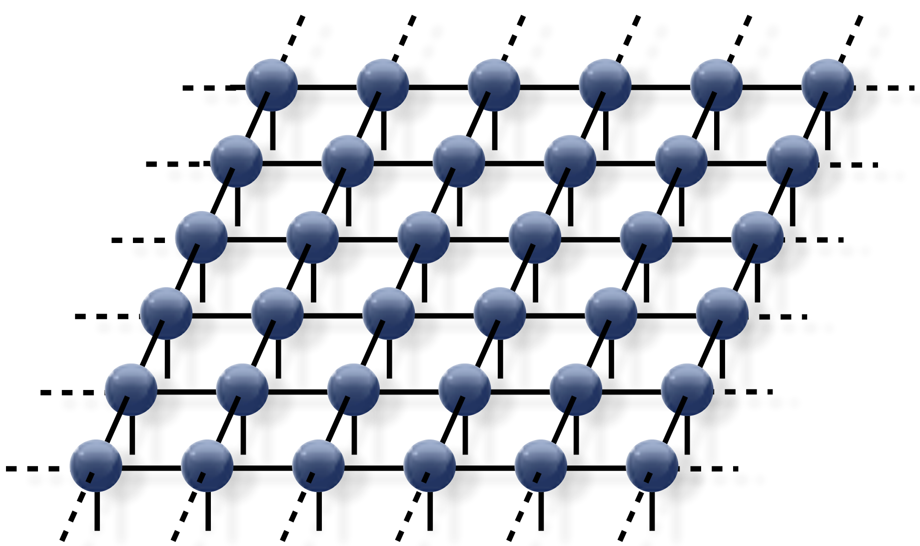
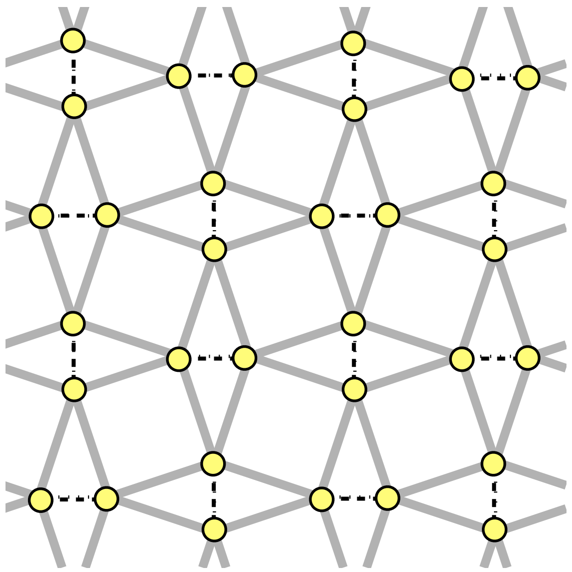
Tensor network studies of $SrCu_2(BO_3)_2$ under pressure and in a magnetic field

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam





iPEPS
2D tensor network ansatz

Shastry-Sutherland model

Delta Institute for Theoretical Physics

European Research Council

QuSoft

Outline

- Part I: SCBO under pressure at finite temperature
  - ✦ *Critical point at finite temperature, analogous 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, Nature 592, 370 (2021)

- Part II: SCBO under extreme conditions of field & pressure
  - ✦ *New type of 1/5 plateau and supersolid phases in the (p, H) phase diagram*

    Z. Shi, S. Dissanayake, PC, W. Steinhardt, D. Graf, D. M. Silevitch, H. A. Dabkowska, T. F. Rosenbaum, F. Mila, S. Haravifard, Nat Commun 13, 1 (2022)

- Part III: SCBO up to the saturation magnetic field
  - ✦ *Close agreement between iPEPS and experiments & insights into ultrasound velocity*

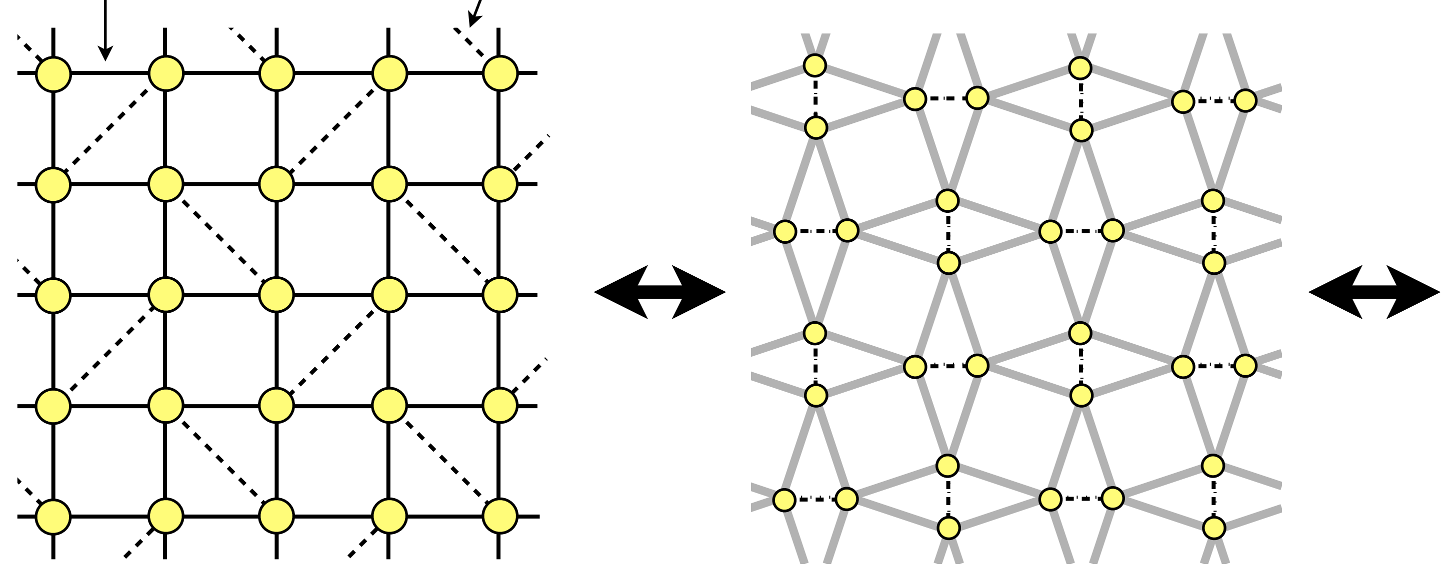
    T. Nomura, PC, A. Miyata, S. Zherlitsyn, Y. Ishii, Y. Kohama, Y. Matsuda, A. Ikeda, C. Zhong, H. Kageyama, F. Mila, arXiv:2209.07652 (to appear in Nat. Comm.)

- Part IV: Role of interlayer coupling in SCBO
  - ✦ *Phase diagram of the SSM with interlayer coupling with new iPEPS approach*

    P. Vlaar, PC, PRL 130, 130601 (2023); arxiv:2302.07894

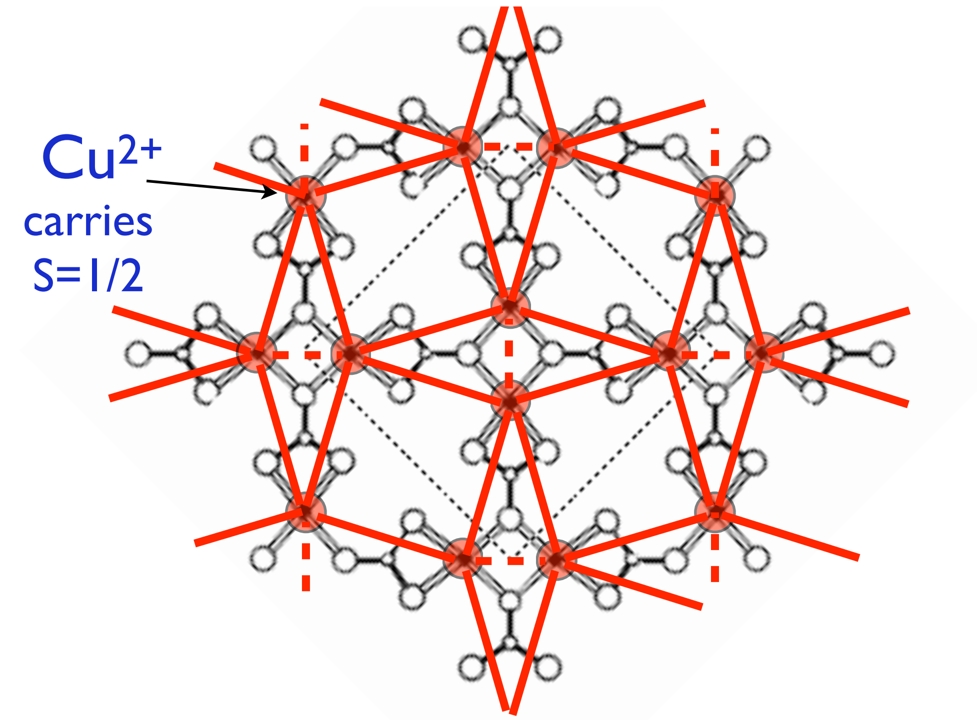
The Shastry-Sutherland model and $SrCu_2(BO_3)_2$

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

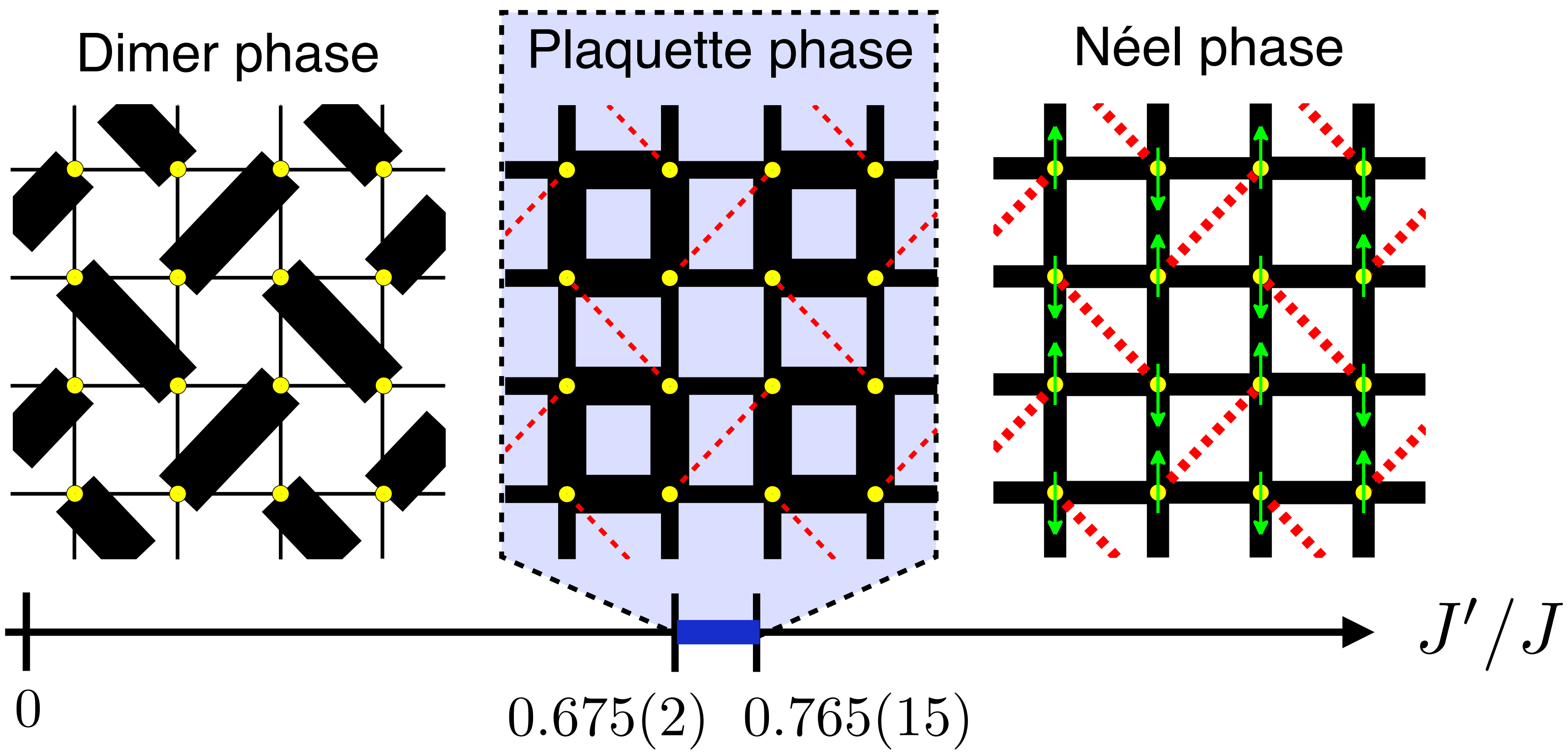


$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



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



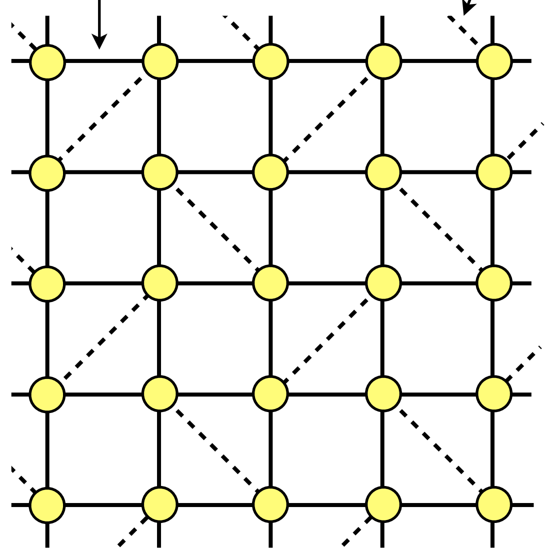
Corboz and Mila, PRB **87** (2013)

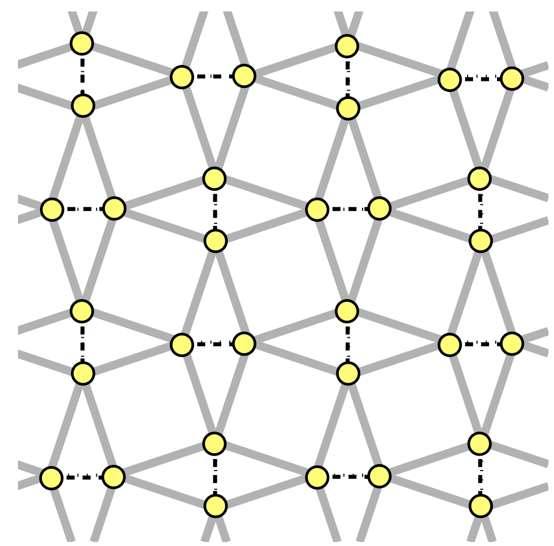
previously found in:

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

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

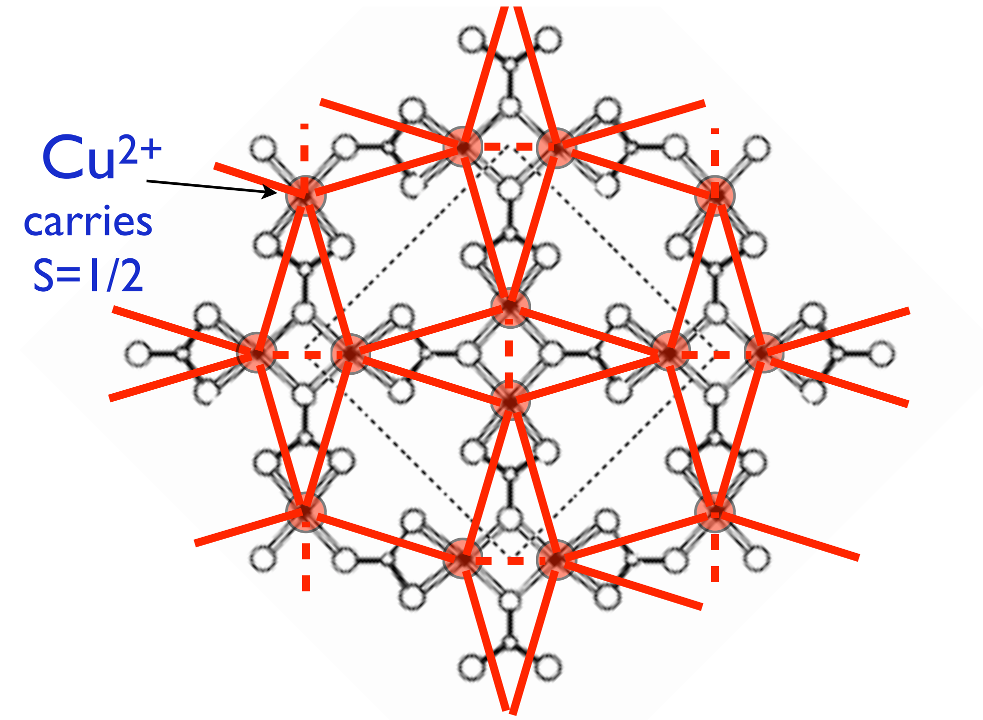
$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\mathrm{dimer}}} S_i \cdot S_j$$



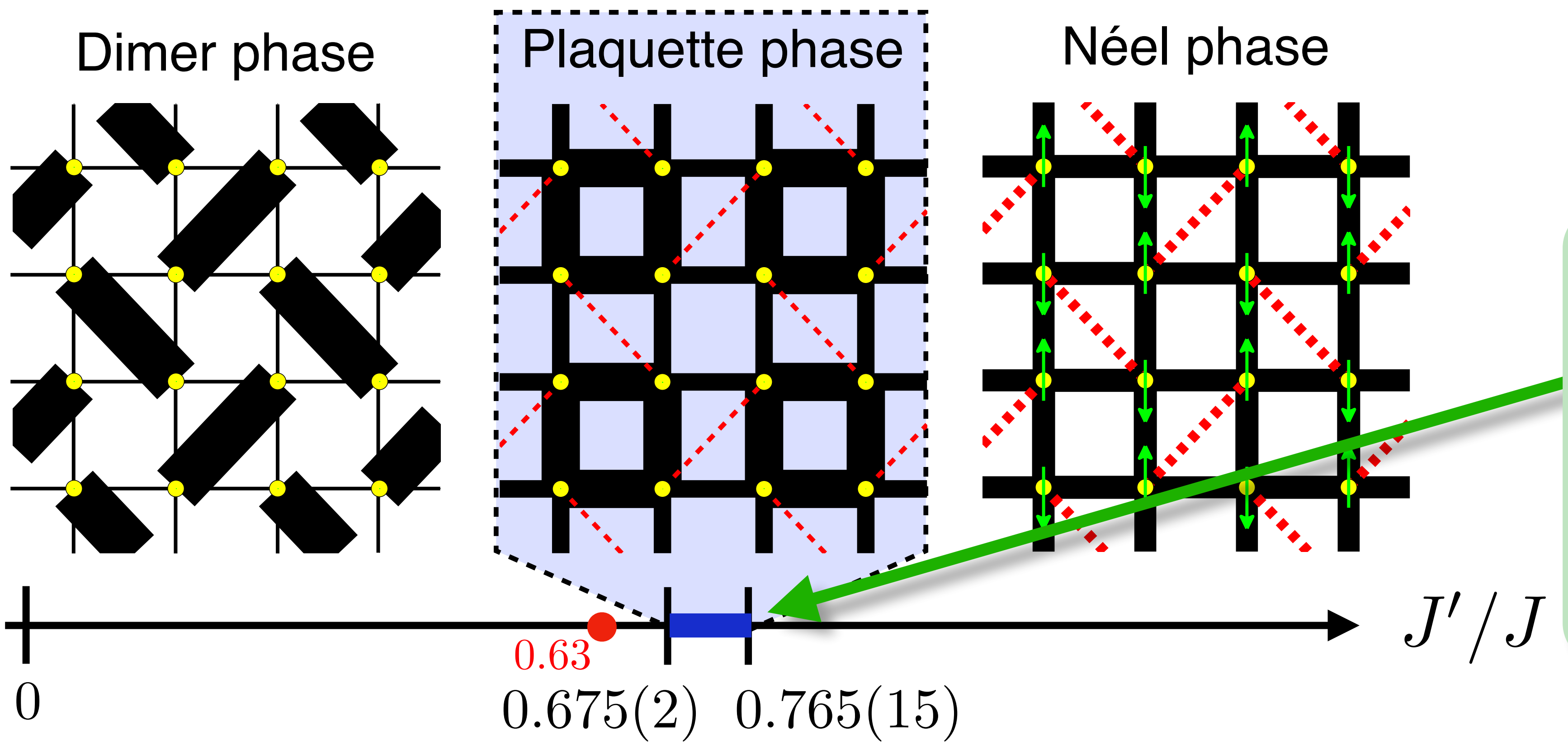


$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



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



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

Deconfined QCP?

