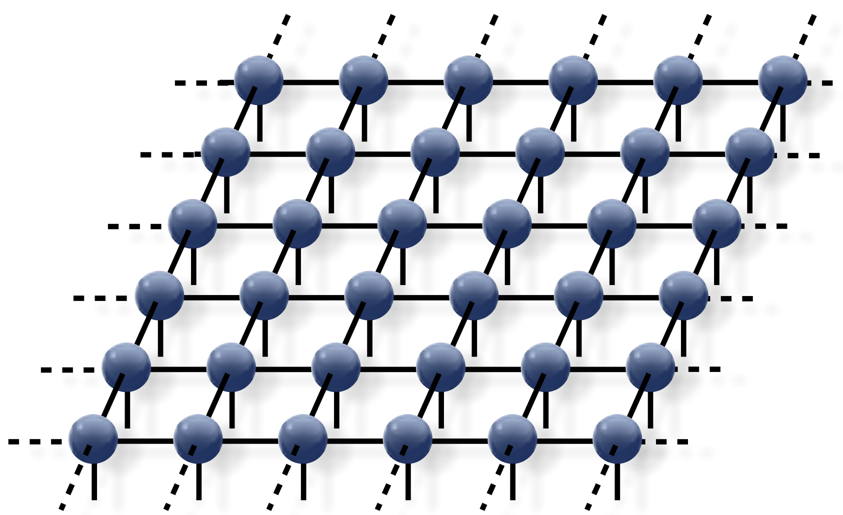
Tensor network study of $SrCu_2(BO_3)_2$ under pressure

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam



iPEPS

2D tensor network ansatz

A quantum magnetic analogue to the critical point of water

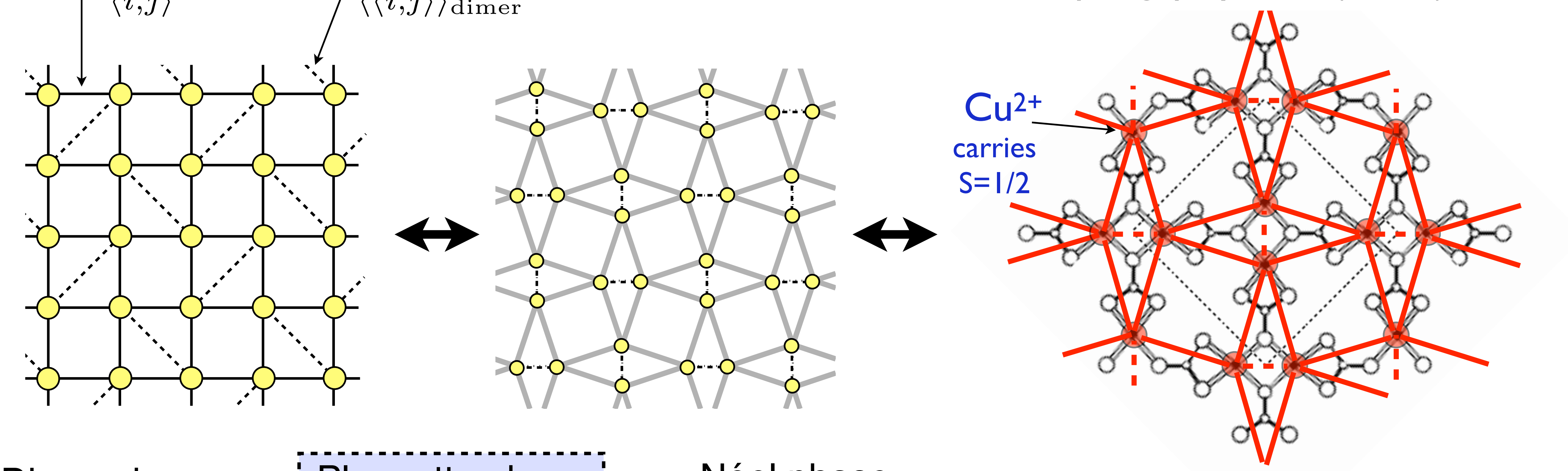
J. L. Jiménez, **S. P. G. Crone**, E. Fogh, M. E. Zayed, R. Lortz, E. Pomjakushina, K. Conder, A. M. Läuchli, L. Weber, S. Wessel, A. Honecker, B. Normand, C. Rüegg, PC, H. M. Rønnow, and F. Mila, arXiv:2009.14492 (accepted in Nature)

The Shastry-Sutherland model and $SrCu_2(BO_3)_2$

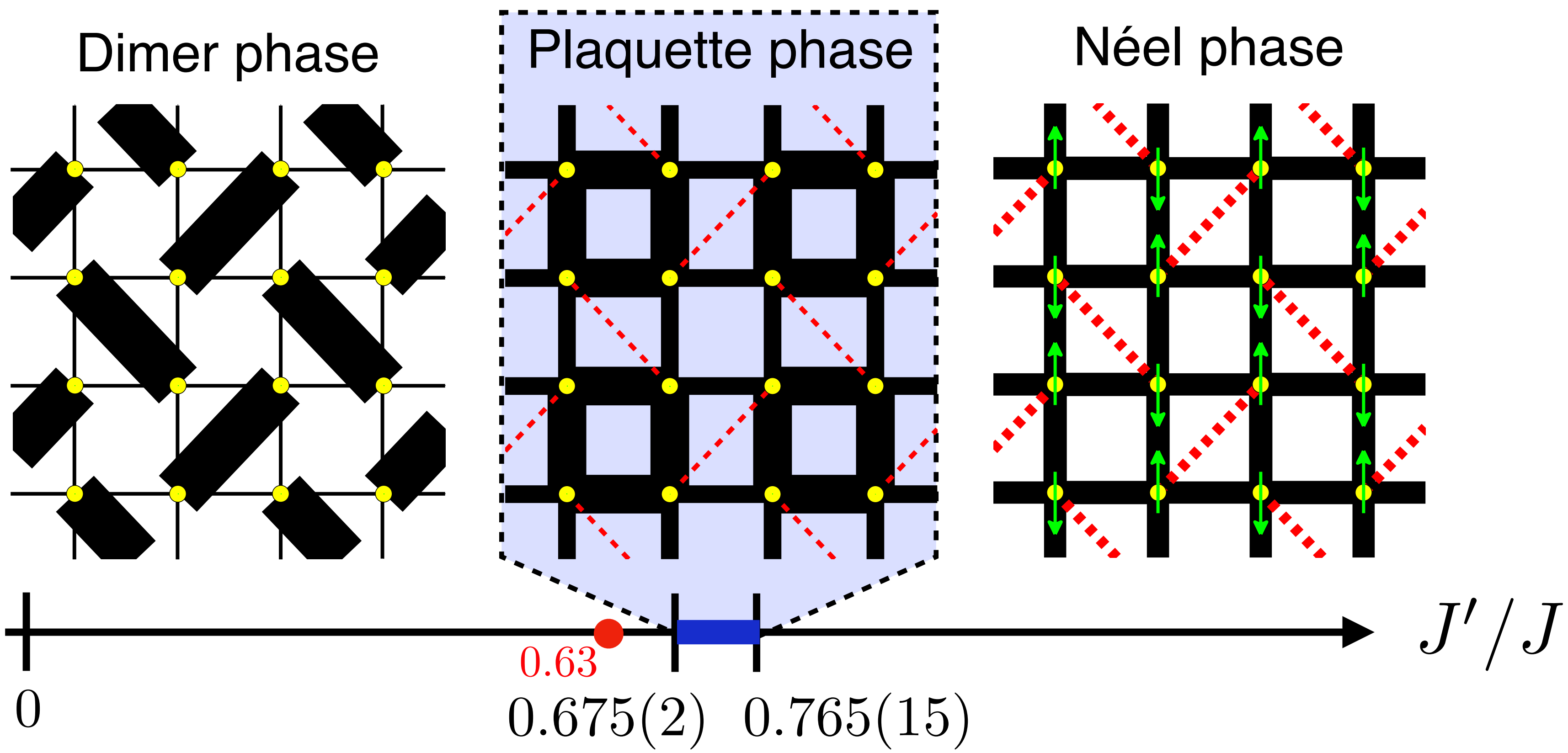
$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\mathrm{dimer}}} S_i \cdot S_j$$

$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



Kageyama et al. PRL **82** (1999)

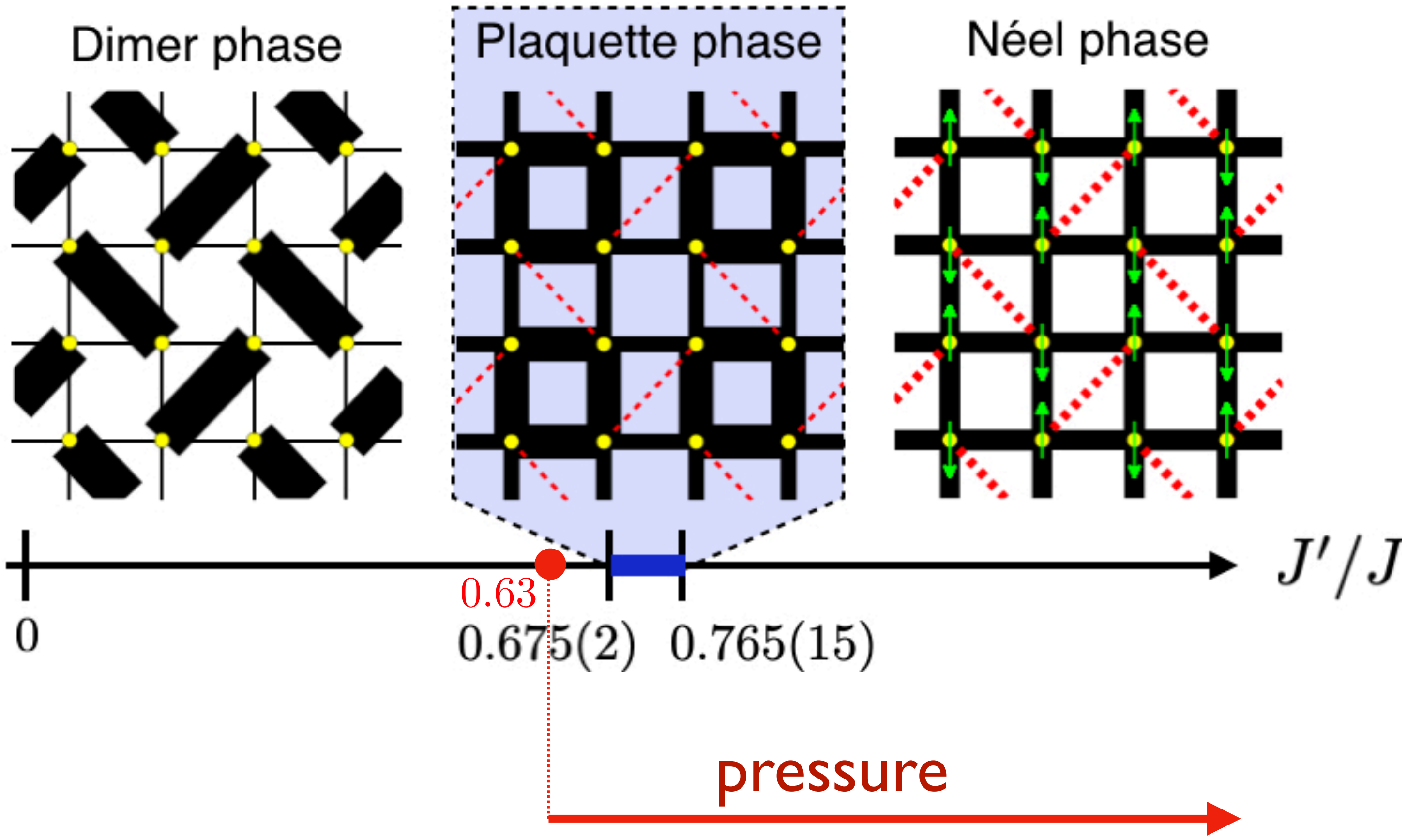


Corboz and Mila, PRB **87** (2013)

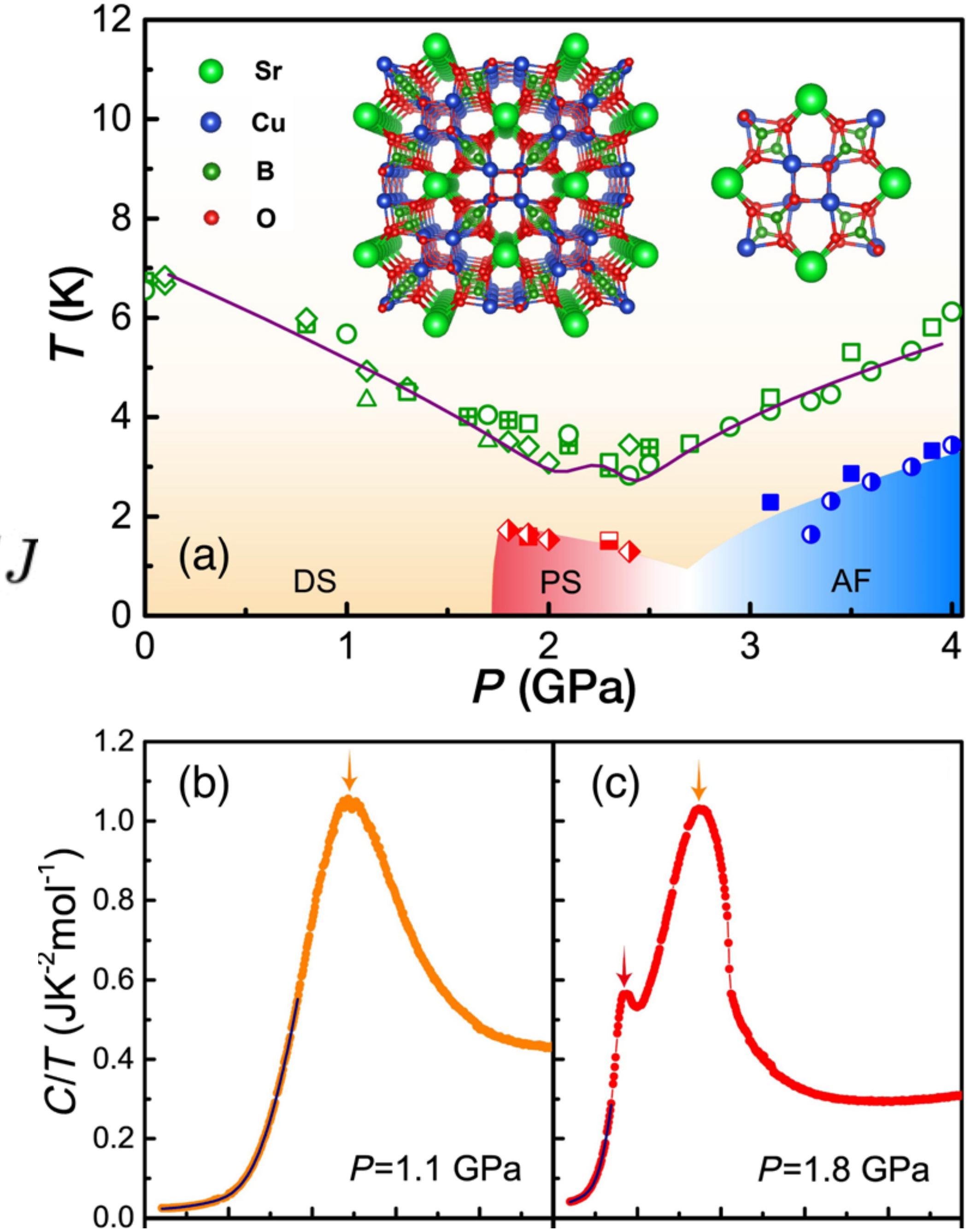
previously found in:

Koga and Kawakami, PRL **84** (2000)
Takushima et al., JPSJ **70** (2001)
Chung et al, PRB **64** (2001)
Läuchli et al, PRB **66** (2002)

$SrCu_2(BO_3)_2$ under pressure



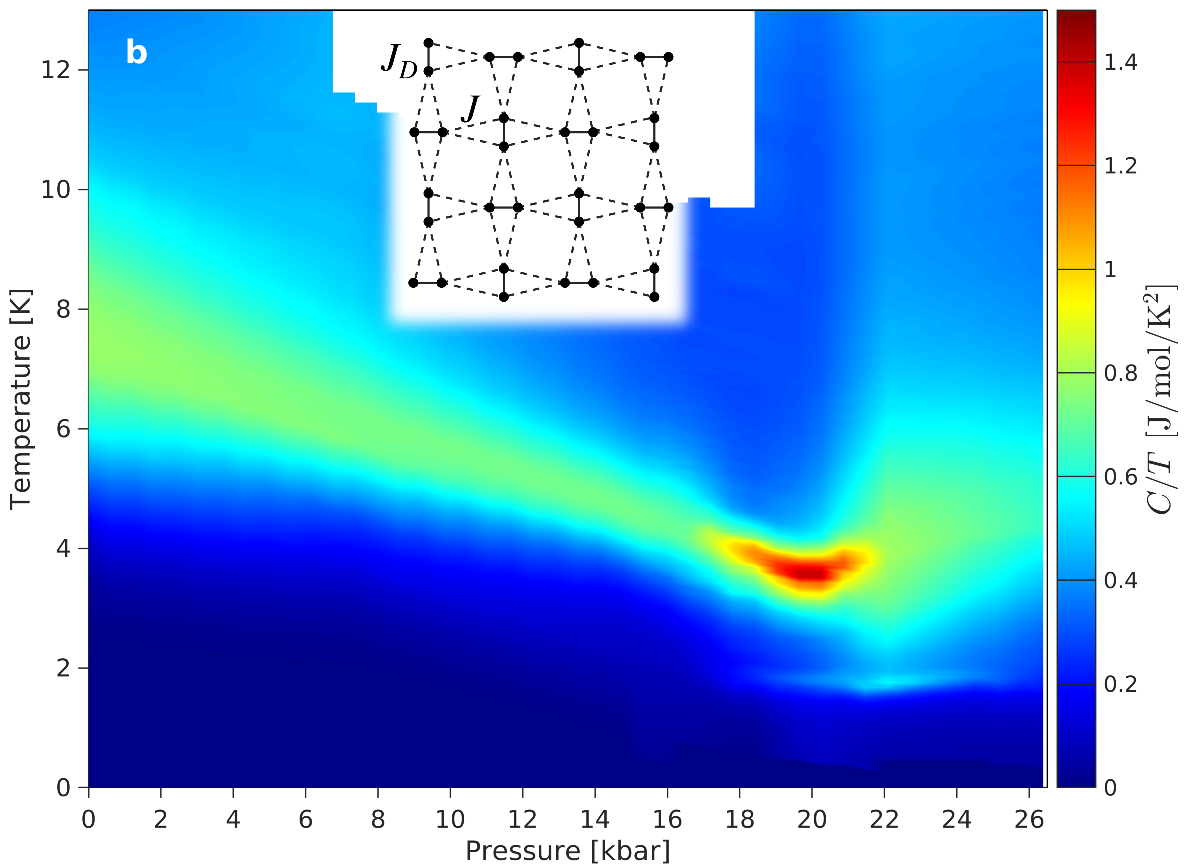
Drive system across the phase transitions!

