Finite temperature iPEPS simulations of $SrCu_2(BO_3)_2$ under pressure

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam

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

Time evolution of an infinite projected entangled pair state: An efficient algorithm
P. Czarnik, J. Dziarmaga, and PC, Phys. Rev. B 99, 035115 (2019)

Institute for Theoretical Physics

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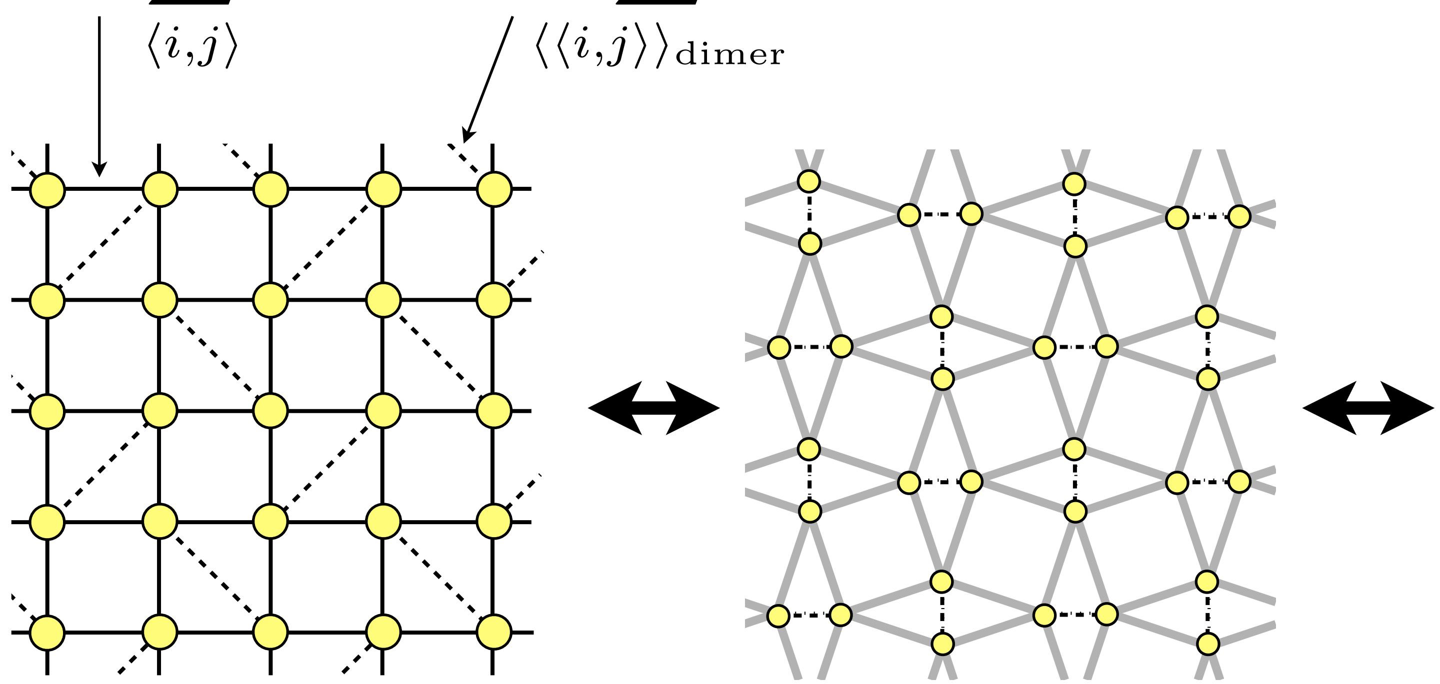
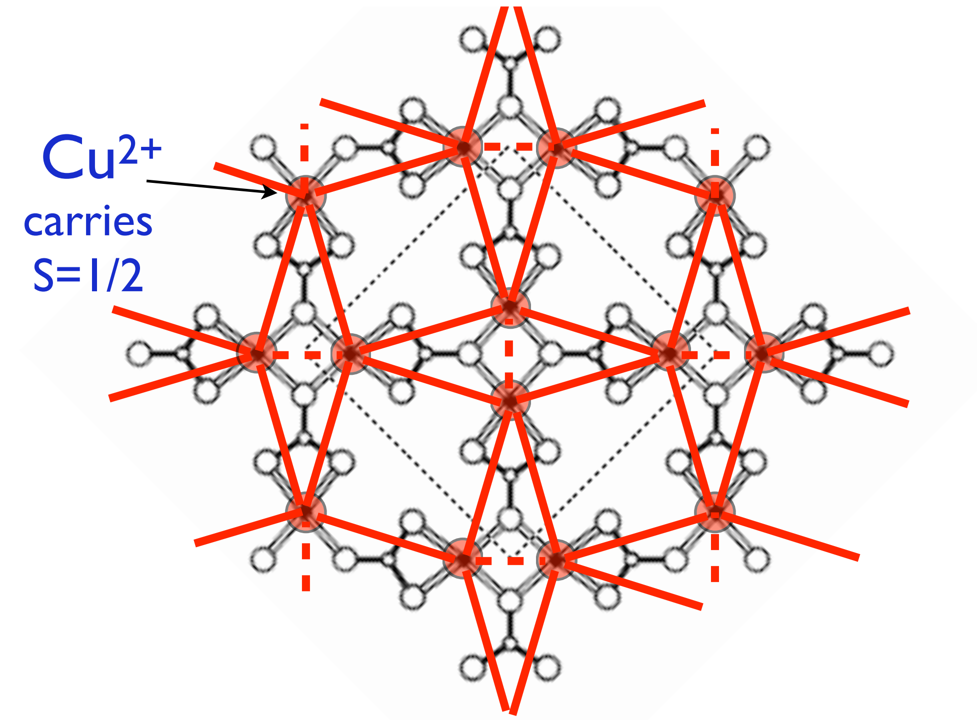
The Shastry-Sutherland model and $SrCu_2(BO_3)_2$

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

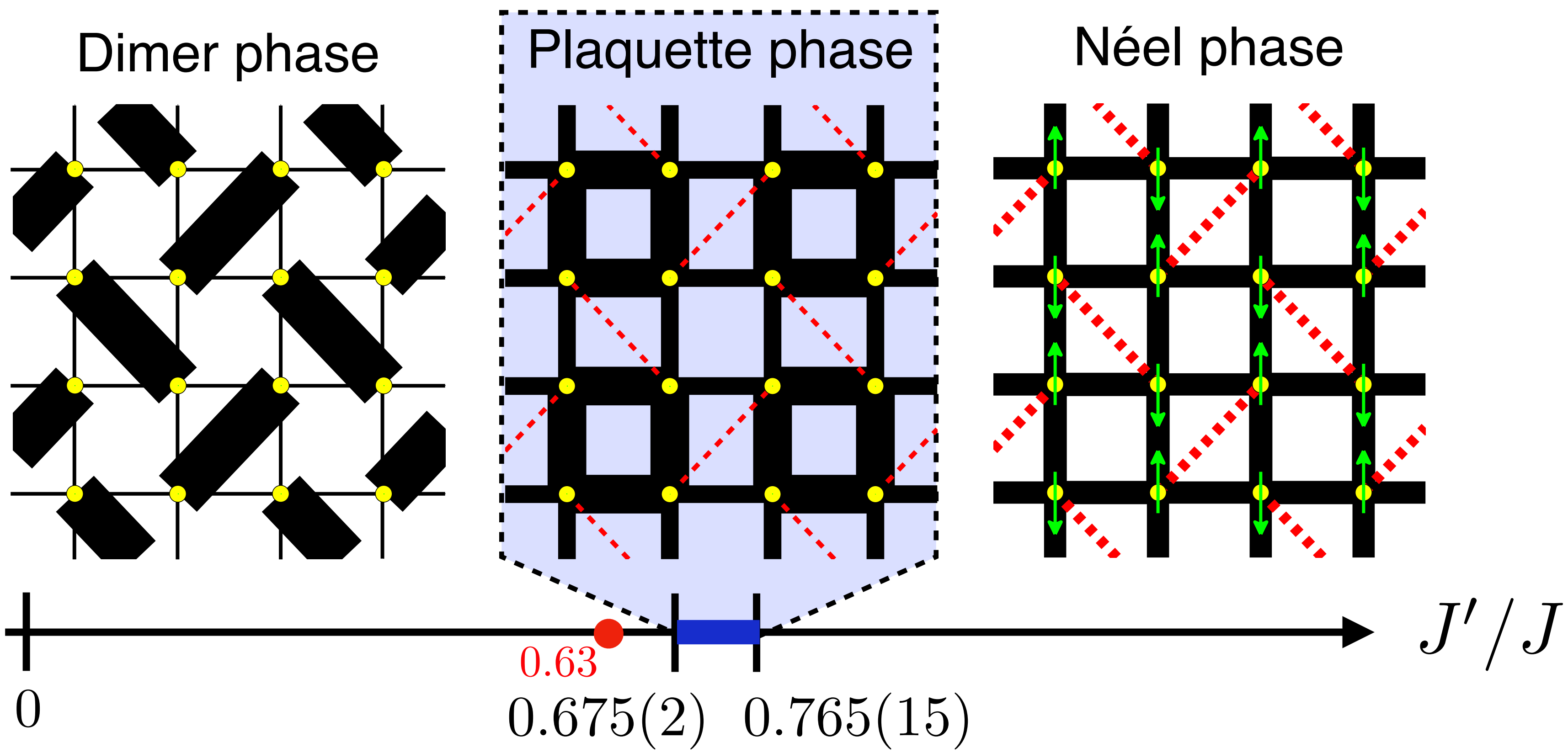


$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



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

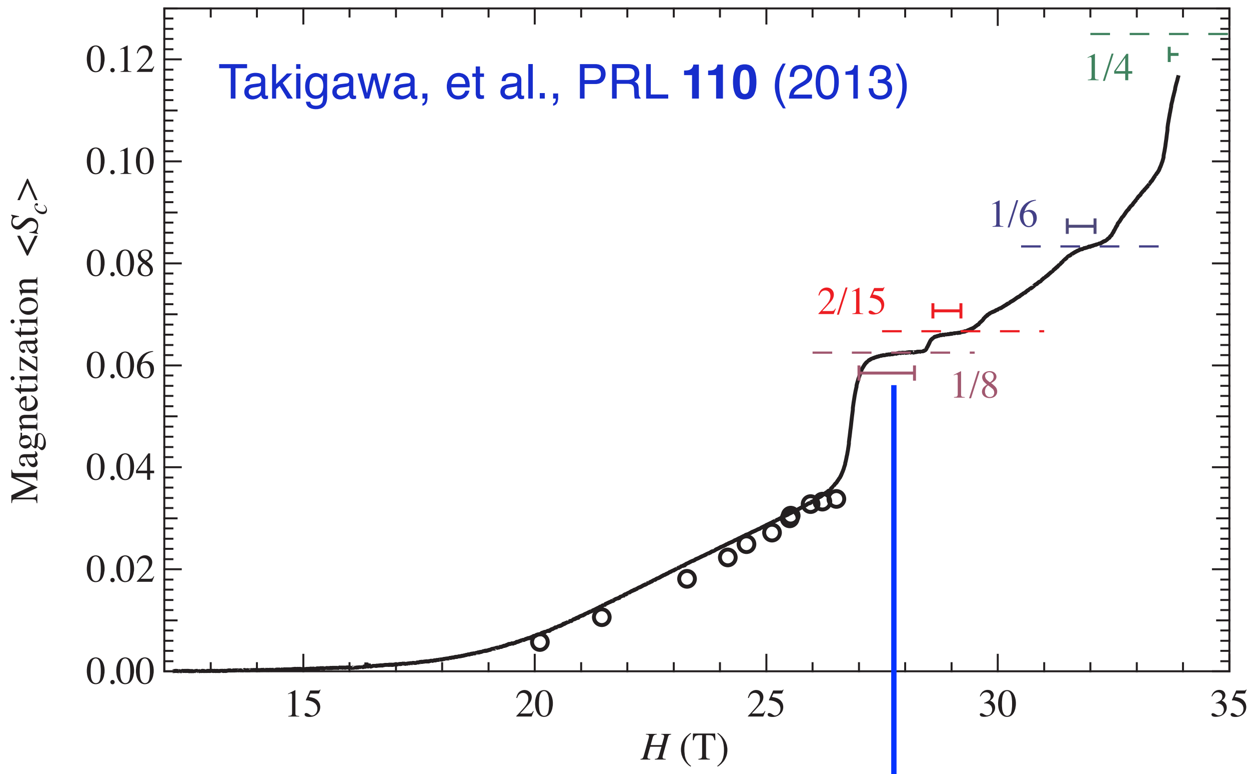


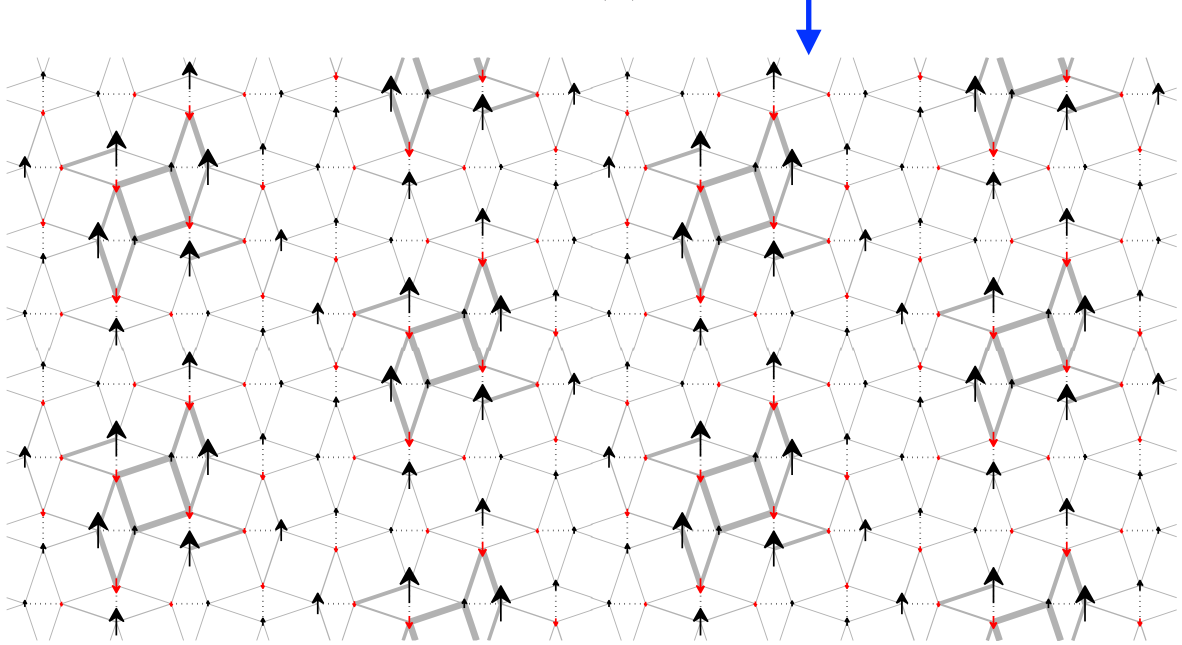
Corboz and Mila, PRB **87** (2013)

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)