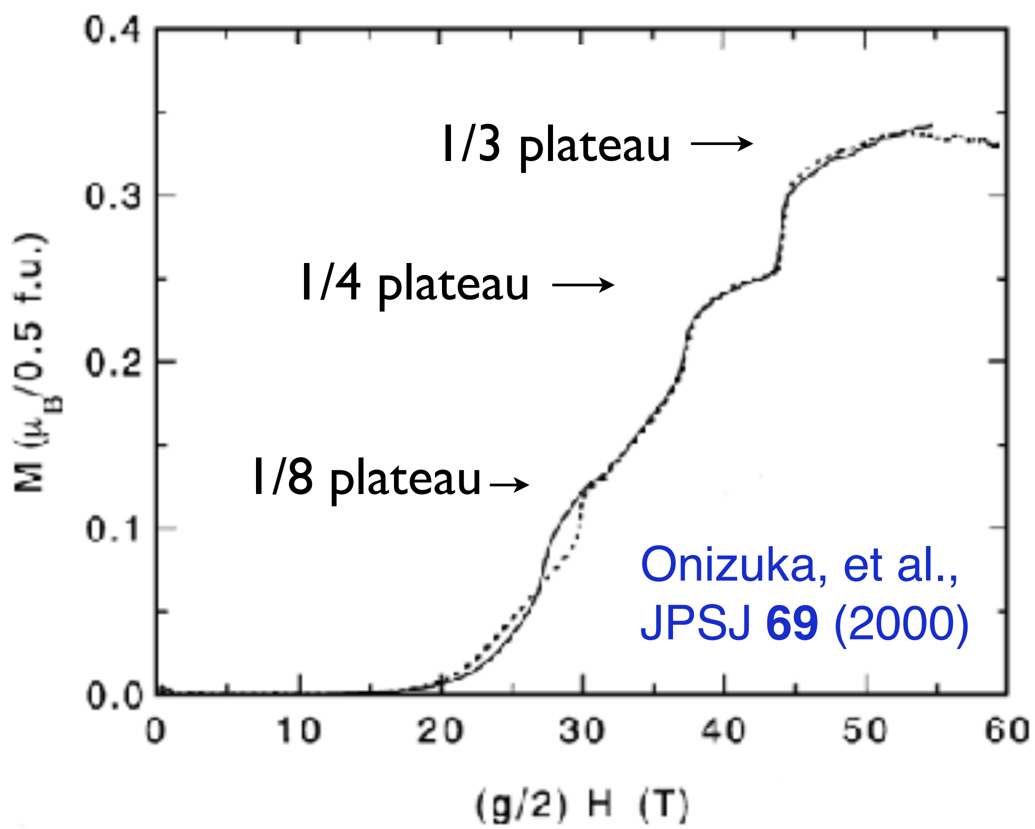
Lee, You, Sachdev & Vishwanath, PRX 9 (2019)

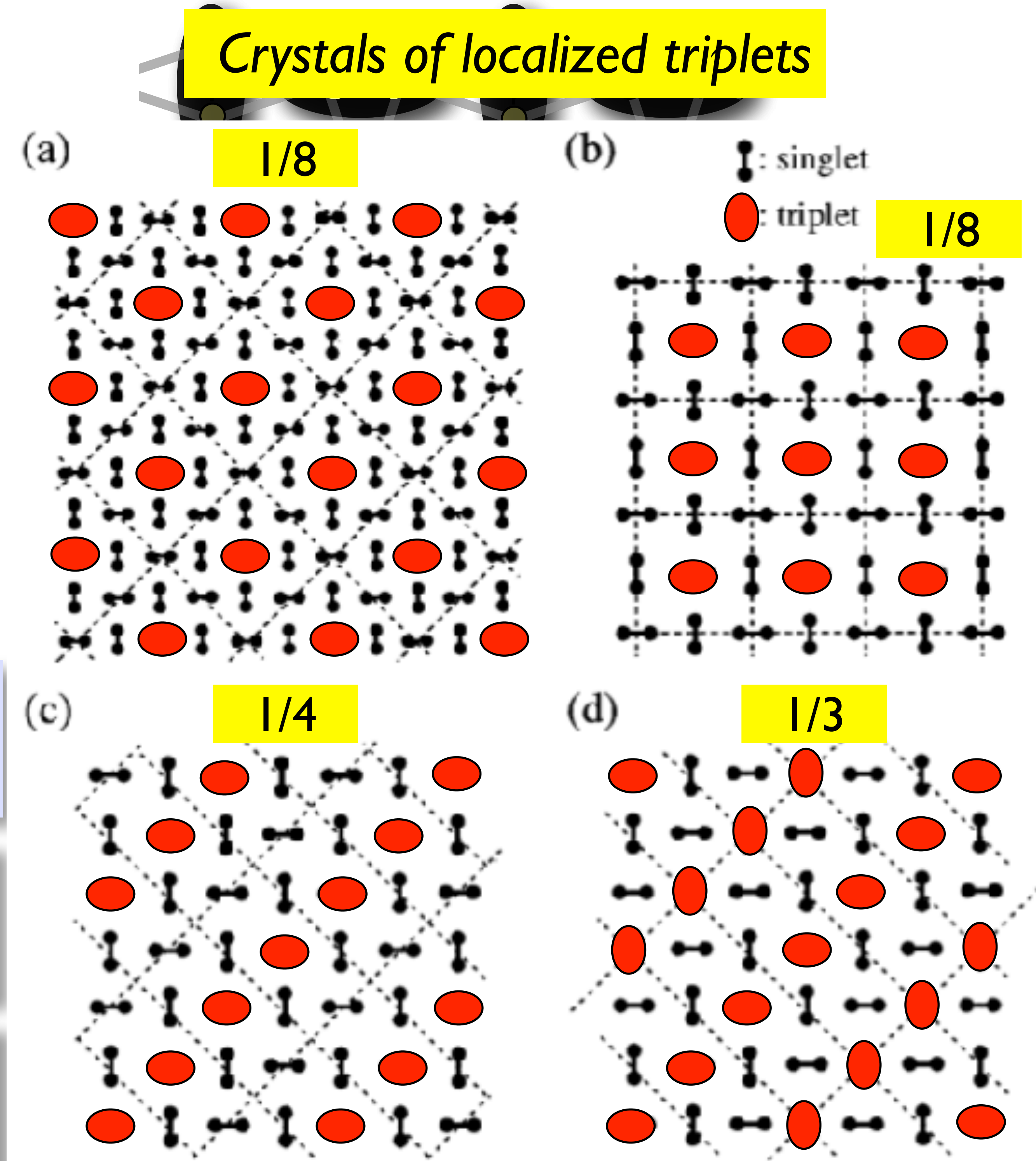
Intermediate QSL phase?

Yang, Sandvik & Wang, PRB 105 (2022)

Magnetization plateaus

$SrCu_2(BO_3)_2$ in a magnetic field exhibits several magnetization plateaus





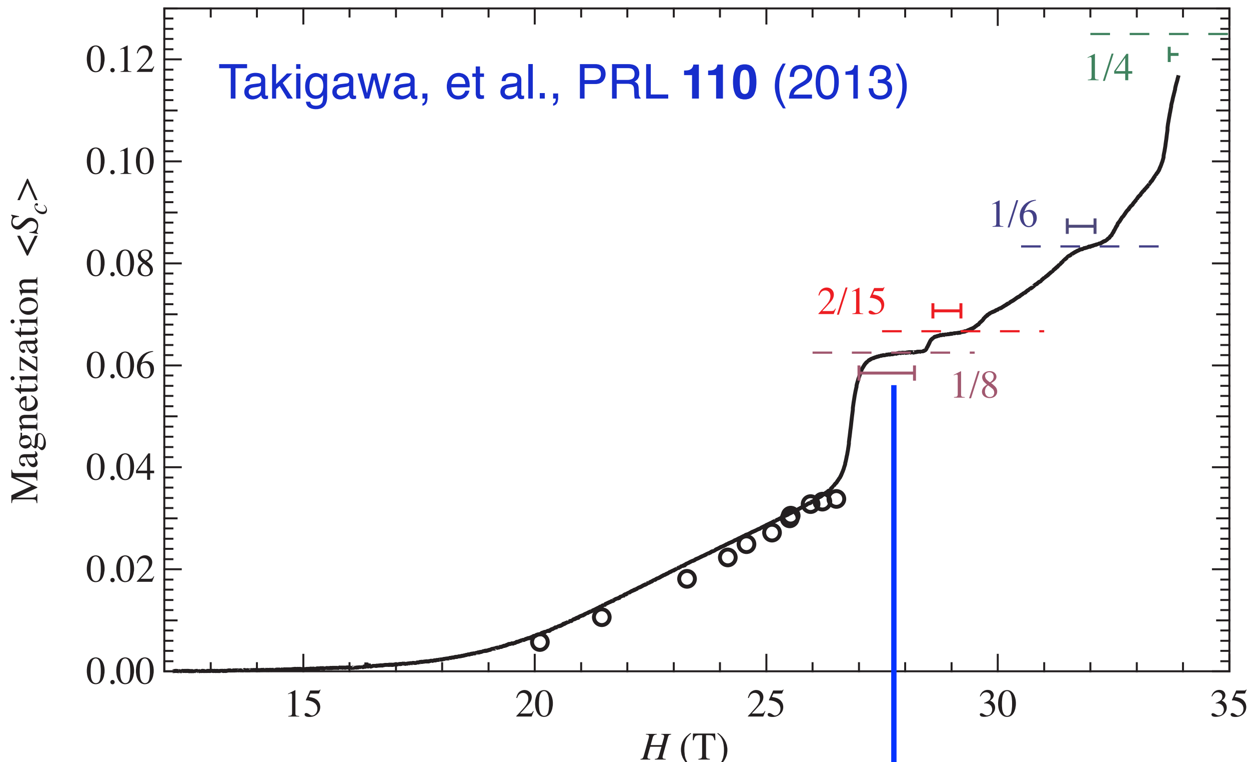
Onizuka, et al., JPSJ **69** (2000)

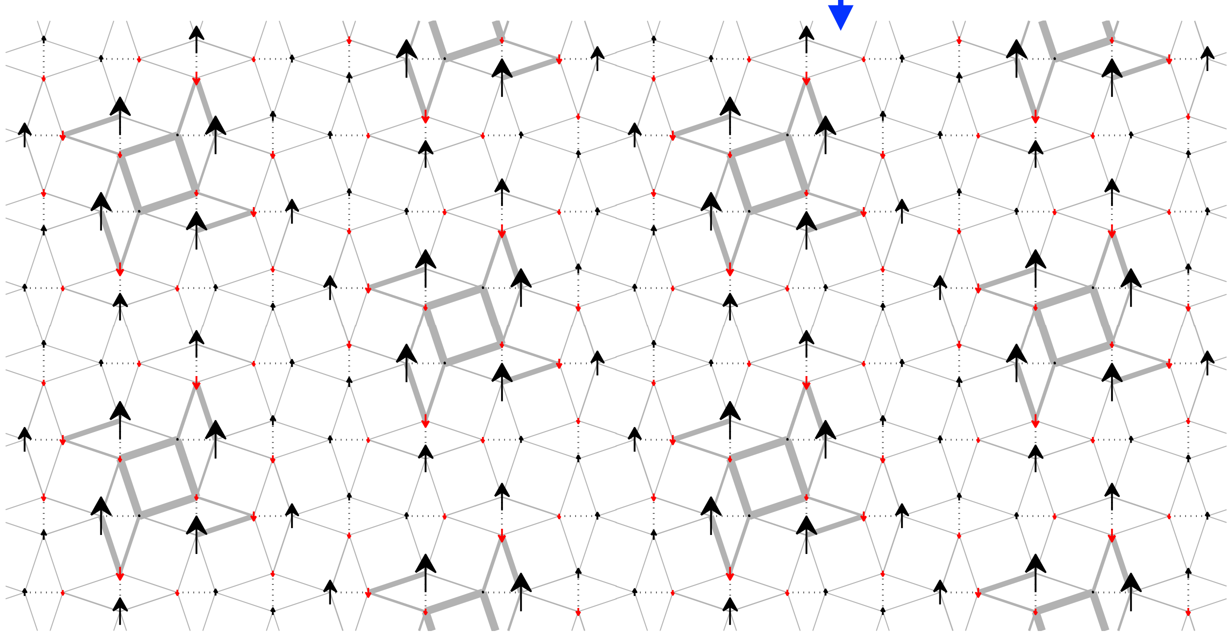
The SSM has almost localized triplet excitations [Miyahara&Ueda'99, Kageyama et al. '00]

Triplets repel each other
(on the mean-field level)

Common assumption:
magnetization plateaus correspond to *crystals of localized triplets*!