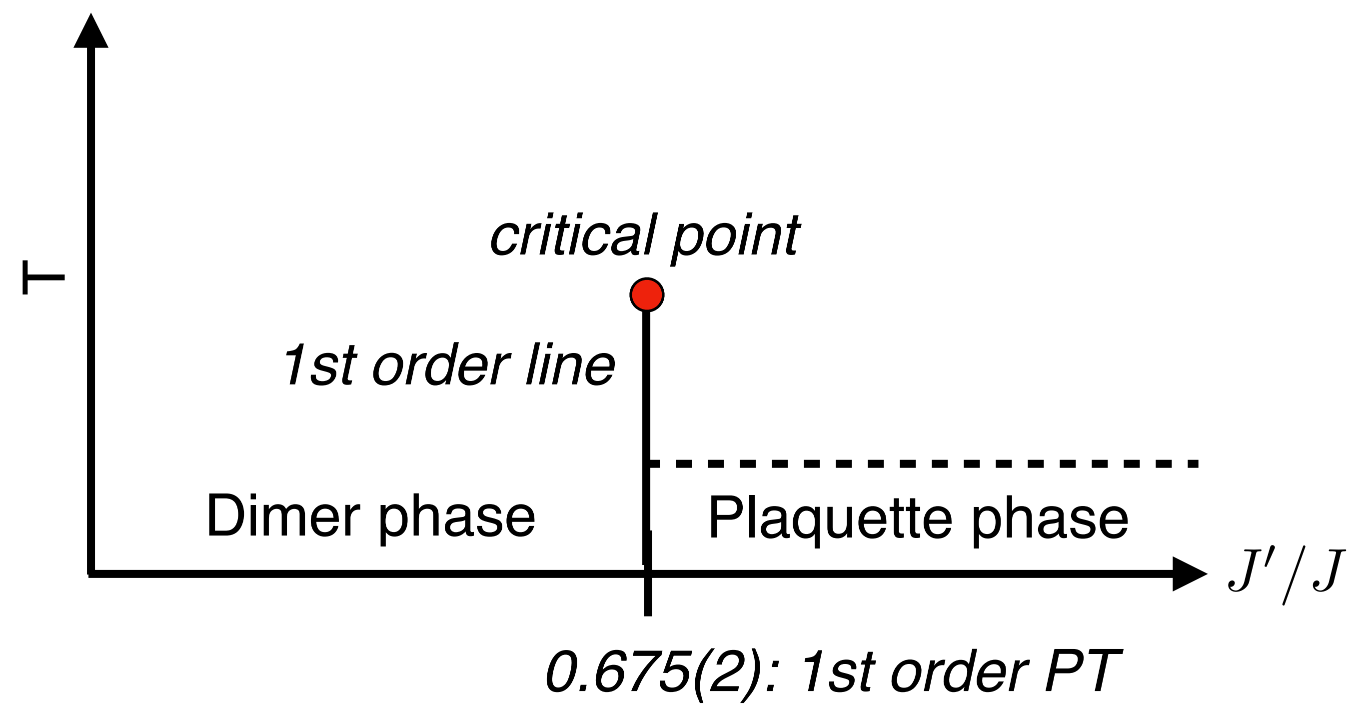


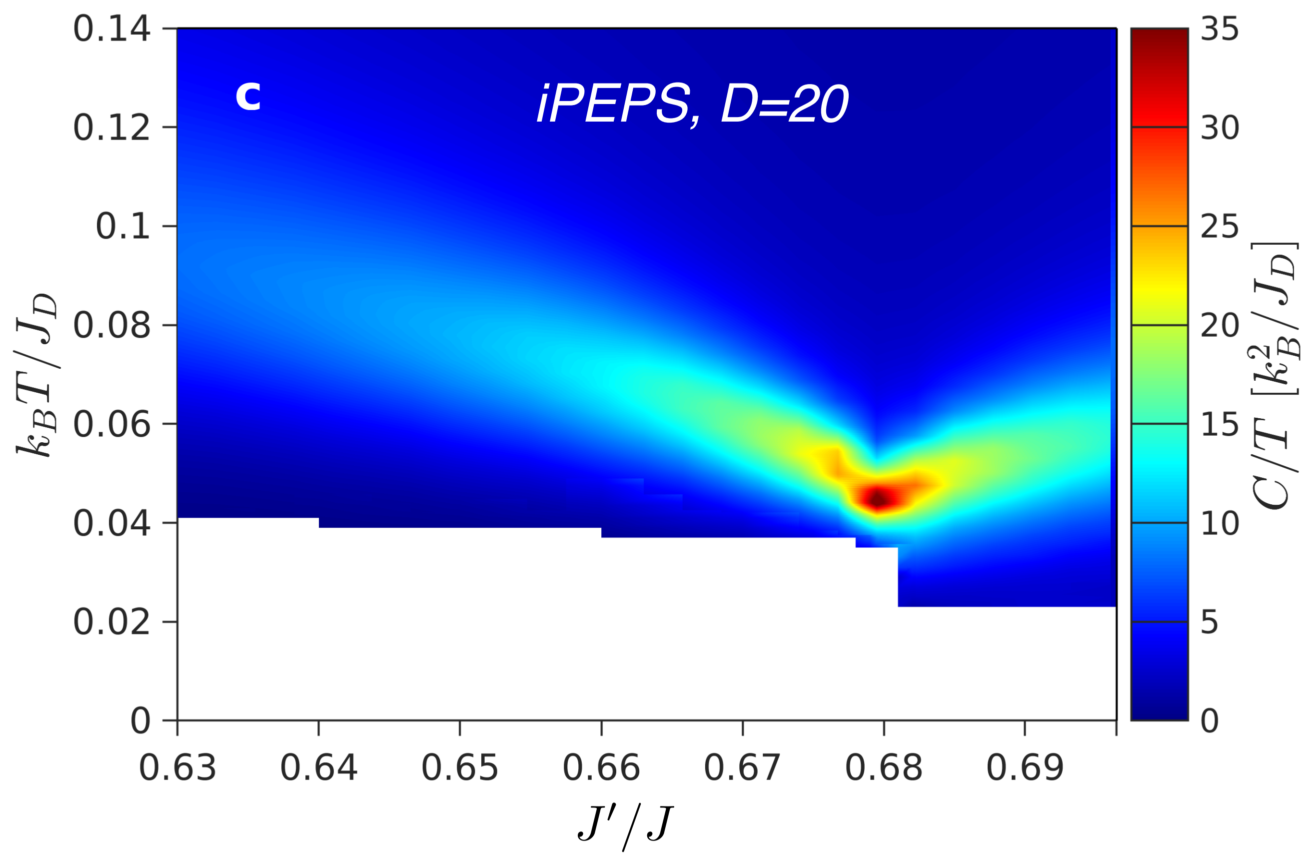
Guo, et al., PRL 124, 206602 (2020)

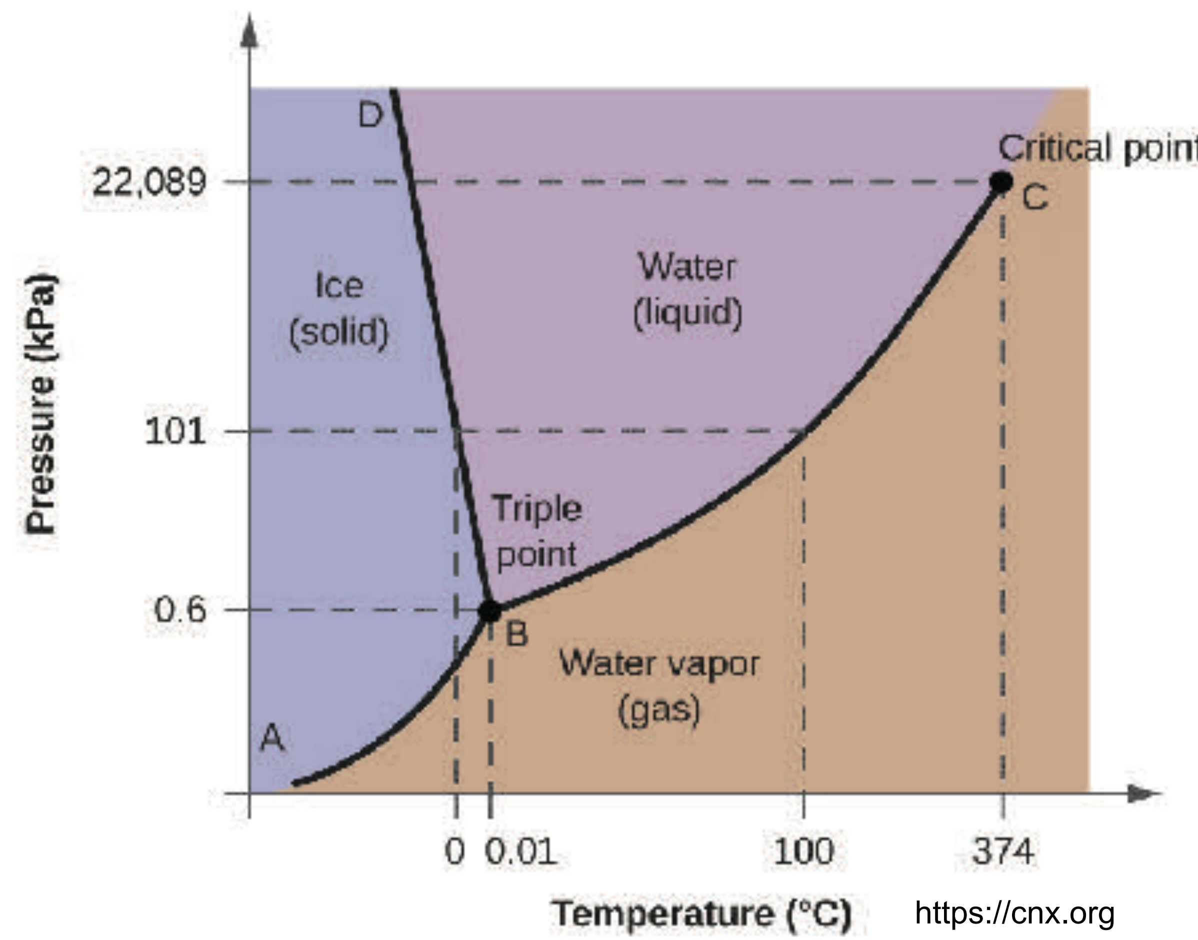
Waki, et al. J. Phys. Soc. Jpn. 76, 073710 (2007)
Haravifard, et al. Nat. Commun. 7, 11956 (2016)
Zayed, et al., Nat. Phys. 13, 962 (2017)
Sakurai, et al., J. Phys. Soc. Jpn. 87, 033701 (2018)
Guo, et al., PRL 124, 206602 (2020)
Bettler, et al,. Phys. Rev. Research 2, 012010 (2020)

Specific heat data (group of H. M. Rønnow)