Magnetization plateaus in $SrCu_2(BO_3)_2$





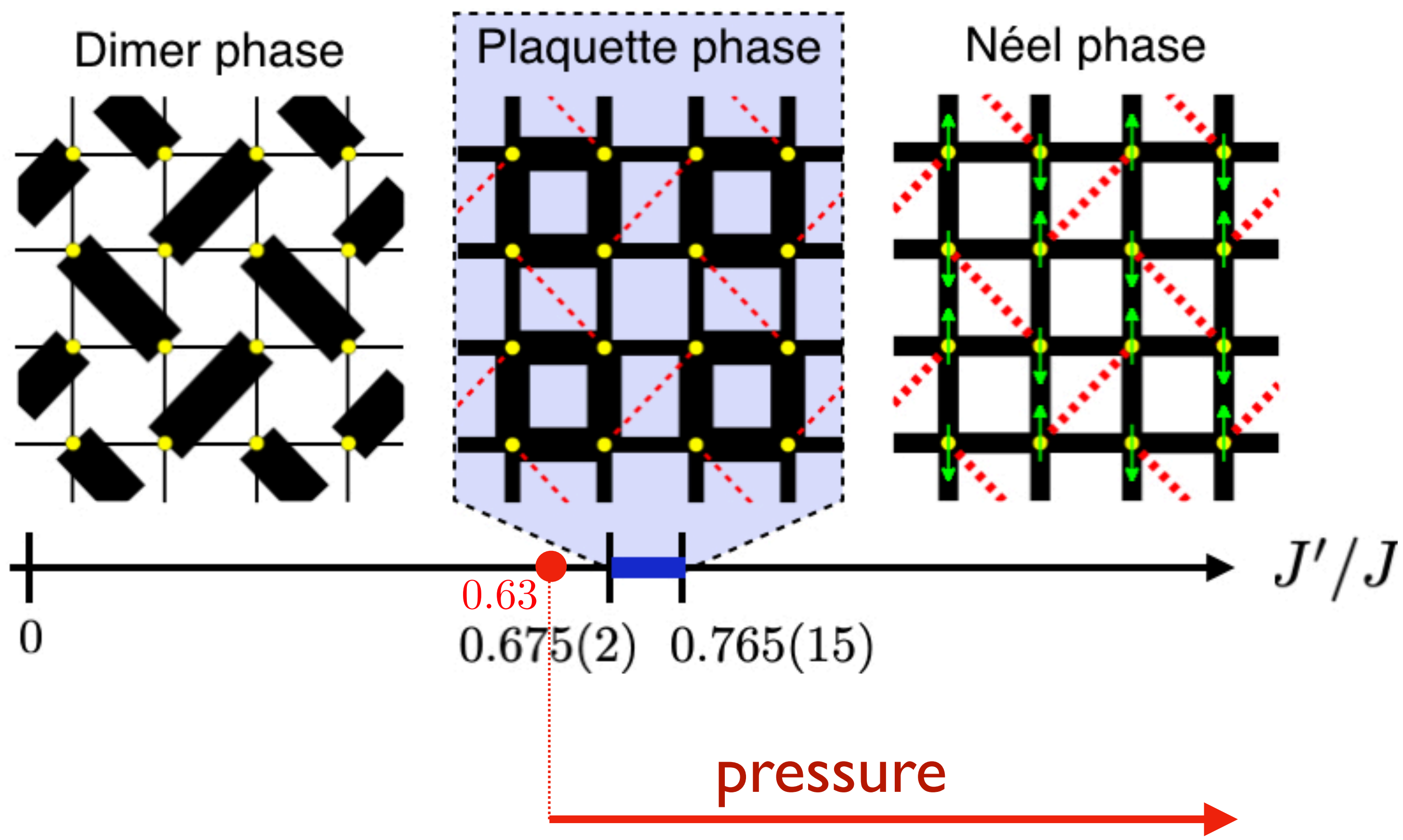
★ Crystals of triplet-bound states

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

Many experimental / theoretical studies

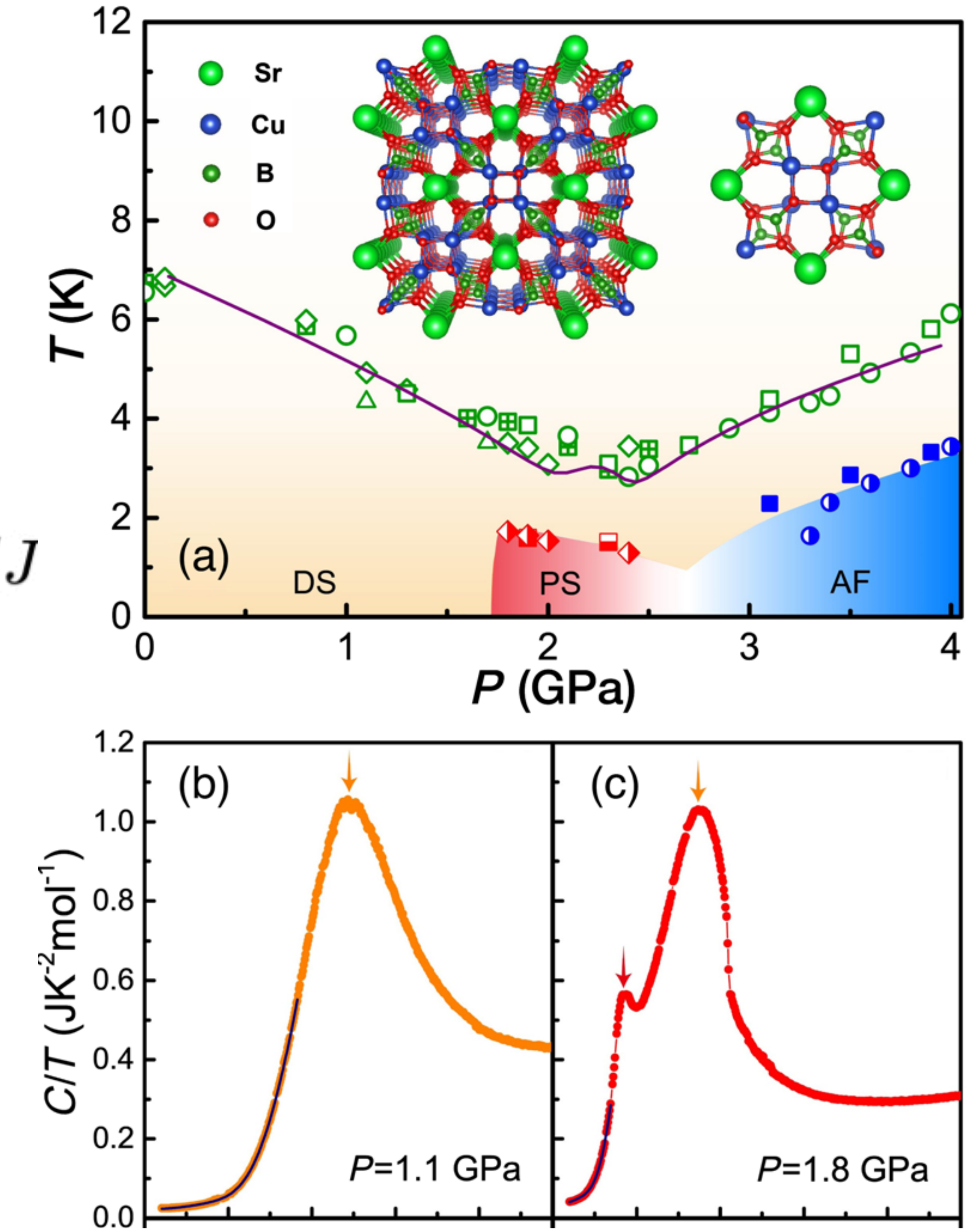
Kageyama et al, PRL **82** (1999)
Onizuka et al, JPSJ **69** (2000)
Kageyama et al, PRL **84** (2000)
Kodama et al, Science **298** (2002)
Takigawa et al, Physica **27** (2004)
Levy et al, EPL **81** (2008)
Sebastian et al, PNAS **105** (2008)
Isaev et al, PRL **103** (2009)
Jaime et al, PNAS **109** (2012)
Takigawa et al, PRL **110** (2013)
Matsuda et al, PRL **111** (2013)
Miyahara and K. Ueda, PRL **82** (1999)
Momoi and Totsuka, PRB **61** (2000)
Momoi and Totsuka, PRB **62** (2000)
Fukumoto and Oguchi, JPSJ **69** (2000)
Fukumoto, JPSJ **70** (2001)
Miyahara and Ueda, JPCM **15** (2003)
Miyahara, Becca and Mila, PRB **68** (2003)
Dorier, Schmidt, and Mila, PRL **101** (2008)
Abendschein & Capponi, PRL **101** (2008)
Takigawa et al, JPSJ **79** (2010)
Nemec et al, PRB **86** (2012)
Matsuda et al., PRL 111 (2013)
...

$SrCu_2(BO_3)_2$ under pressure



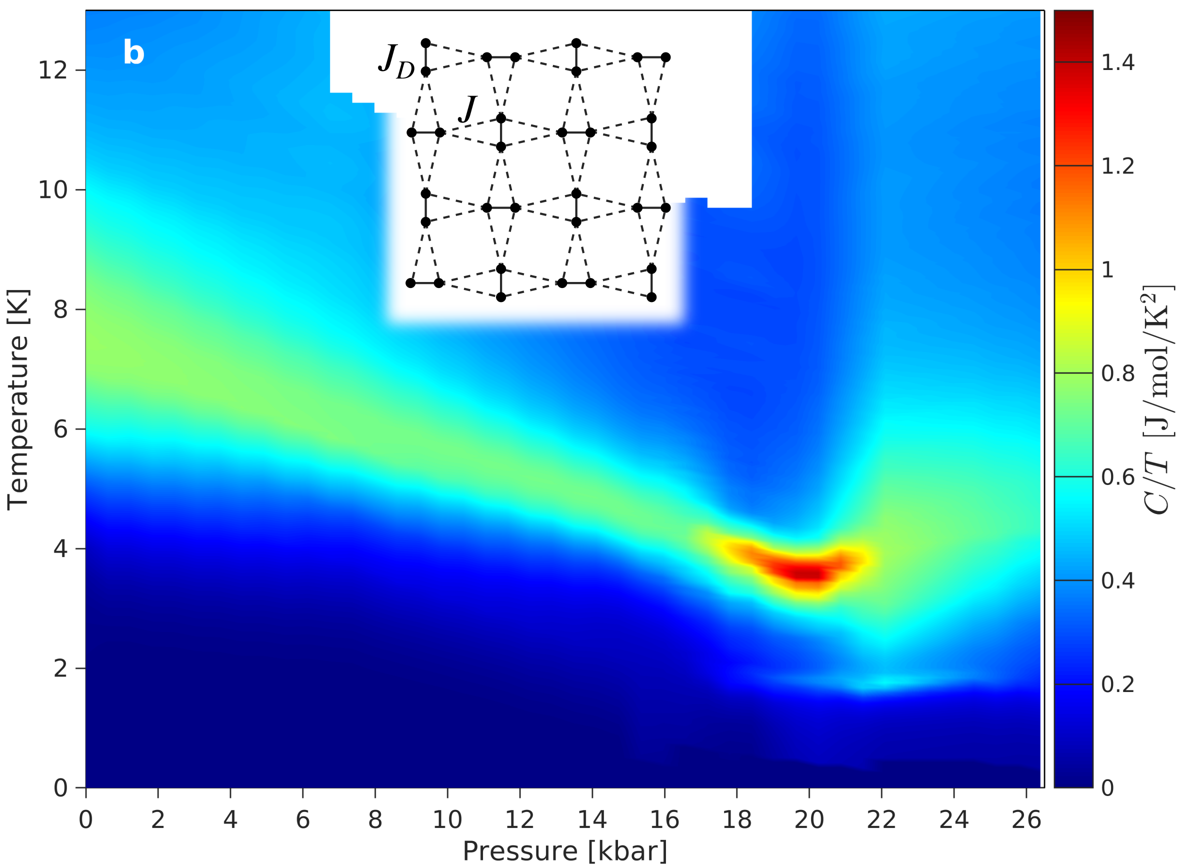
Drive system across the phase transitions!

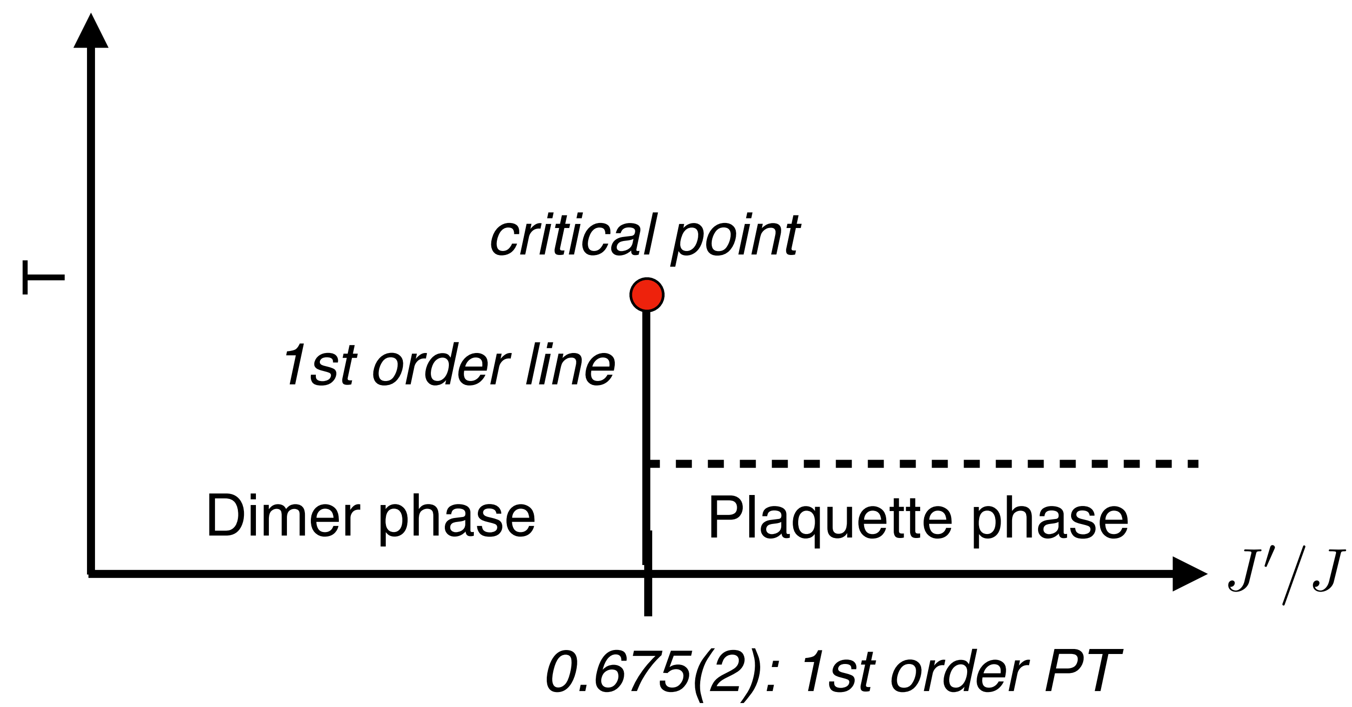
Waki, et al. J. Phys. Soc. Jpn. 76, 073710 (2007)
Haravifard, et al. Nat. Commun. 7, 11956 (2016)
Zayed, et al., Nat. Phys. 13, 962 (2017)
Sakurai, et al., J. Phys. Soc. Jpn. 87, 033701 (2018)
Guo, et al., PRL 124, 206602 (2020)
Bettler, et al,. Phys. Rev. Research 2, 012010 (2020)