Magnetization plateaus below the 1/4 plateau





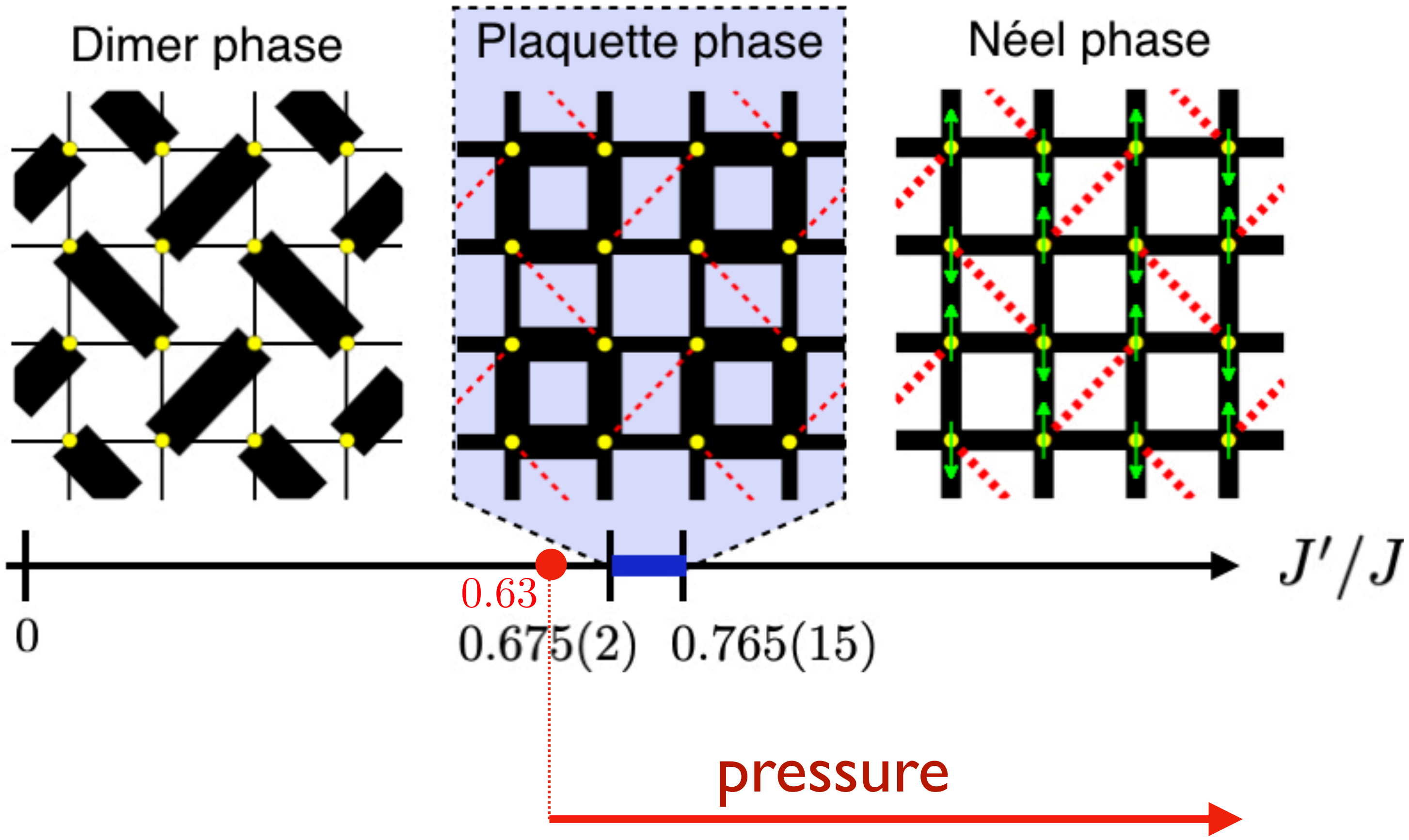
★ Crystals of triplet-bound states

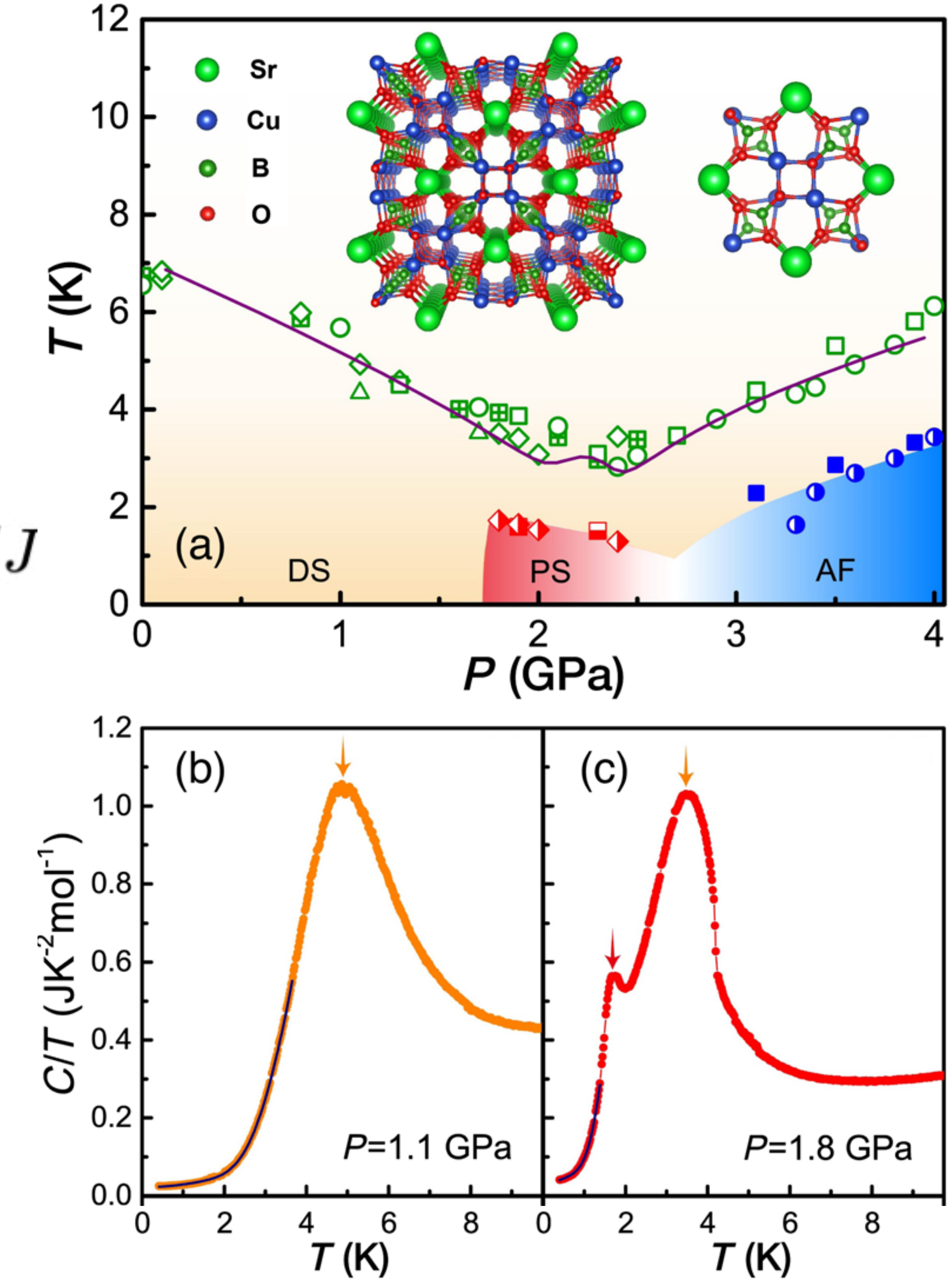
PC, F. Mila, PRL **112** (2014)

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





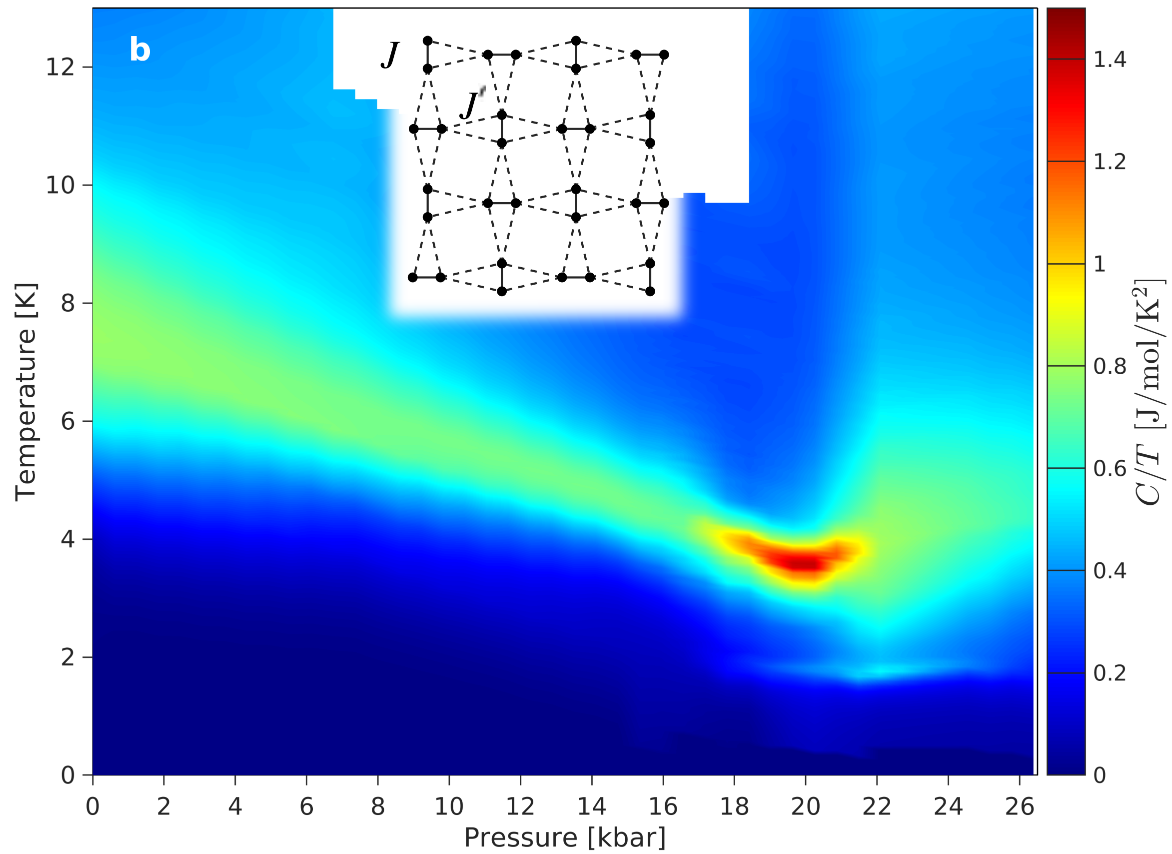
Guo, et al., PRL 124, 206602 (2020)

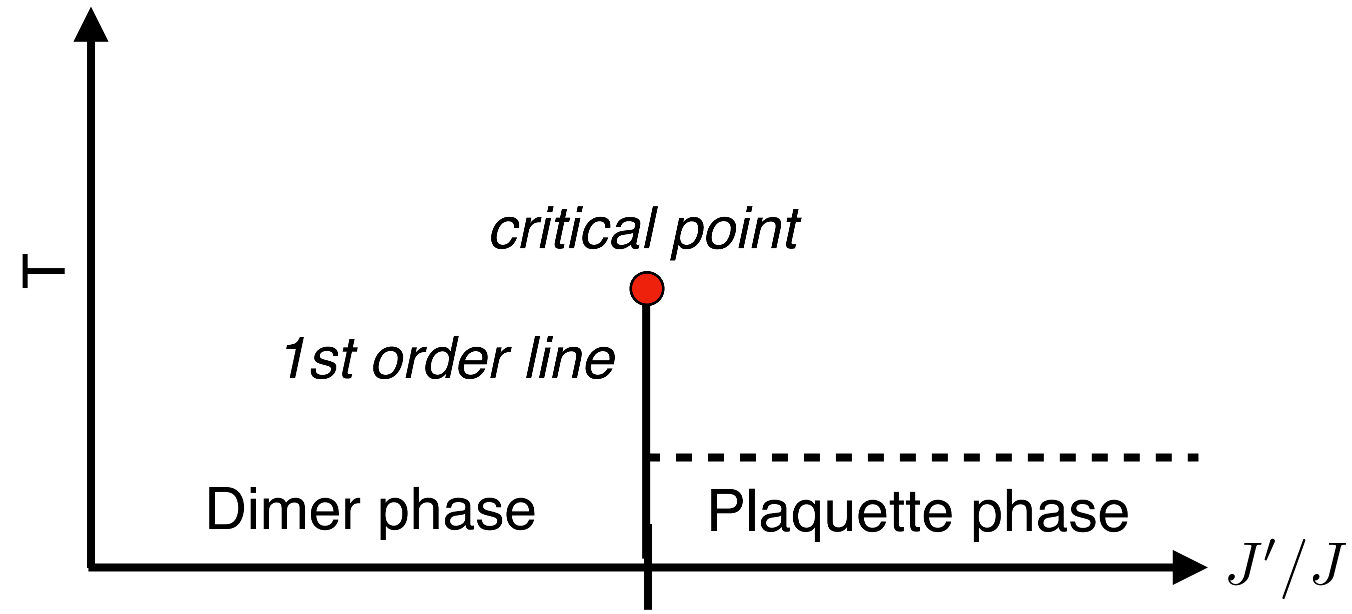
Drive system across the phase transitions!

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)
Cui et al., arxiv:2204.08133
…

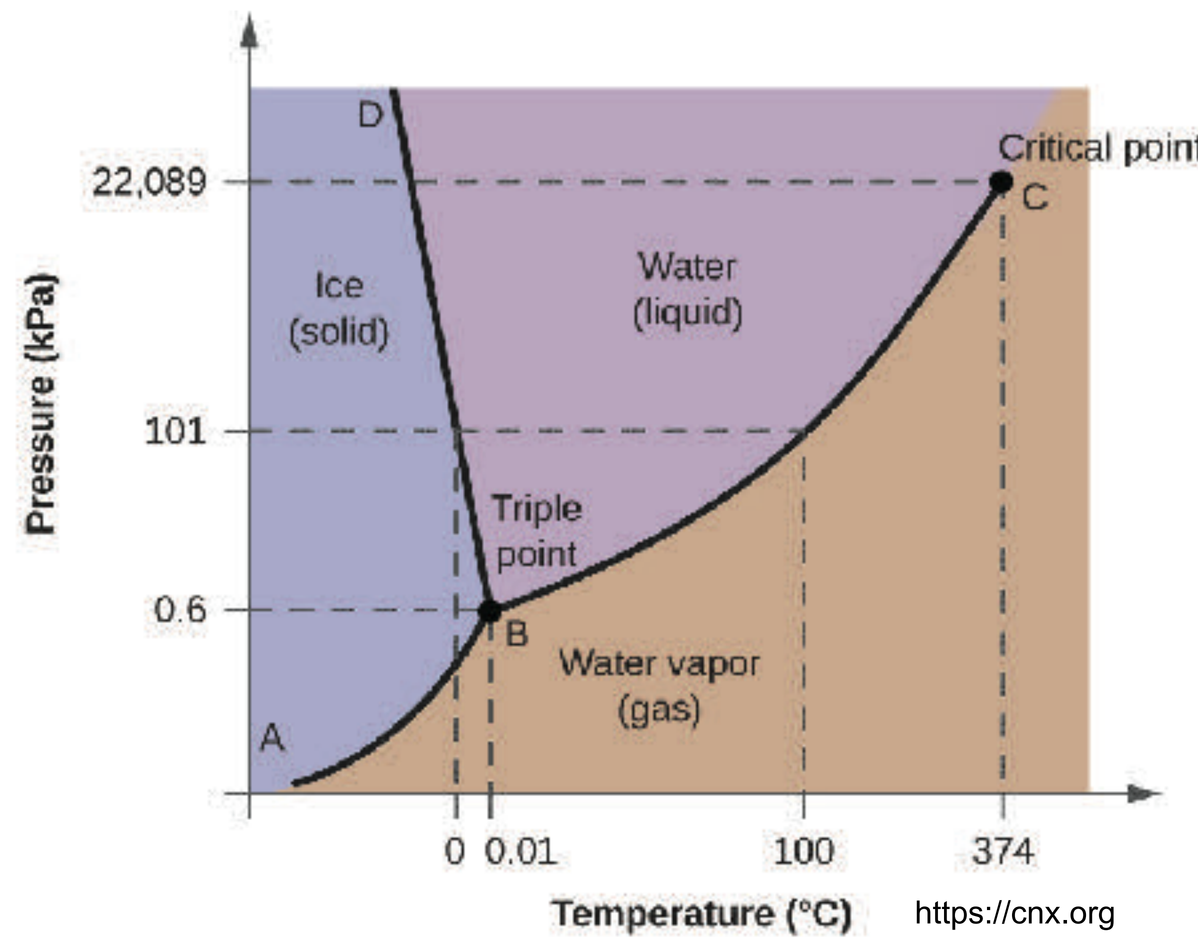
Specific heat data (group of H. M. Rønnow)

Jiménez, Crone, et al., Nature 592, 370 (2021)





Can we reproduce this with iPEPS?



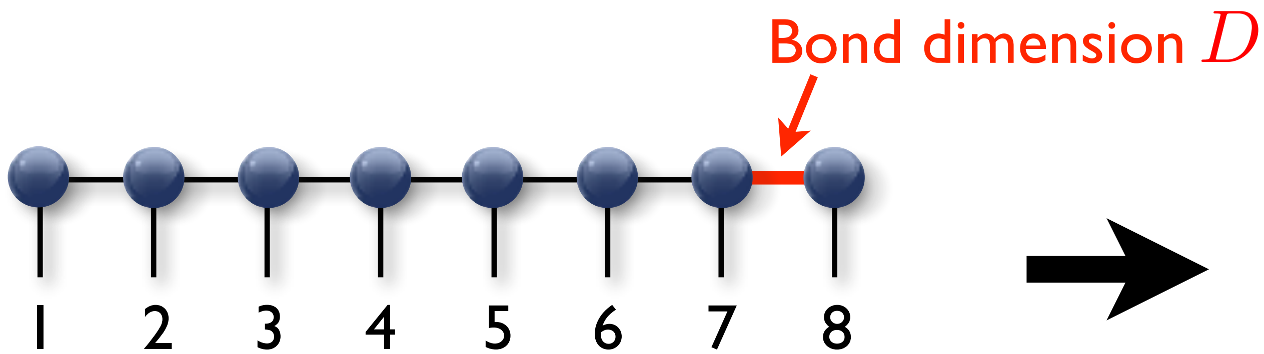
https://cnx.org

MPS & PEPS

1D

MPS

Matrix-product state



Physical indices (lattices sites)

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

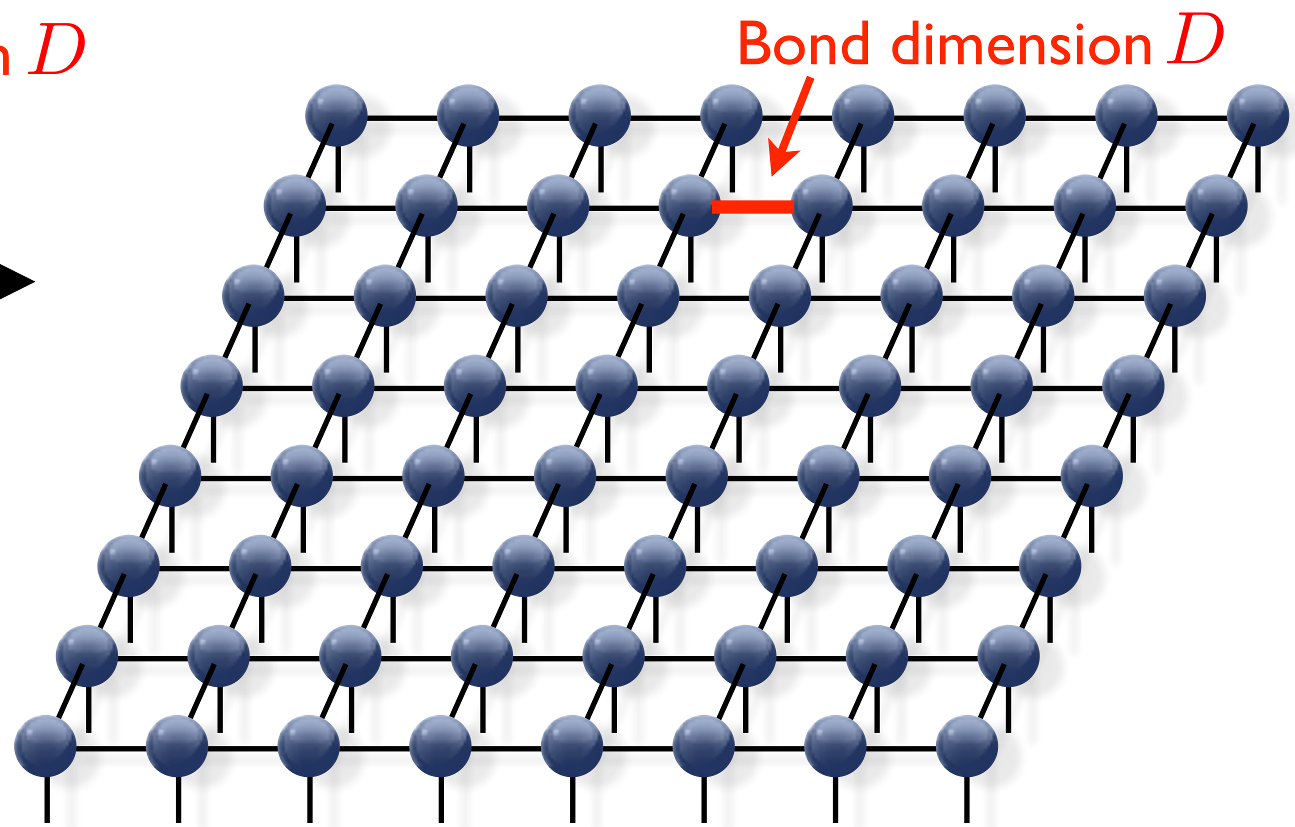
Fannes et al., CMP 144, 443 (1992)

Östlund, Rommer, PRL 75, 3537 (1995)

2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)



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

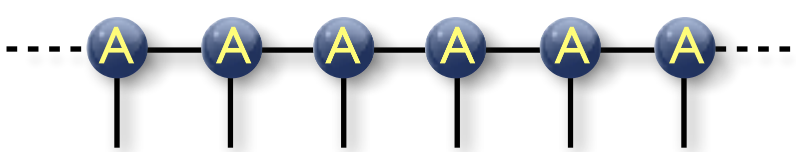
Nishio, Maeshima, Gendiar, Nishino, cond-mat/0401115

Infinite PEPS (iPEPS)