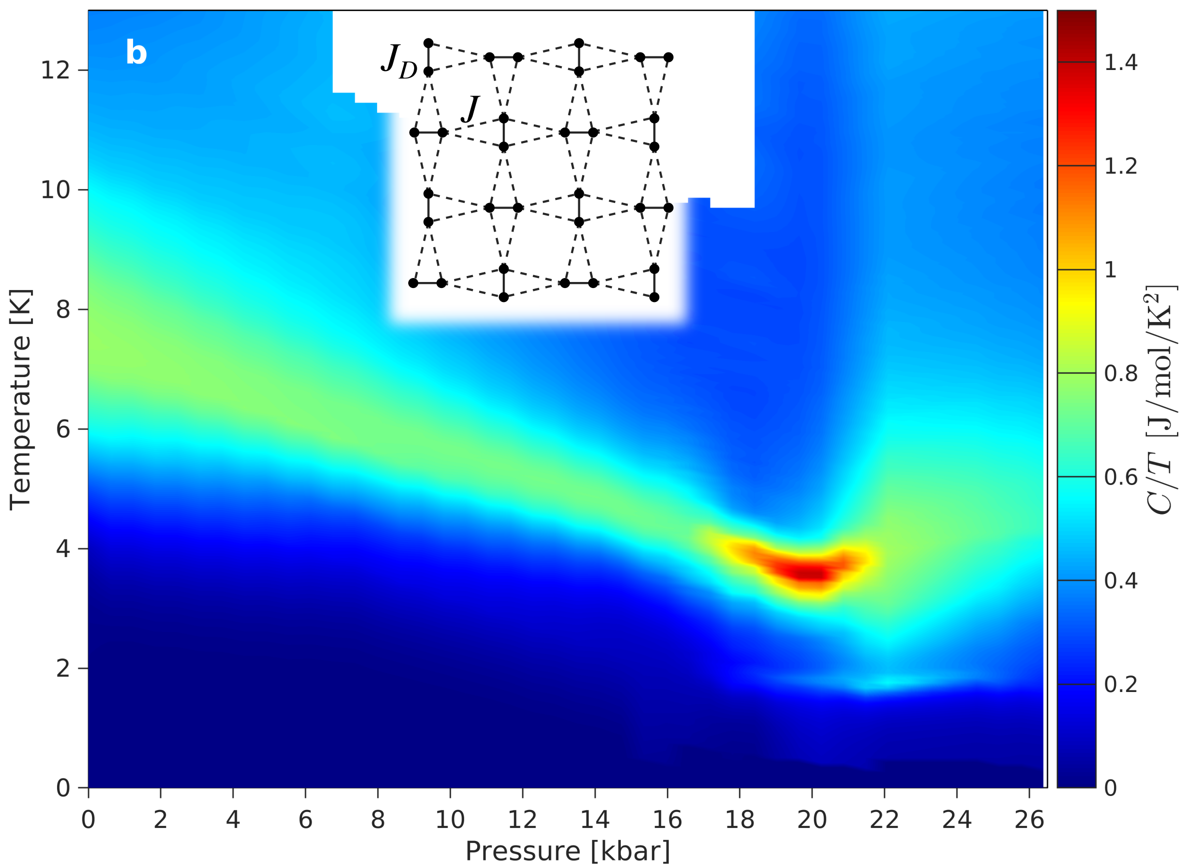


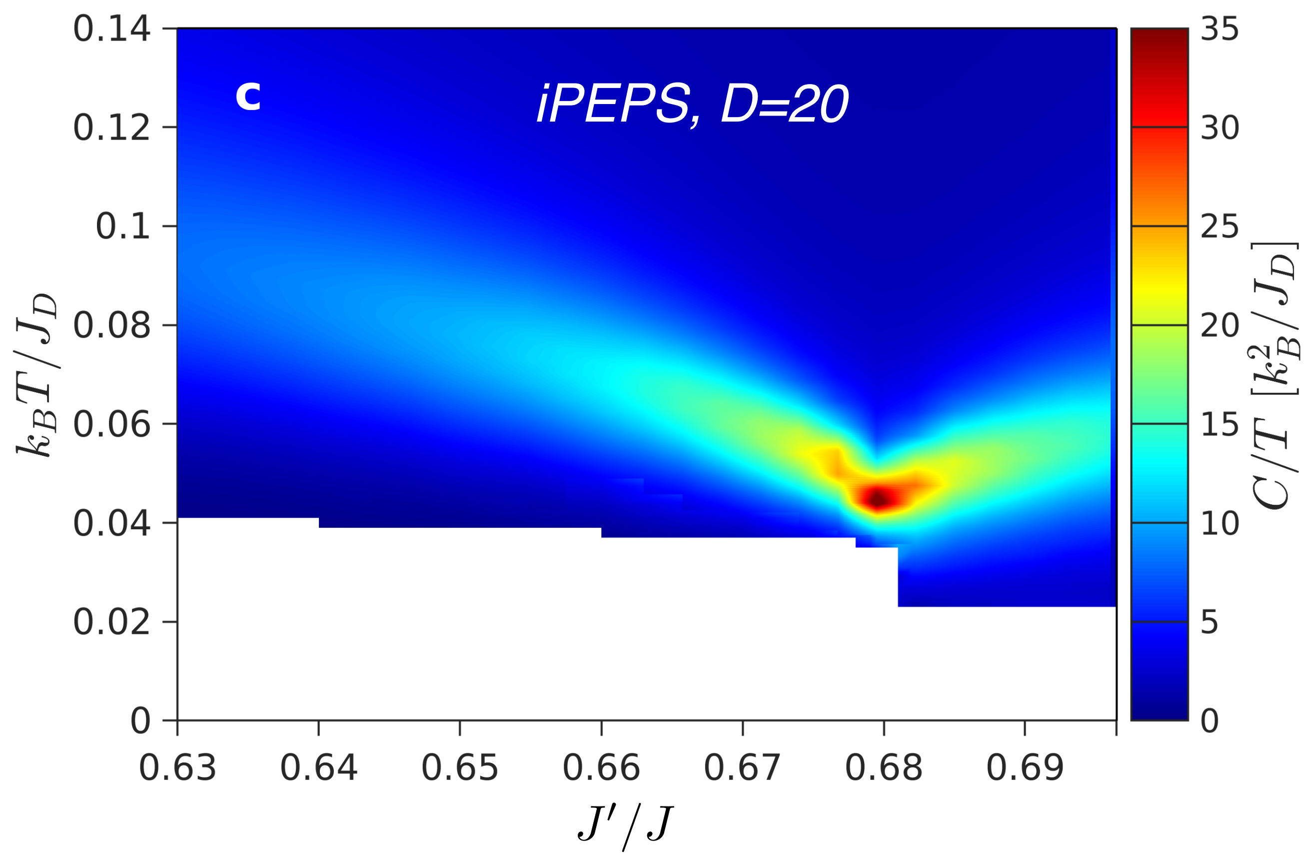


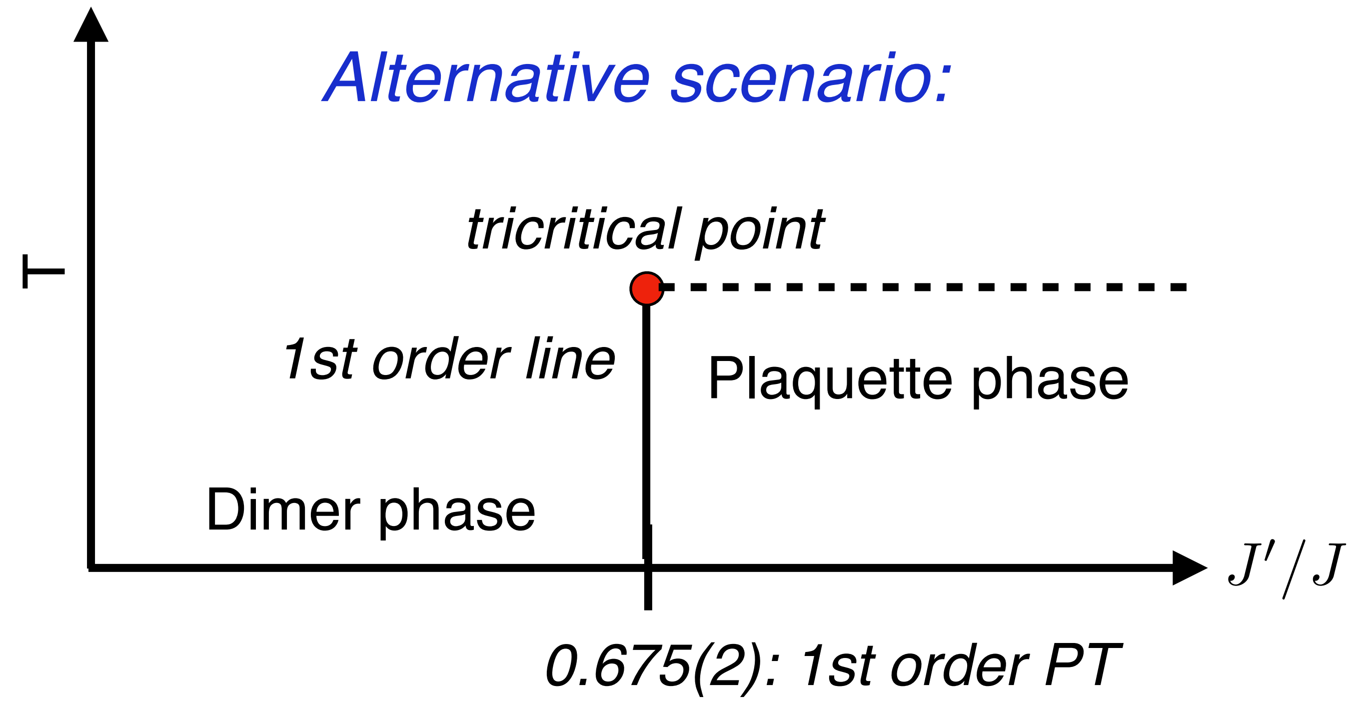


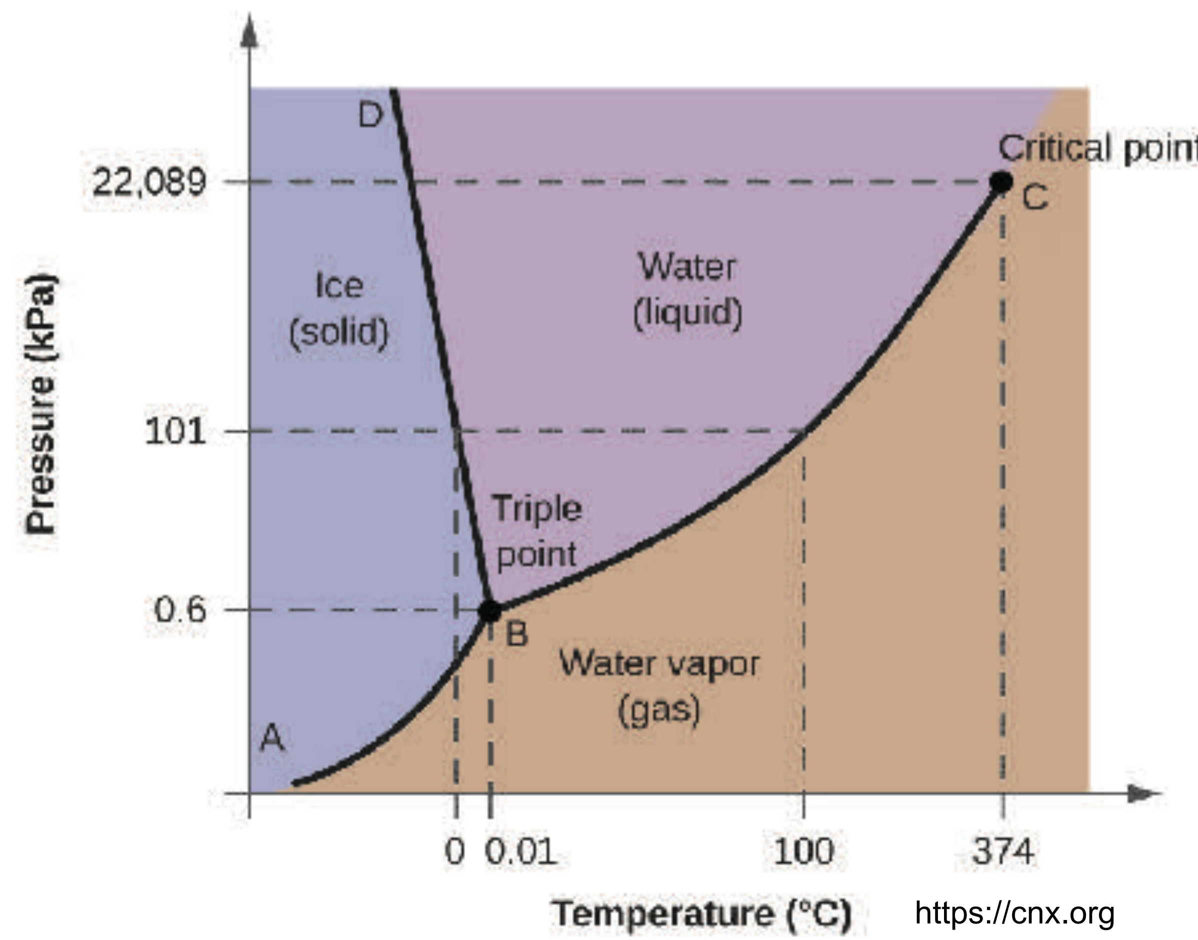


Specific heat data (group of H. M. Rønnow)





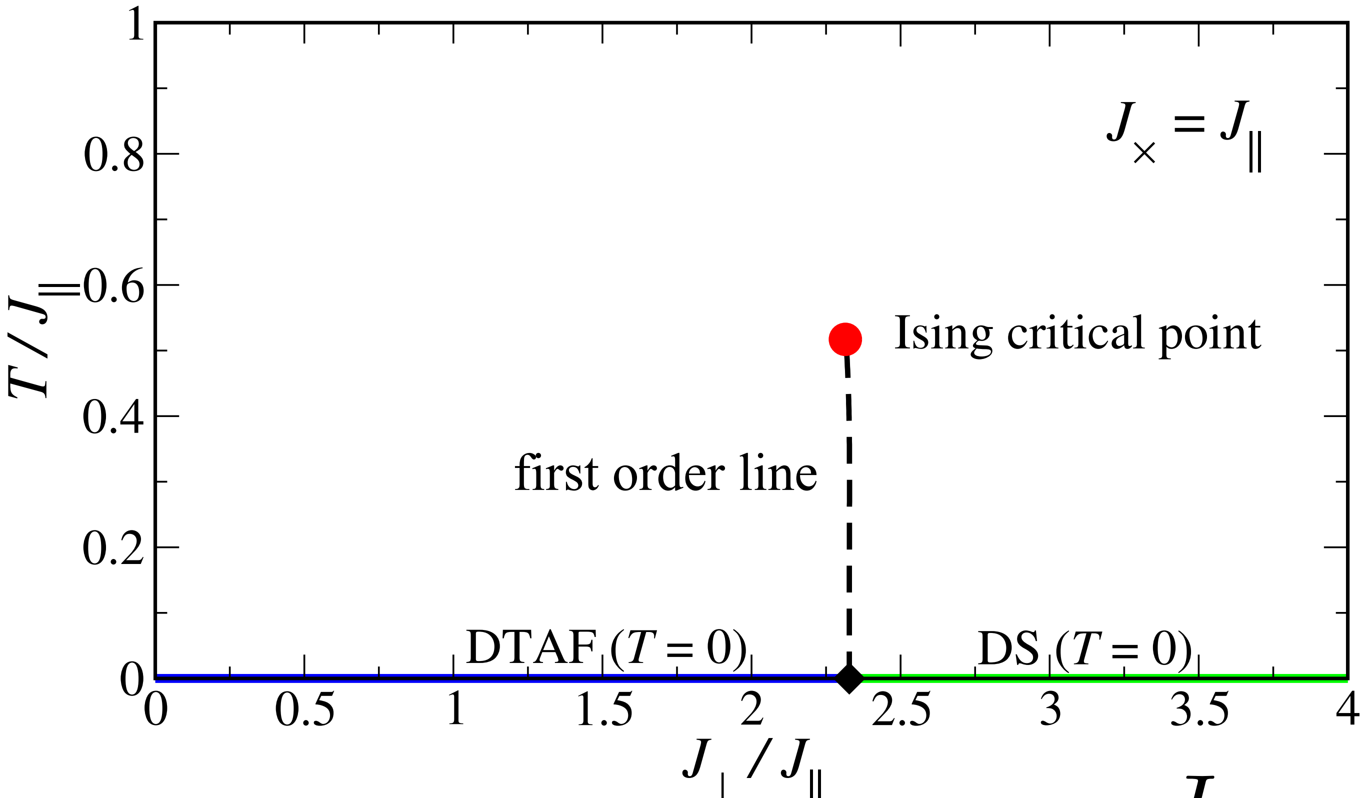


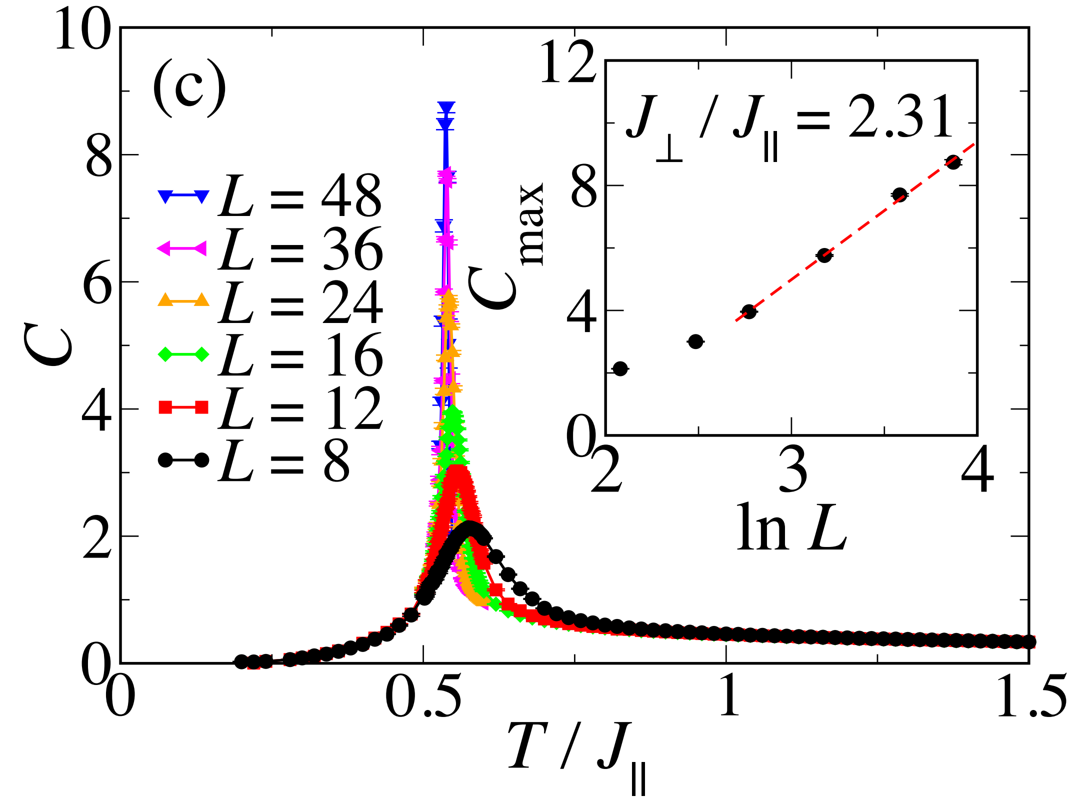


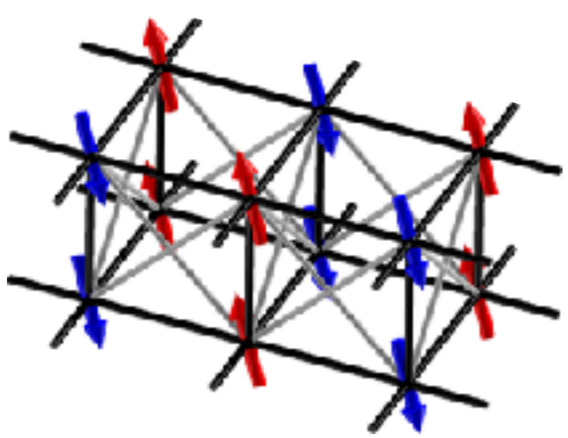
https://cnx.org

Inspiration: fully frustrated Heisenberg bilayer model

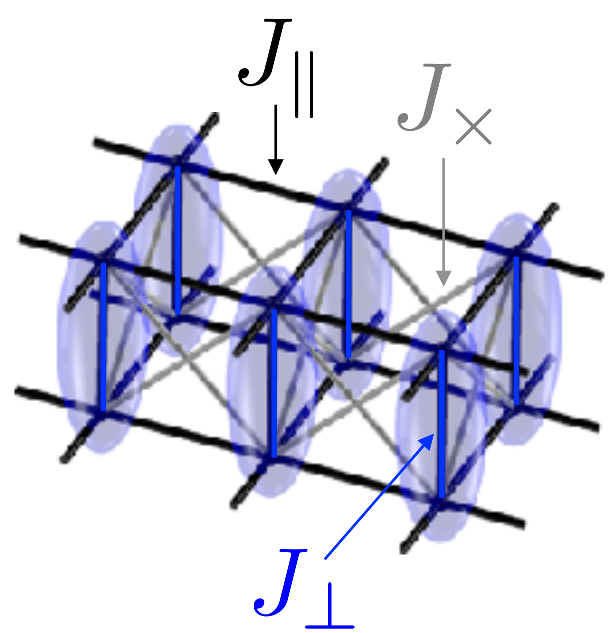
Stapmanns, PC, Mila, Honecker, Normand, and Wessel, PRL 121 (2018)







Dimer triplets

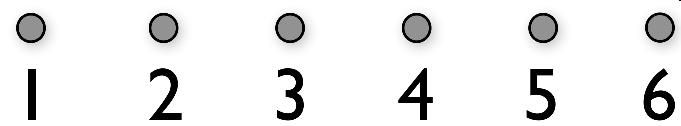


Dimer singlets

Jump in $\langle S \cdot S \rangle$ on a dimer at the phase transition

Tensor network ansatz for a wave function

Lattice:



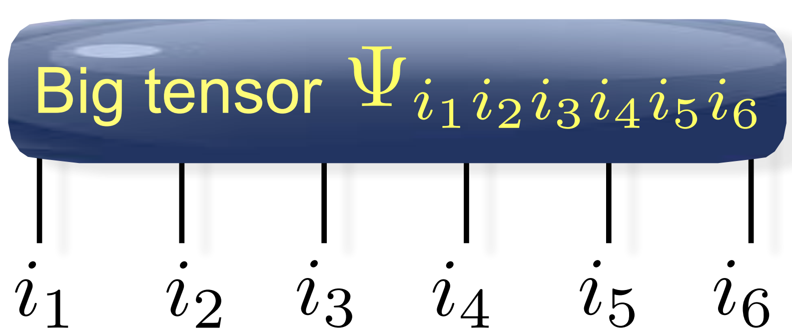
2 basis states per site: $\{|\uparrow\rangle, |\downarrow\rangle\}$

2^6 basis states

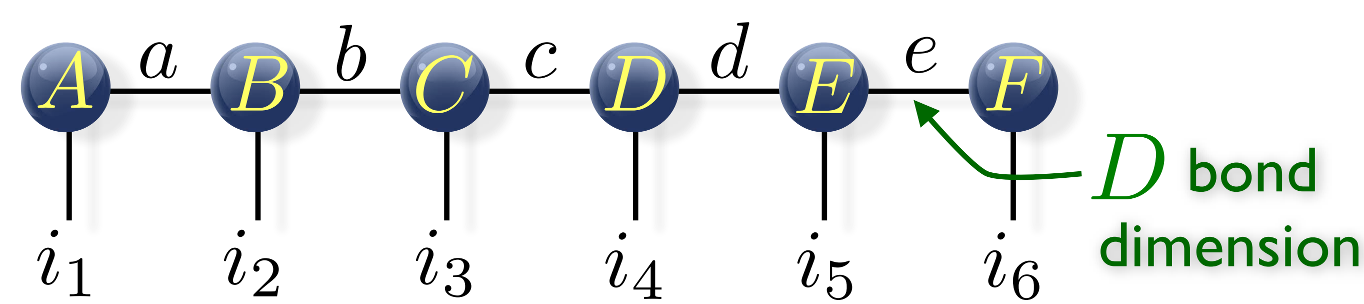
2^6 coefficients

State: $$|\Psi\rangle = \sum_{i_1 i_2 i_3 i_4 i_5 i_6} \Psi_{i_1 i_2 i_3 i_4 i_5 i_6} |i_1 \otimes i_2 \otimes i_3 \otimes i_4 \otimes i_5 \otimes i_6\rangle$$

Tensor/multidimensional array



Tensor network: matrix product state (**MPS**)



$$\Psi_{i_1 i_2 i_3 i_4 i_5 i_6} \approx \sum_{abcde} A^{a}_{i_1} B^{ab}_{i_2} C^{bc}_{i_3} D^{cd}_{i_4} E^{de}_{i_5} F^{e}_{i_6} = \tilde{\Psi}_{i_1 i_2 i_3 i_4 i_5 i_6}$$

exp(N) many numbers ***vs*** poly(D,N) numbers

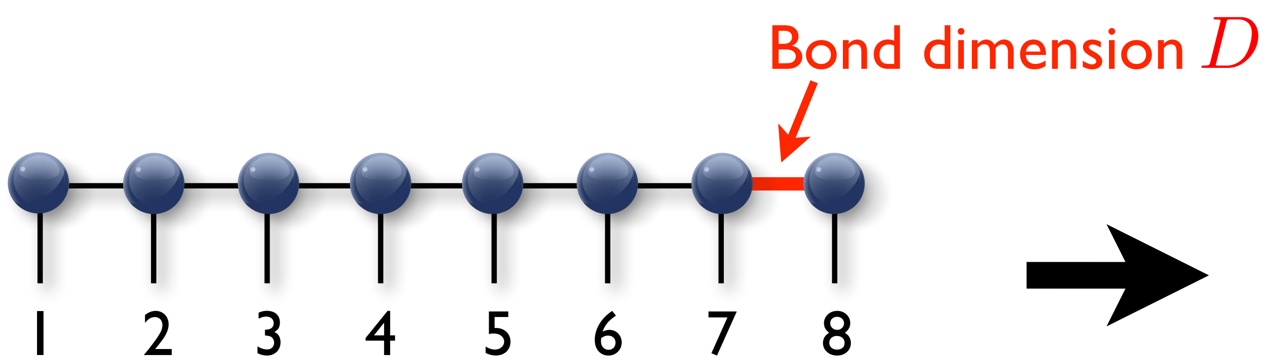
Efficient representation!