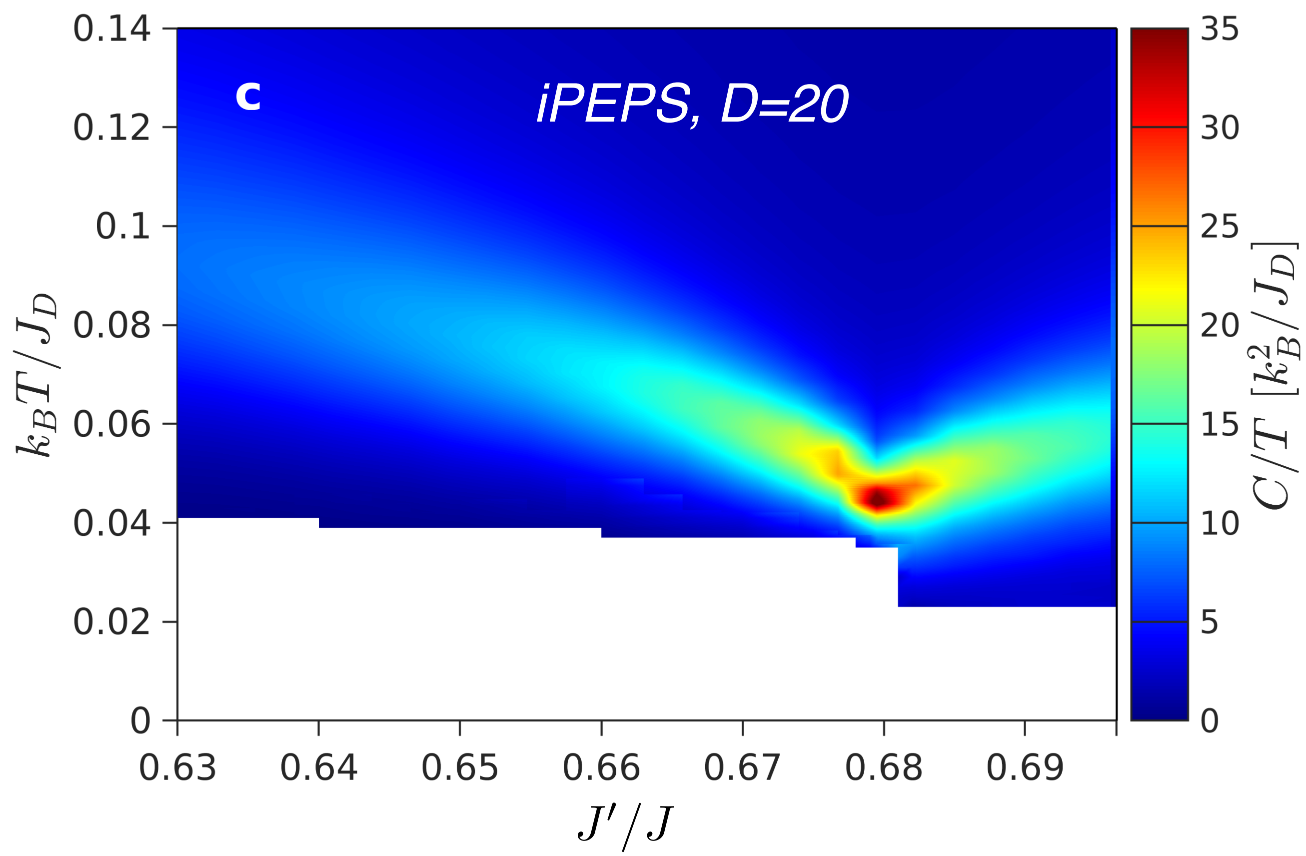


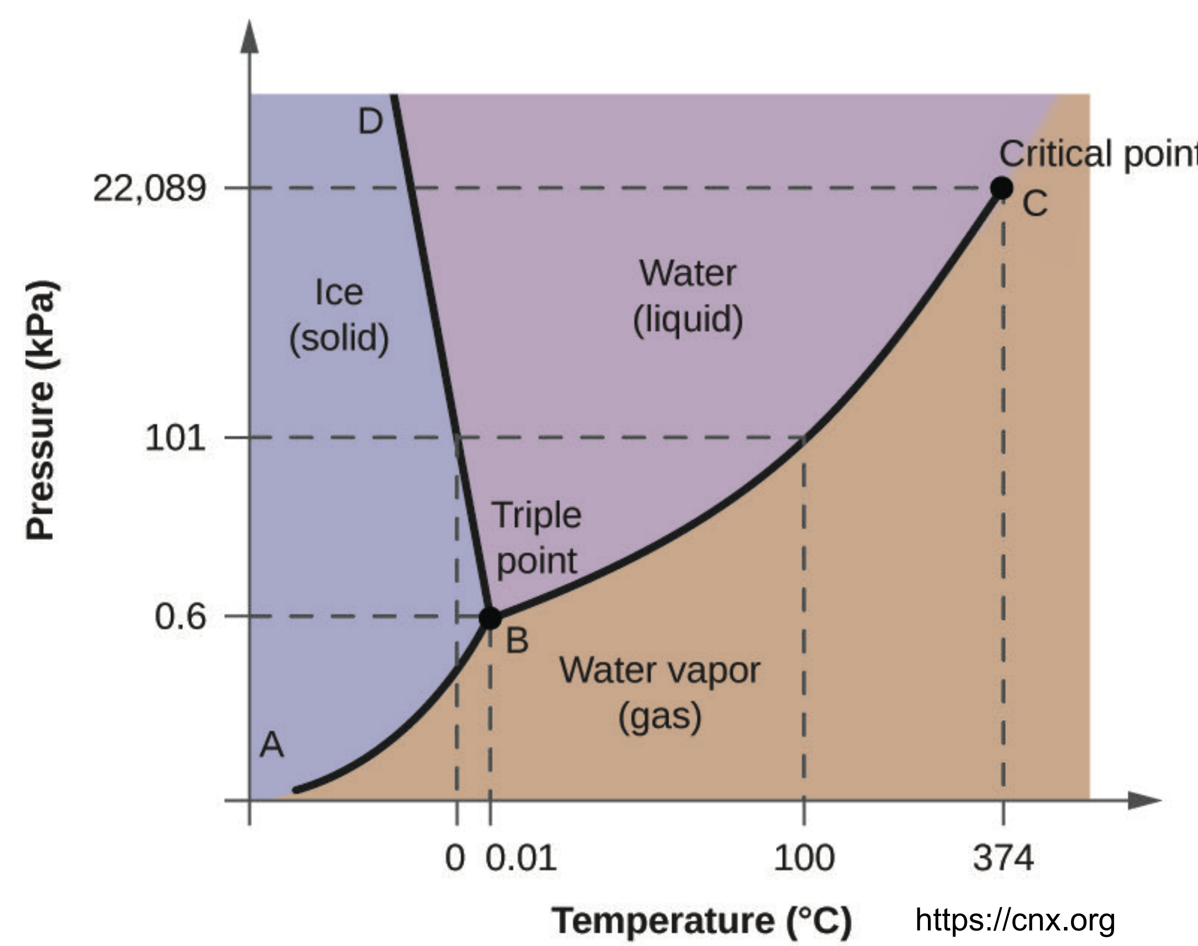
Guo, et al., PRL 124, 206602 (2020)

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

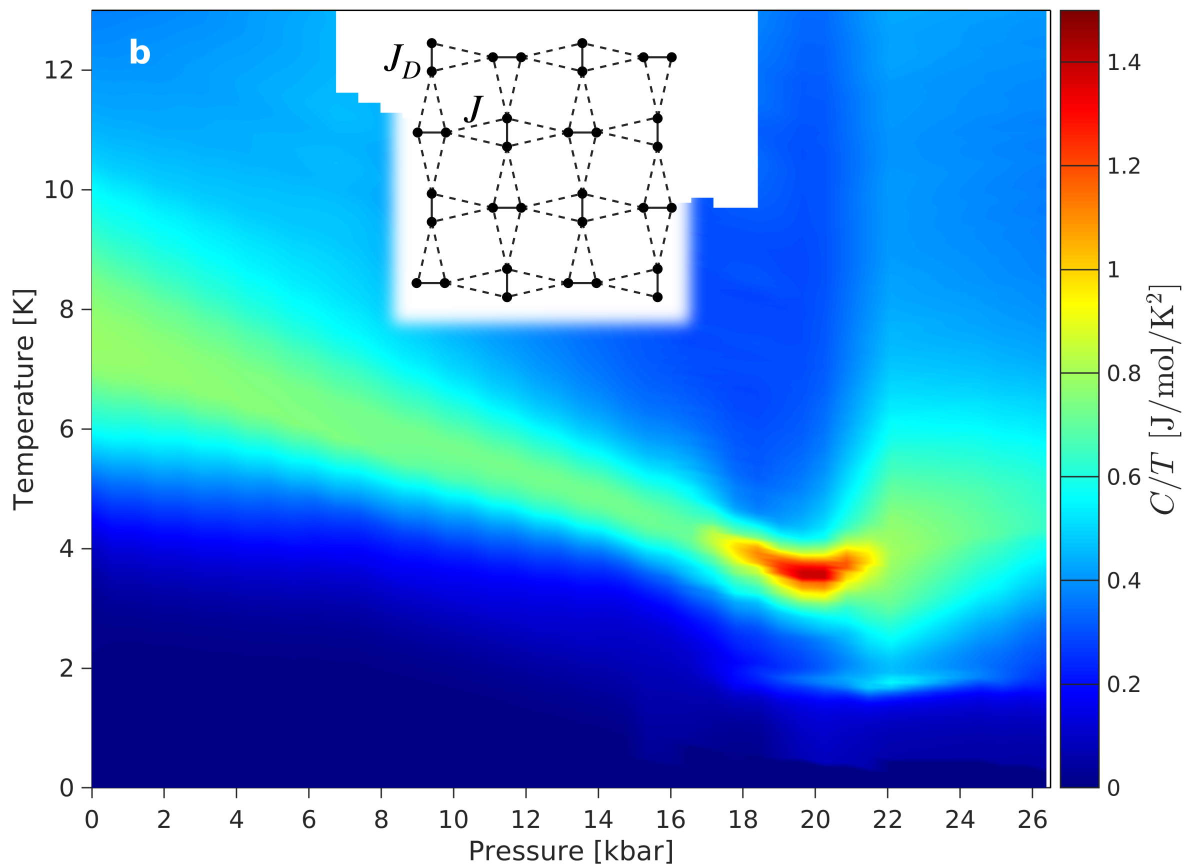


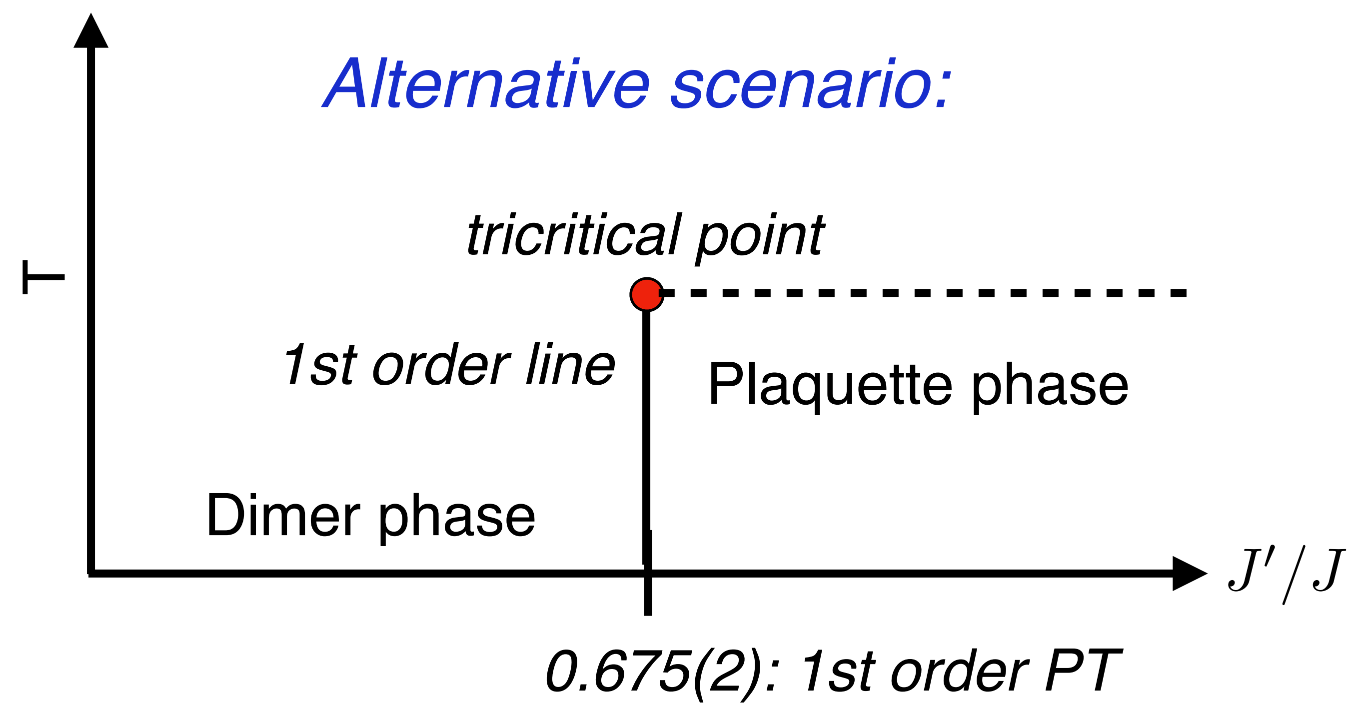


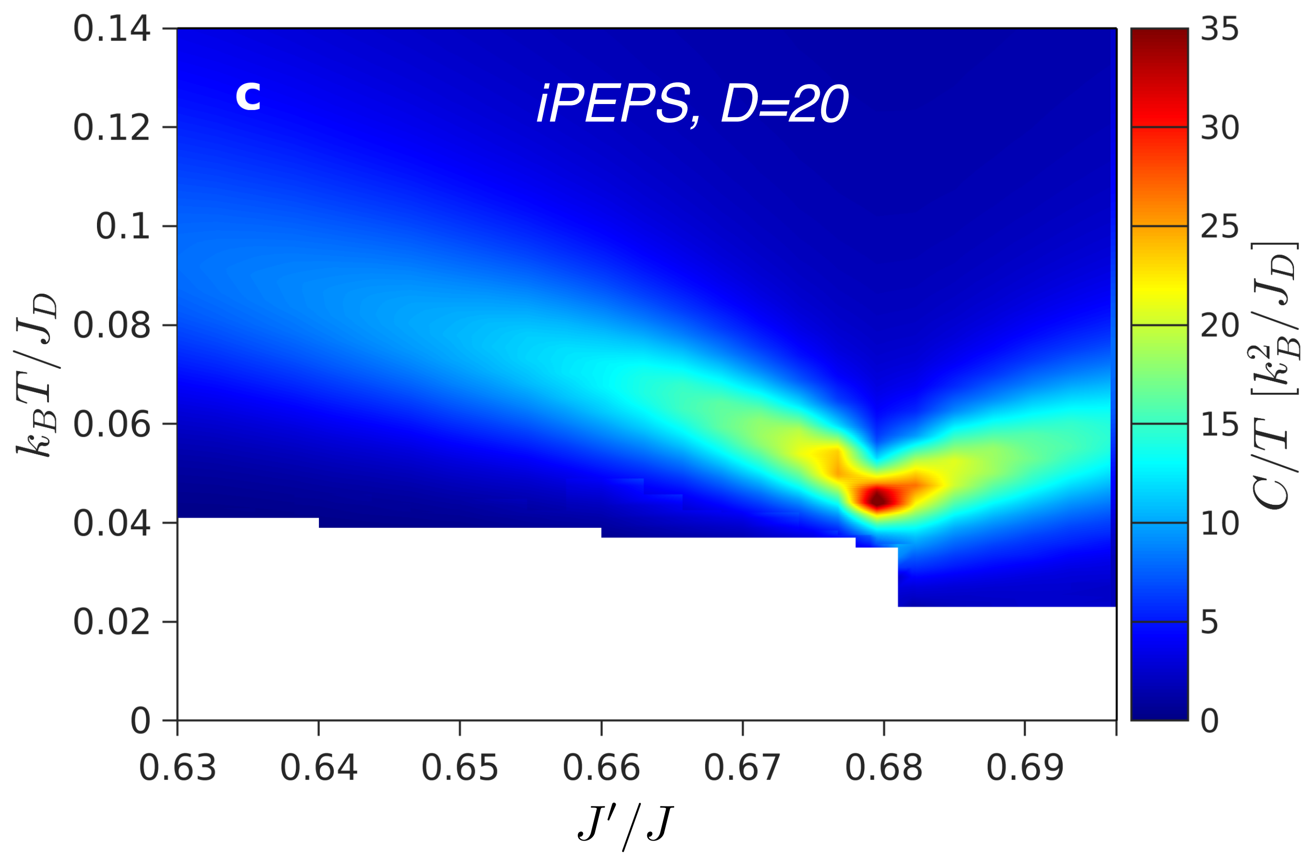


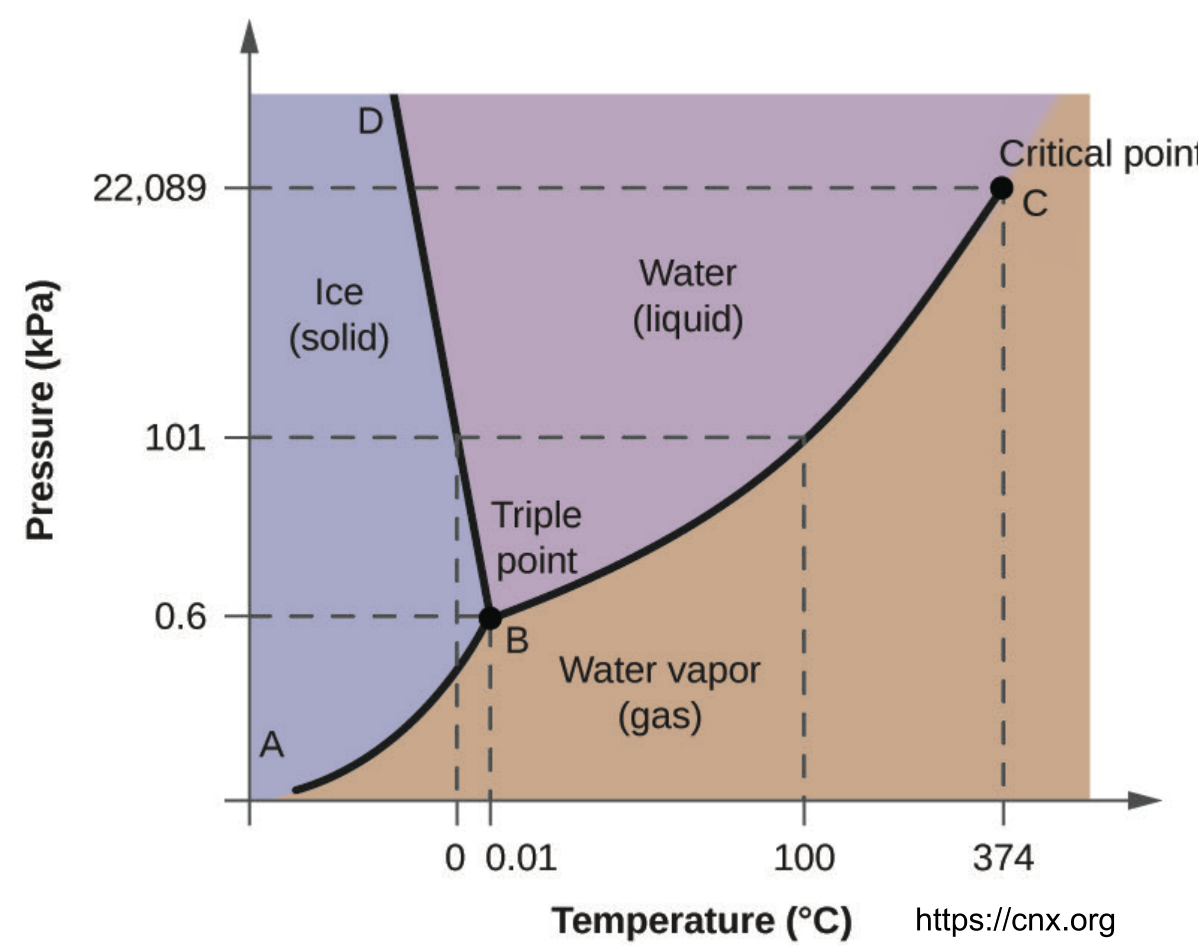


Specific heat data (group of H. M. Rønnow)