1D

iMPS

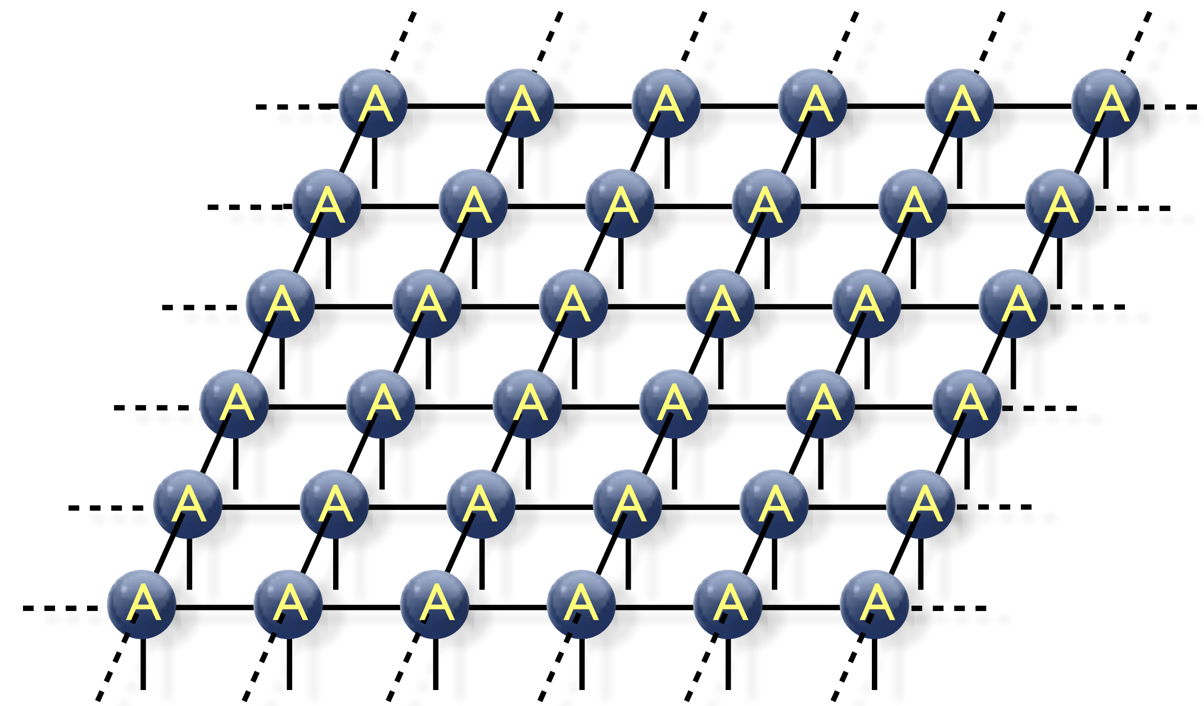
infinite matrix-product state



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

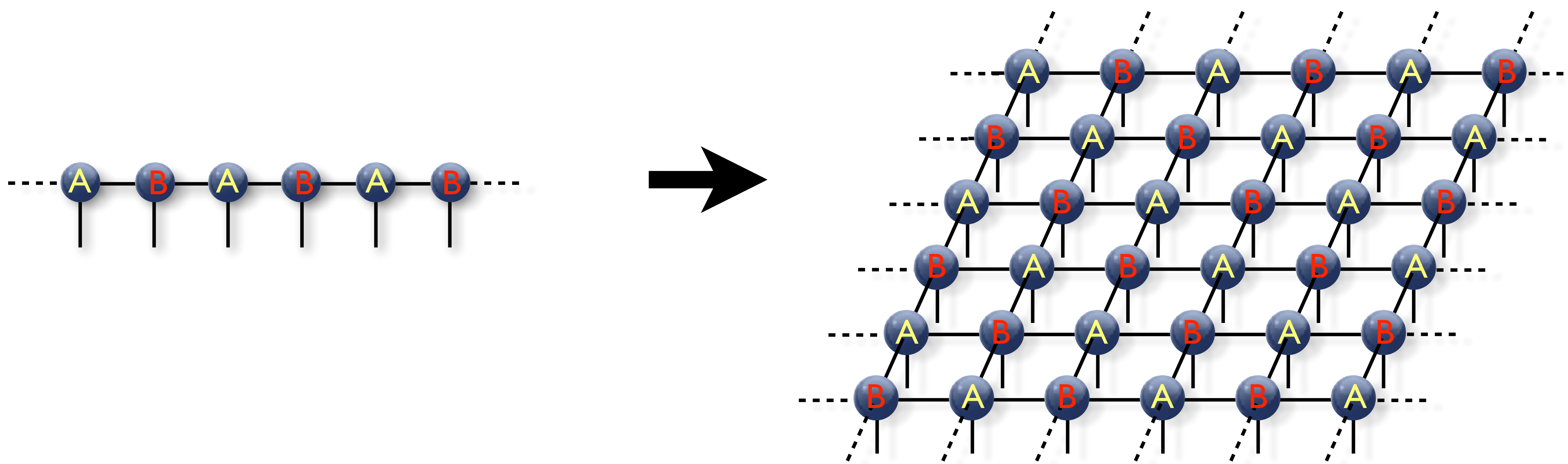
iMPS

infinite matrix-product state

2D

iPEPS

infinite projected entangled-pair state



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

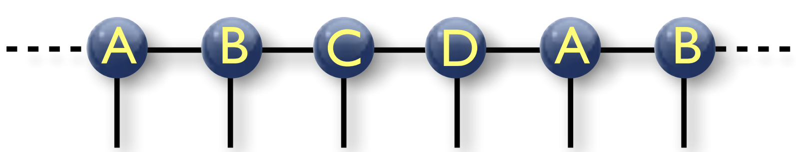
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

iPEPS with arbitrary unit cells

1D

iMPS

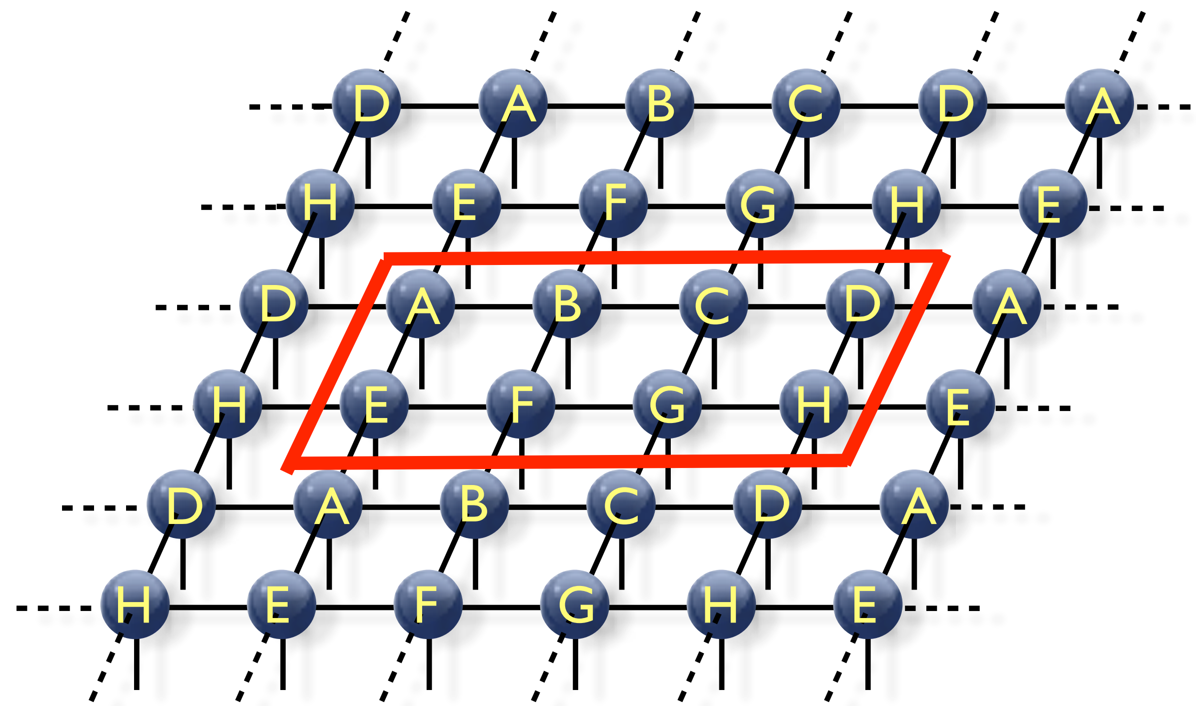
infinite matrix-product state



2D

iPEPS

with arbitrary unit cell of tensors



here: 4x2 unit cell

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

★ Run simulations with different unit cell sizes and compare variational energies

iPEPS ground state simulations

- Many applications to challenging problems, including frustrated spin, SU(N), bosonic systems, t-J / Hubbard models, and more, see e.g.:

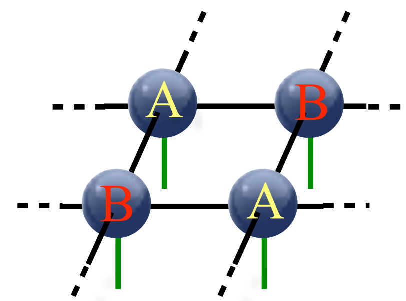
S. Dusuel, M. Kamfor, R. Orús, K. P. Schmidt, and J. Vidal, PRL 106, 107203 (2011)
P. Corboz, A. M. Läuchli, K. Penc, M. Troyer and F. Mila, PRL 107 (2011)
H. H. Zhao, C. Xu, Q. N. Chen, Z. C. Wei, M. P. Qin, G. M. Zhang and T. Xiang, PRB 85 (2012)
P. Corboz, M. Lajkó, A. M. Läuchli, K. Penc and F. Mila, PRX 2 (2012)
P. Corboz and F. Mila, PRB 87 (2013); PRL 112 (2014)
Z.-C. Gu, H.-C. Jiang, D. N. Sheng, H. Yao, L. Balents and X.-G. Wen, PRB 88 (2013)
J. Osorio Iregui, P. Corboz and M. Troyer, PRB 90 (2014)
P. Corboz, T. Rice and M. Troyer, PRL 113 (2014)
T. Picot and D. Poilblanc, PRB 91 (2015)
T. Picot, M. Ziegler, R. Orús and D. Poilblanc, PRB 93 (2016)
P. Nataf, M. Lajkó, P. Corboz, A. M. Läuchli, K. Penc and F. Mila, PRB 93 (2016)
H. Liao, Z. Xie, J. Chen, Z. Liu, H. Xie, R. Huang, B. Normand and T. Xiang, PRL 118 (2017)
B.-X. Zheng, et al., Science 358, 1155 (2017)
I. Niesen and P. Corboz, PRB 95 (2017); SciPost Physics 3, 030 (2017); Rev. B 97, 245146 (2018)
R. Haghshenas, W.-W. Lan, S.-S. Gong, and D. N. Sheng, PRB 97 (2018)
J.-Y. Chen, L. Vanderstraeten, S. Capponi, and D. Poilblanc, PRB 98 (2018)
S. S. Jahromi and R. Orús, PRB 98 (2018)
H.-Y. Lee and N. Kawashima, PRB 97 (2018)
H. Yamaguchi, Y. Sasaki, T. Okubo, et al.,PRB 98, 094402 (2018)
R. Haghshenas, S.-S. Gong, and D. N. Sheng, PRB 99, 174423 (2019)
S. S. Chung and P. Corboz, PRB 100 (2019)
B. Ponsioen, S. S. Chung, and P. Corboz, PRB 100 (2019)
C. Boos, S. P. G. Crone, I. A. Niesen, P. Corboz, K. P. Schmidt, and F. Mila, PRB 100 (2019)
Z. Shi, et al, Nature Communications 10, 2439 (2019)
A. Kshetrimayum, C. Balz, B. Lake, and J. Eisert, ArXiv:1904.00028 (2019)
H.-Y. Lee, R. Kaneko, T. Okubo, and N. Kawashima, PRL 123, 087203 (2019)
O. Gauthé, S. Capponi, M. Mambrini, and D. Poilblanc, PRB 101, 205144 (2020)
H.-Y. Lee, R. Kaneko, L. E. Chern, T. Okubo, Y. Yamaji, N. Kawashima, and Y. B. Kim, Nature Communications 11 (2020)
W.-Y. Liu, S.-S. Gong, Y.-B. Li, D. Poilblanc, W.-Q. Chen, and Z.-C. Gu, ArXiv:2009.01821 (2020)
J.-Y. Chen, S. Capponi, A. Wietek, M. Mambrini, N. Schuch, and D. Poilblanc, PRL 125, 017201 (2020)
J. Hasik, D. Poilblanc, and F. Becca, SciPost Physics 10, 012 (2021)
… and many more …

Finite temperature simulations with iPEPS

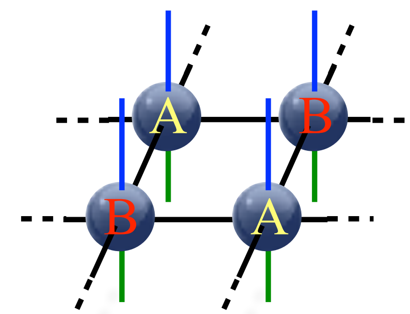
- Methodological developments (2D):

  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), …

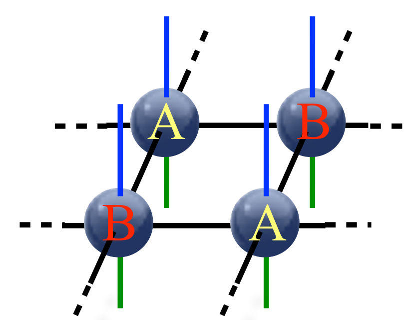
- Wave-function: $|\Psi\rangle \approx$



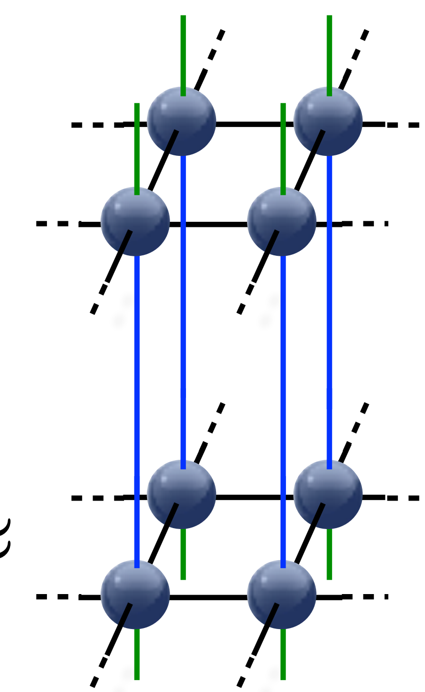
- Density-operator: $\hat{\rho} = e^{-\beta \hat{H}} \approx$



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



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

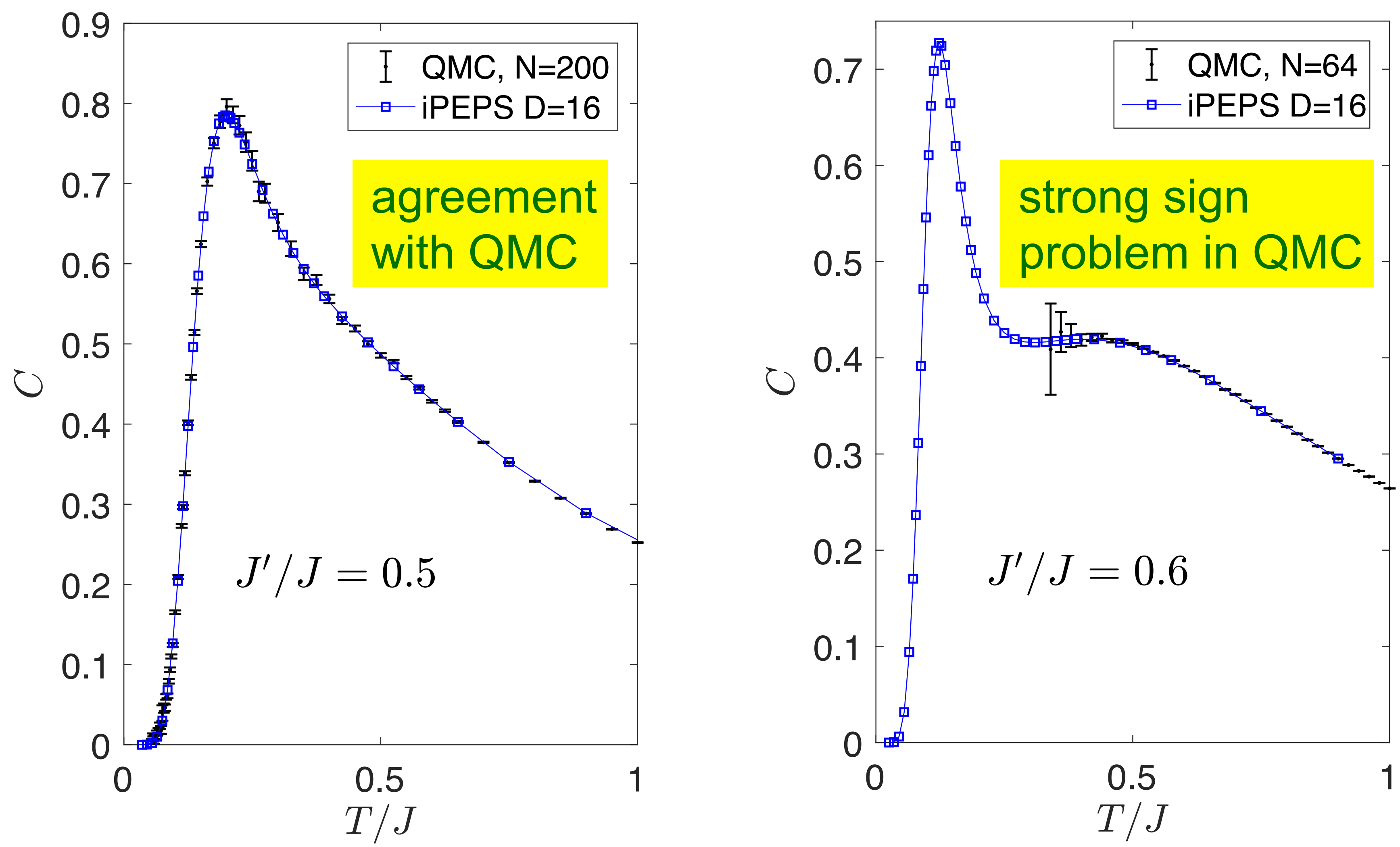


$$\hat{\rho}(\beta) = \hat{\rho}^{\dagger}(\beta)$$ by construction

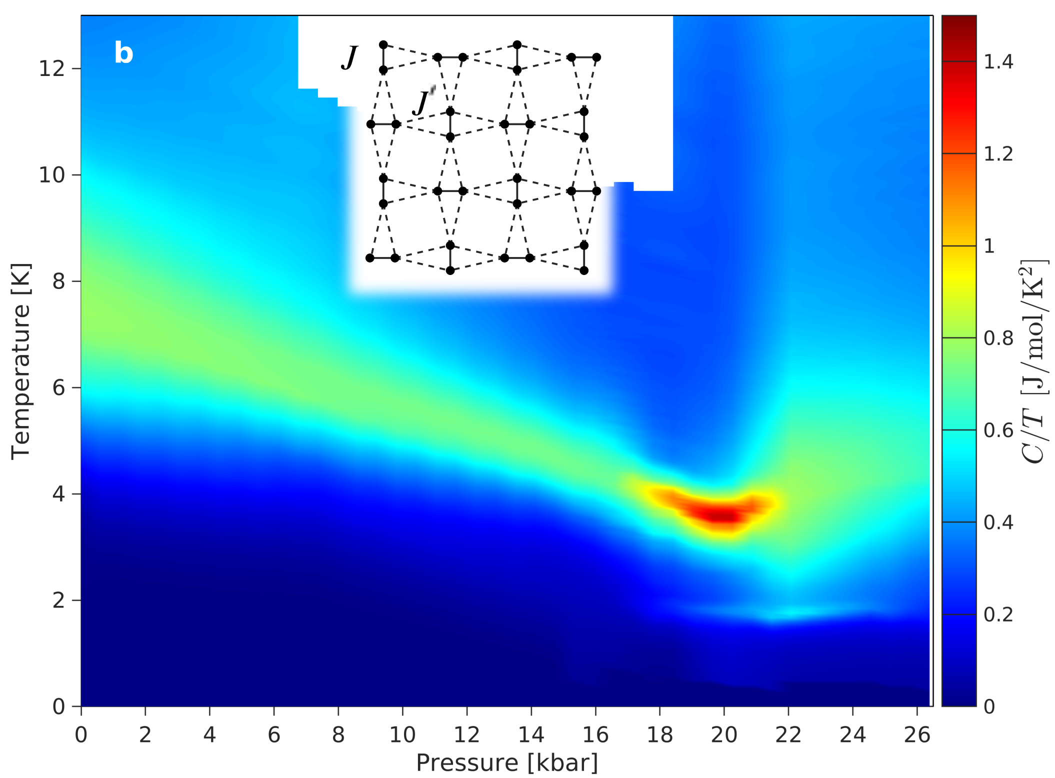
Finite temperature simulation benchmarks