MPS & PEPS

1D

MPS

Matrix-product state



Physical indices (lattices sites)

S. R. White, PRL 69, 2863 (1992)

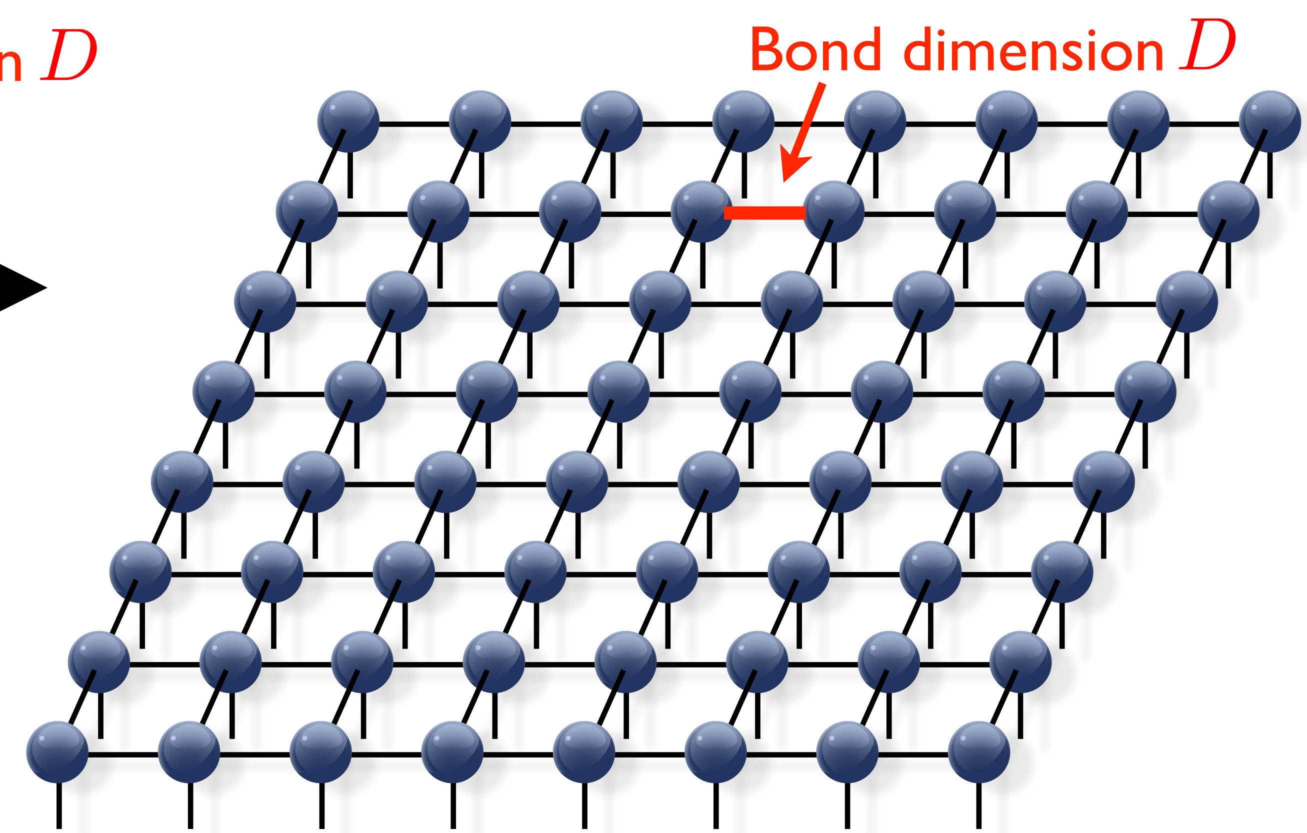
Fannes et al., CMP 144, 443 (1992)

Östlund, Rommer, PRL 75, 3537 (1995)

2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)



F. Verstraete, J. I. Cirac, cond-mat/0407066

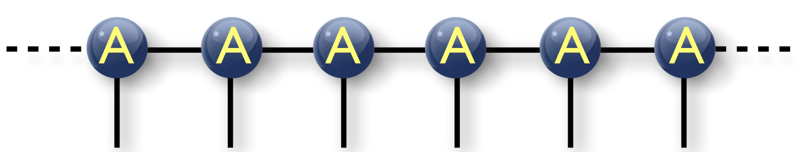
Nishio, Maeshima, Gendiar, Nishino, cond-mat/0401115

Infinite PEPS (iPEPS)

1D

iMPS

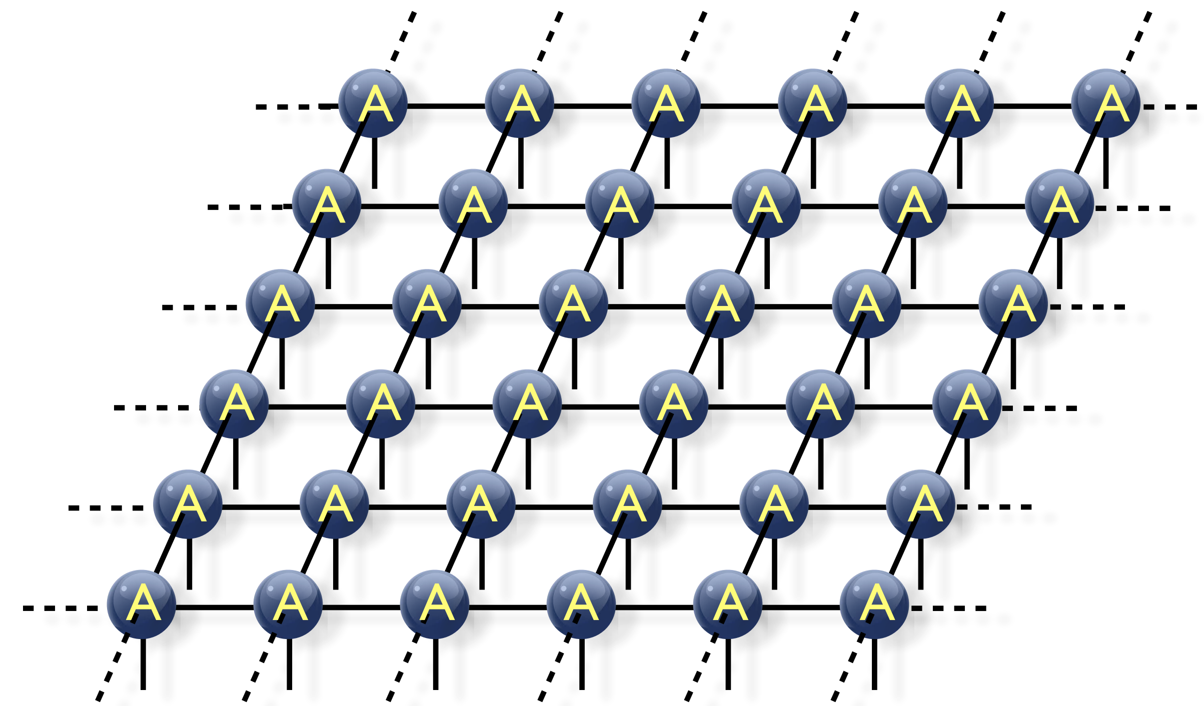
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



Jordan, Orus, Vidal, Verstraete, Cirac, PRL (2008)

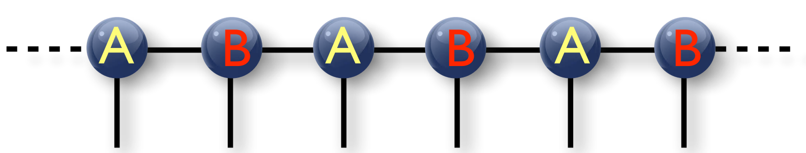
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

Infinite PEPS (iPEPS)

1D

iMPS

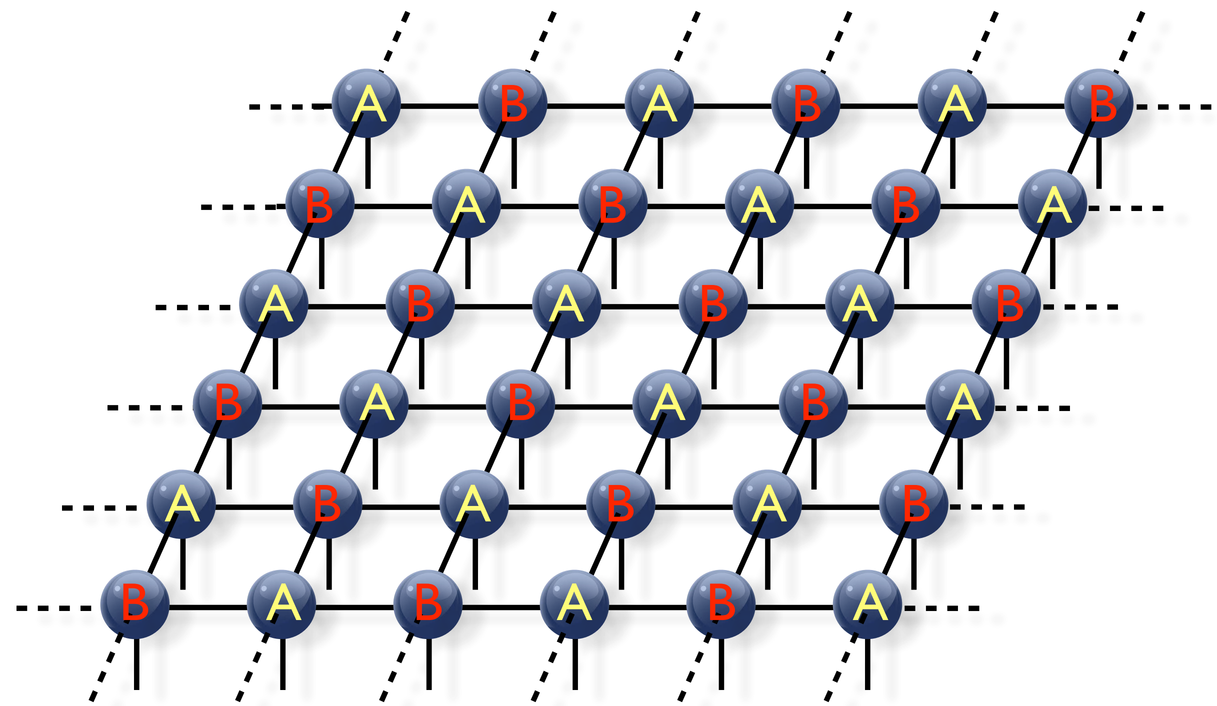
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



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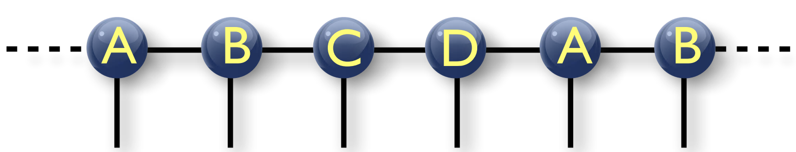
infinite PEPS (iPEPS)

1D

iMPS

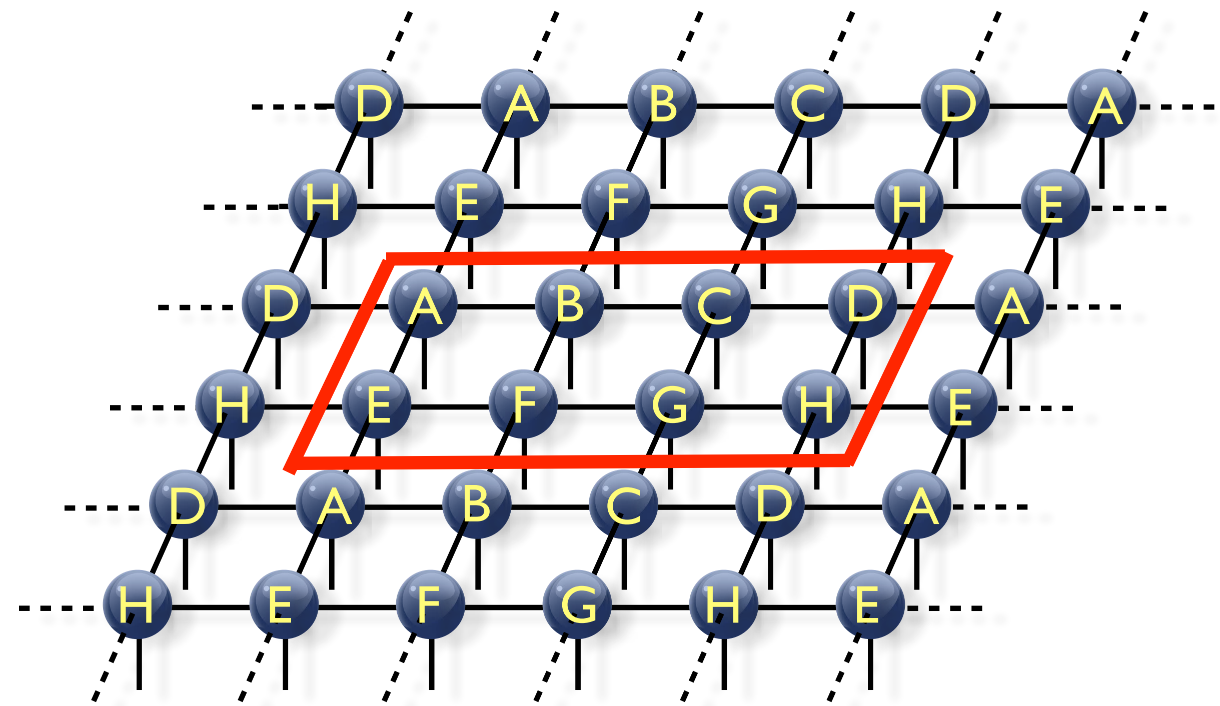
infinite matrix-product state



2D

iPEPS

with arbitrary unit cell of tensors

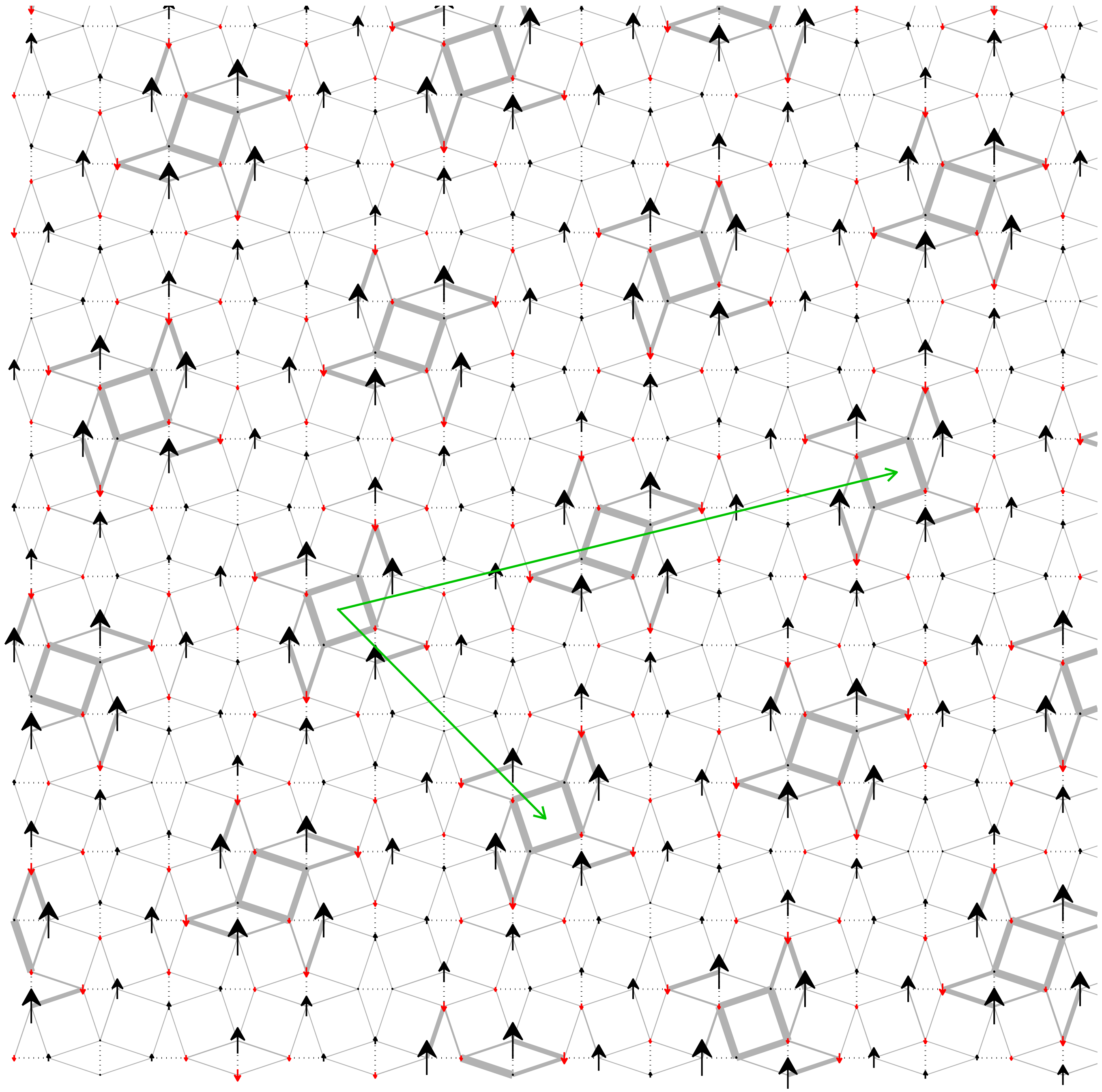


here: 4x2 unit cell

Jordan, Orus, Vidal, Verstraete, Cirac, PRL (2008)