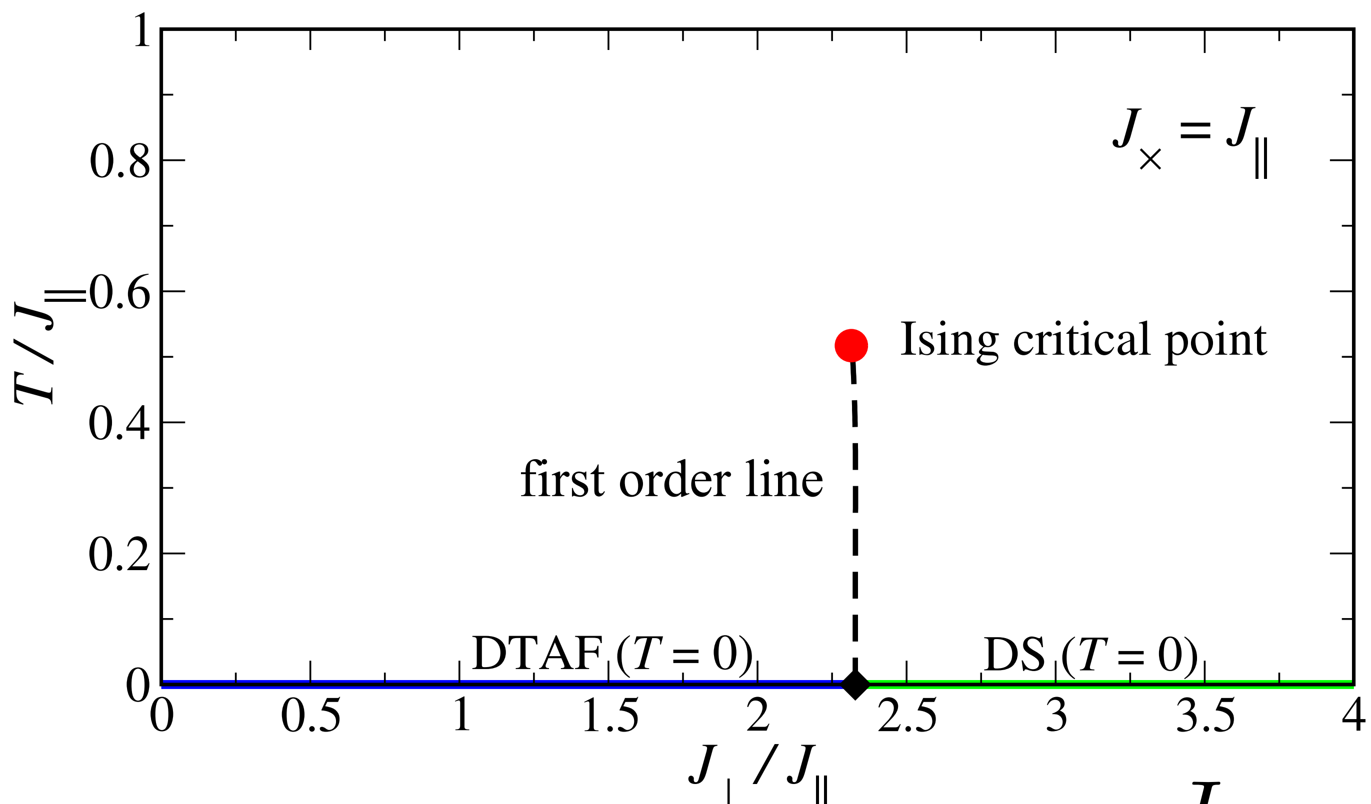


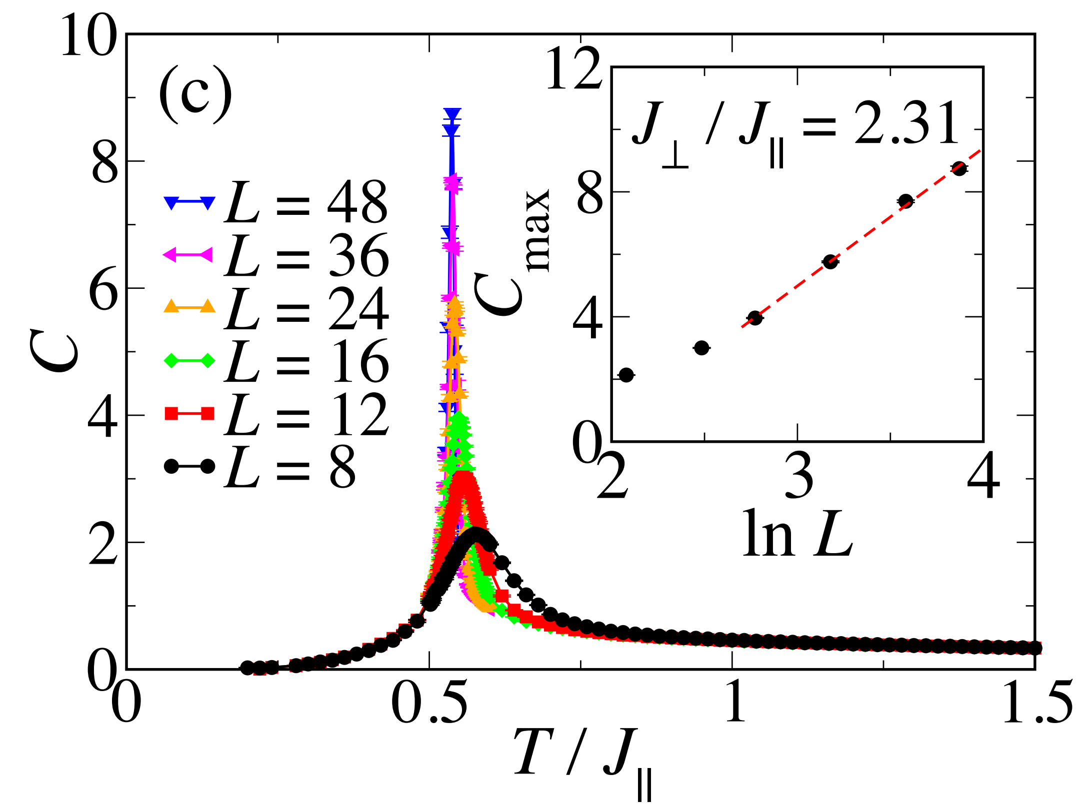


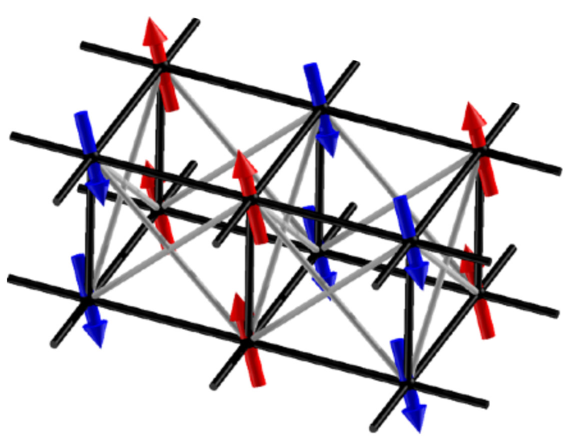


Inspiration: fully frustrated Heisenberg bilayer model

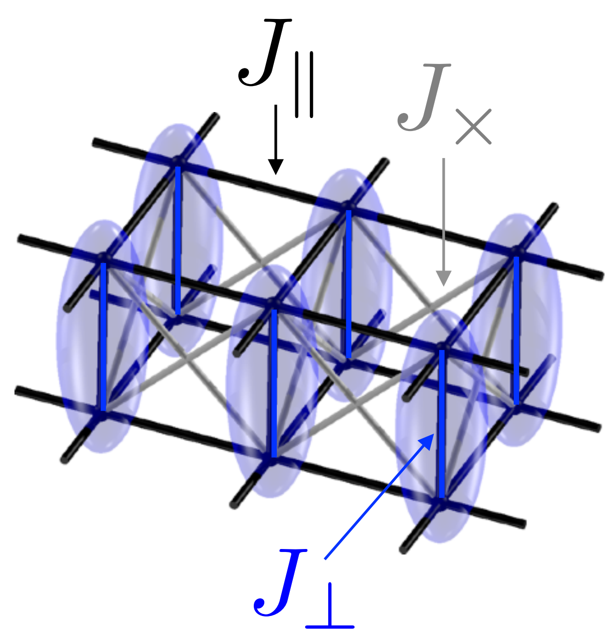
Stapmanns, PC, Mila, Honecker, Normand, and Wessel, PRL 121 (2018)







Dimer triplets



Dimer singlets

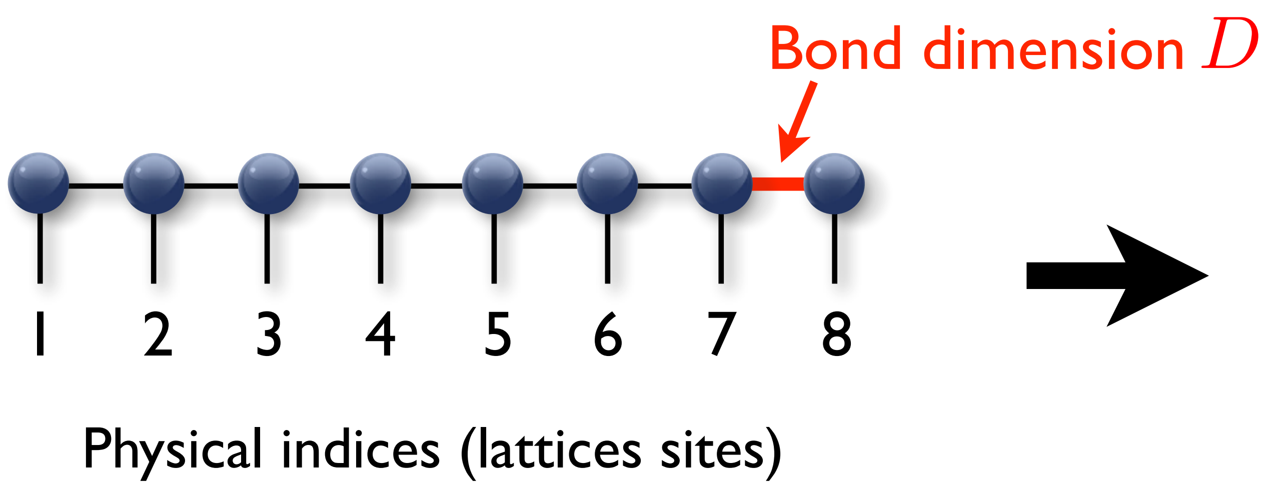
Jump in $\langle S \cdot S \rangle$ on a dimer at the phase transition

MPS & PEPS

1D

MPS

Matrix-product state



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

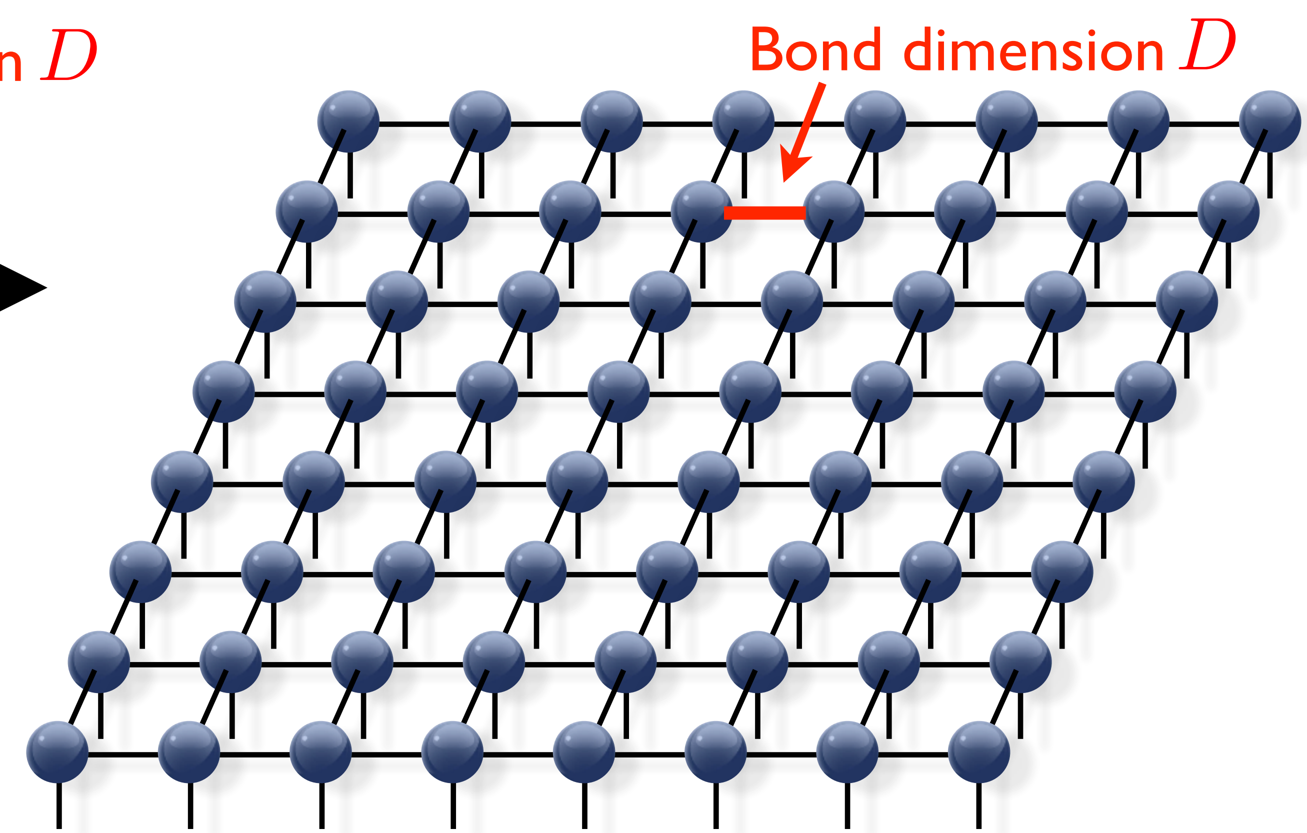
Fannes et al., CMP 144, 443 (1992)

Östlund, Rommer, PRL 75, 3537 (1995)

2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)



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

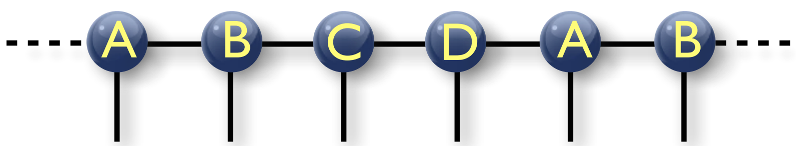
Nishio, Maeshima, Gendiar, Nishino, cond-mat/0401115

infinite PEPS (iPEPS)

1D

iMPS

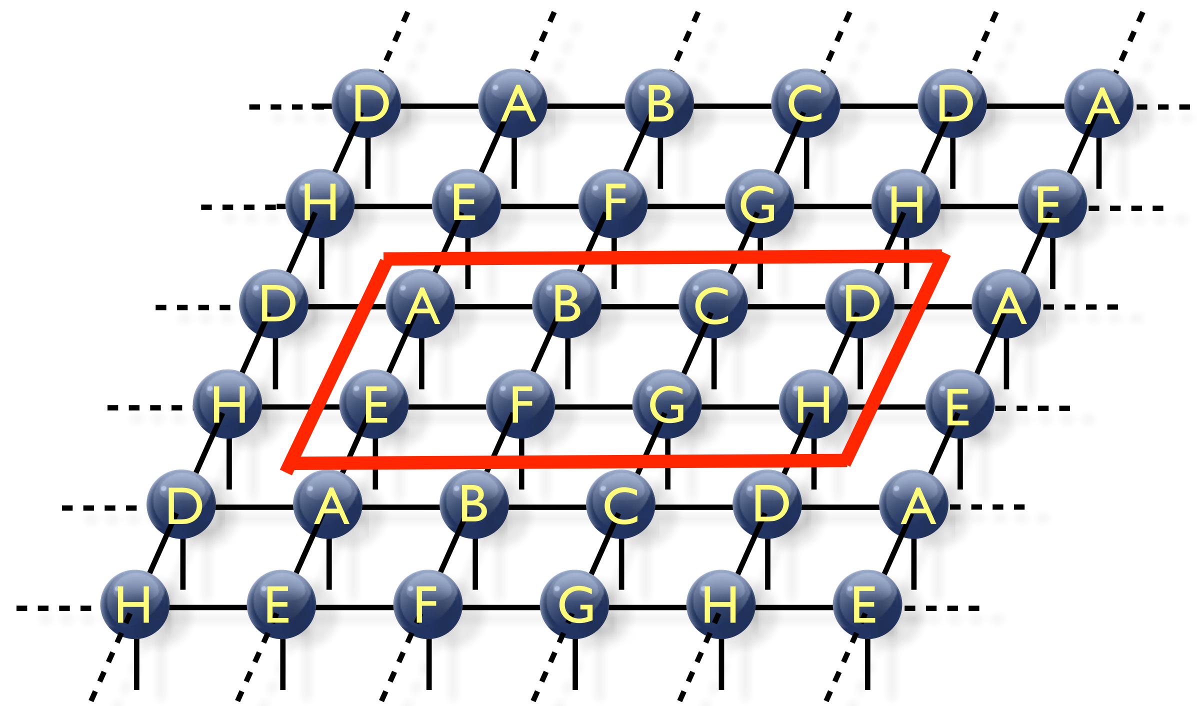
infinite matrix-product state



2D

iPEPS

with arbitrary unit cell of tensors



here: 4x2 unit cell

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

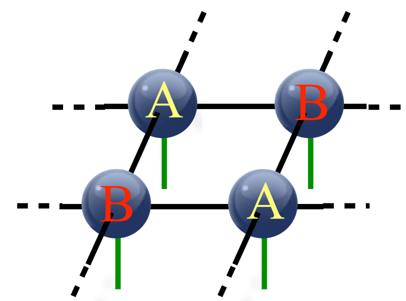
PC, White, Vidal, Troyer, PRB **84** (2011)

Finite temperature simulations with iPEPS

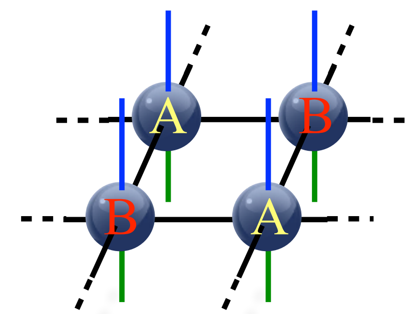
- Methodological developments (2D):