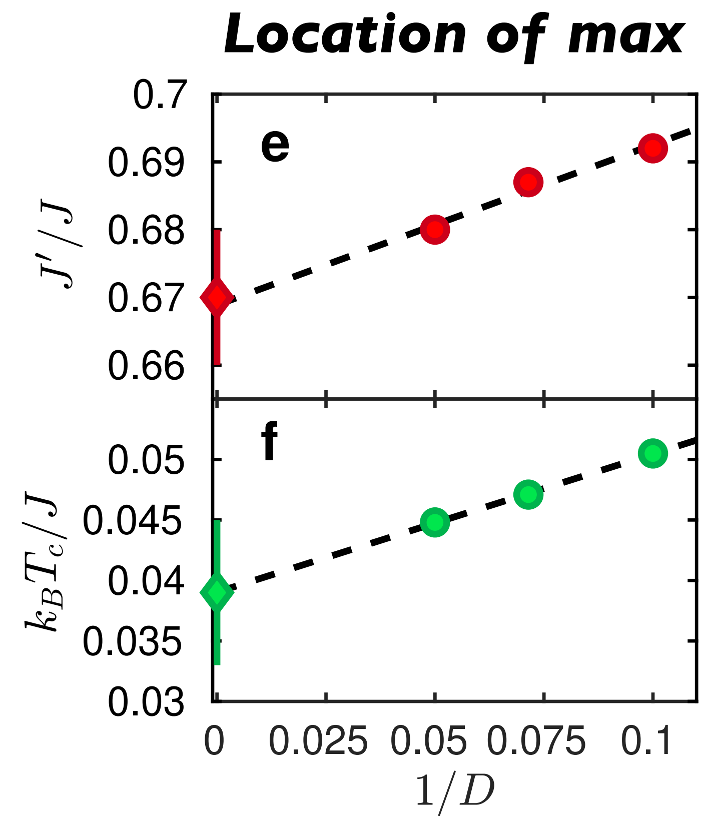
Wietek, PC, Wessel, Normand, Mila, and Honecker, PRR 1 (2019)

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

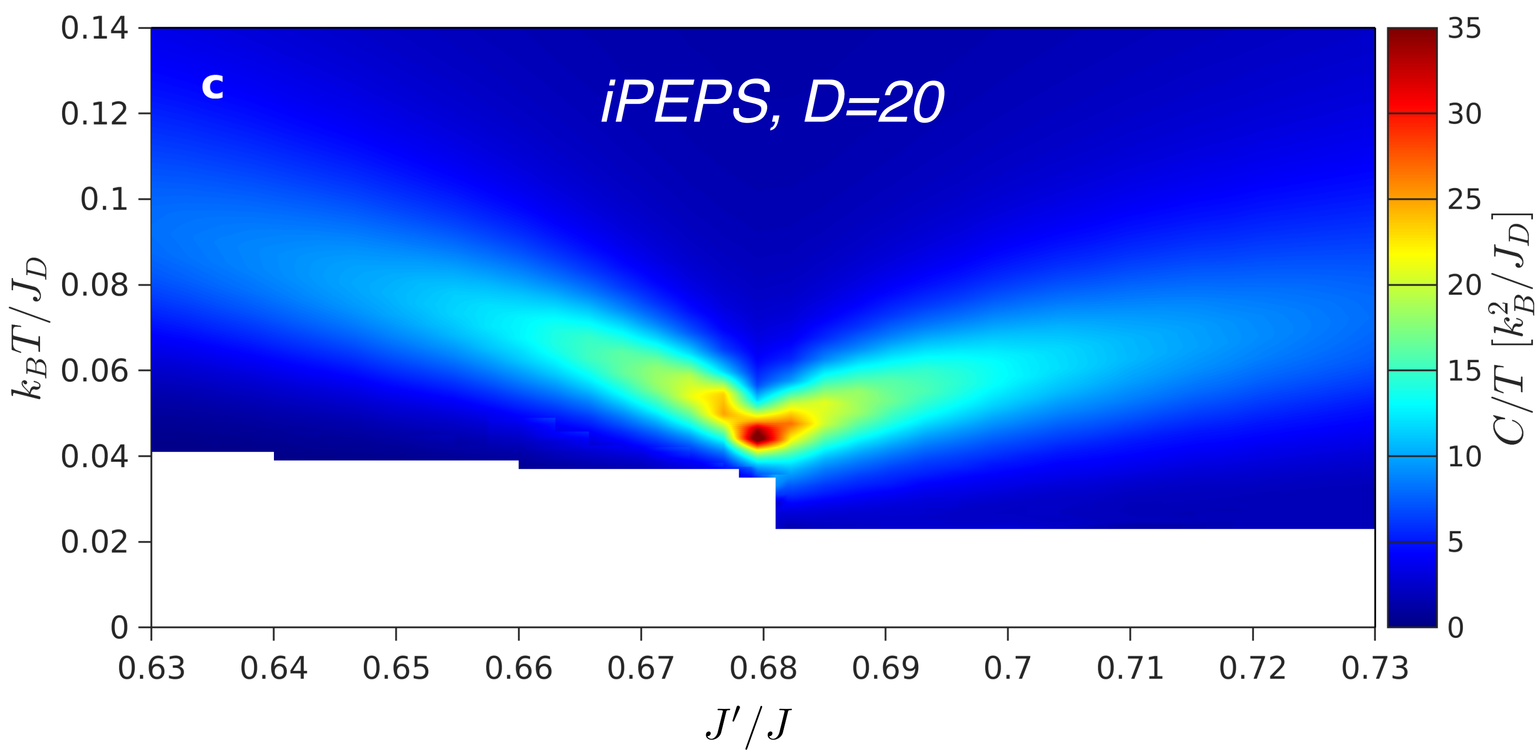


Specific heat: experiments vs iPEPS



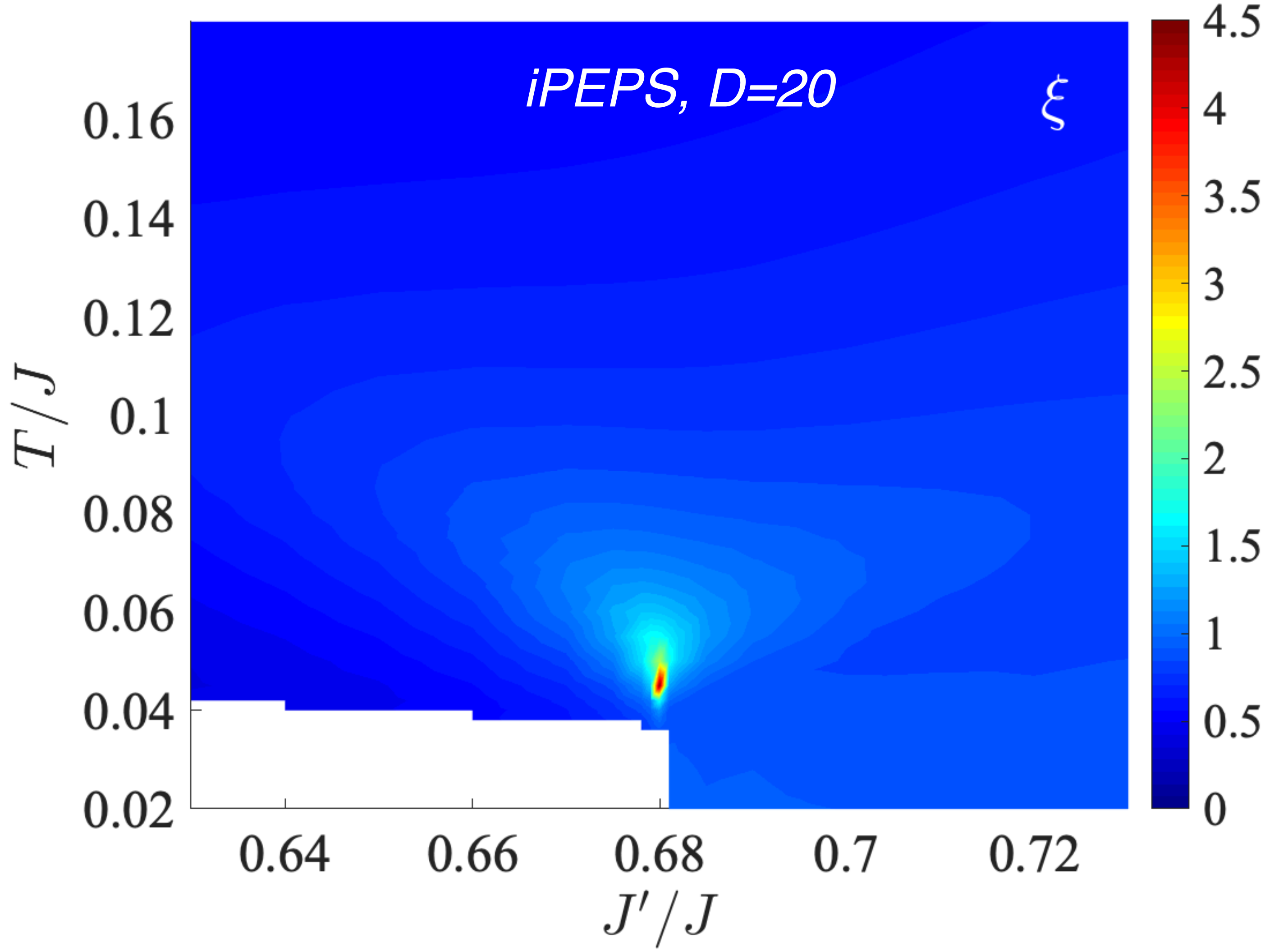


$$T_c = 3.0(6)K$$

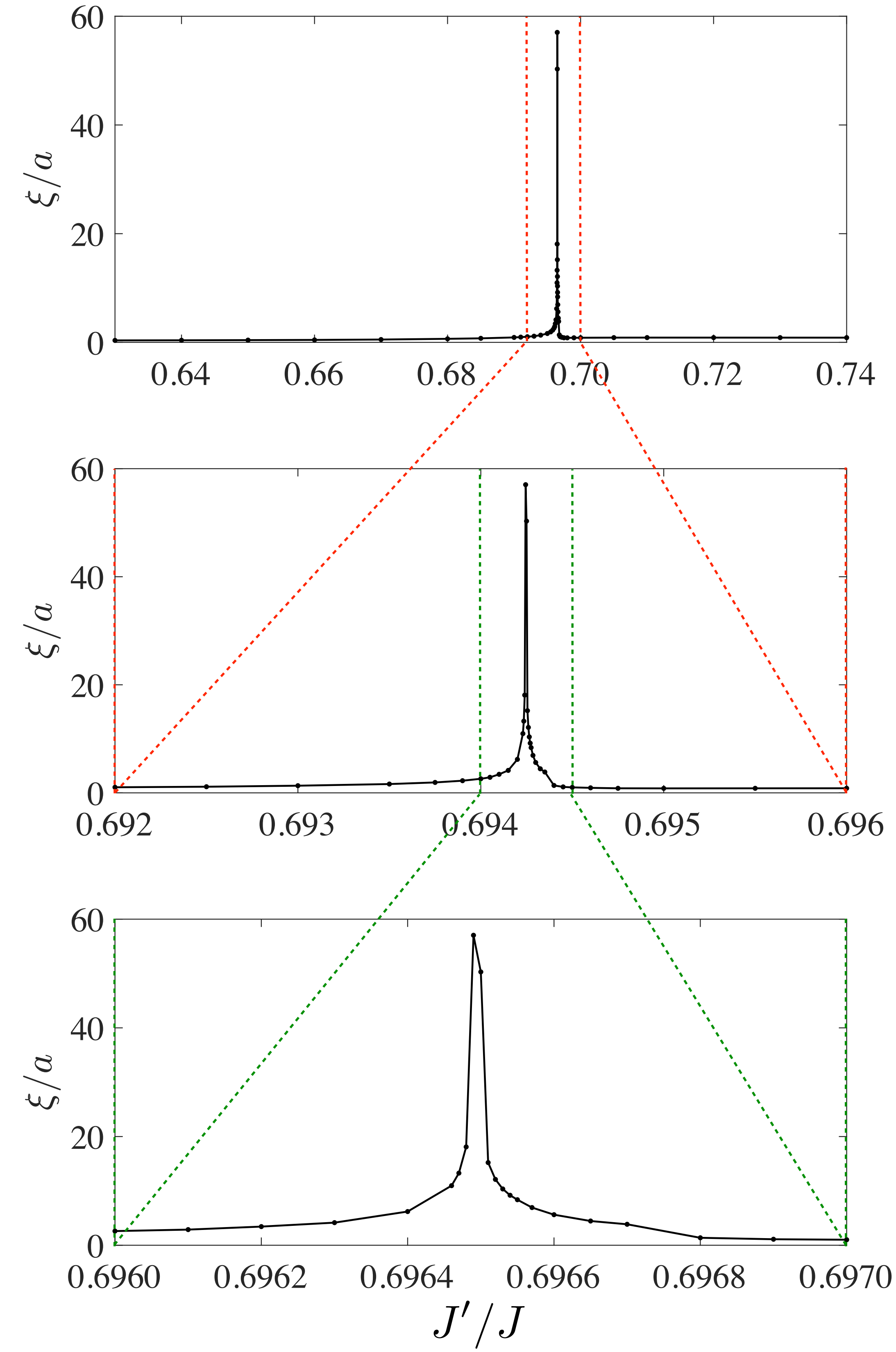


Jiménez, Crone, et al., Nature 592, 370 (2021)

Correlation length



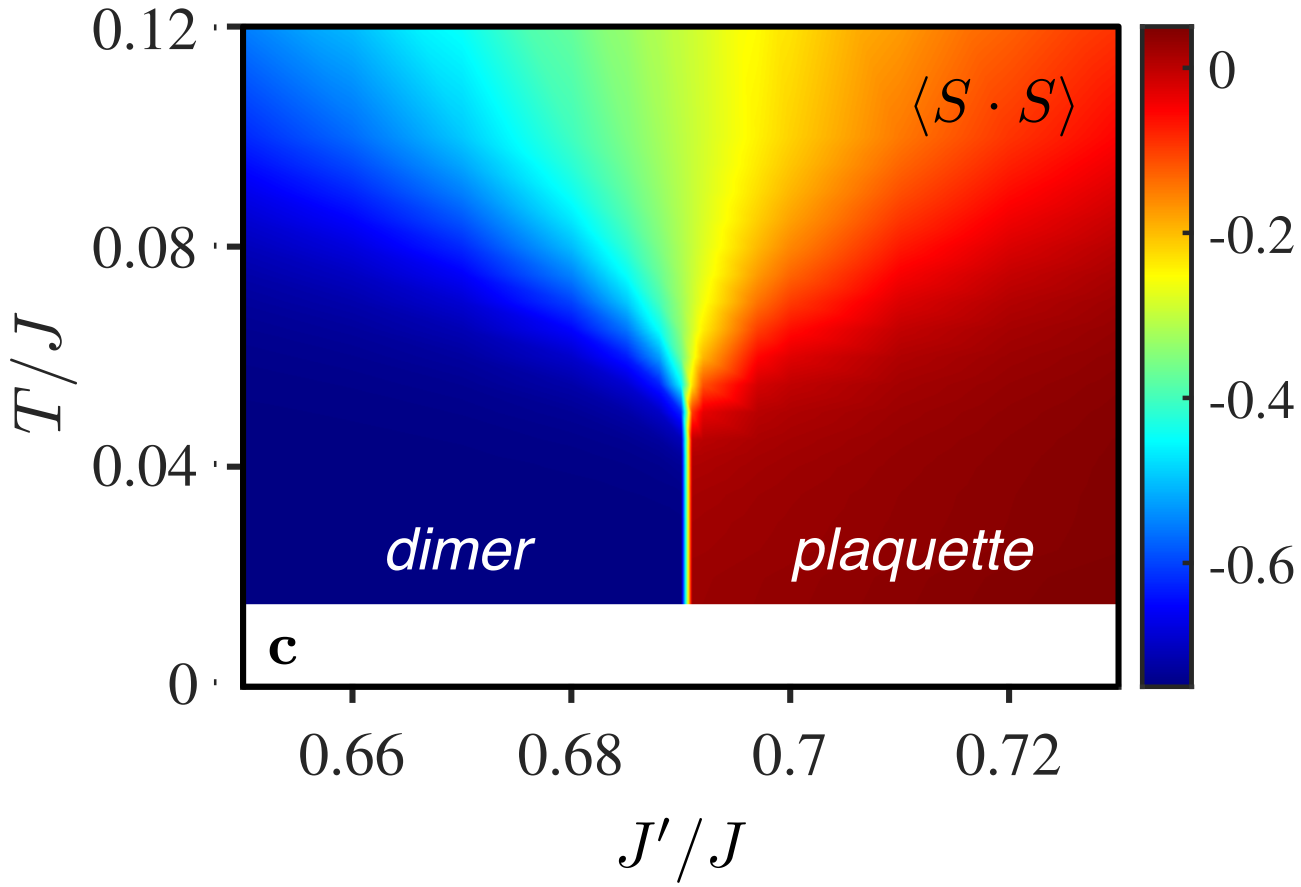
Zooming-in (D=8)