PC, White, Vidal, Troyer, PRB **84** (2011)

2/15 plateau in the Shastry-Sutherland model



Unit cell with 30 tensors (60 sites)

★ Crystal of triplet bound states

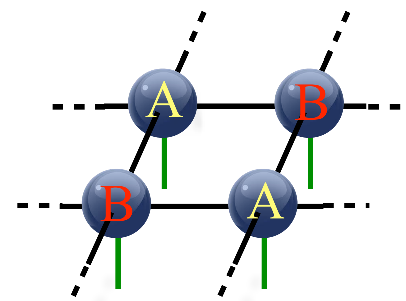
PC, F. Mila, PRL **112** (2014)

Finite temperature simulations with iPEPS

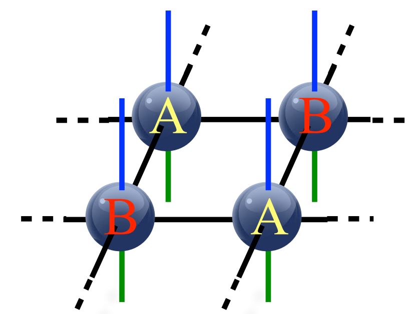
- Methodological developments (2D):

  Li et al. PRL 106 (2011); Czarnik et al. PRB 86 (2012); Czarnik & Dziarmaga PRB 90 (2014); Czarnik & Dziarmaga PRB 92 (2015); Czarnik et al. PRB 94 (2016); Dai et al PRB 95 (2017); Kshetrimayum, Rizzi, Eisert, Orus, PRL 122 (2019), P. Czarnik, J. Dziarmaga, PC, PRB 99 (2019), …

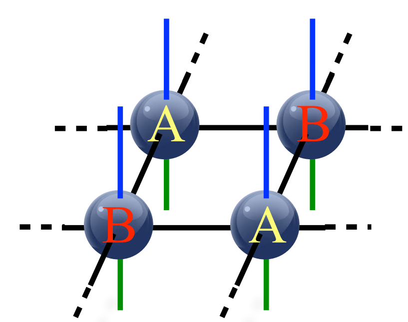
- Wave-function: $|\Psi\rangle \approx$



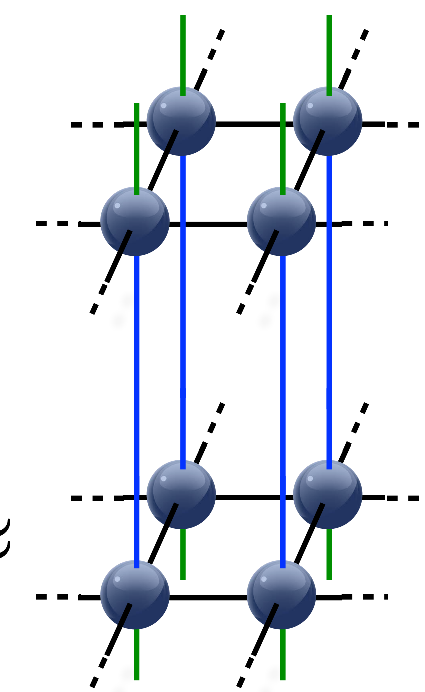
- Density-operator: $\hat{\rho} = e^{-\beta \hat{H}} \approx$



- Symmetric form: $e^{-\beta \hat{H}/2} \approx$



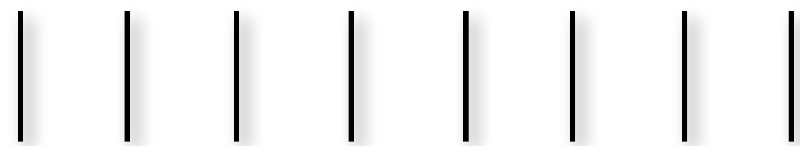
$\hat{\rho}(\beta) \approx$



$$\hat{\rho}(\beta) = \hat{\rho}^{\dagger}(\beta)$$ by construction

Imaginary time evolution

- Start at infinite temperature: $\hat{\rho}(\beta = 0) = \mathbb{I}$

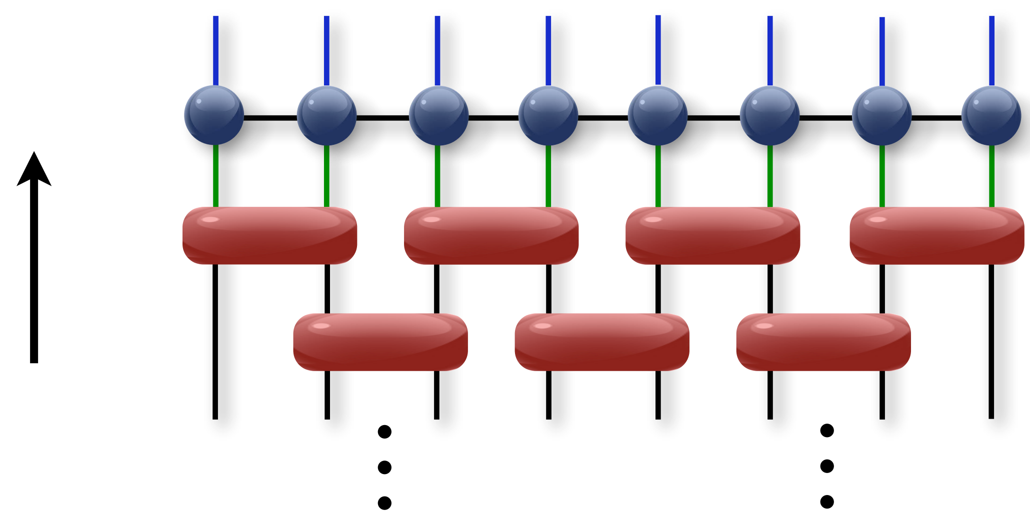
- Initial state:  exact!

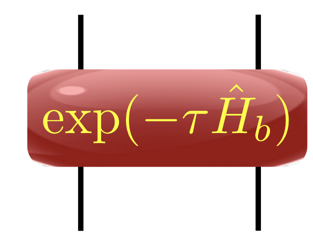
- Evolve in imaginary time: $\hat{\rho}(\beta) = e^{-\beta \hat{H}/2} \hat{\rho}(0) e^{-\beta \hat{H}/2}$

Trotter-Suzuki decomposition:

$$\tau = \beta/n$$

$$\exp(-\beta \hat{H}) = \exp(-\beta \sum_b \hat{H}_b) = \left(\exp(-\tau \sum_b \hat{H}_b) \right)^n \approx \left(\prod_b \exp(-\tau \hat{H}_b) \right)^n$$





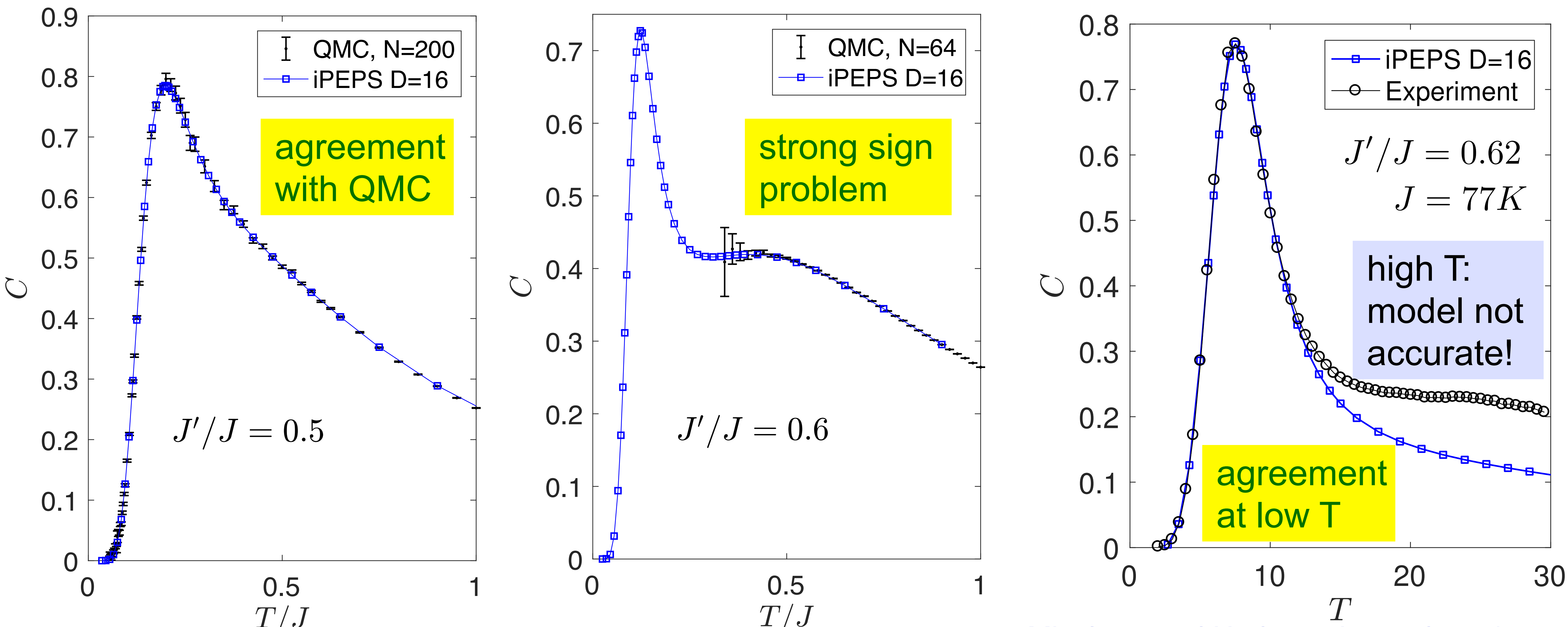
- Truncate after each step using e.g. simple / full update

- Evolve up to target $\beta/2$

Finite temperature simulations examples

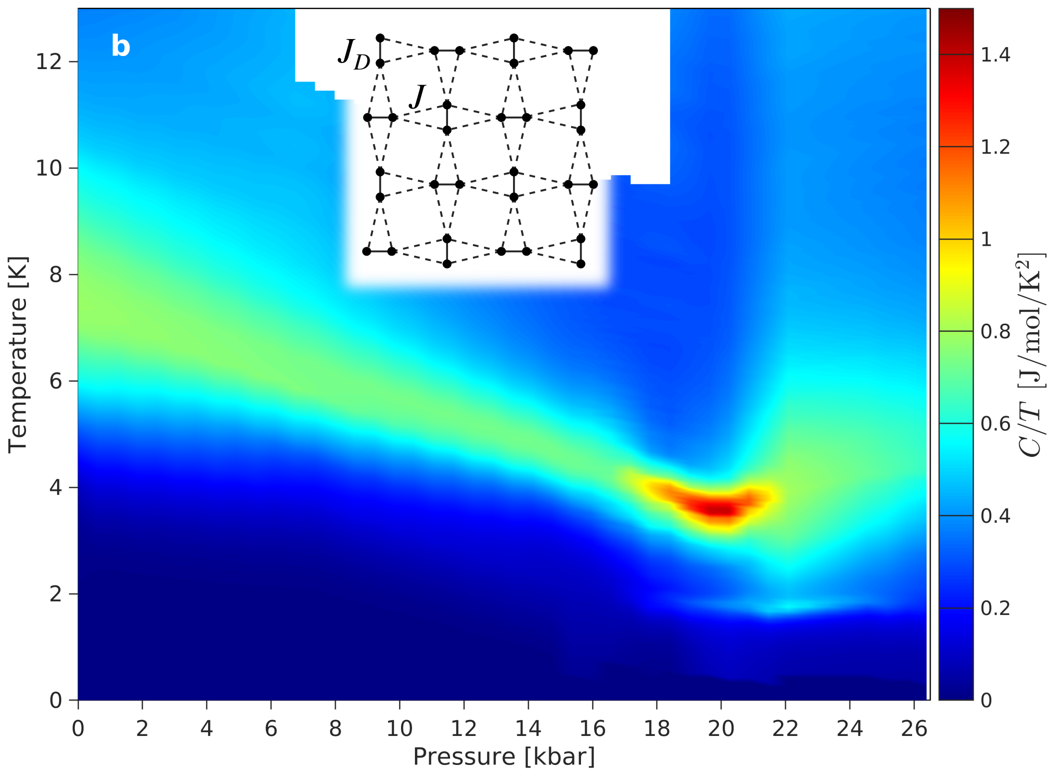
Wietek, PC, Wessel, Normand, Mila, and Honecker, PRR 1 (2019)

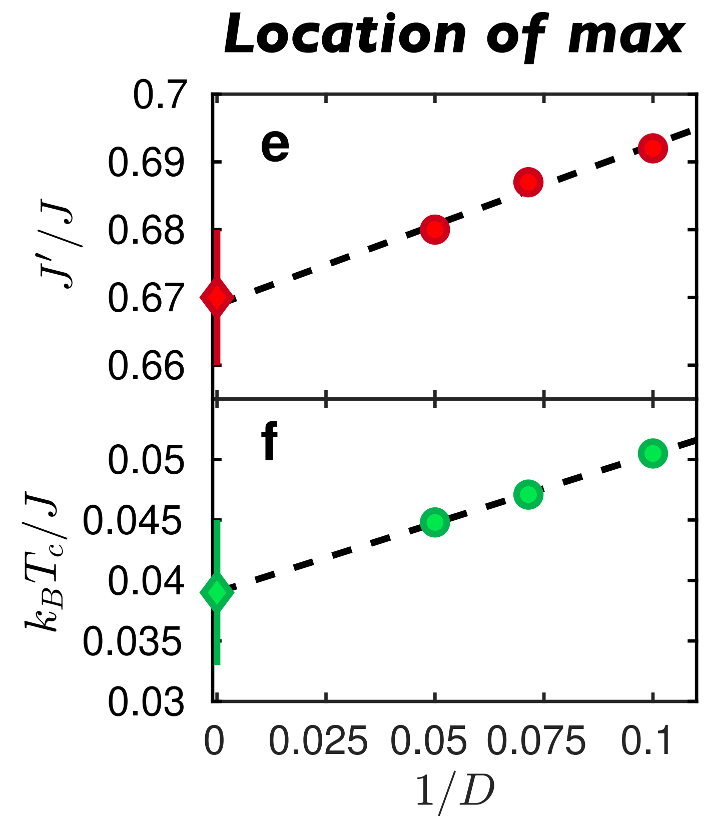
- Benchmarks in the dimer phase of the Shastry-Sutherland model
- Comparison between ED, TPQ, QMC, iPEPS