  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), …

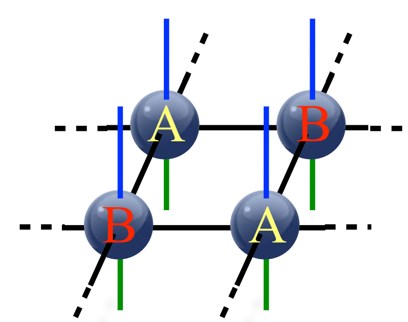
- Wave-function: $|\Psi\rangle \approx$



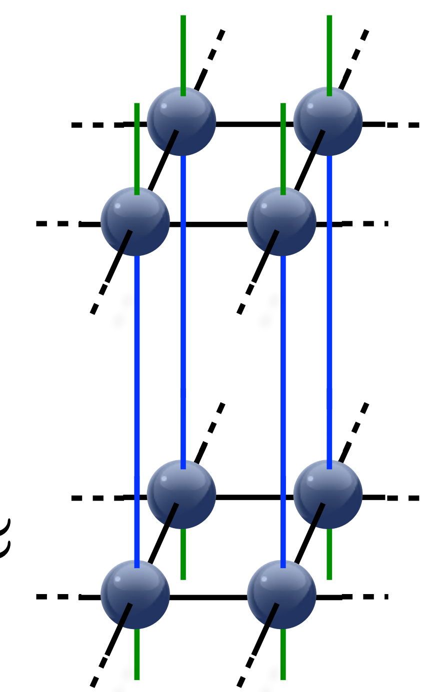
- Density-operator: $\hat{\rho} = e^{-\beta \hat{H}} \approx$



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



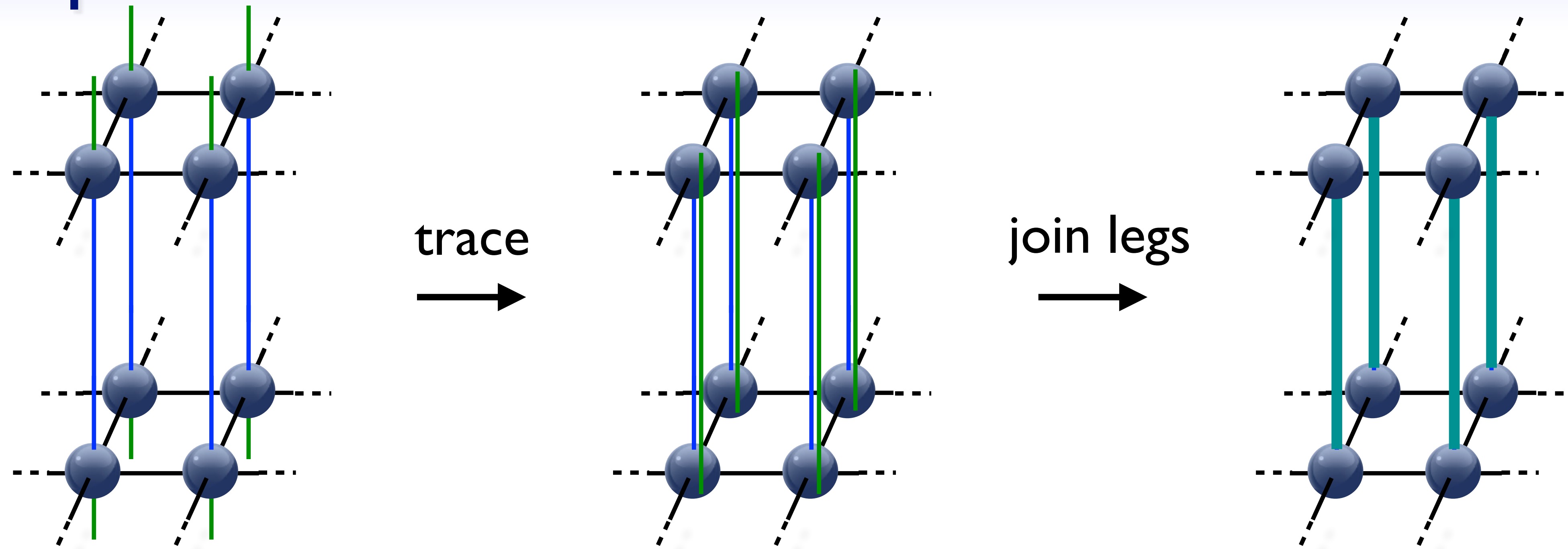
$\hat{\rho}(\beta) \approx$



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

Finite temperature simulations with iPEPS

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



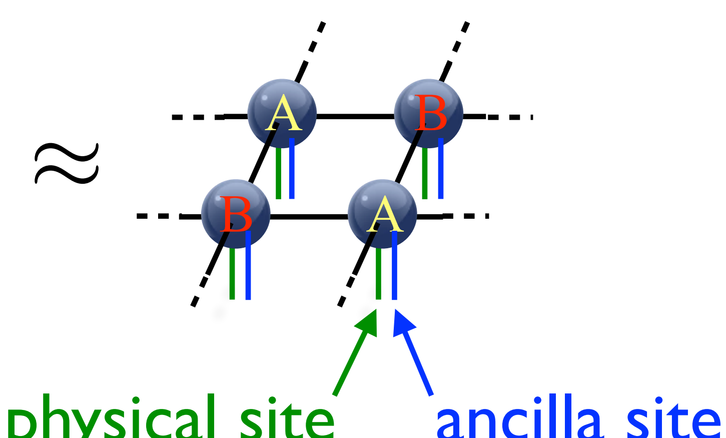
$$\langle\tilde{\Psi}|\tilde{\Psi}\rangle$$

same structure as for wave functions

Recycle algorithms for wave functions!
(CTM + imaginary time evolution)

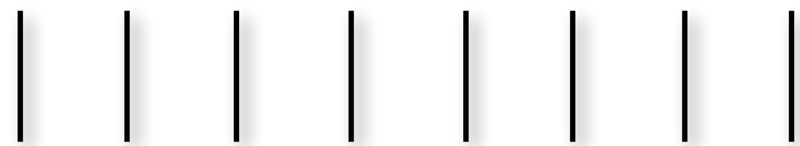
Other (equivalent) formulation using purification:

$$|\tilde{\Psi}\rangle \approx$$



$$\hat{\rho}(\beta) = \mathrm{Tr}_a|\tilde{\Psi}\rangle\langle\tilde{\Psi}|$$

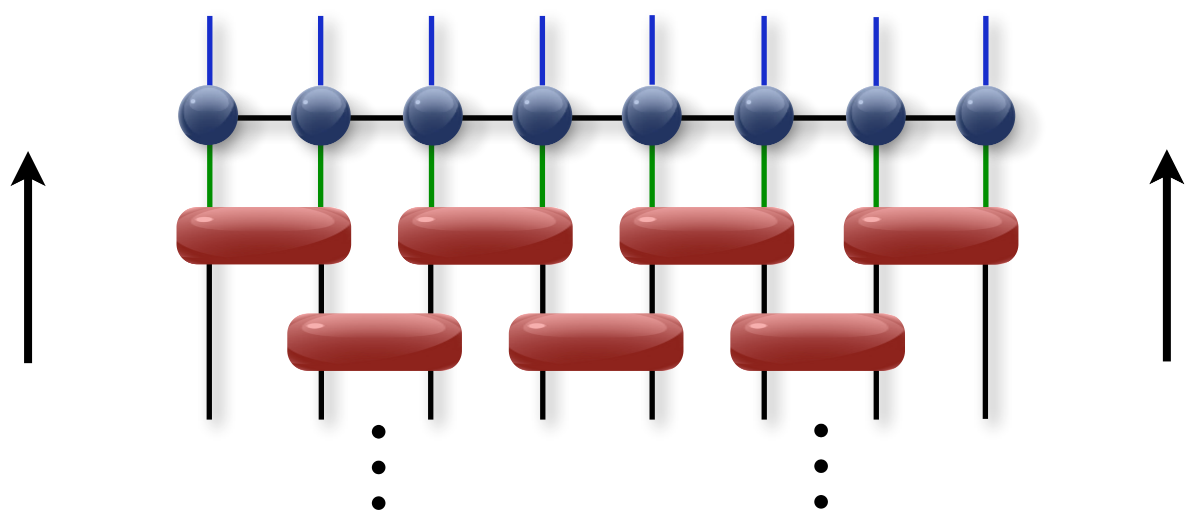
Imaginary time evolution

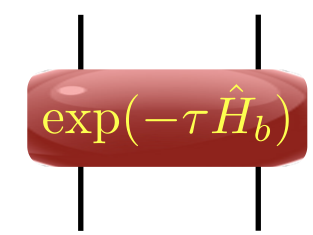
- Start at infinite temperature: $\hat{\rho}(\beta = 0) = \mathbb{I}$
- Initial state:  exact!
- Evolve in imaginary time: $\hat{\rho}(\beta) = e^{-\beta \hat{H}/2} \hat{\rho}(0) e^{-\beta \hat{H}/2}$

Trotter-Suzuki decomposition:

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

$\tau = \beta / n$



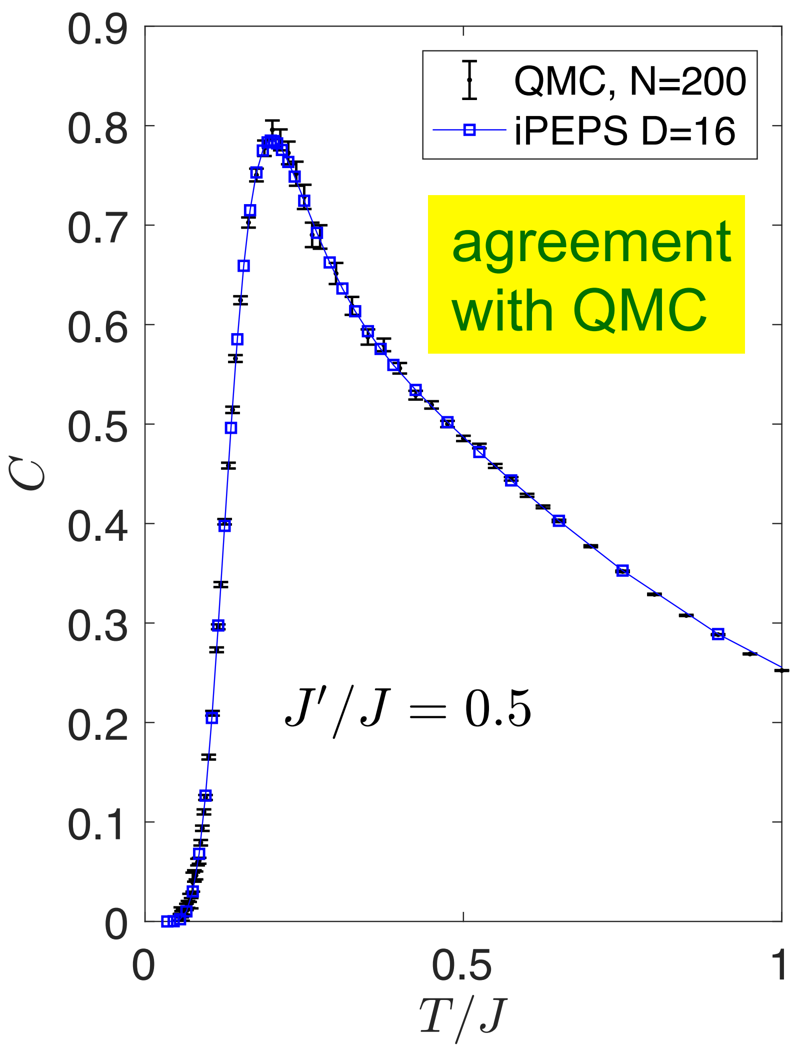


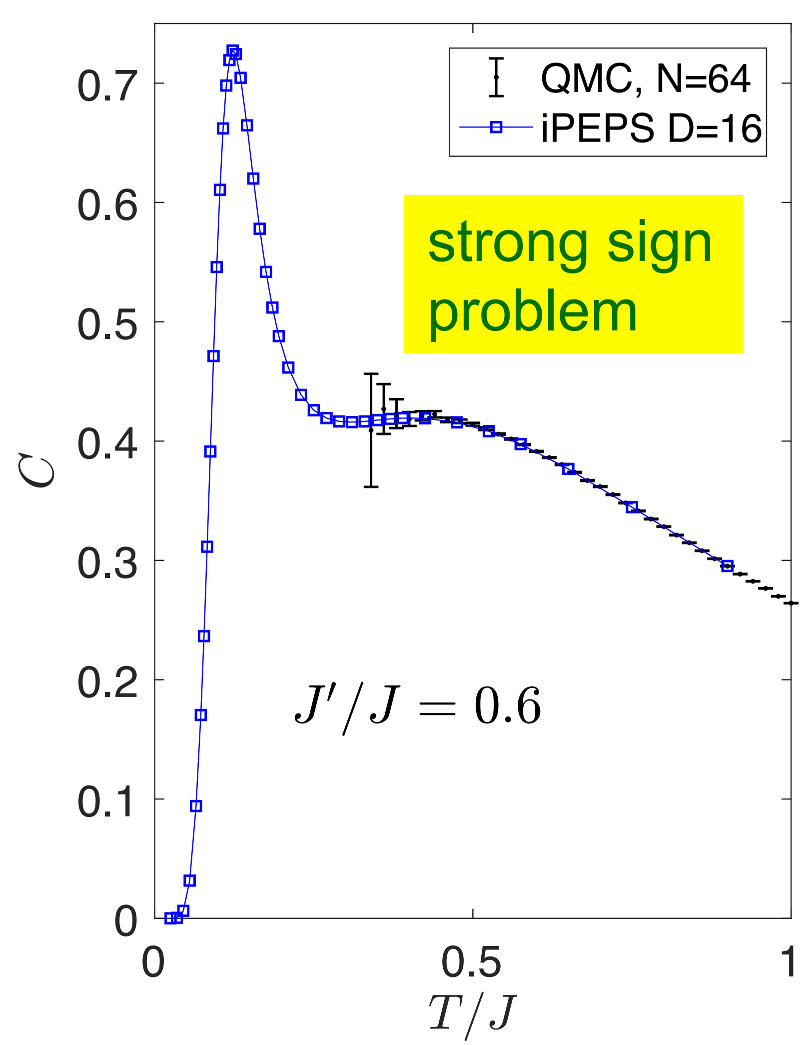
- Truncate after each step using e.g. simple / full update
- Evolve up to target $\beta/2$