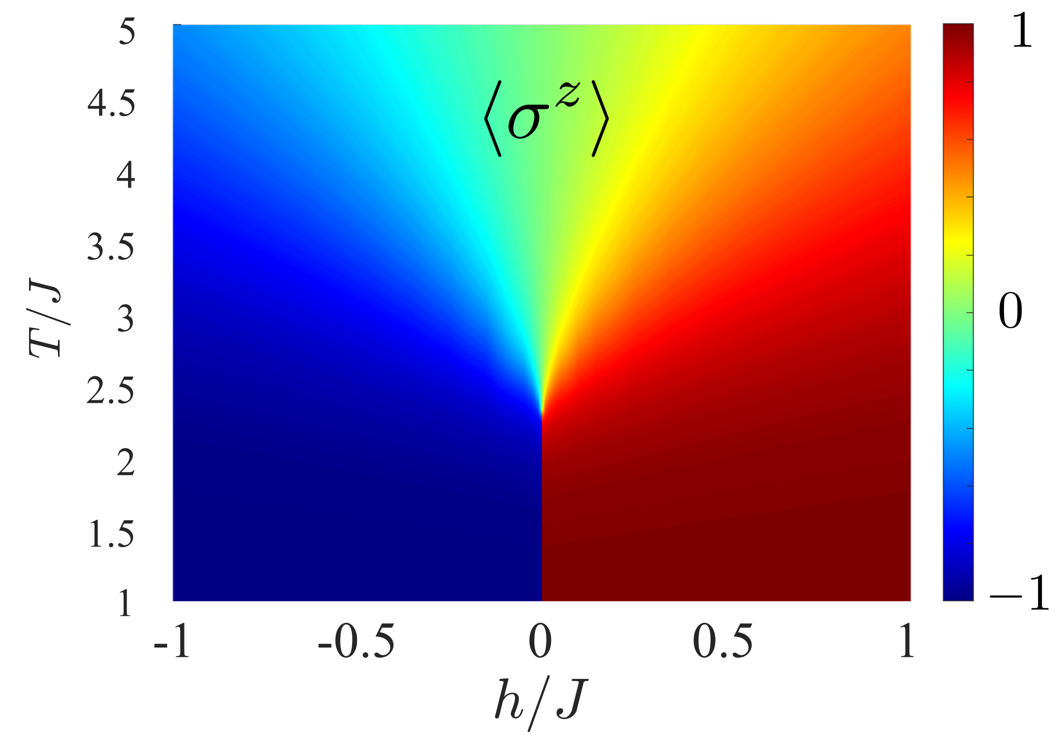
Diverging correlation length compatible with a critical point

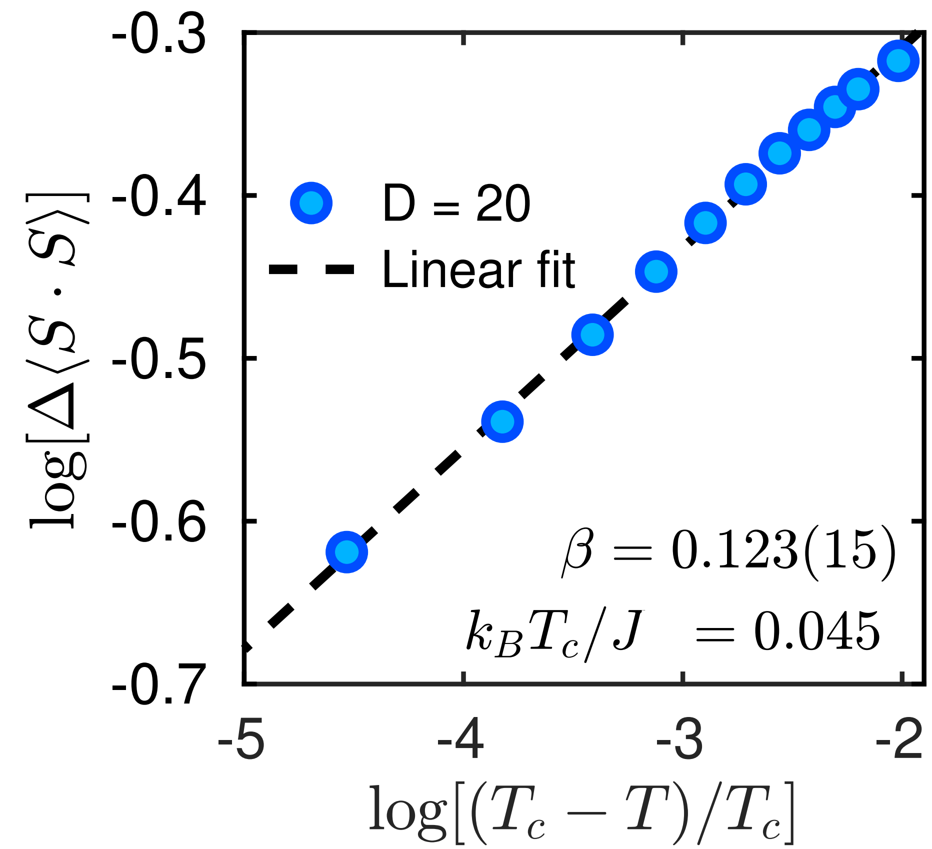
Jump in <S · S> on dimer

iPEPS D=10 (with DM)



2D classical Ising model in a field

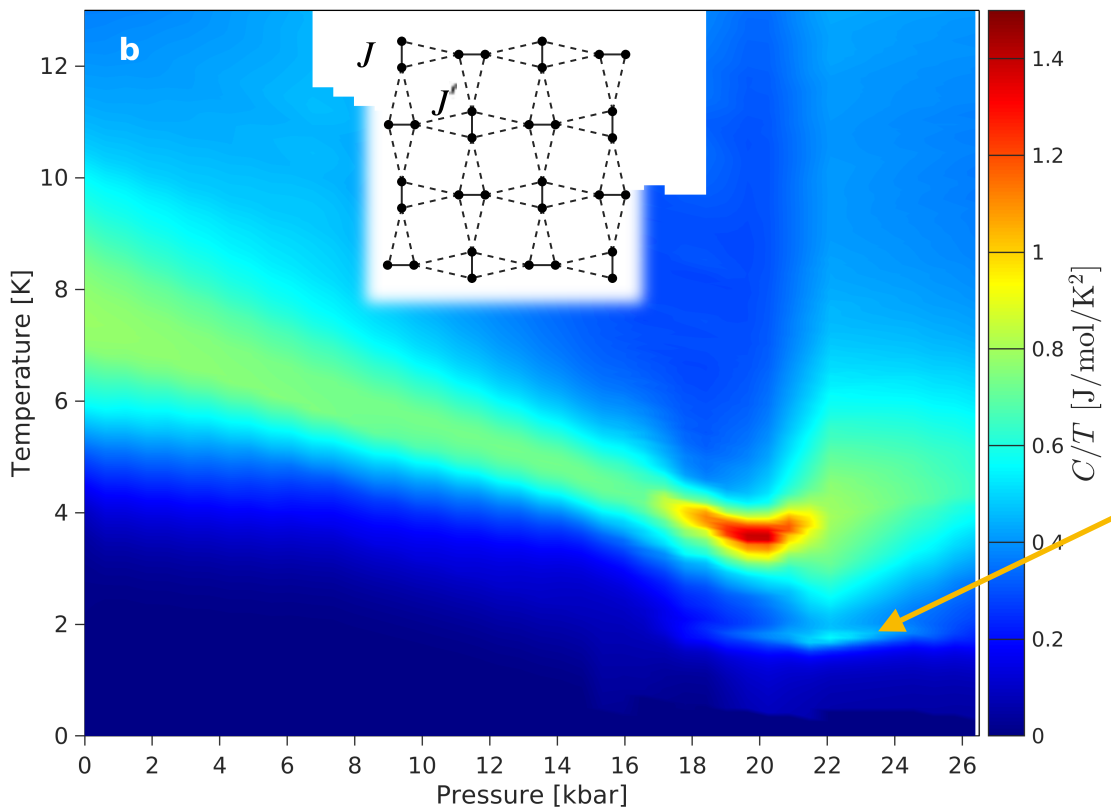




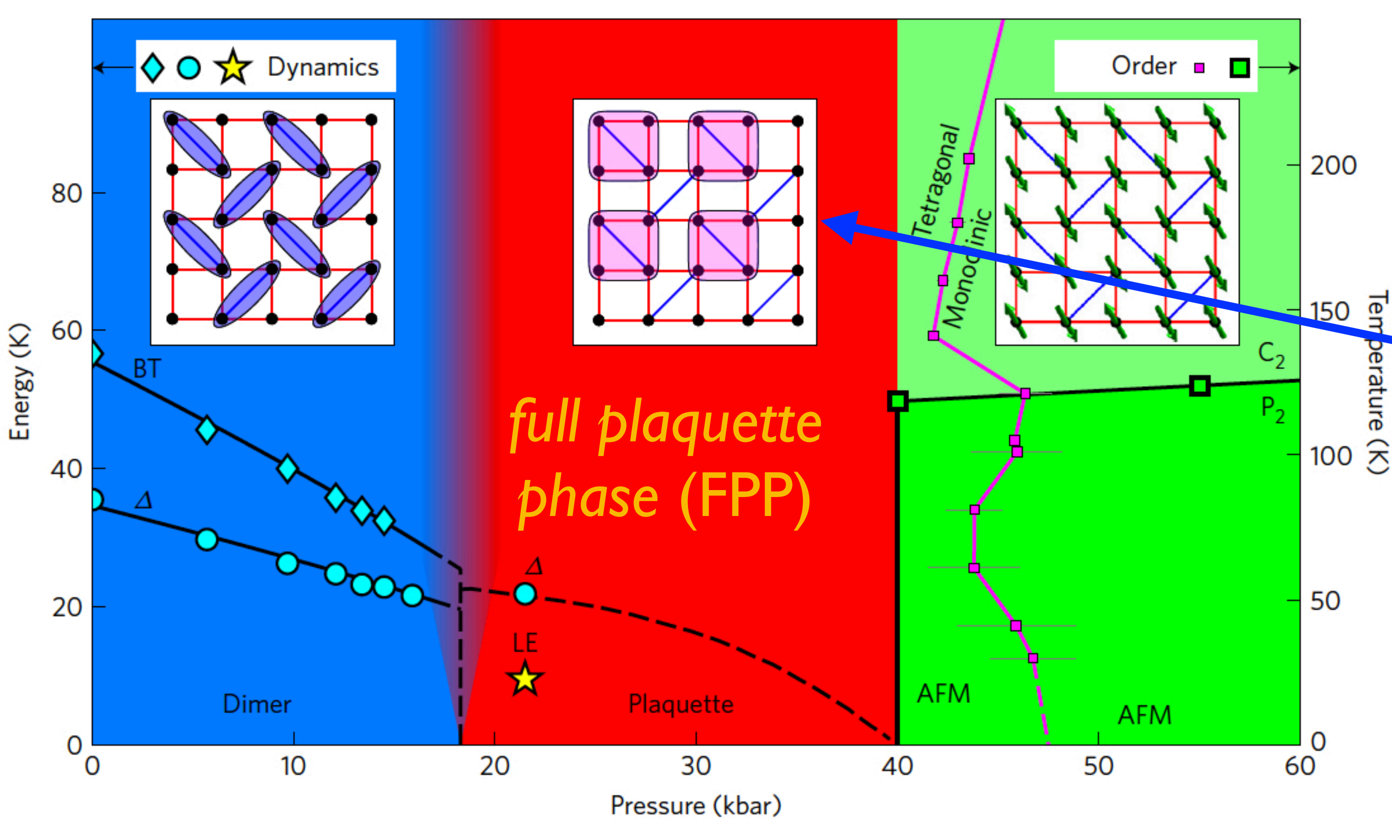
Clear evidence of a first order line with a critical point compatible with the 2D Ising universality class

exact value:
$\beta = 0.125$

Open challenges

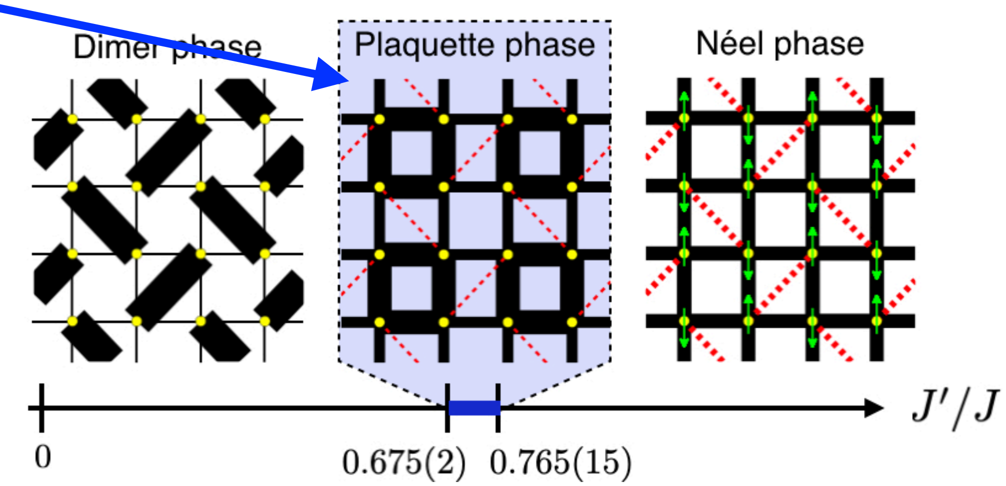


too low T to obtain reliable data with iPEPS (currently)



- NMR & INS experiments: *full plaquette phase* (FPP), not *empty plaquette phase* (EPP)

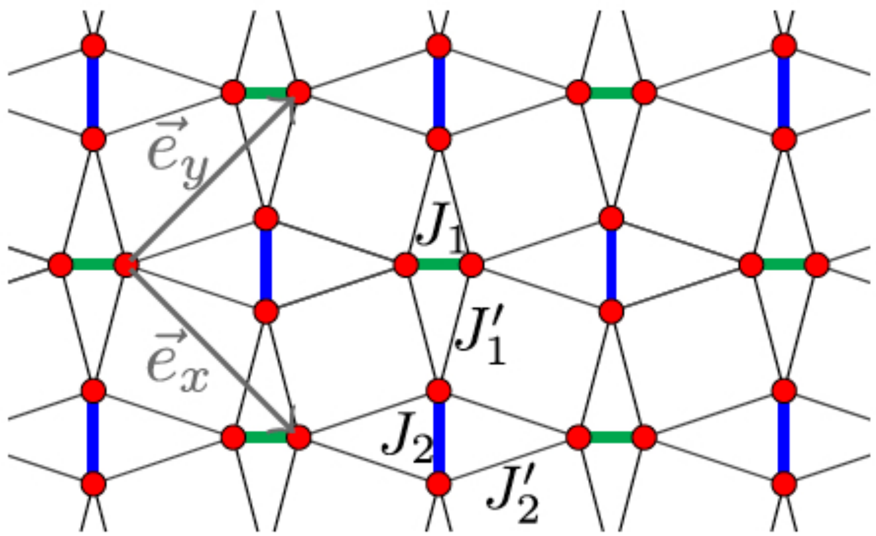
Zayed, et al., Nat. Phys. 13, 962 (2017)
Waki, et al. JPSJ 76 (2007)
Cui et al., arxiv:2204.08133

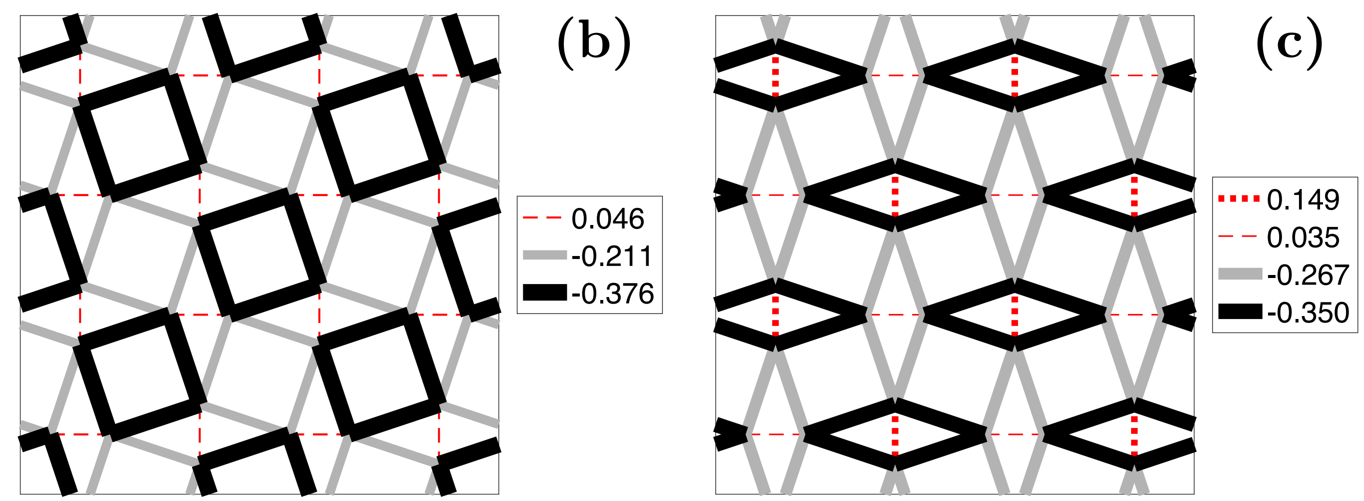


Competing plaquette phases

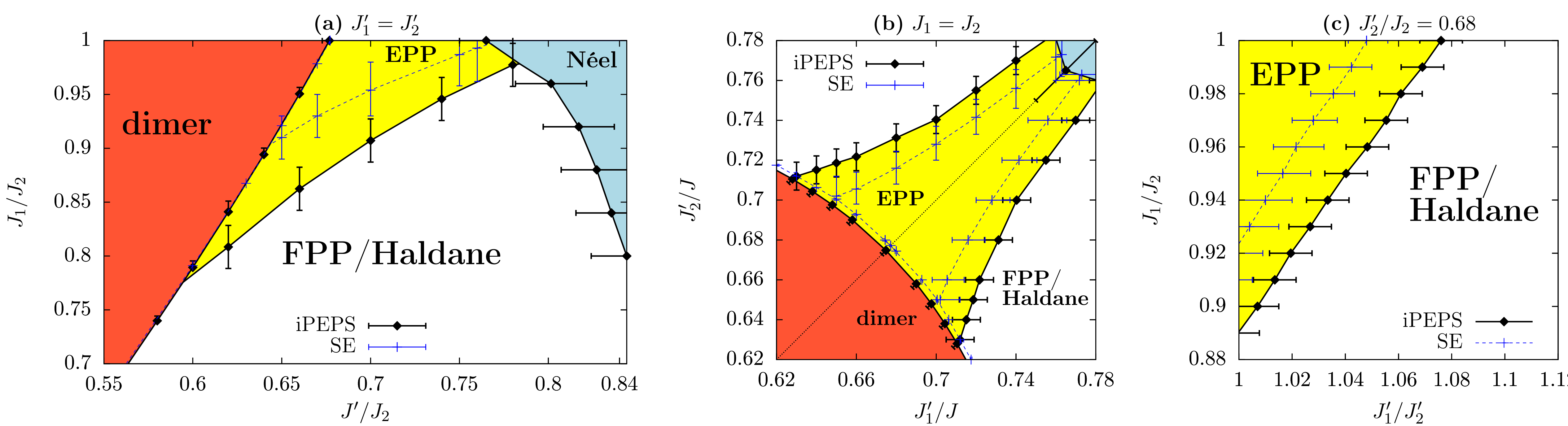
Boos, Crone, Niesen, PC, Schmidt & Mila, PRB 100 (2019)

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





EPP *vs* *FPP*



- Small deformation leads to FPP phase!