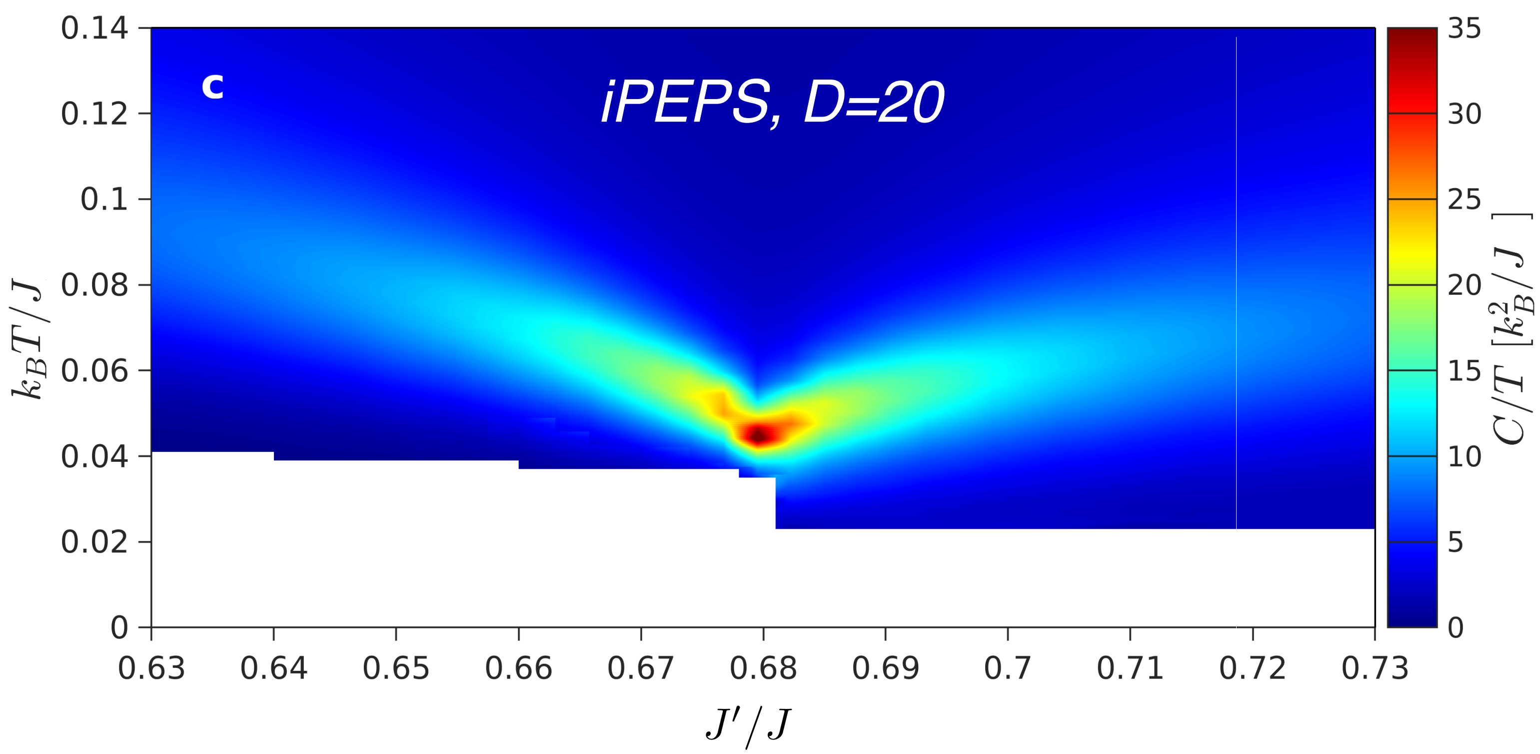
Miyahara and Ueda, arxiv:cond-mat/0004260

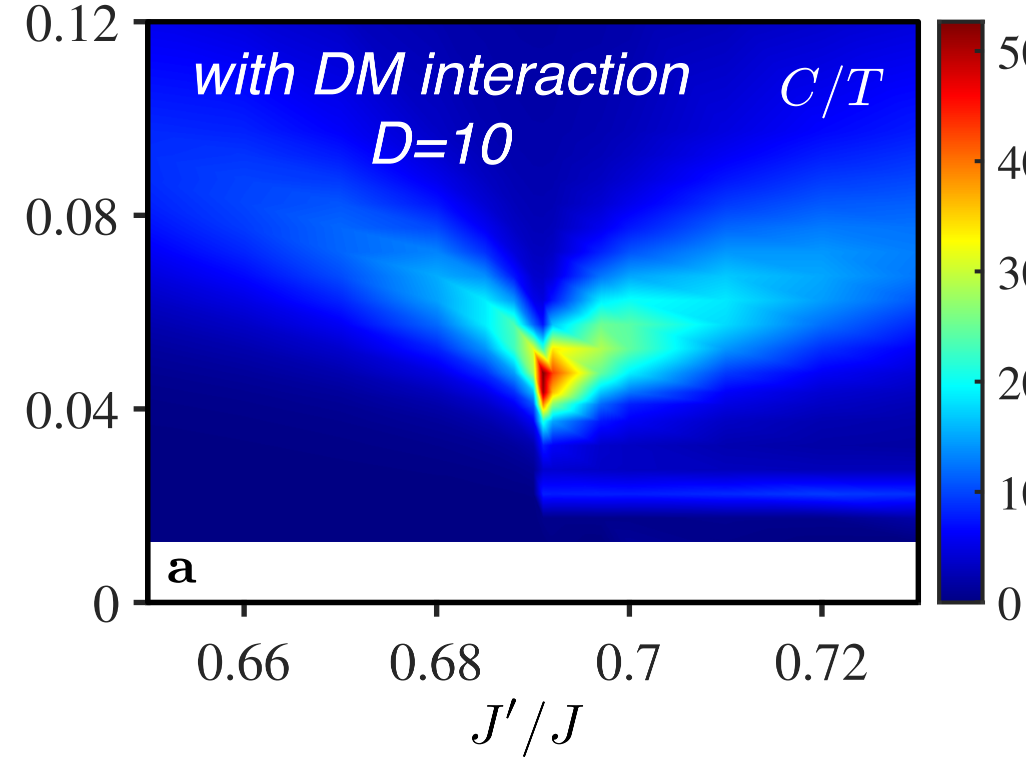
Specific heat: experiments vs iPEPS





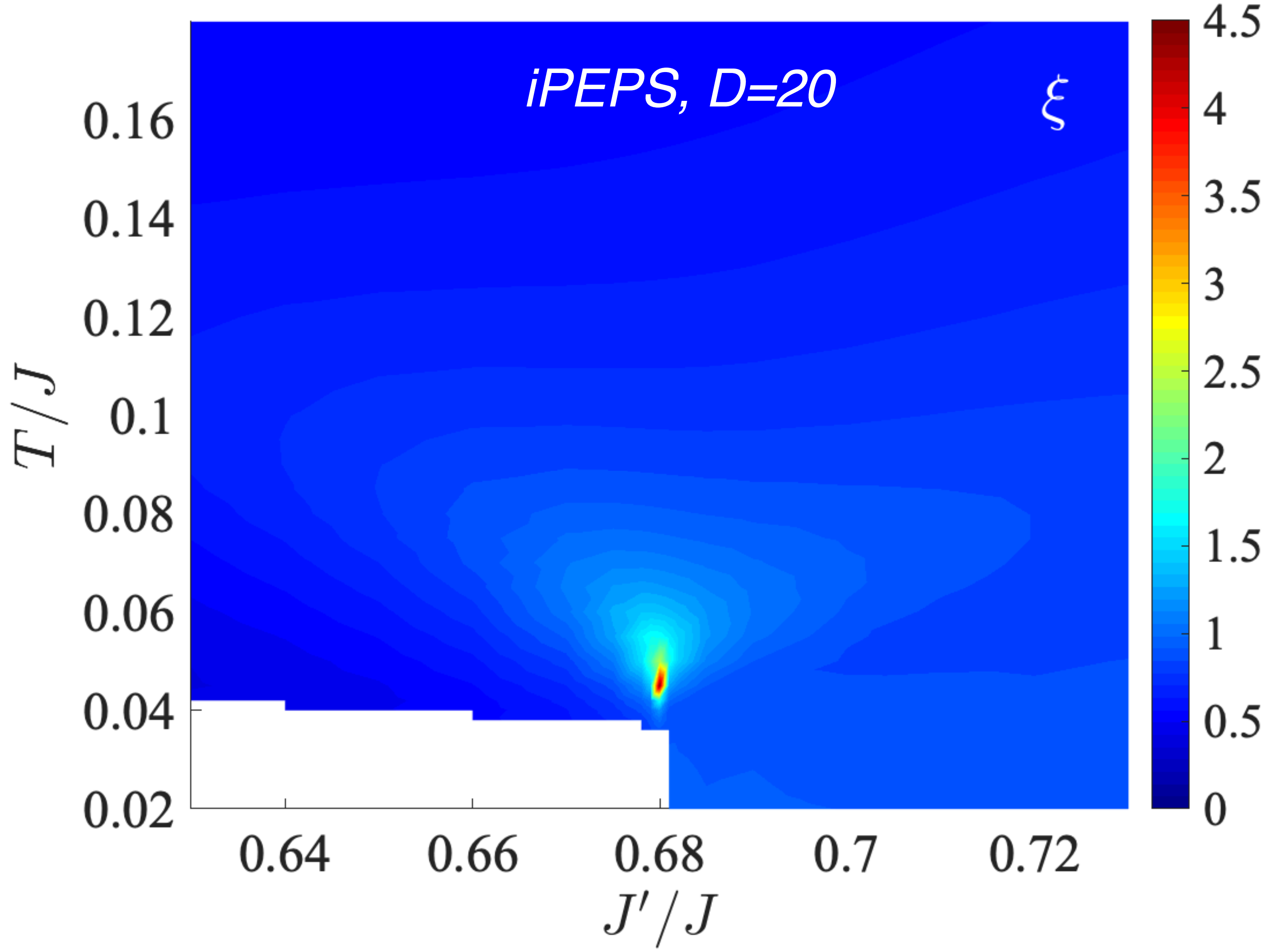
$T_c = 3.0(6)K$



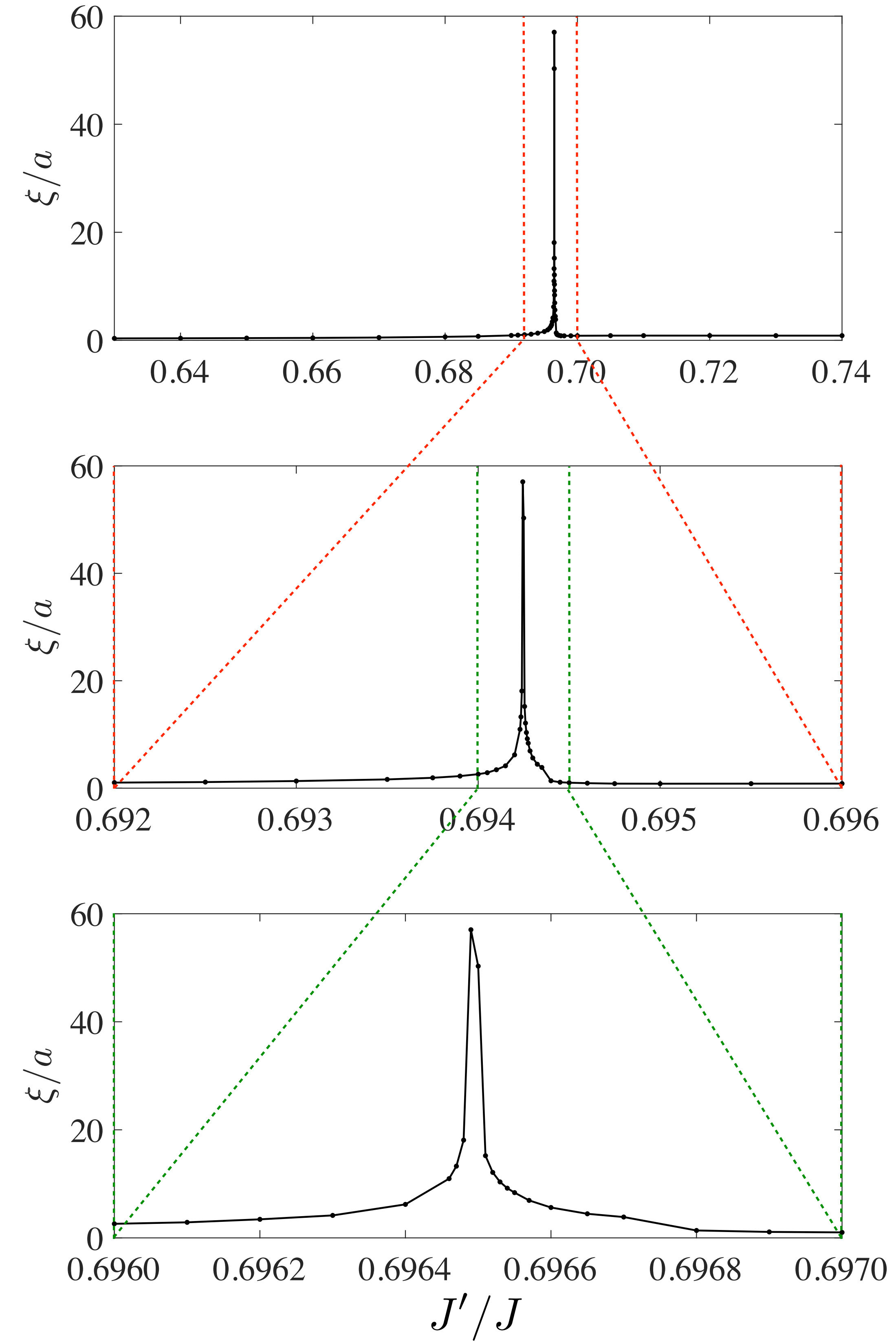


Larrea Jiménez et al., arxiv:2009:14492

Correlation length



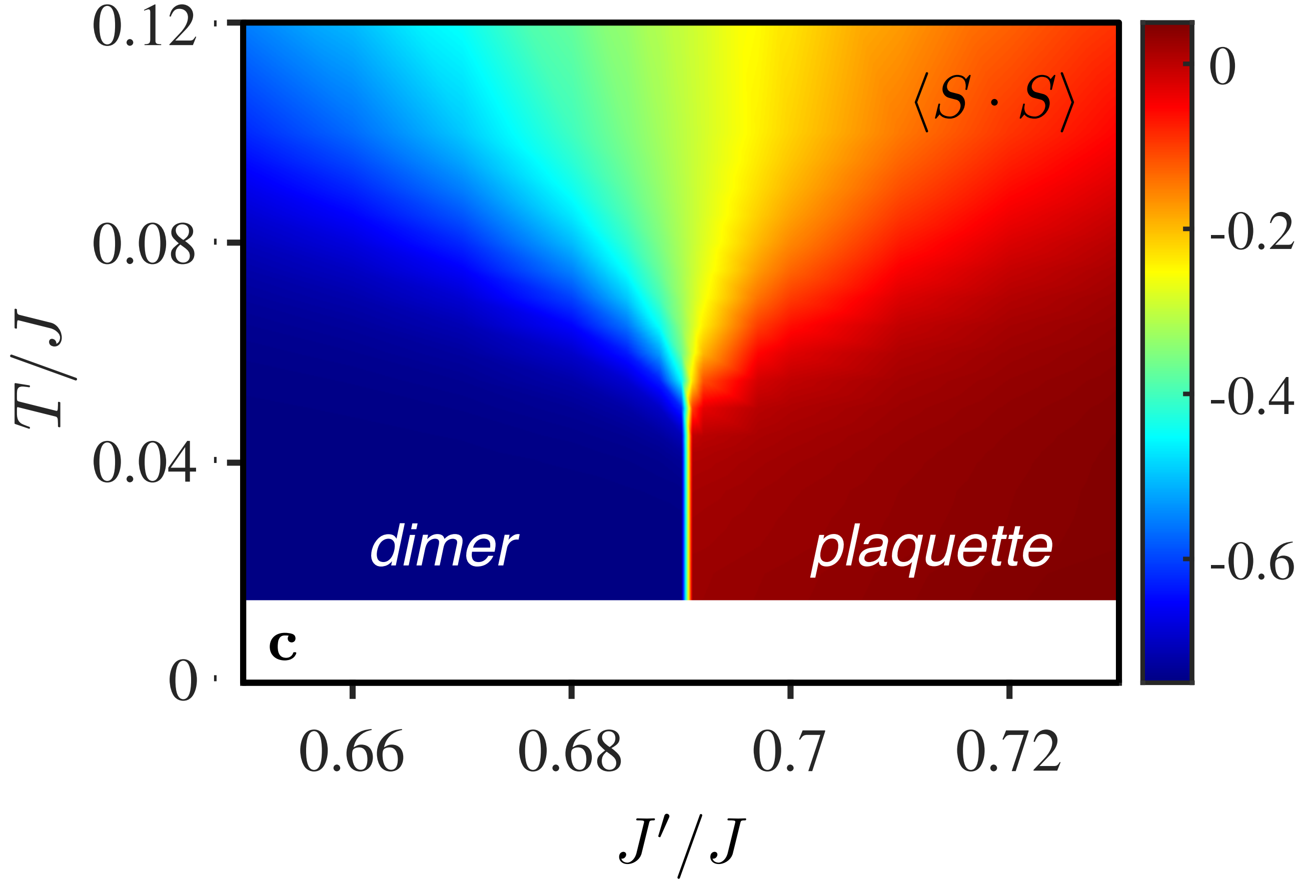
Zooming-in (D=8)



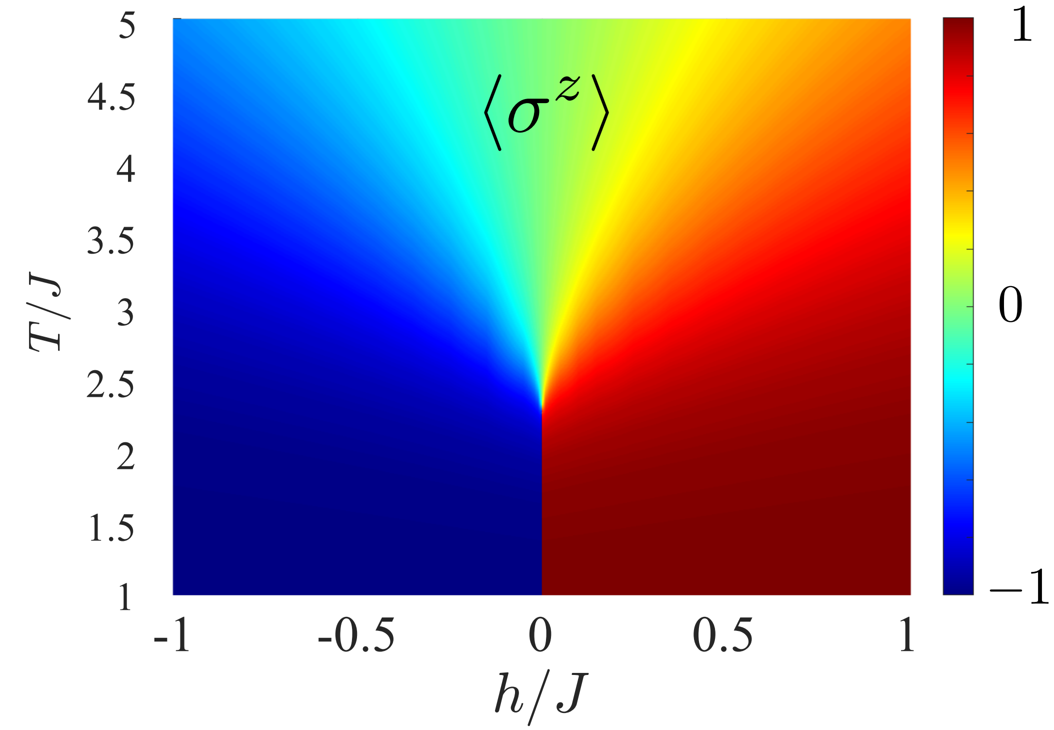
Diverging correlation length compatible with a critical point