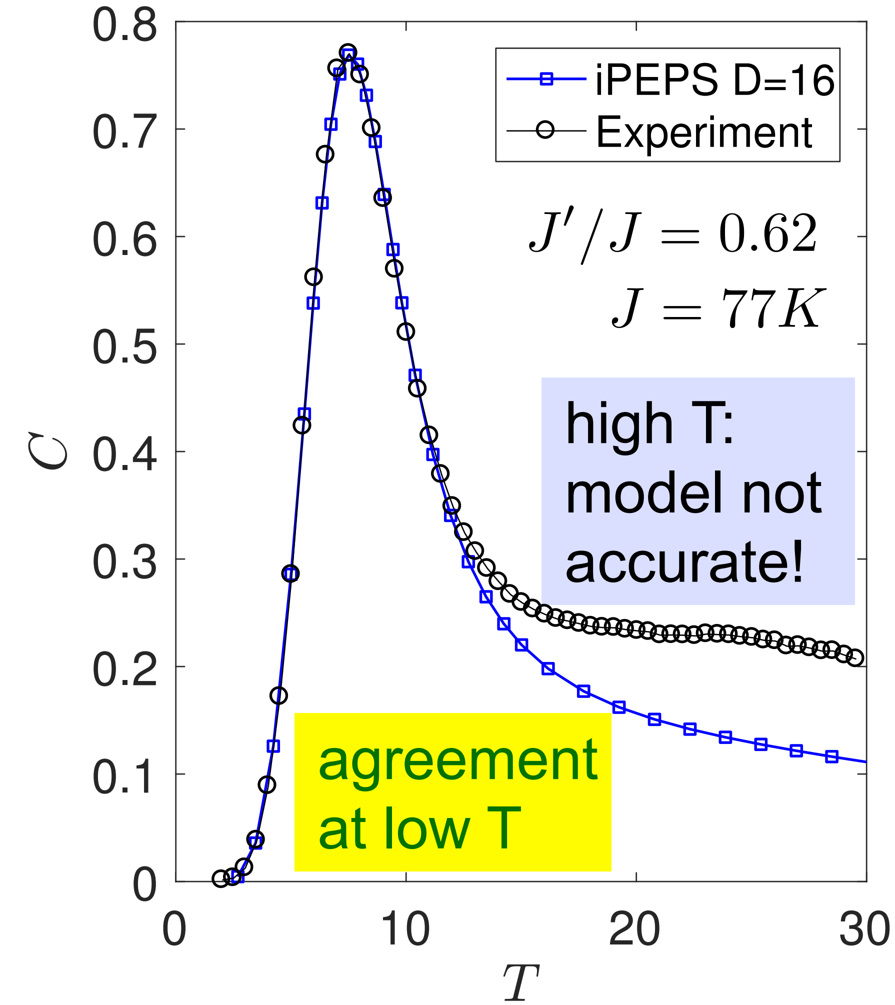
Finite temperature simulations examples

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

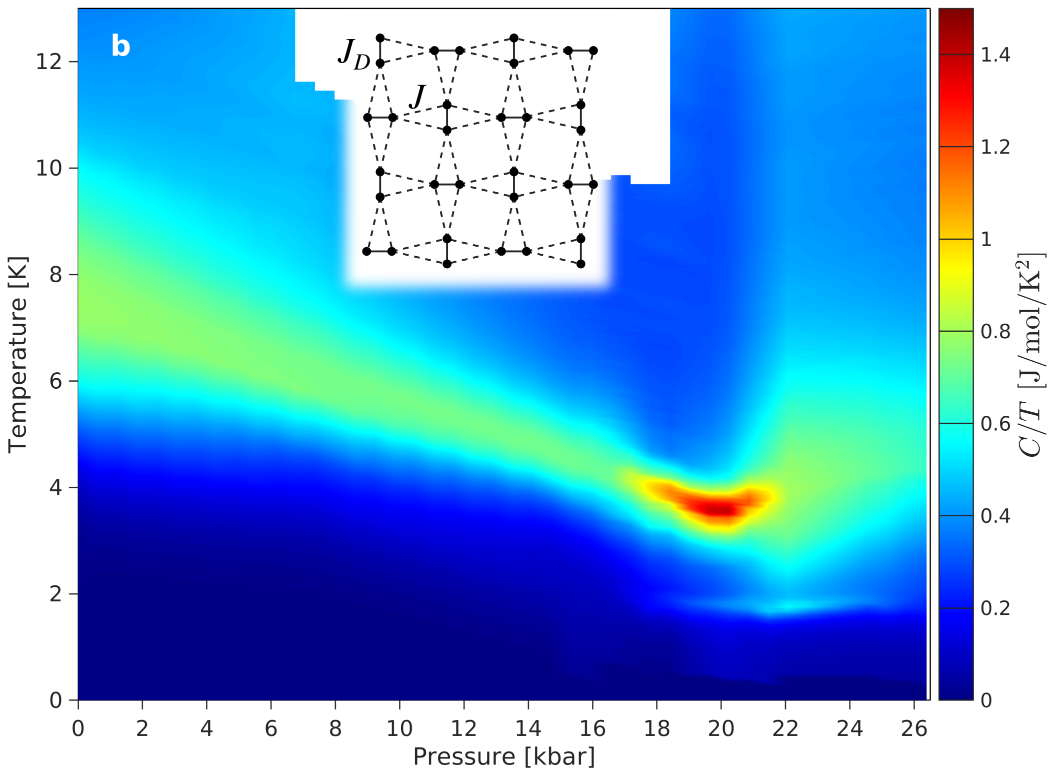


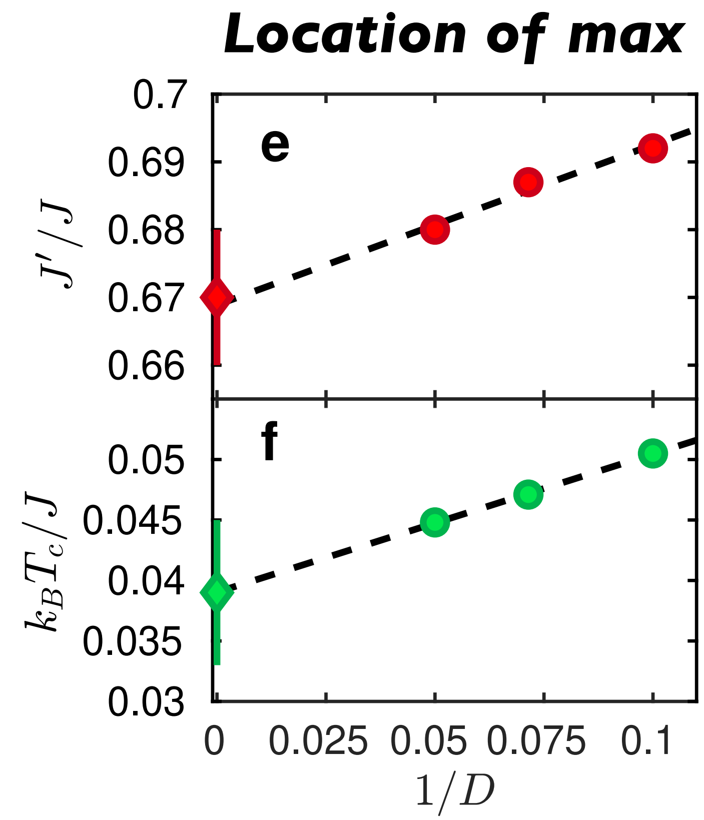




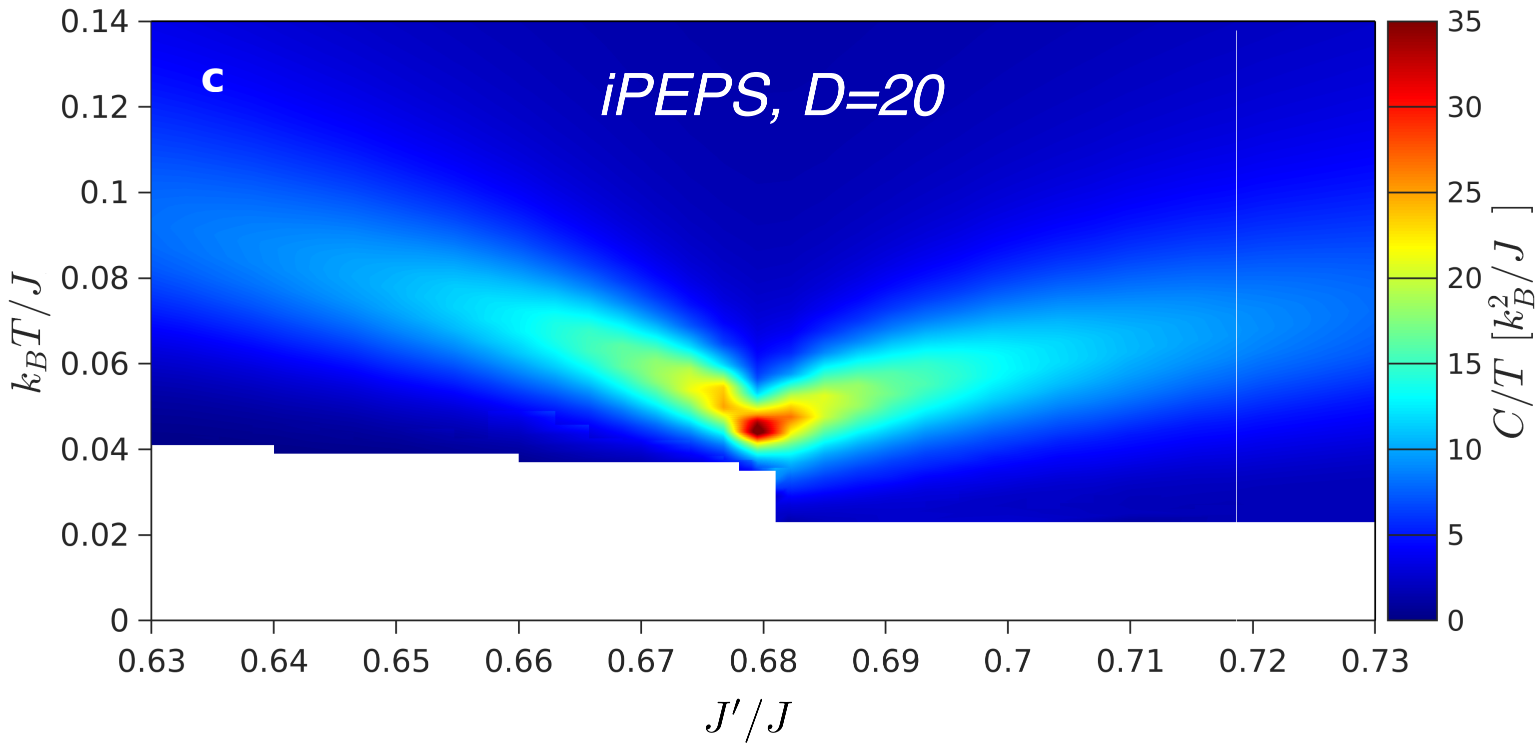
Miyahara and Ueda, arxiv:cond-mat/0004260