But precise model still unclear…

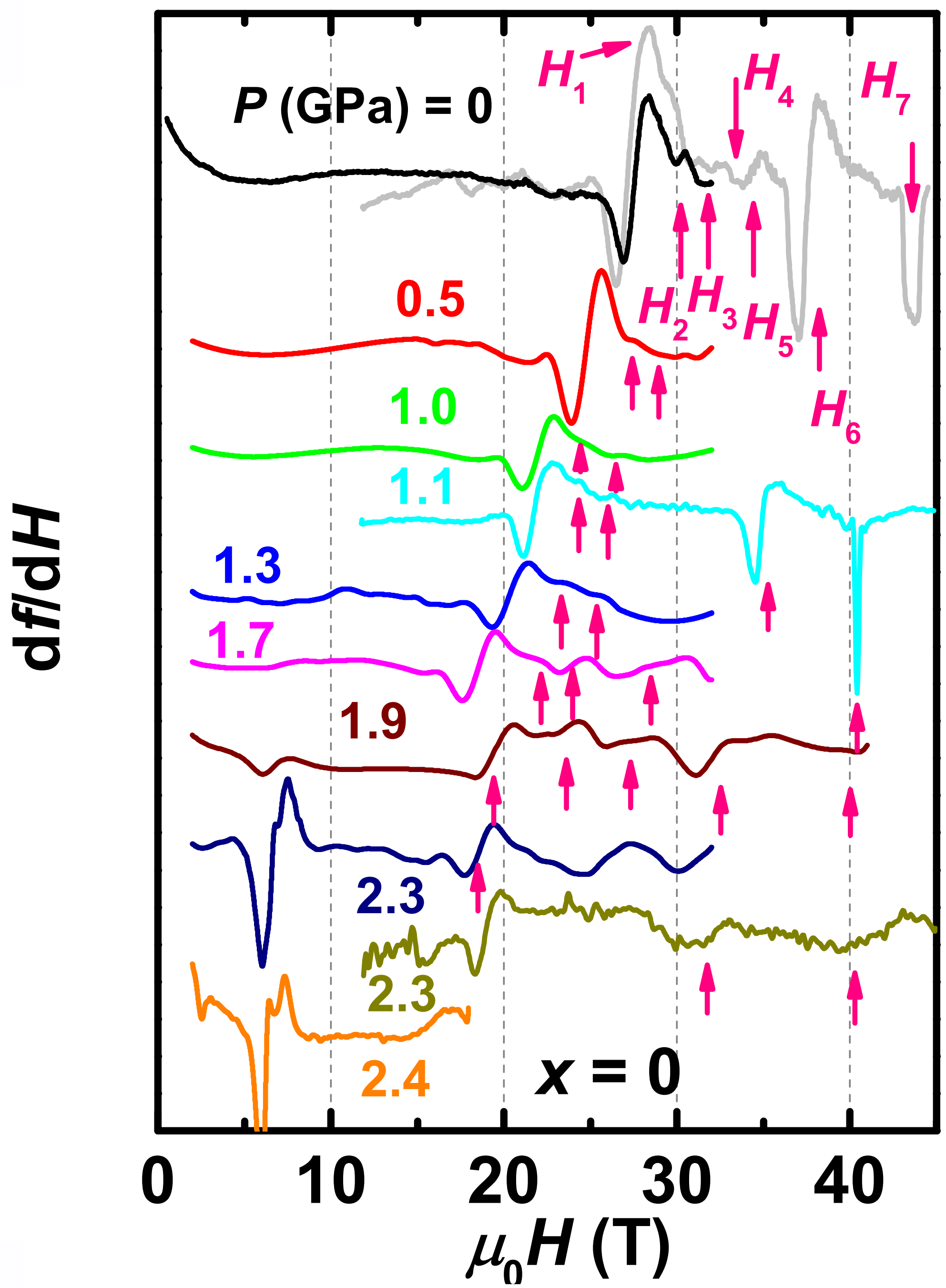
Part II: SCBO under extreme conditions of field & pressure

Shi, Dissanayake, PC, William Steinhardt, Graf, Silevitch, Dabkowska, Rosenbaum, Mila, Haravifard, Nat Commun 13, 1 (2022)

- Experiments:
  tunnel diode oscillator (TDO) technique

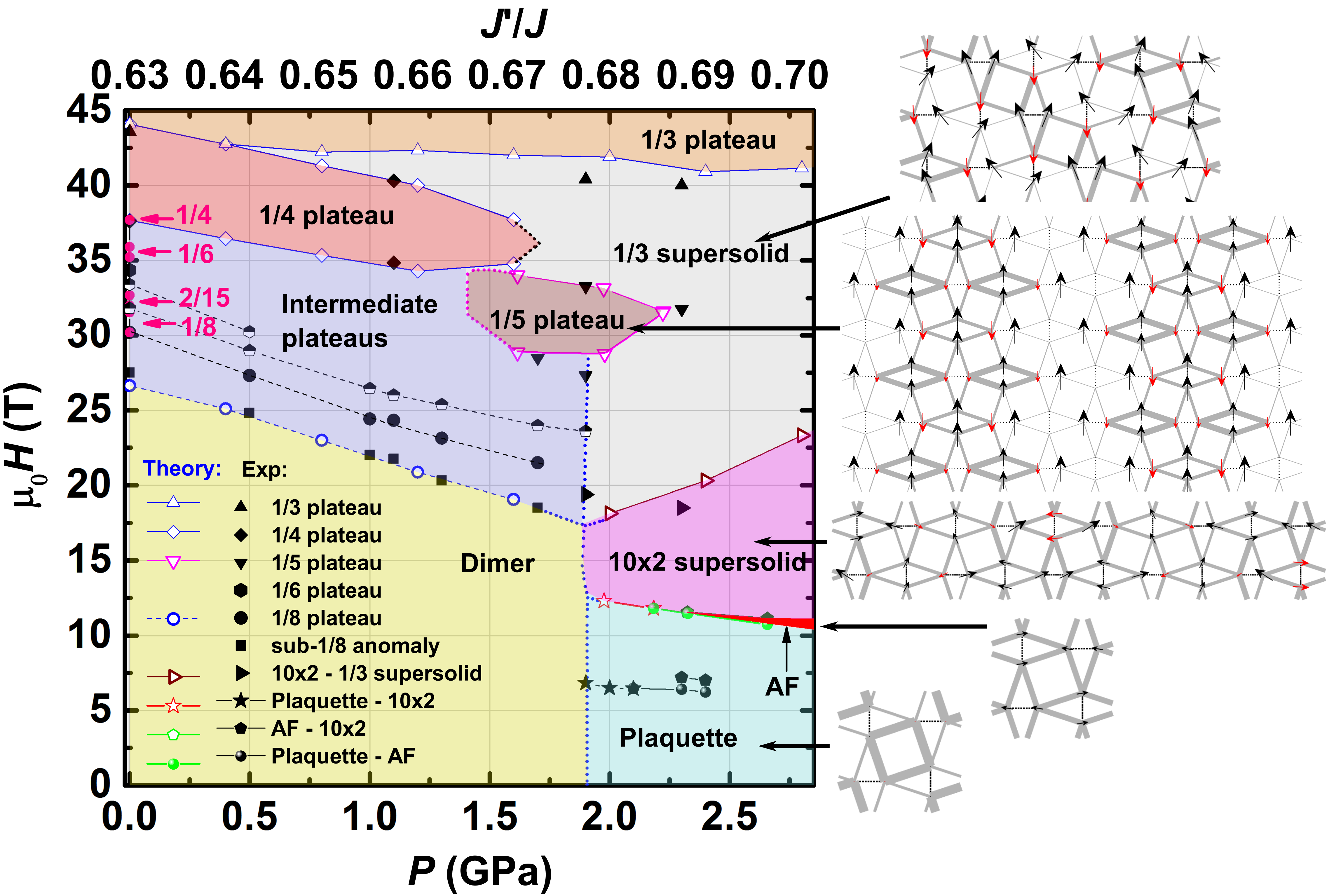
$$\frac{df}{dH} \propto -\frac{d^2M}{dH^2}$$

- Non-zero df/dH ↔ slope change in M
- Identify anomalies → *phase transitions*
- Compare with iPEPS phase diagram

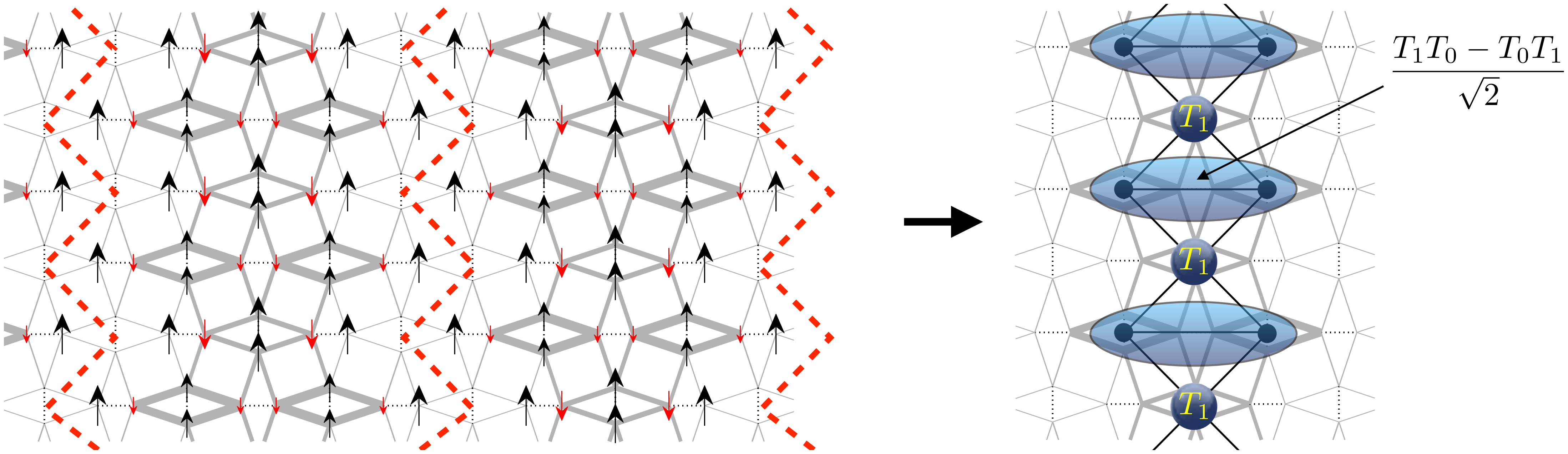


$SrCu_2(BO_3)_2$ under extreme conditions of field & pressure

Shi, Dissanayake, PC, William Steinhardt, Graf, Silevitch, Dabkowska, Rosenbaum, Mila, Haravifard, Nat Commun 13, 1 (2022)



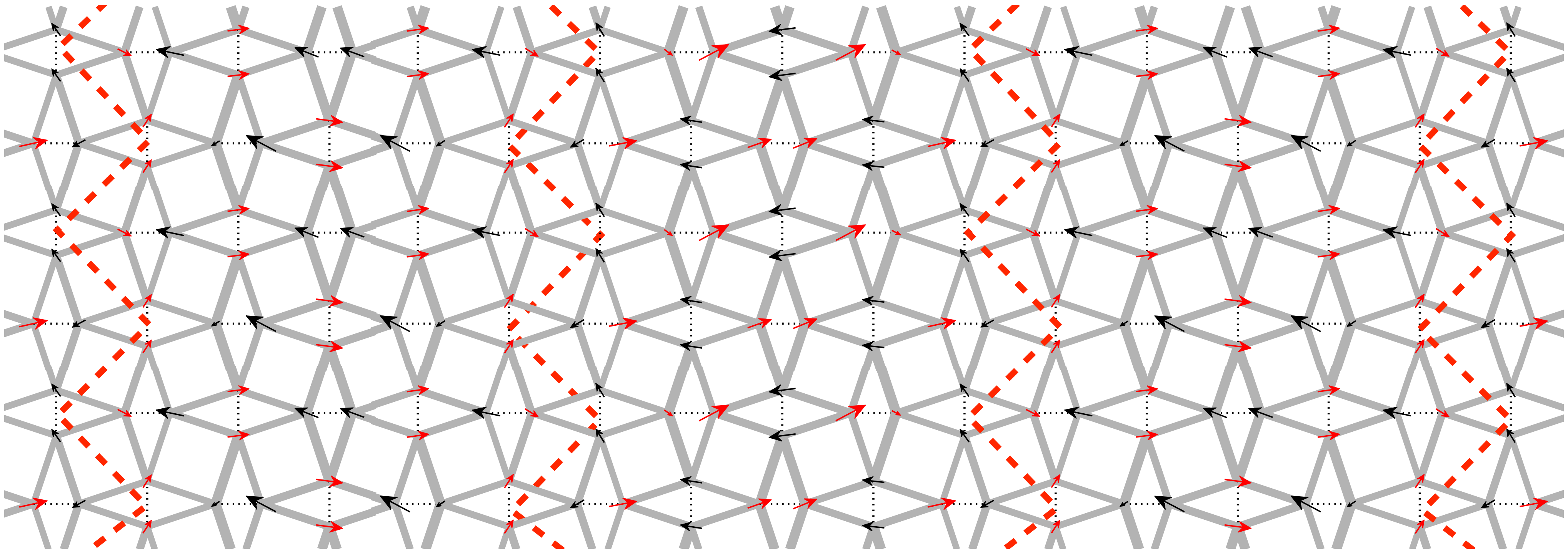
Nature of the 1/5 plateau



- Vertical stripes separated by dimer singlets (along red dashed lines)
- Strong triplets in the center of each stripe, with a weaker pair of triplets in between
  - ✦ *Neither a crystal of triplets, nor a crystal of triplet bound states!*
- Full-plaquette formation: reminiscent of full plaquette phase (FPP)
  - ✦ *FPP: triplets on dimers within plaquette and singlets on dimers outside of plaquette, where the triplets form effective S=1 Haldane chains*
- Effective description: S=1 diamond chain with m=2/3
- Also found in a thin SSM tube made of 2 orthogonal dimer chains

Manmana, Picon, Schmidt, and Mila, EPL 94, 67004 (2011)

Nature of the 10x2 supersolid



- Descendant of the 1/5 plateau state
- Alternating rotation of the spins of successive stripes clockwise or counterclockwise by 90 degrees
- Finite component in the field direction, also on the boundary between stripes

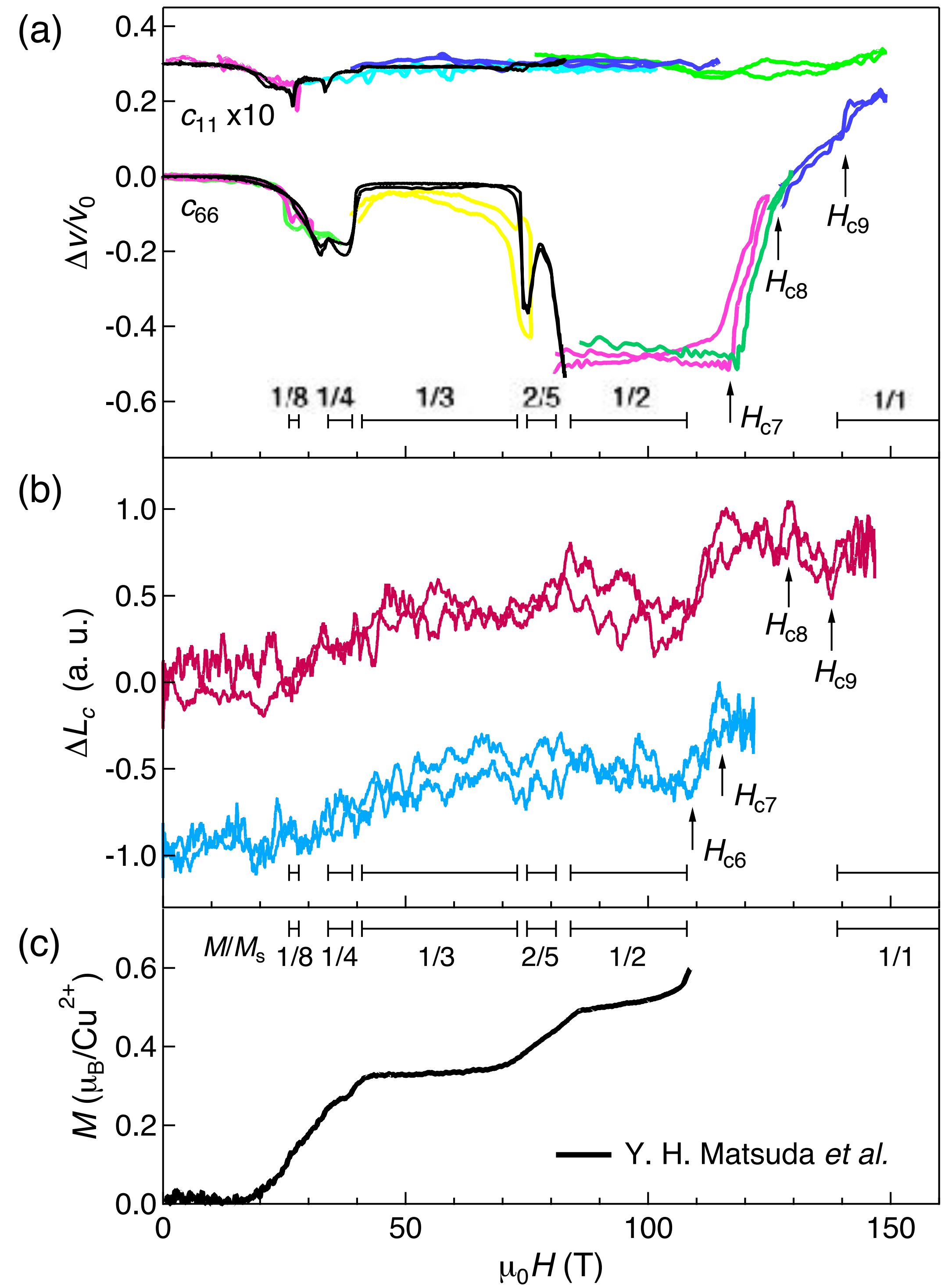
Full plaquette physics appearing at finite magnetic field!