Jump in <S · S> on dimer

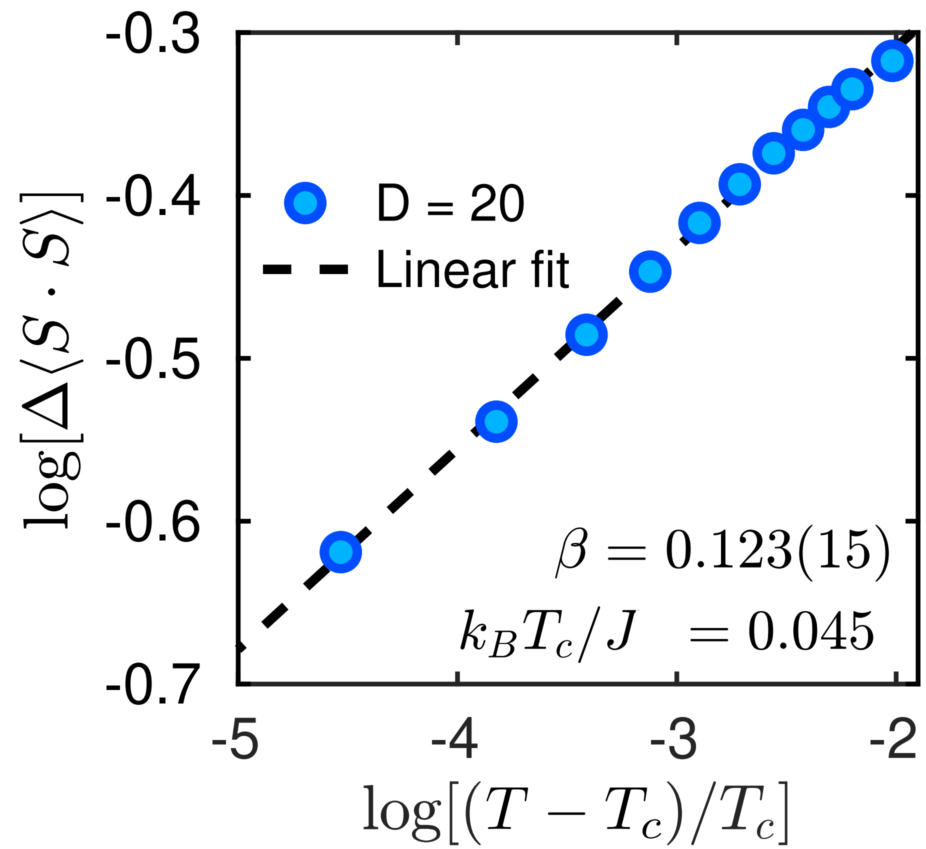
iPEPS D=10 (with DM)



2D classical Ising model in a field

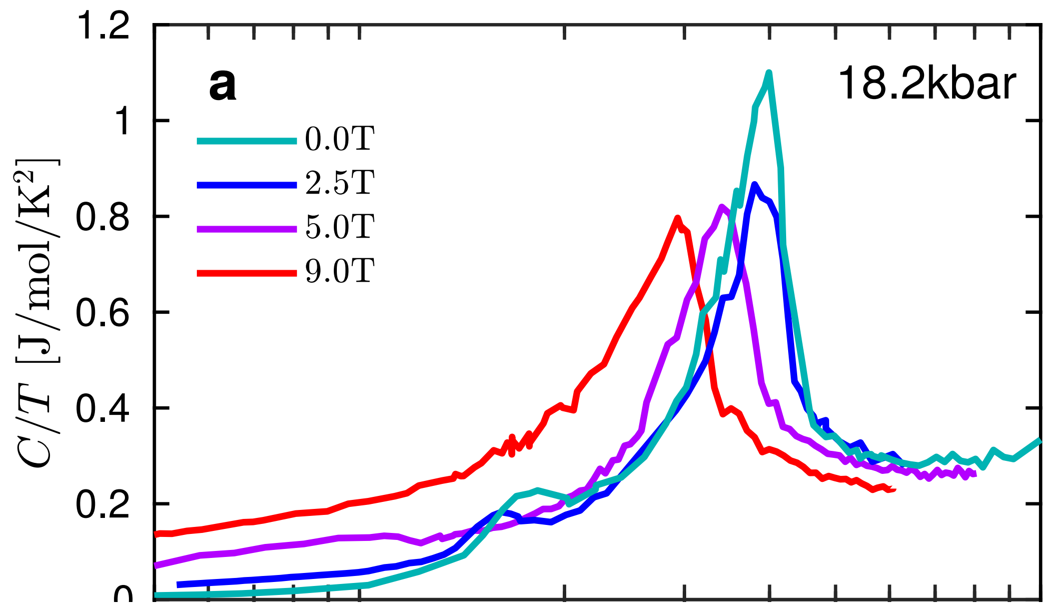


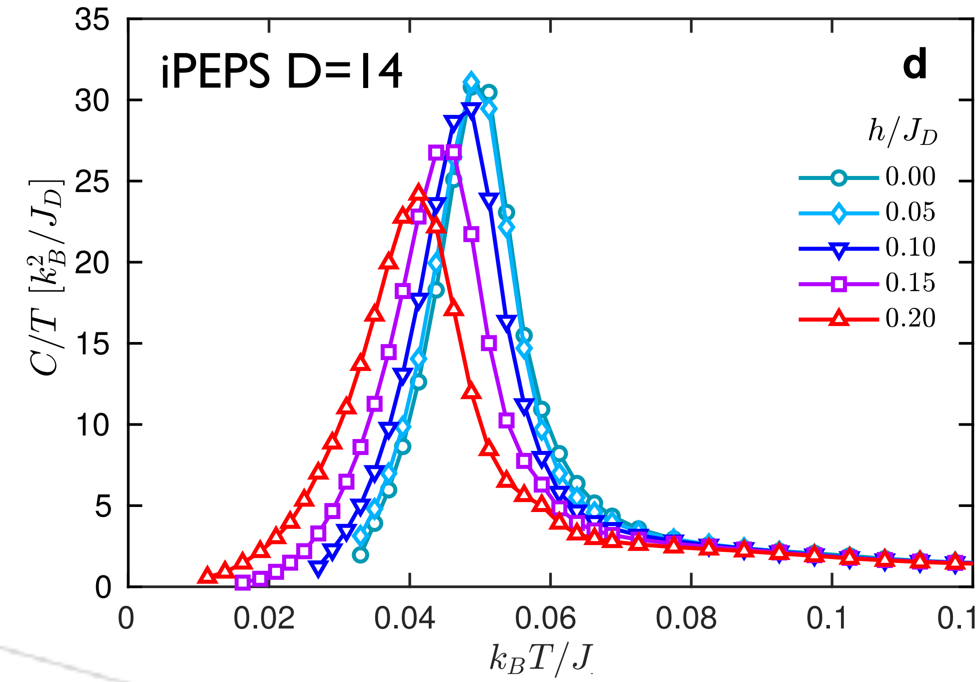
Clear evidence of a first order line with a critical point compatible with the 2D Ising universality class

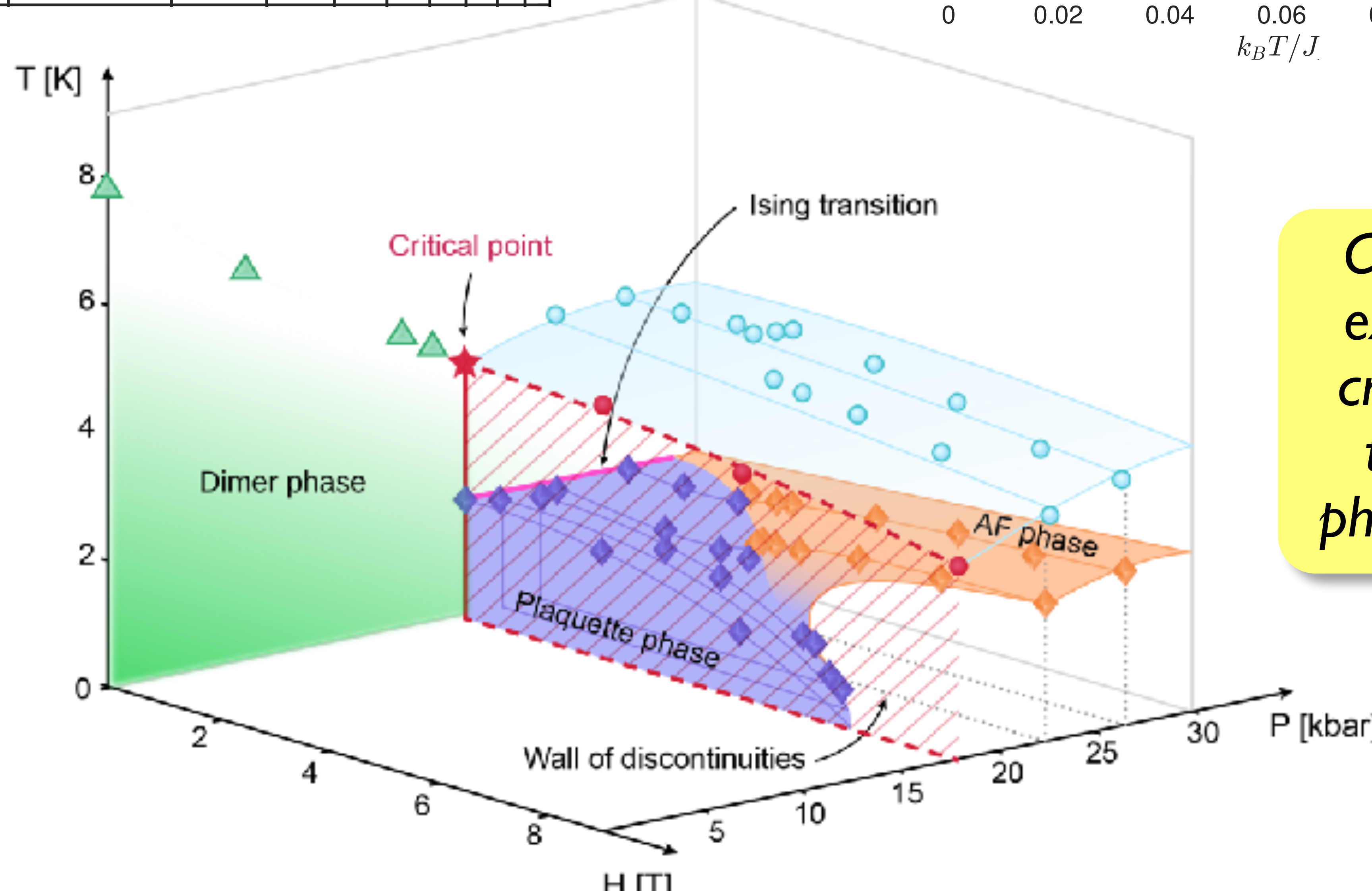


exact value:
$\beta = 0.125$

Effect of a finite magnetic field

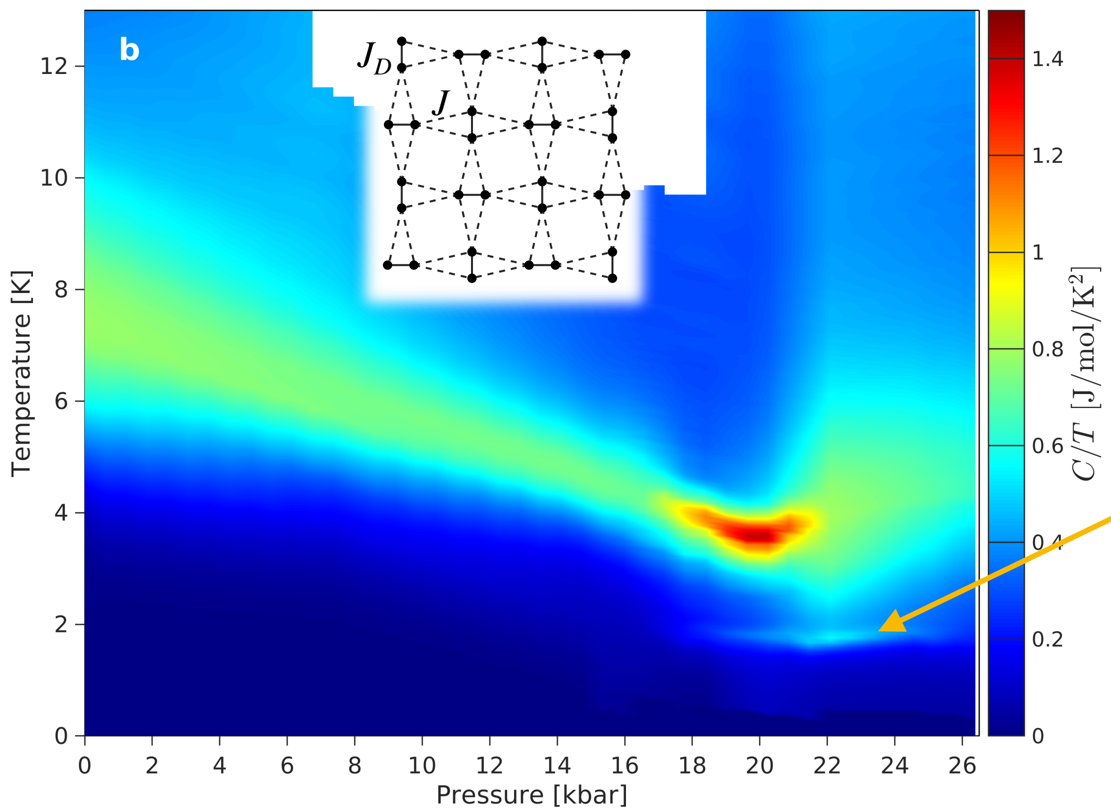




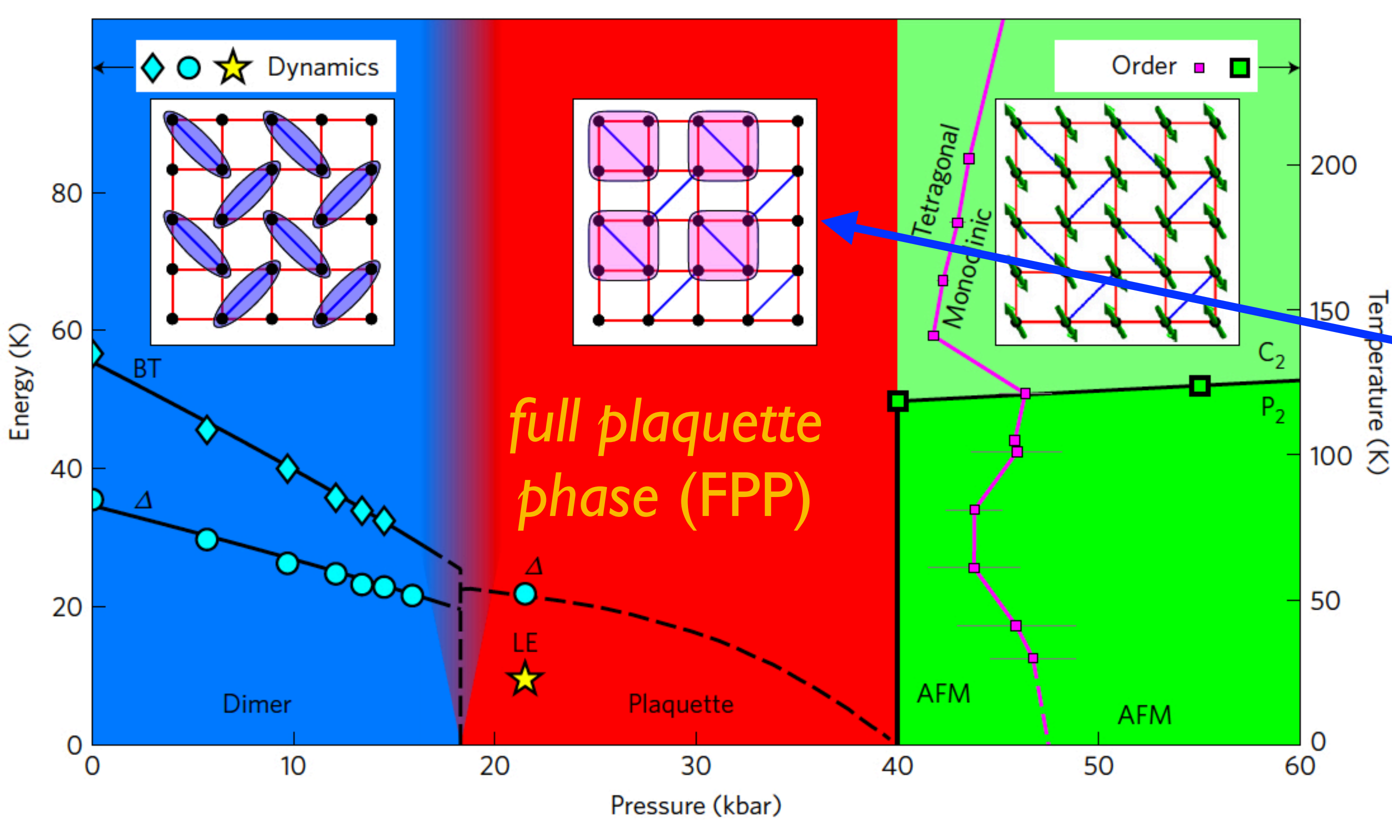


Critical point extends as a critical line in the (H,P,T) phase diagram

Open challenges

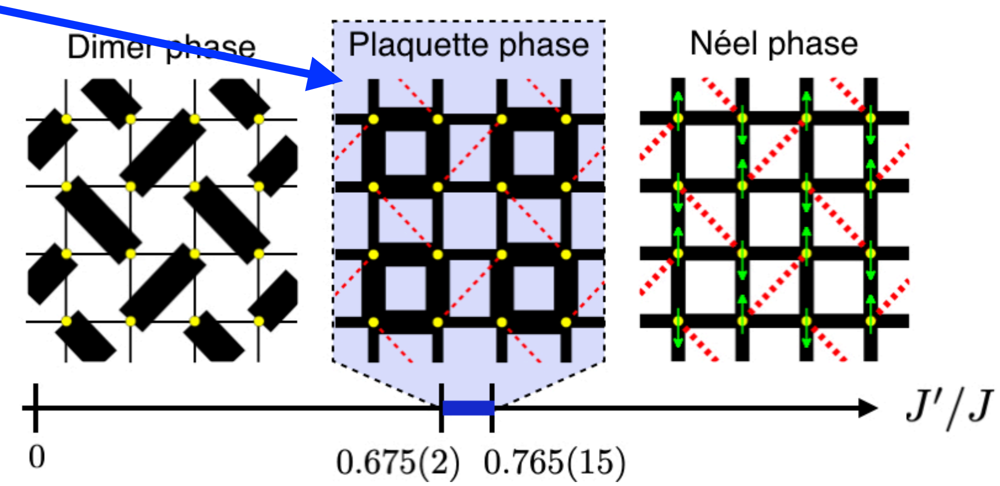


too low T to obtain reliable data with iPEPS (currently)



