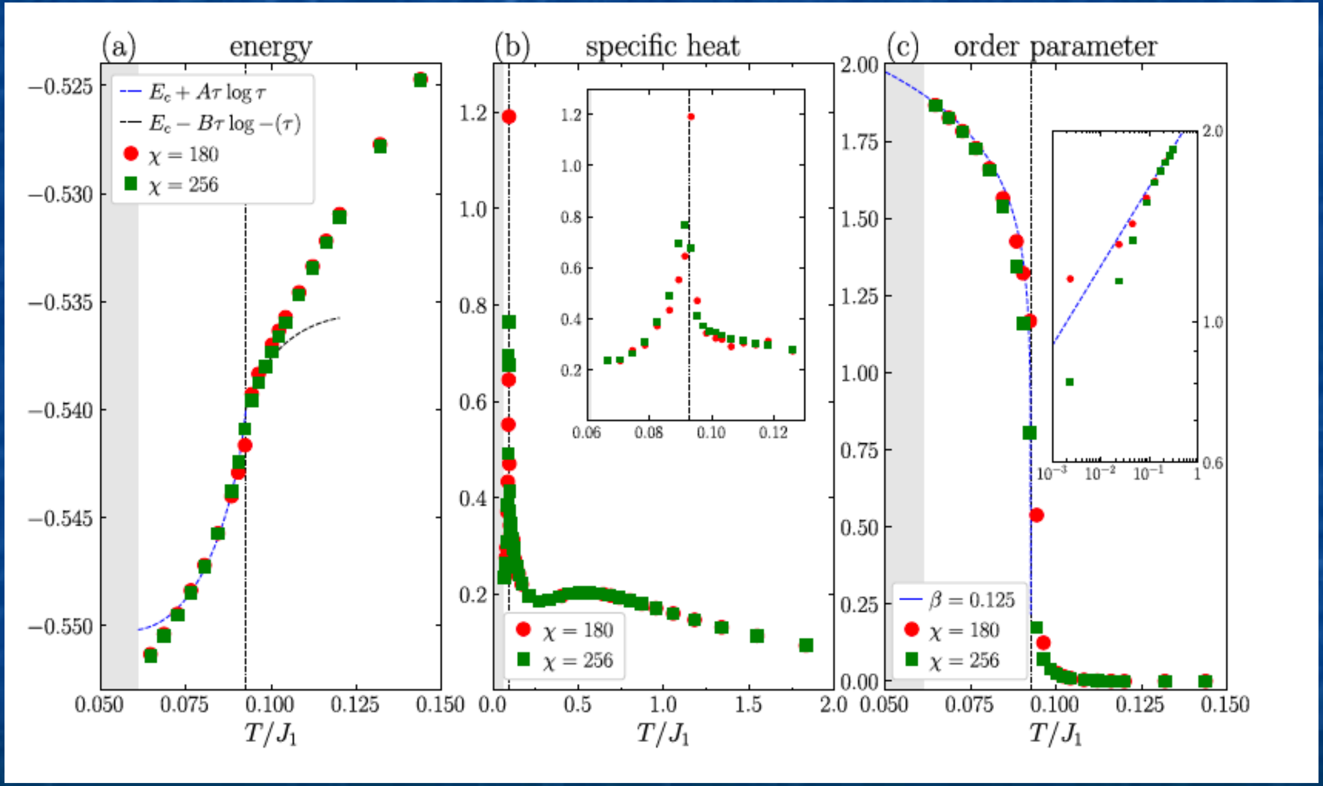
  → QMC: very severe minus sign problem

  → 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

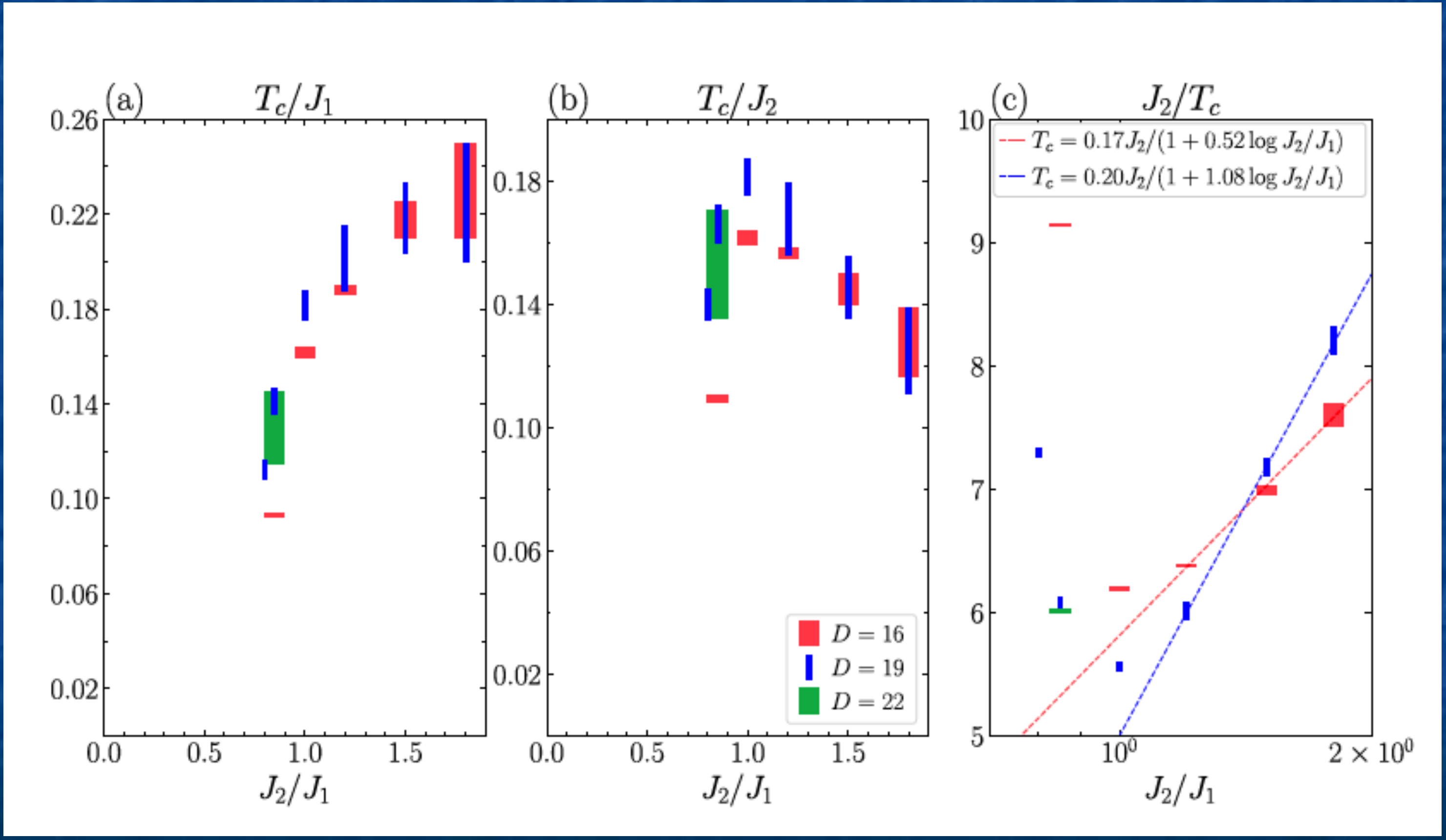
Olivier Gauthé* and Frédéric Mila



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

- Tensor networks contracted with CTMRG

  → Clearly outperforms Monte Carlo for certain 2D classical problems
- Thermal properties of frustrated quantum magnets

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

  → Tensor networks with quantum purification
    - Critical point of Shastry-Sutherland model
    - Ising transition of J_1-J_2 model on square lattice