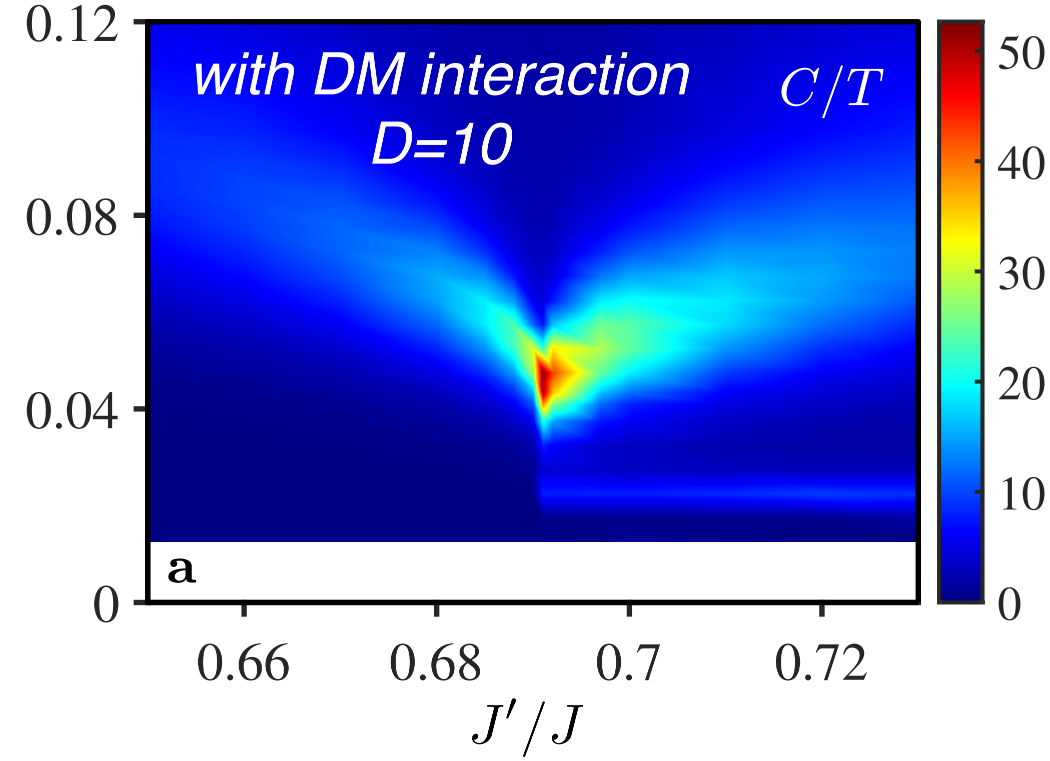
Specific heat: experiments vs iPEPS





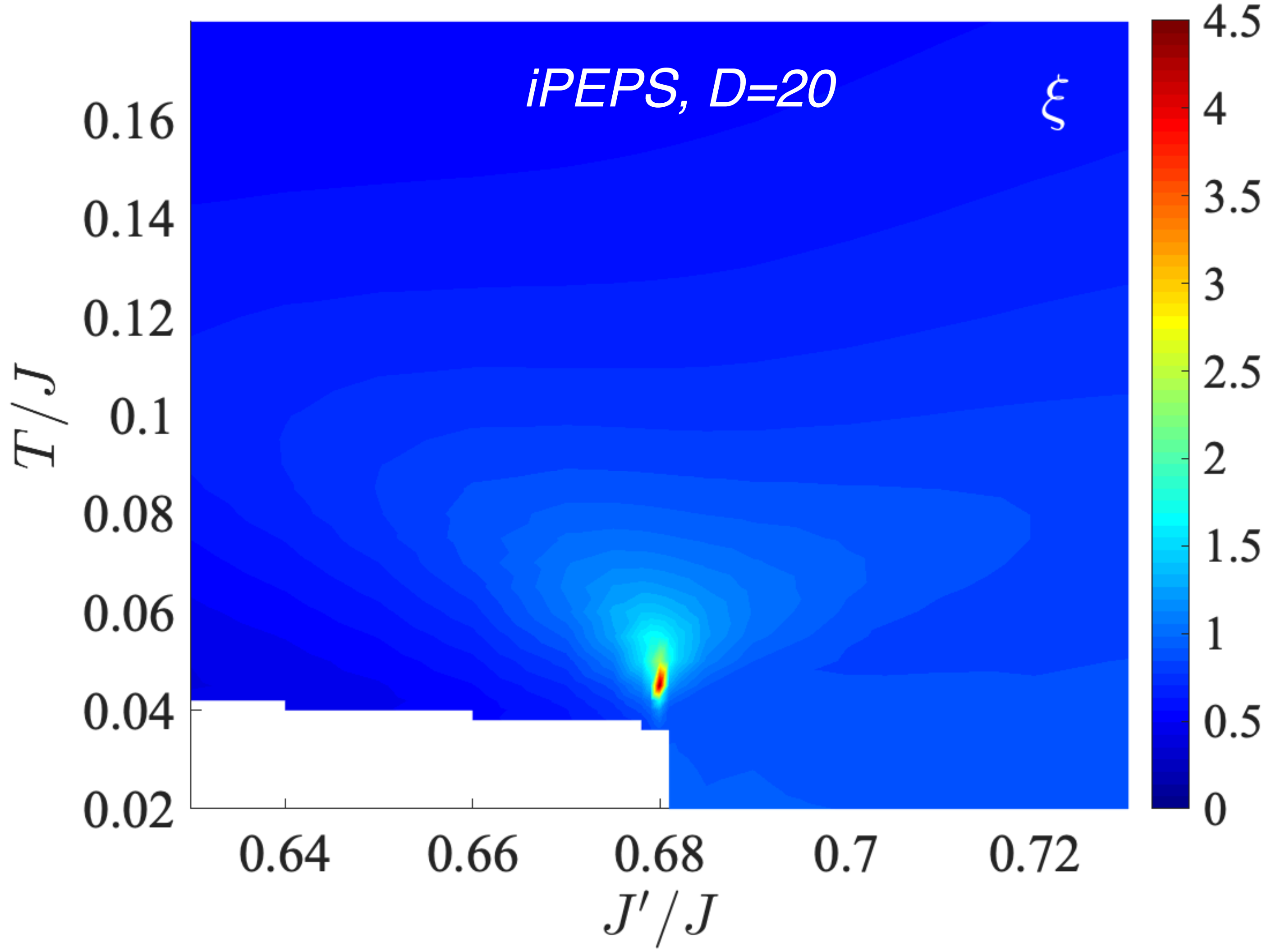
$T_c = 3.0(6)K$



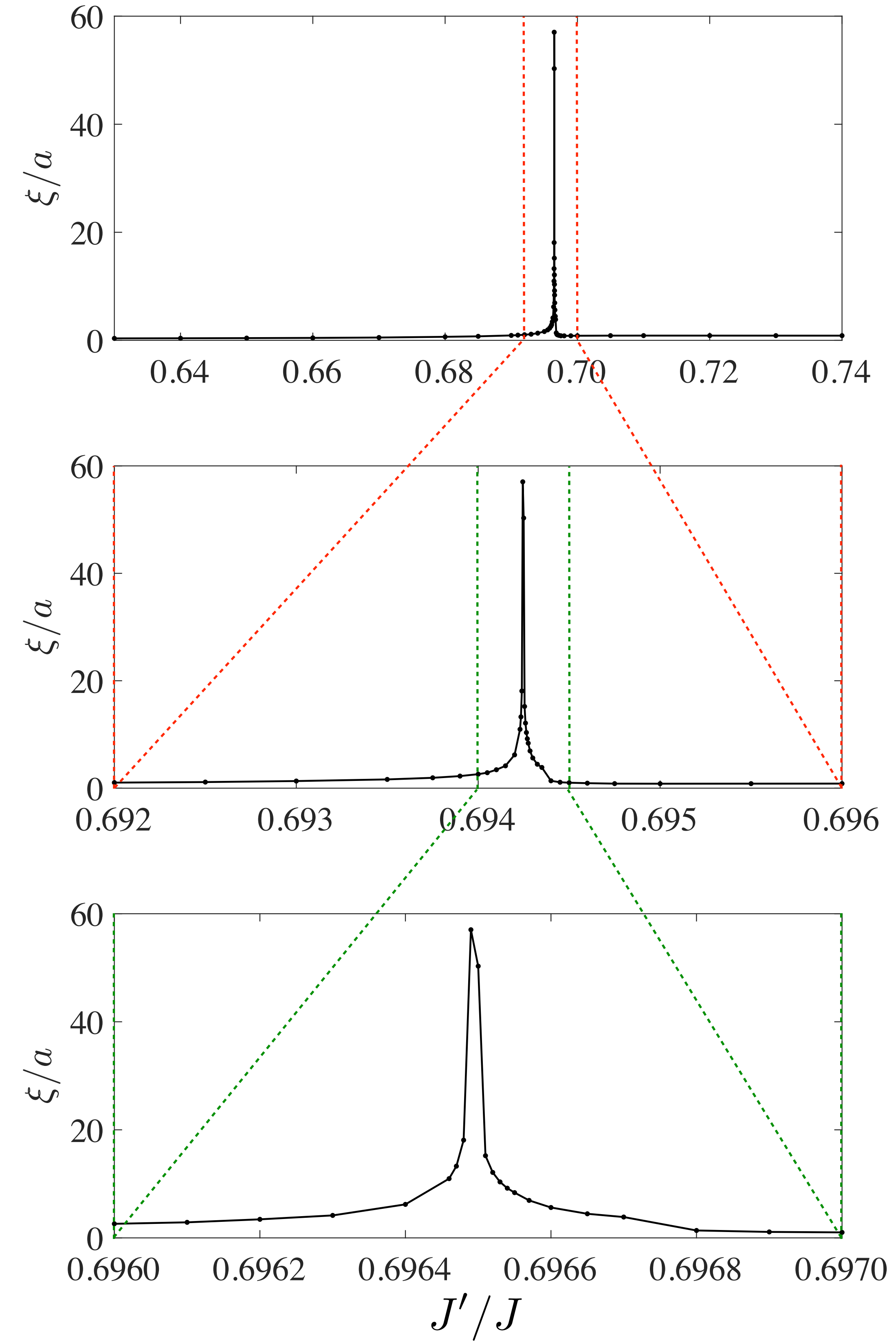


Larrea Jiménez et al., arxiv:2009:14492

Correlation length



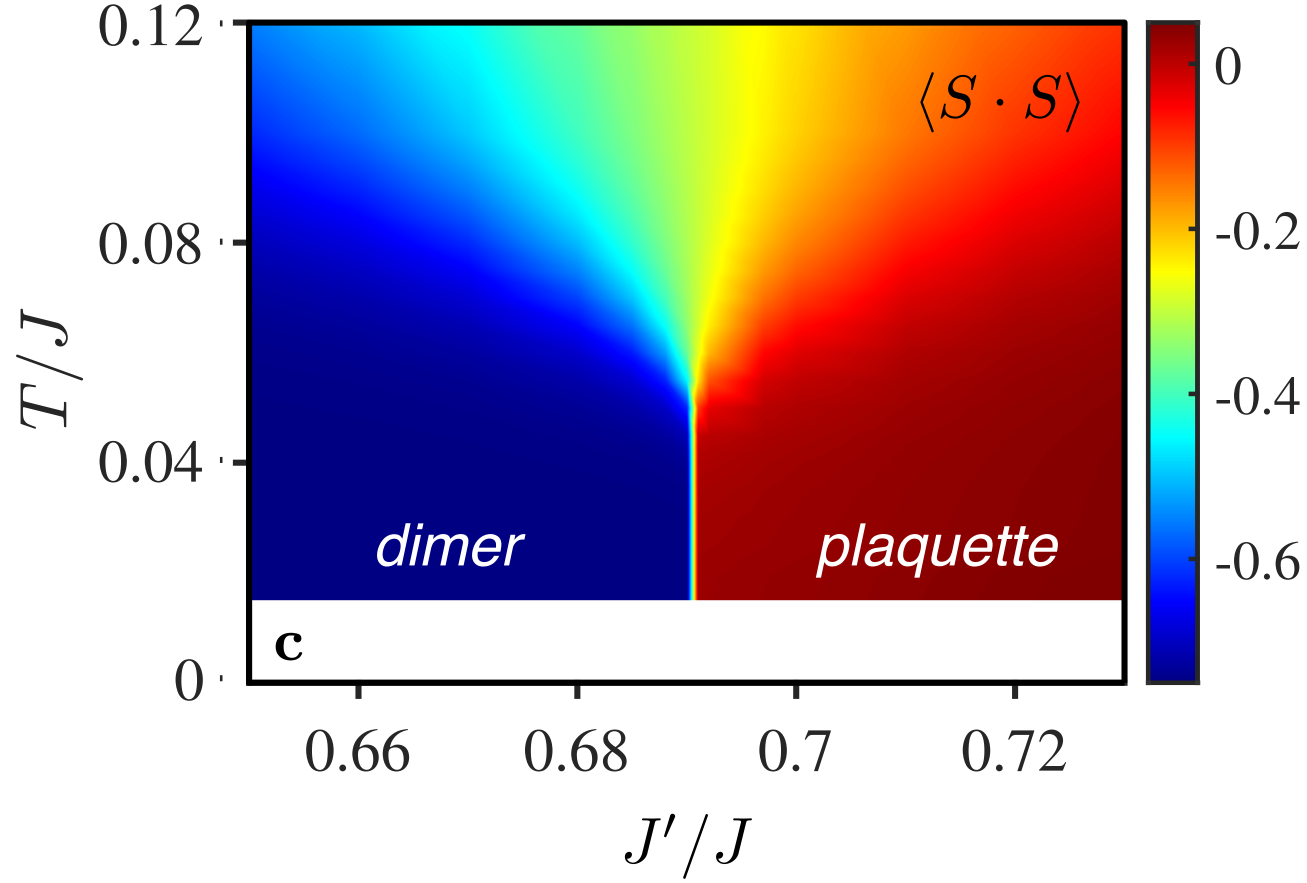
Zooming-in (D=8)



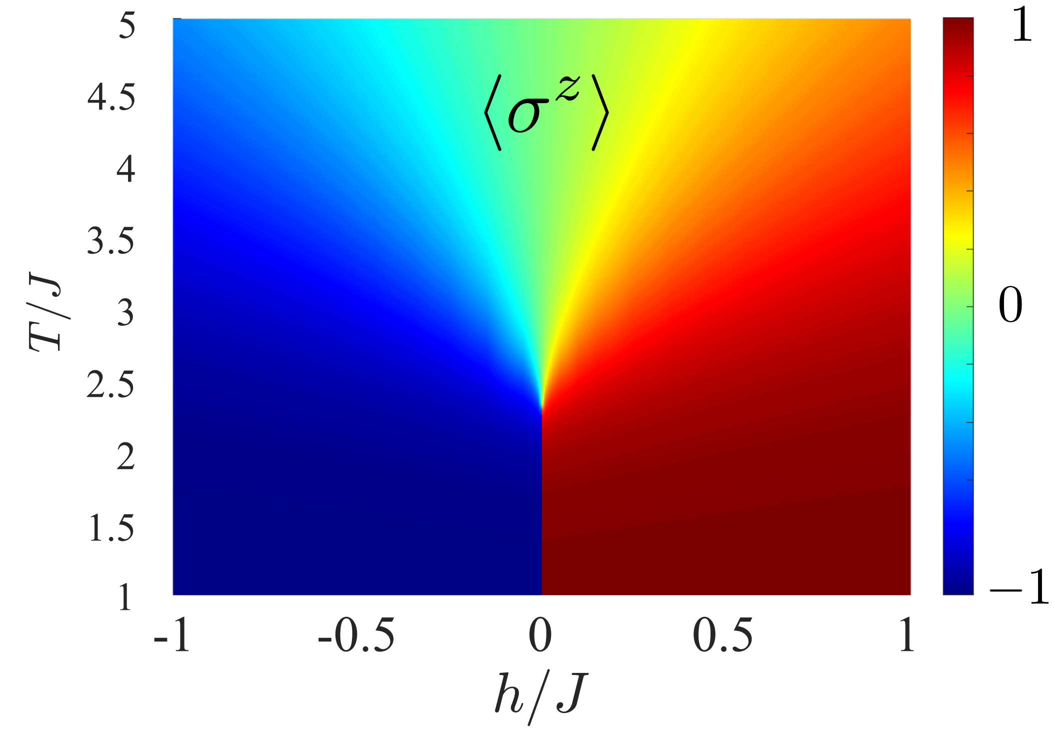
Diverging correlation length compatible with a critical point

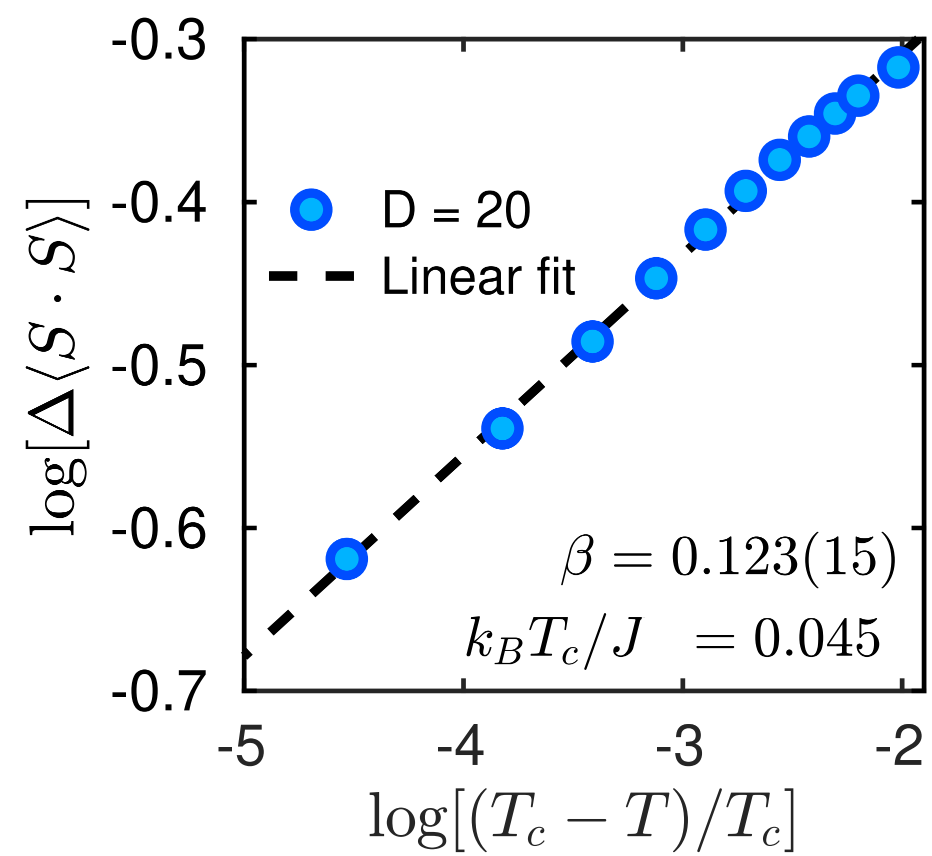
Jump in <S S> on dimer

iPEPS D=10 (with DM)



2D classical Ising model in a field

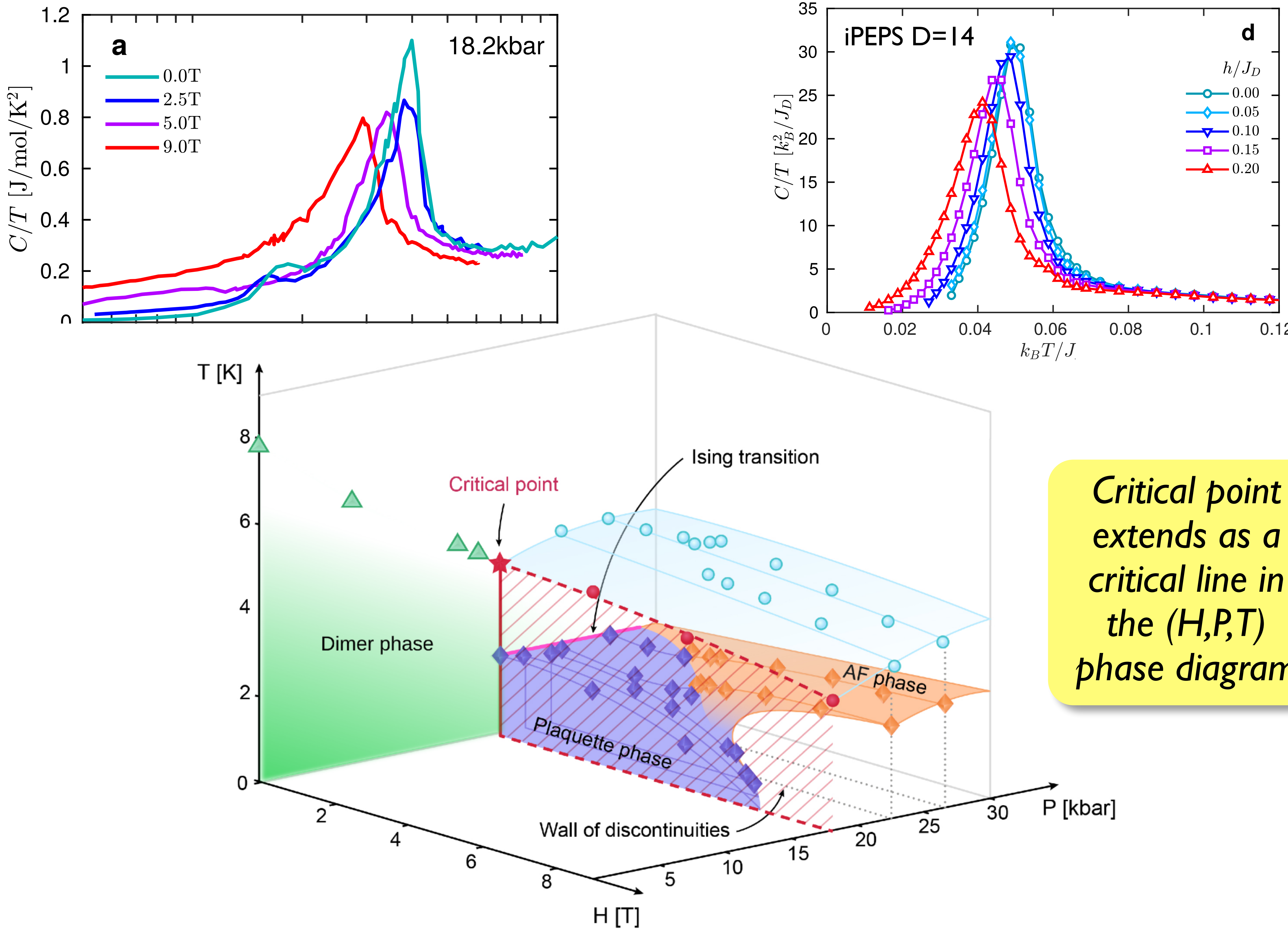




Clear evidence of a first order line with a critical point compatible with the 2D Ising universality class