- Inelastic neutron scattering: *full plaquette phase* (FPP), not *empty plaquette phase* (EPP)

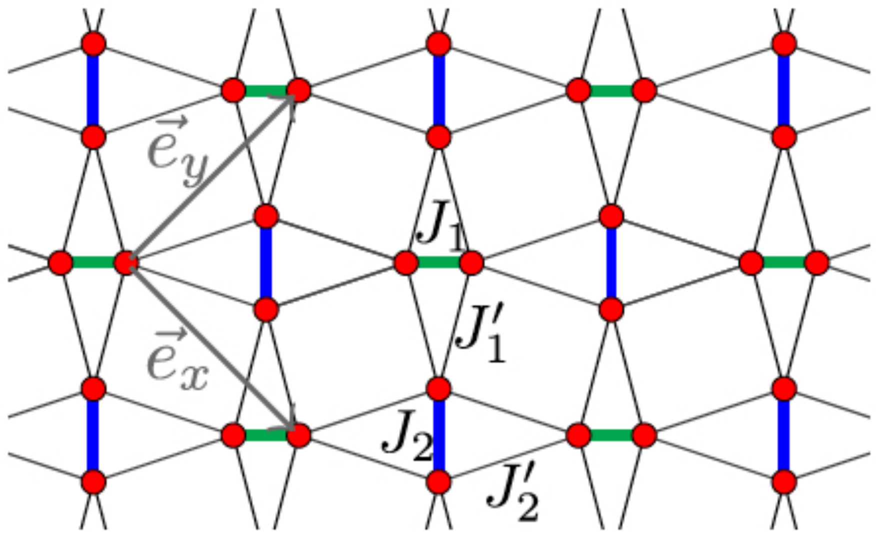
Zayed, et al., Nat. Phys. 13, 962 (2017)

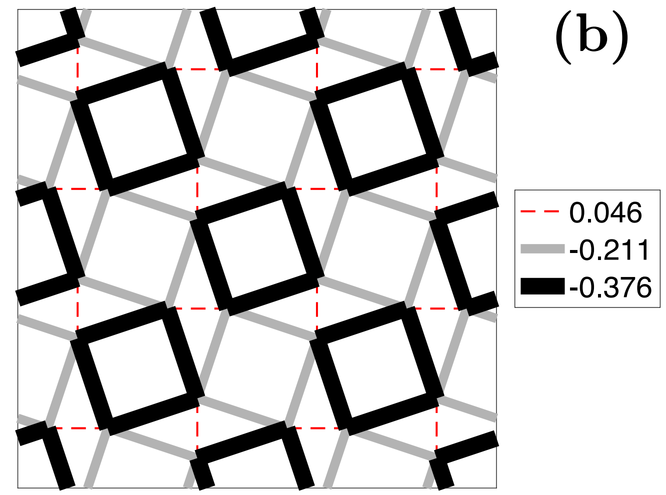


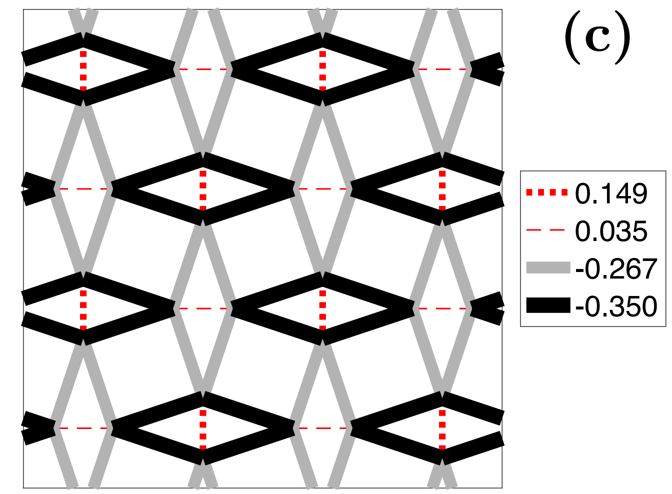
$SrCu_2(BO_3)_2$ under pressure

Boos, Crone, Niesen, PC, Schmidt & Mila, PRB 100 (2019)

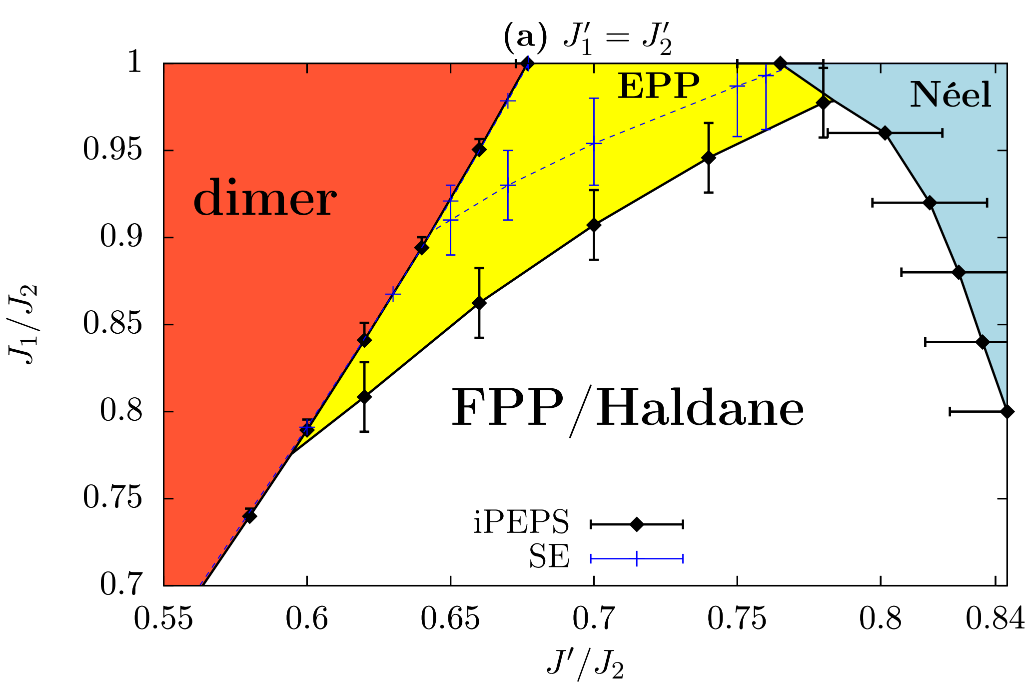
- Distorted Shastry-Sutherland model: *competition between EPP and FPP phase*

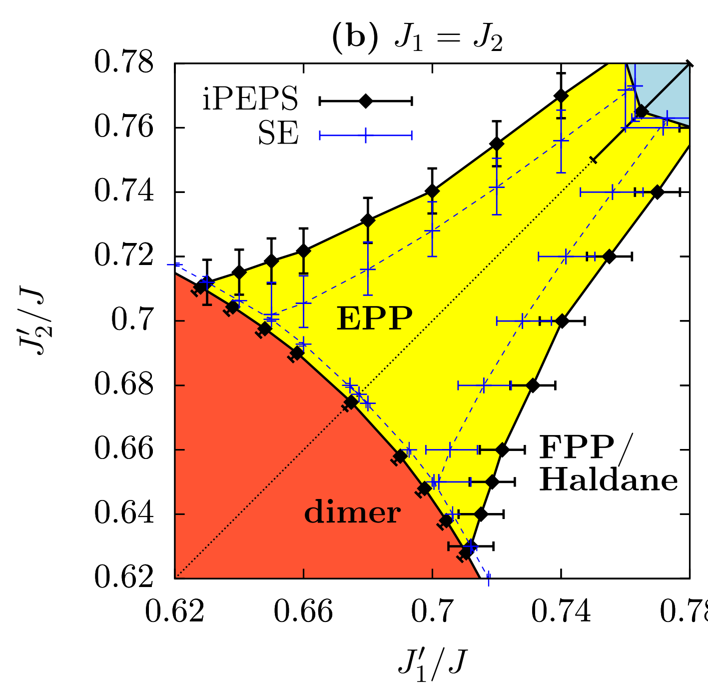


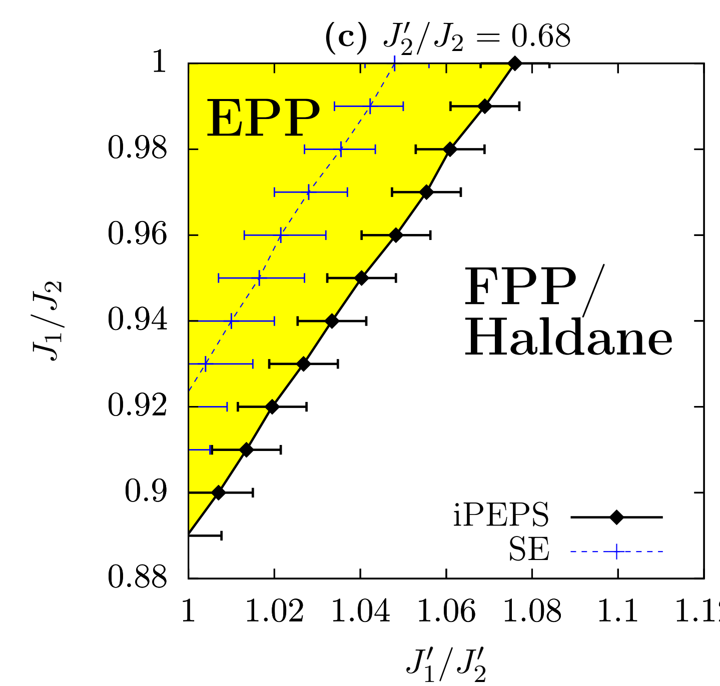




EPP *vs* *FPP*







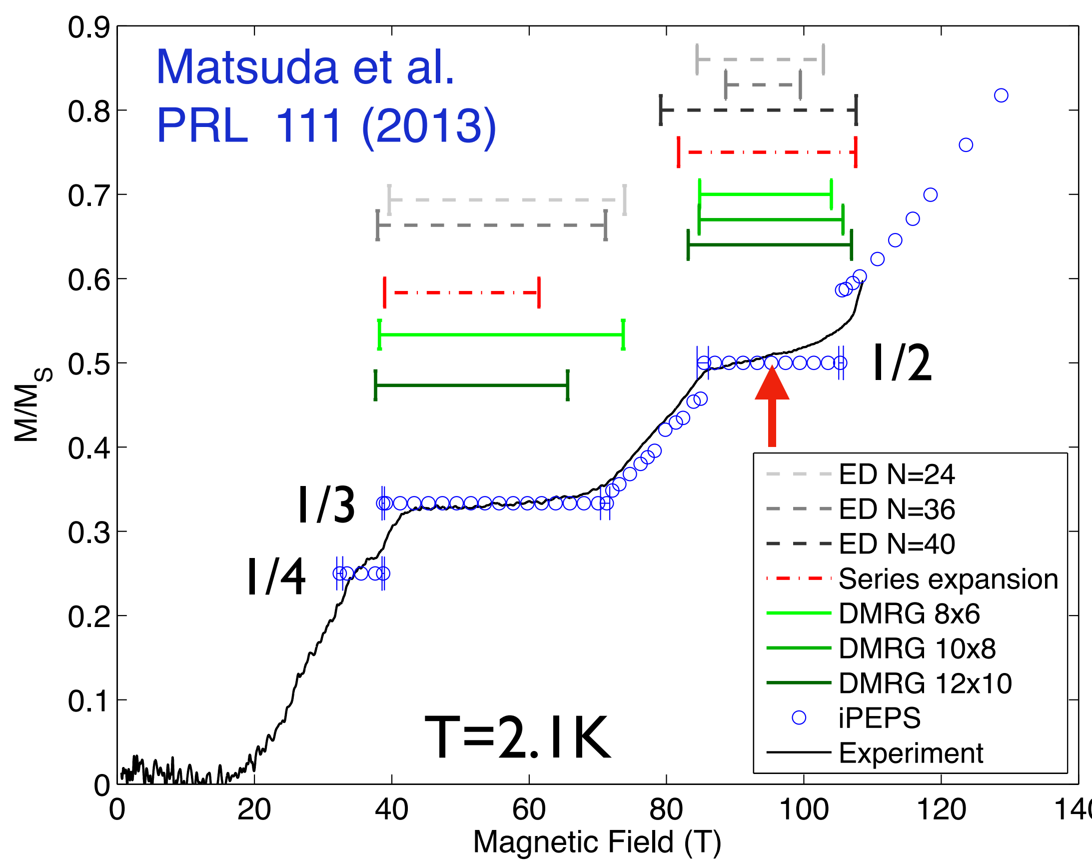
- Small deformation leads to FPP phase!

But precise model still unclear…

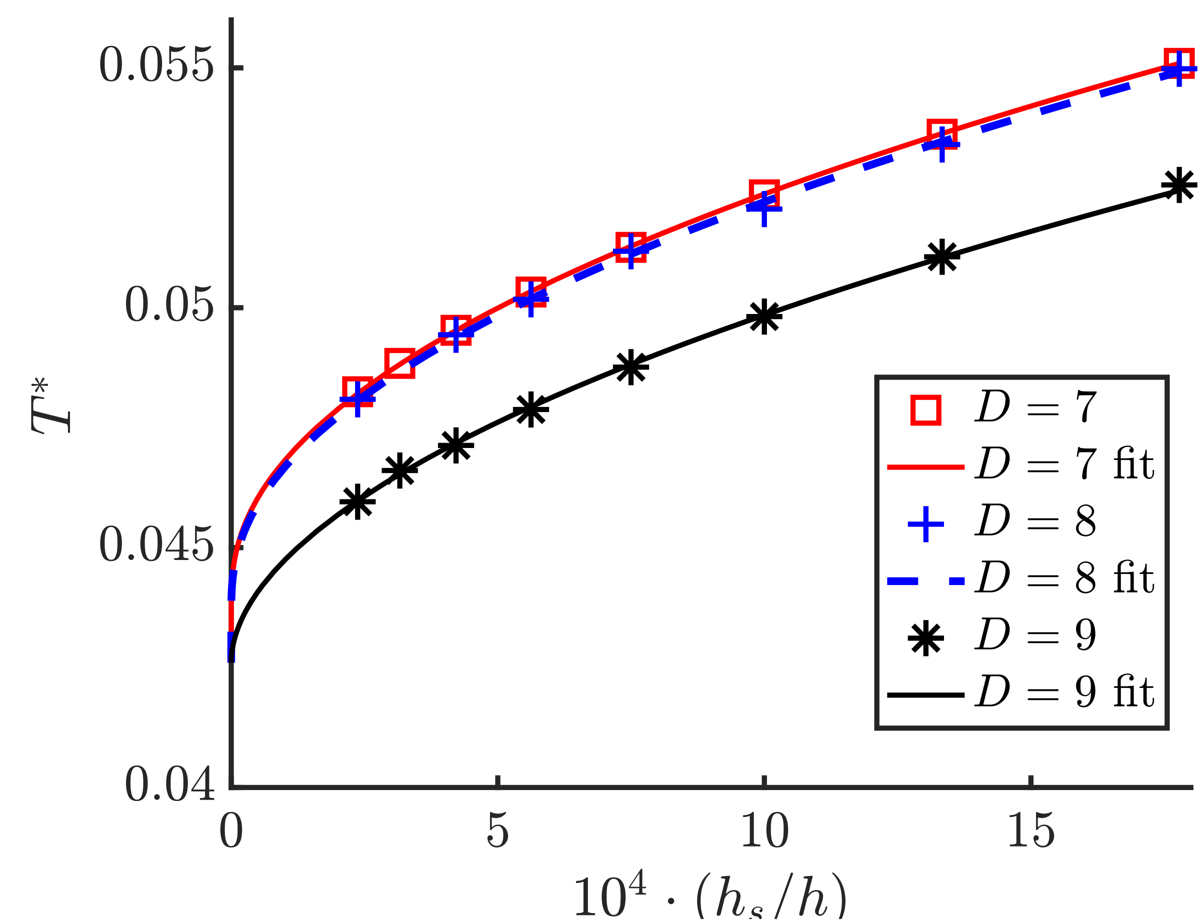
Finite T study of the m=1/2 plateau in $SrCu_2(BO_3)_2$

P. Czarnik, M. M. Rams, PC, and J. Dziarmaga, PRB 103, 075113 (2021)

High-field magnetization data



Systematic scaling analysis



$$T^*(h_s, \xi_D) = T_c + a h_s^{1/\tilde{\beta}\delta} + \frac{b}{\xi_D^c} h_s^{(1-cv)/\tilde{\beta}\delta}$$

Critical exponents compatible with 2D Ising universality class

$$T_c = 0.043(2)J \approx 3.5(2)K$$

Conclusion

- ✓ iPEPS has become a useful tool to study systems at finite T
- ✓ Confirmed the presence of a finite temperature Ising critical point in $SrCu_2(BO_3)_2$, analogous to the critical point of water
- ✓ Similar physics expected in related models / materials

- Open challenges:
  - Improving finite-T iPEPS at low T to study transition into plaquette phase
  - For a quantitative comparison with experiments at low T modified Shastry-Sutherland model may be required

Thank you for your attention!