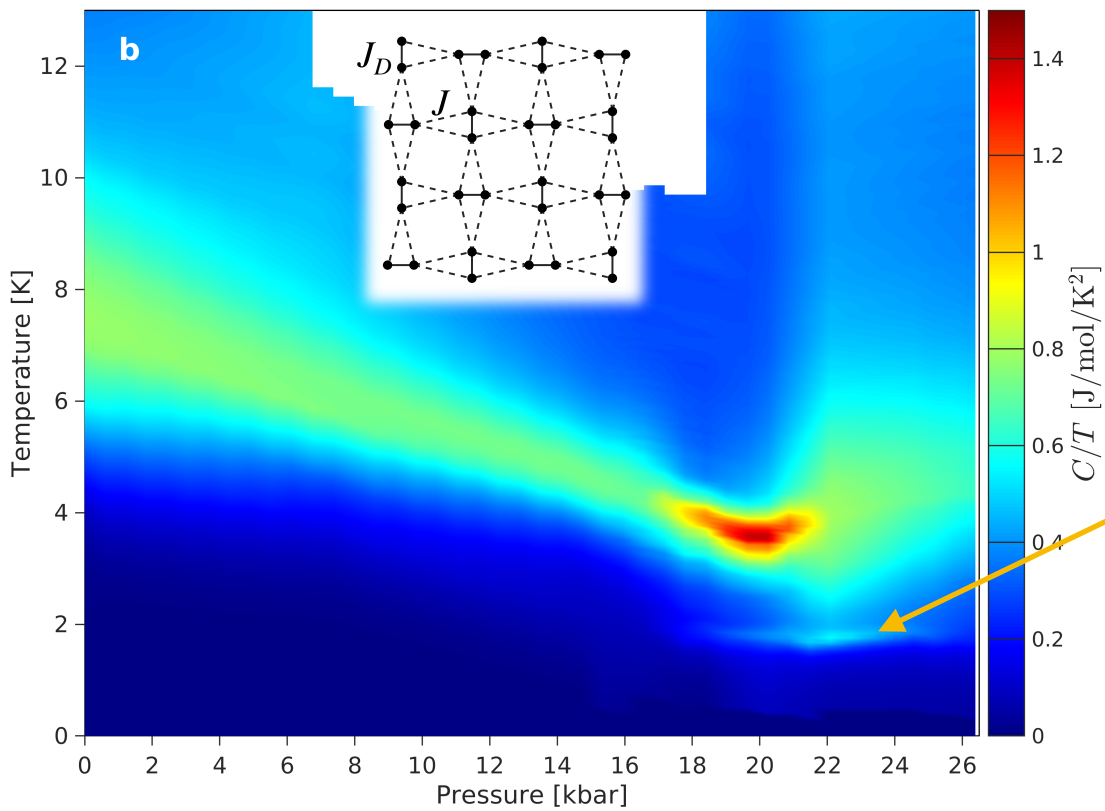
exact value: $\beta = 0.125$

Effect of a finite magnetic field

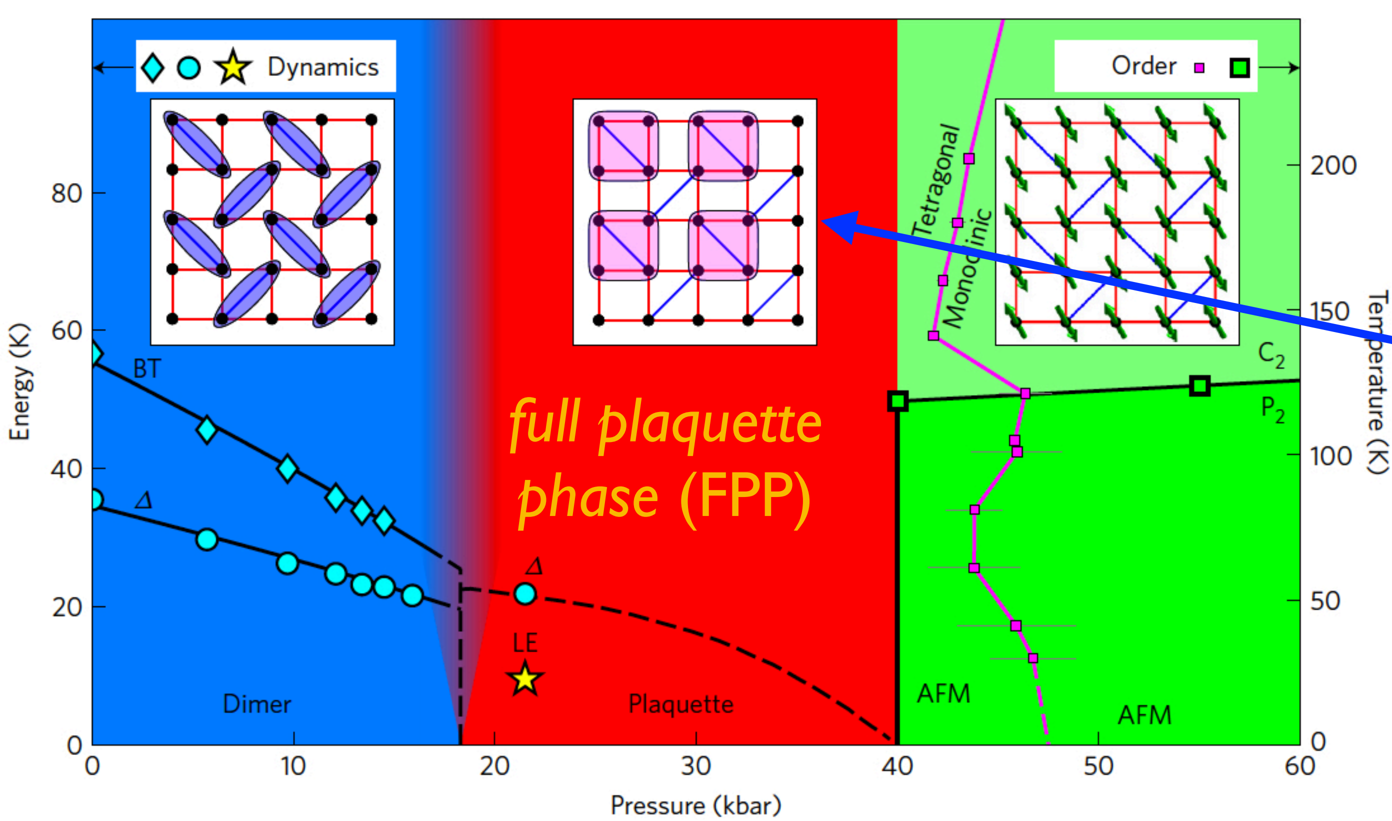


Critical point extends as a critical line in the (H,P,T) phase diagram

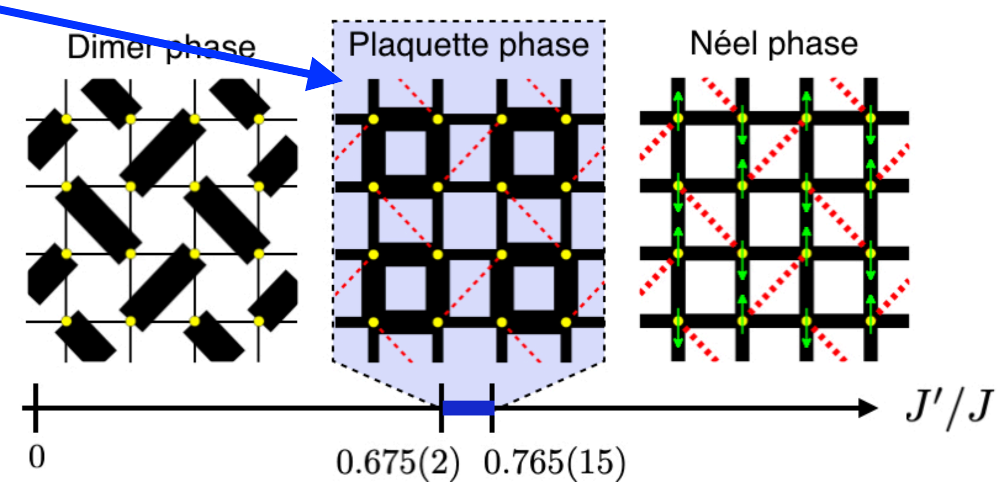
Open challenges



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



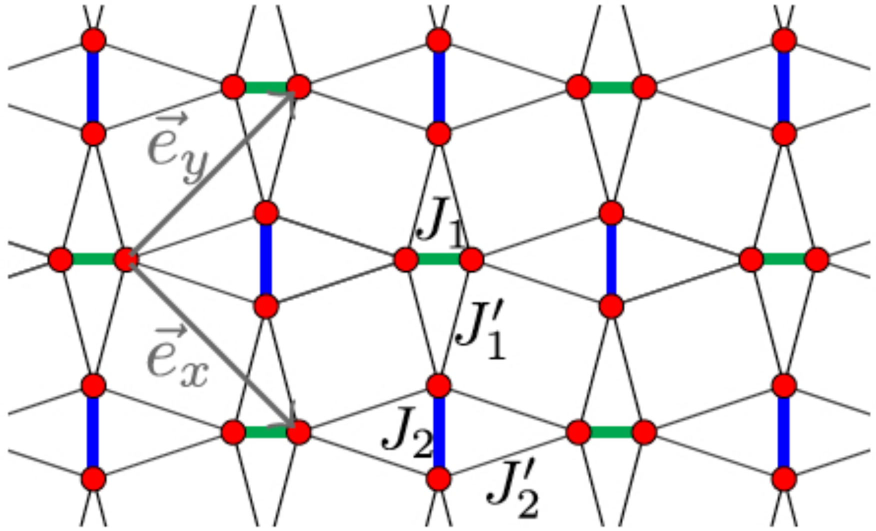
- Inelastic neutron scattering: *full plaquette phase* (FPP), not *empty plaquette phase* (EPP)
  Zayed, et al., Nat. Phys. 13, 962 (2017)

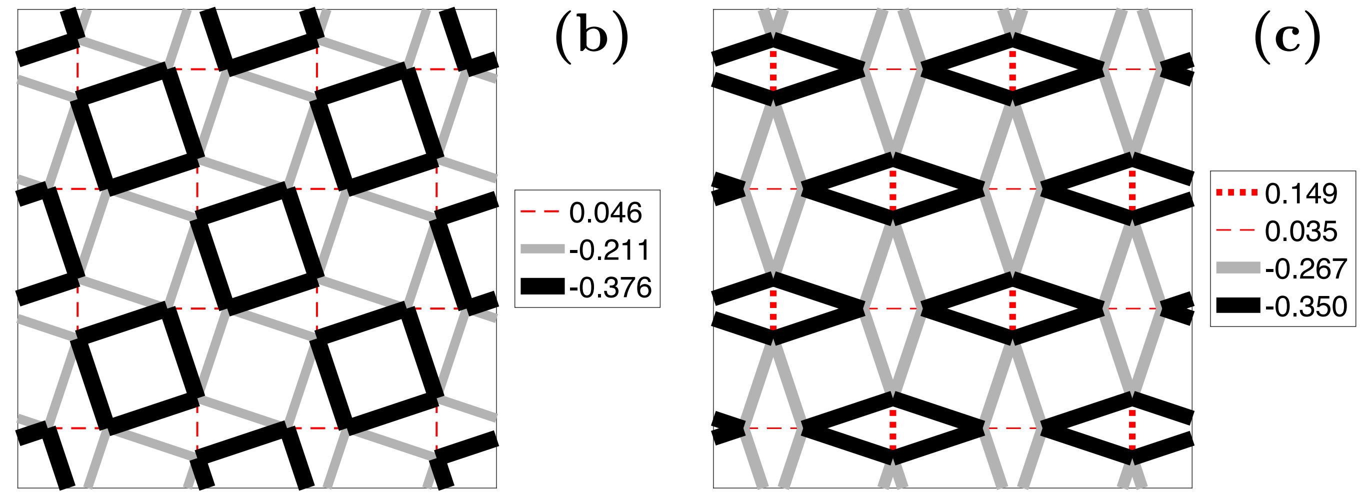


$SrCu_2(BO_3)_2$ under pressure

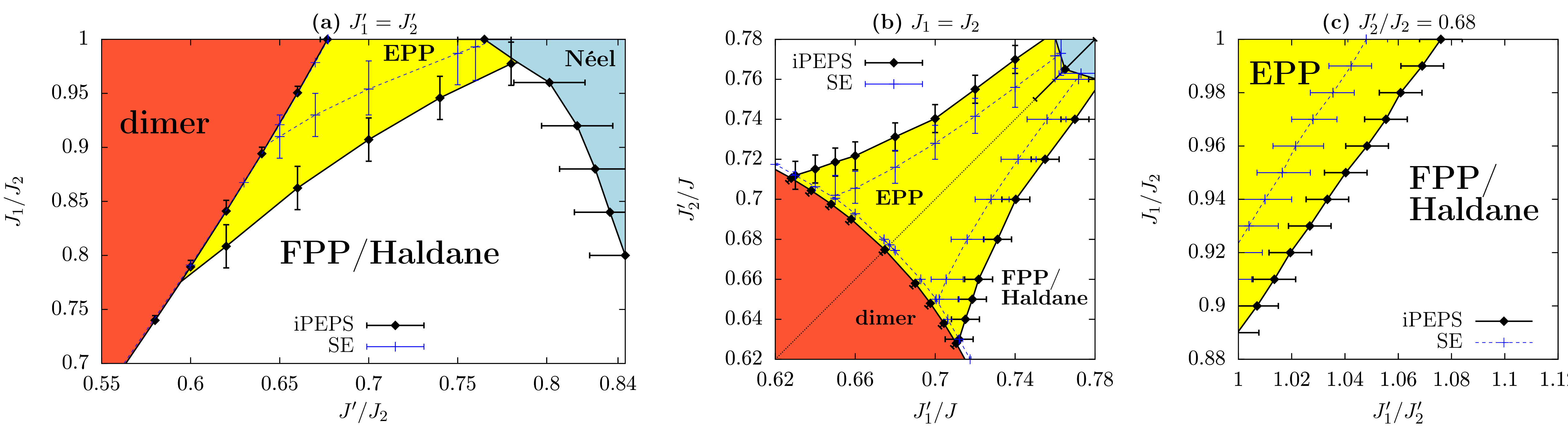
Boos, Crone, Niesen, PC, Schmidt & Mila, PRB 100 (2019)

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





EPP *vs* *FPP*



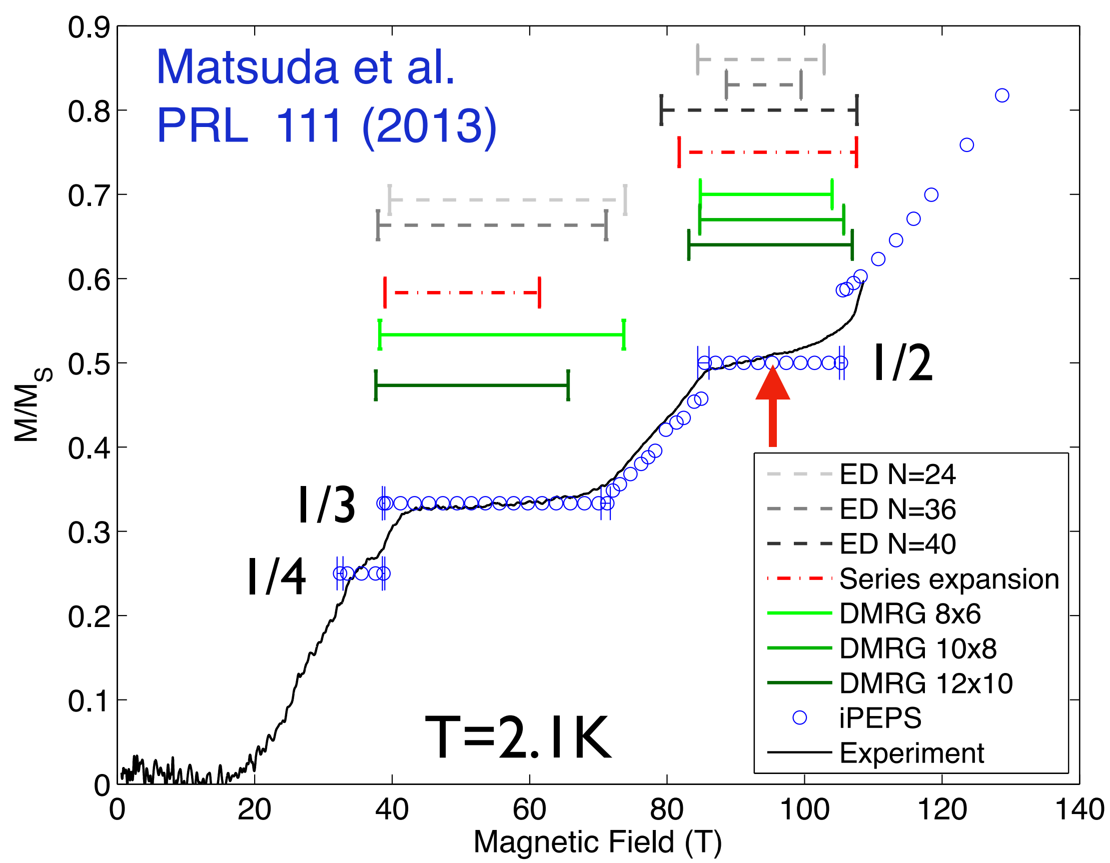
- Small deformation leads to FPP phase!

But precise model still unclear…

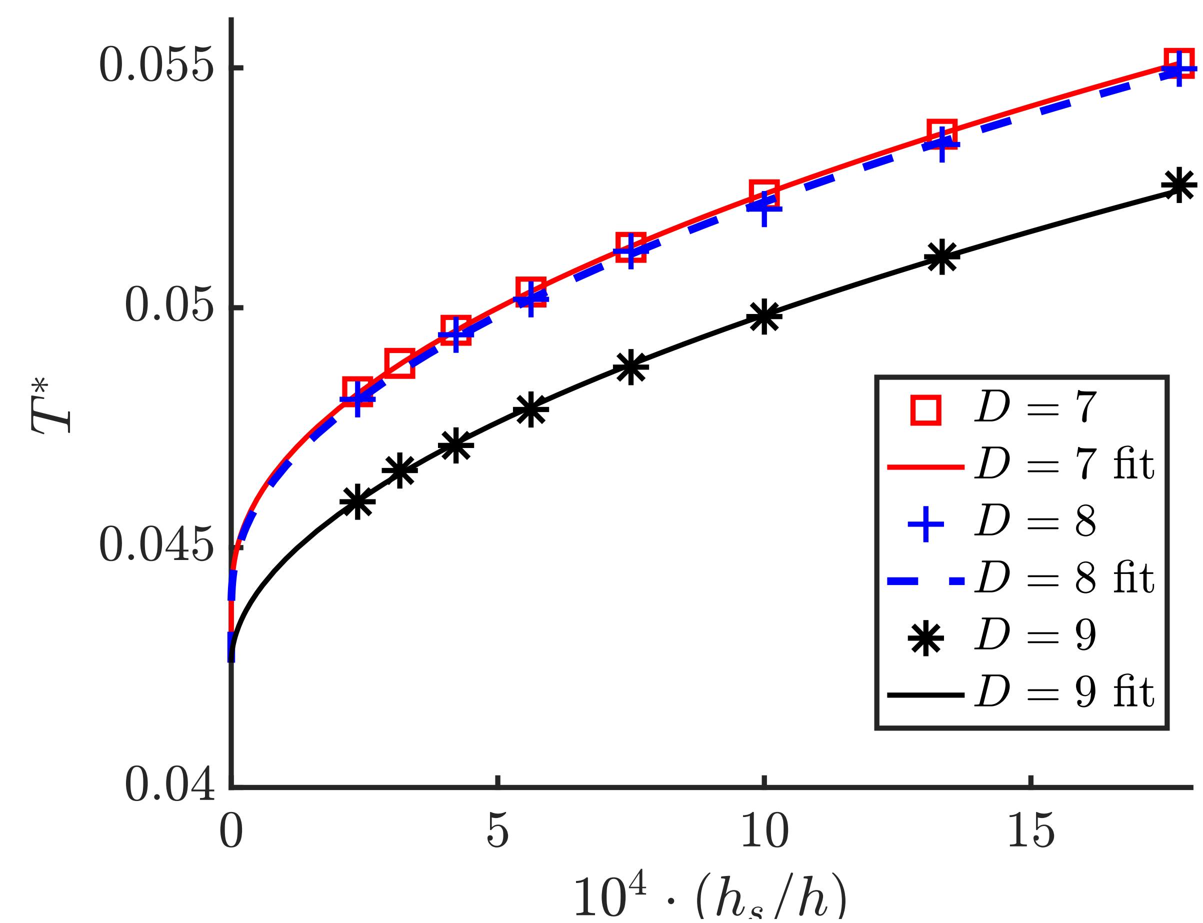
Finite T study of the m=1/2 plateau in $SrCu_2(BO_3)_2$

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

High-field magnetization data



Systematic scaling analysis



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

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!