Part III: $SrCu_2(BO_3)_2$ up to the saturation field

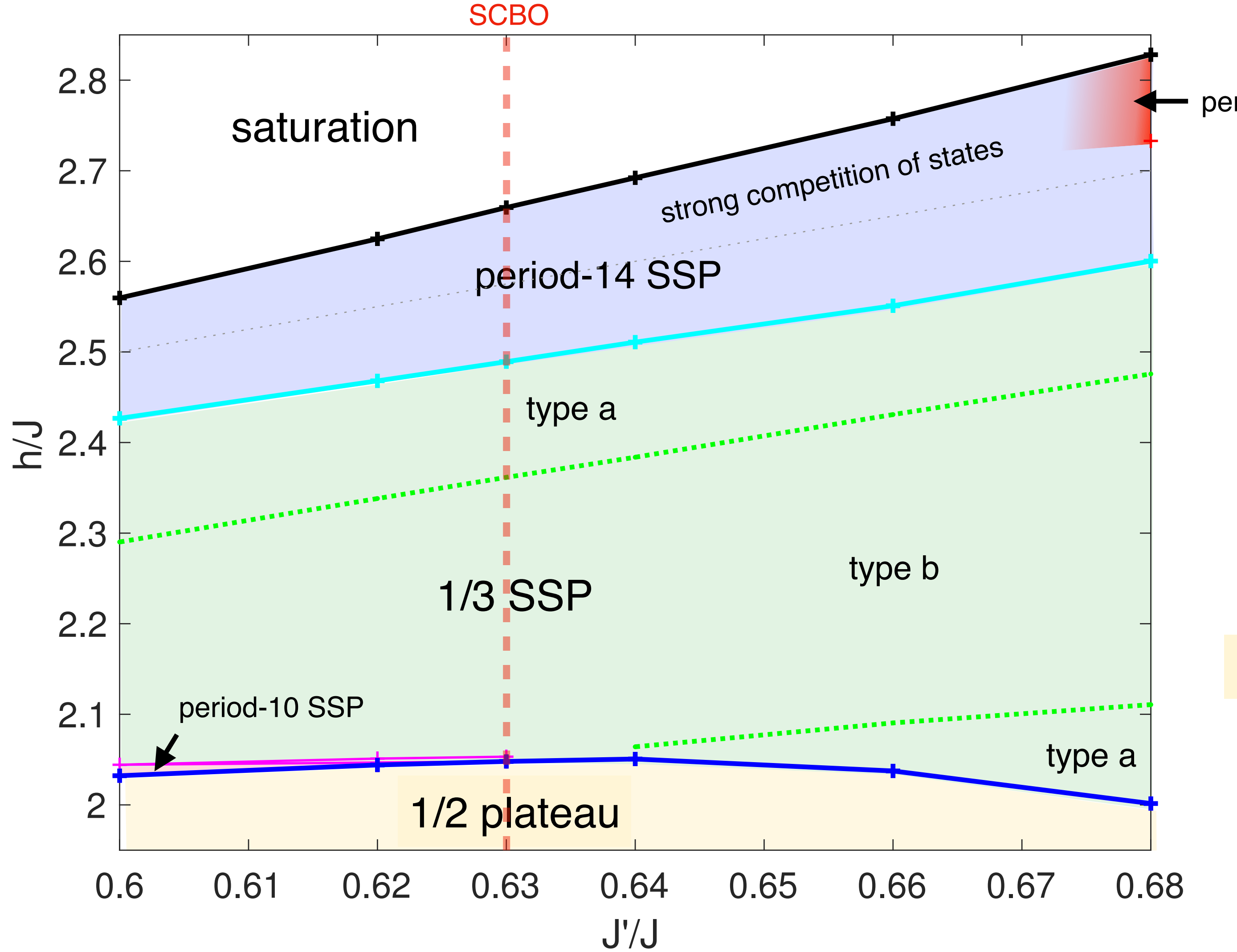
Nomura, PC, Miyata, Zherlitsyn, Ishii, Kohama, Matsuda, Ikeda, Zhong, Kageyama, Mila, arXiv:2209.07652 (to appear in Nat. Comm.)

- Experiments: ultrahigh fields up to **150T!**
- Ultrasound velocity & magnetostriction
- Identified new anomalies above the 1/2 plateau at 116T, 127T, and 139T
- Saturation field: 139T

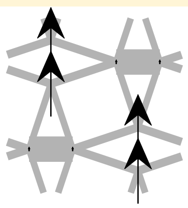
- Comparison with iPEPS results
- Strong decrease of the sound velocity of the c_{66} acoustic in the 1/2 plateau?



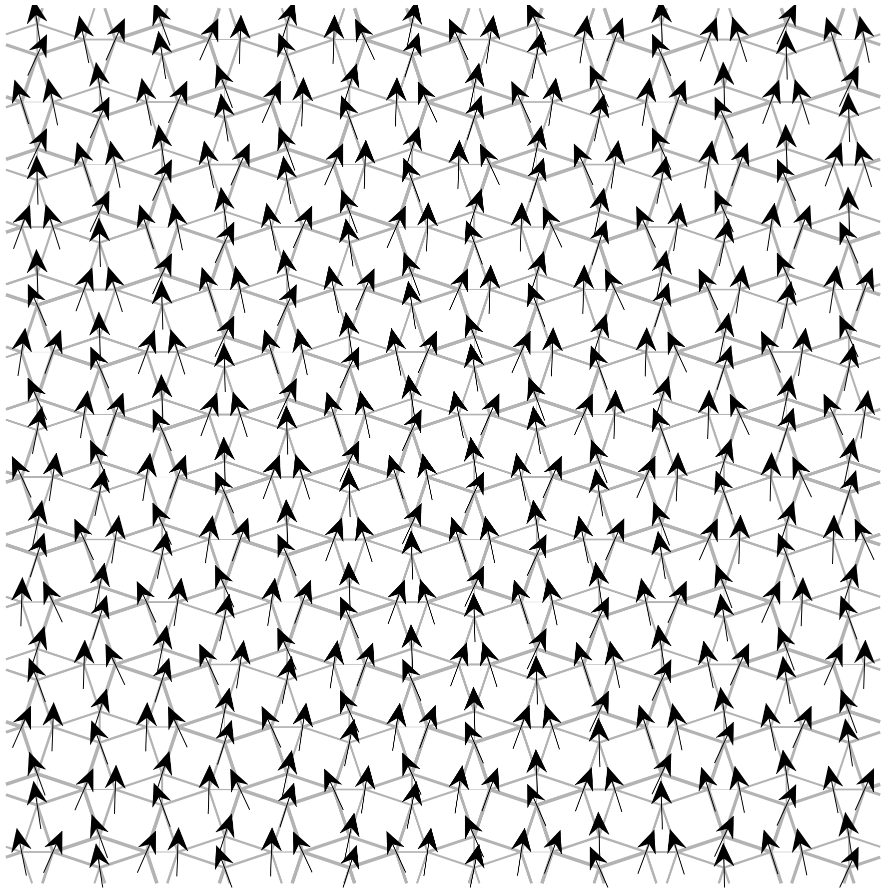
iPEPS phase diagram



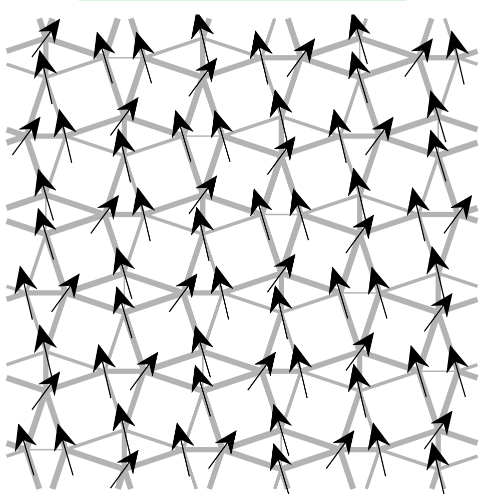
1/2 plateau



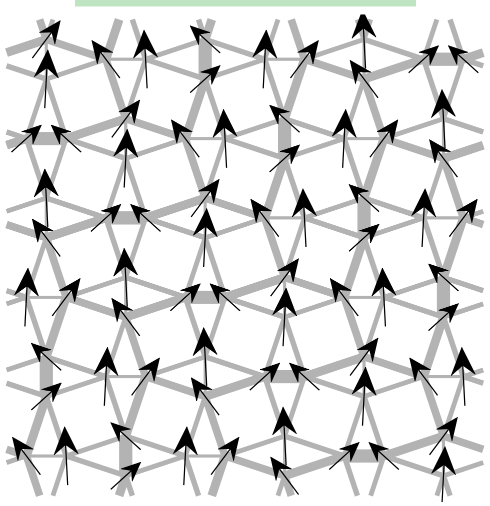
period-14 SSP



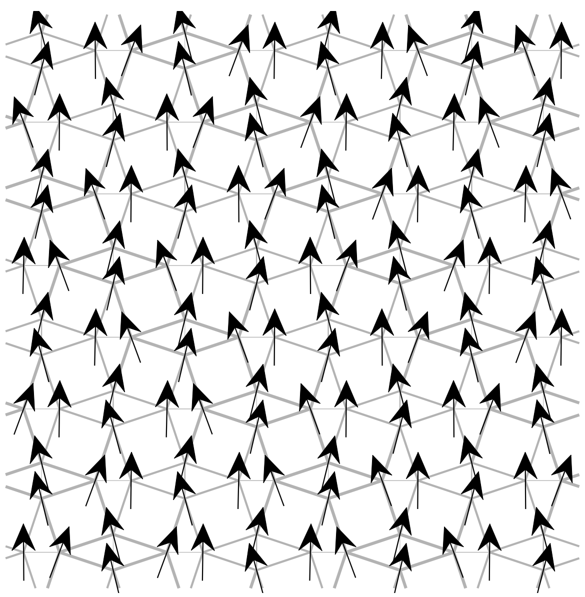
1/3 SSP type a



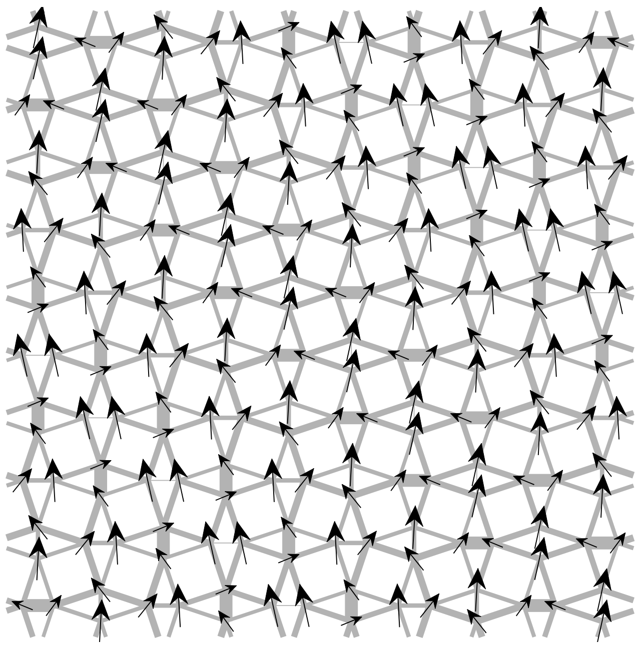
1/3 SSP type b



period-8 SSP



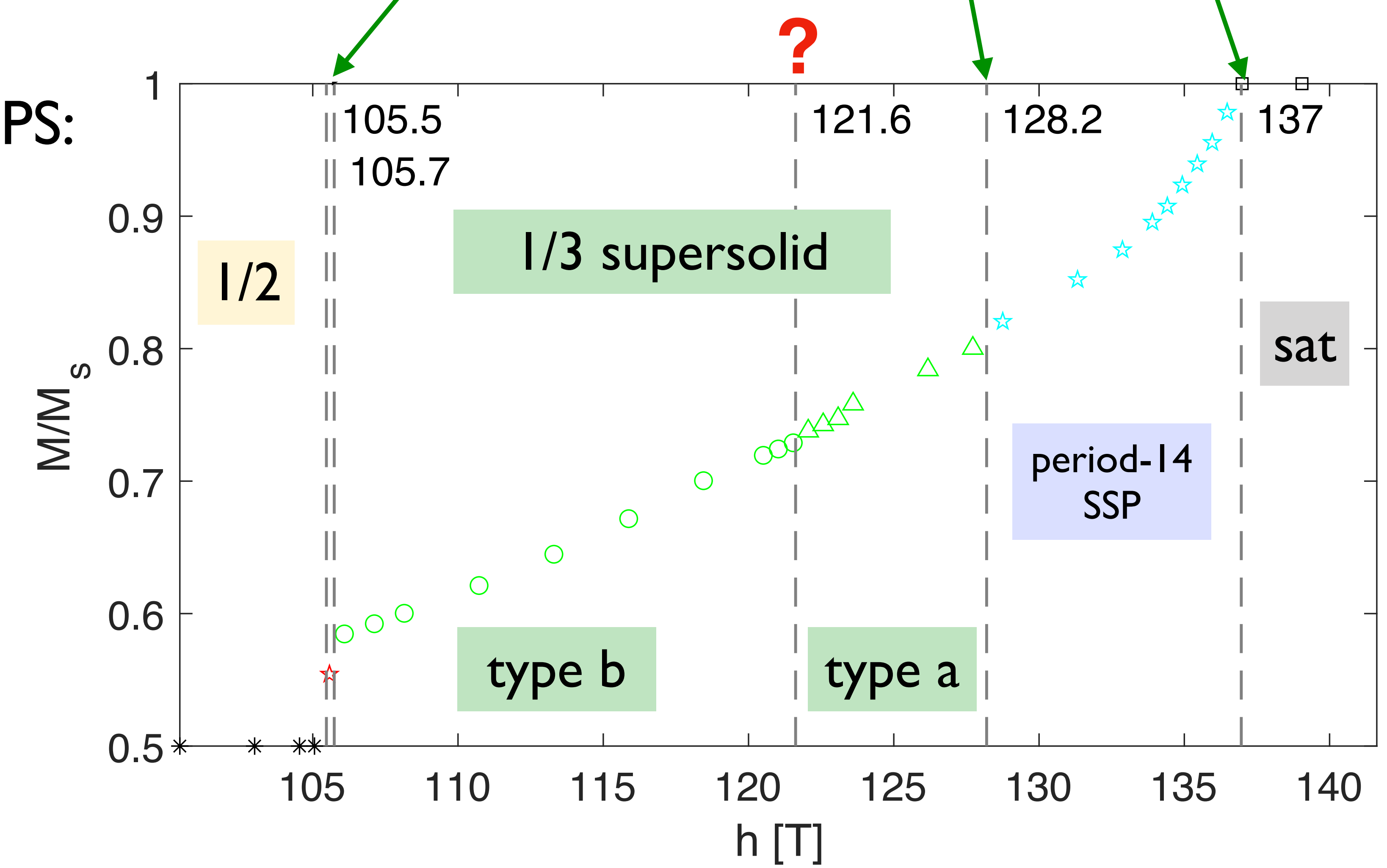
period-10 SSP



Results for J'/J=0.63

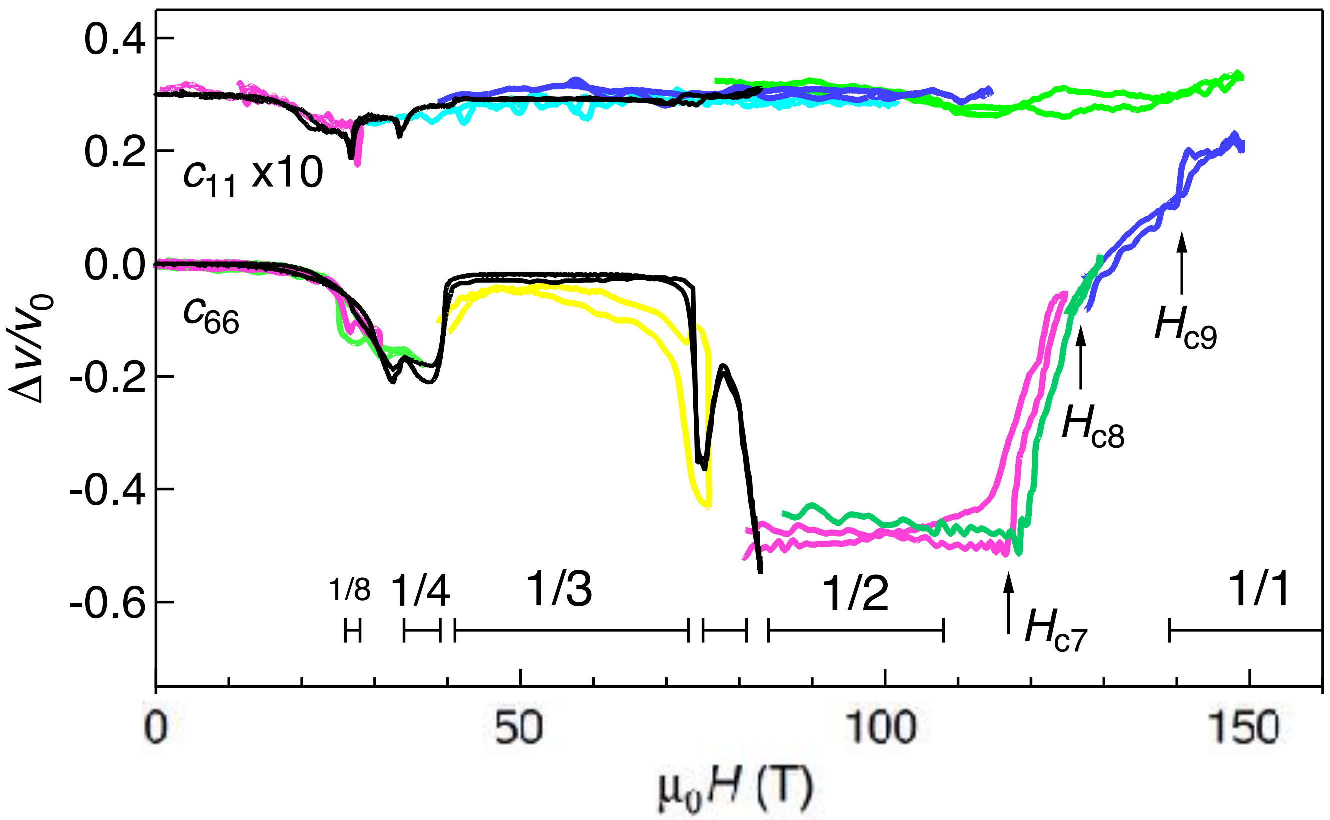
	H_{c6}	H_{c7}	H_{c8}	H_{c9}
Ultrasound		116(3)	126(3)	140(2)
Magnetostriction	108(2)	116(2)	128(3)	138(3)
Magnetization [3]	108(1)	?		

iPEPS:

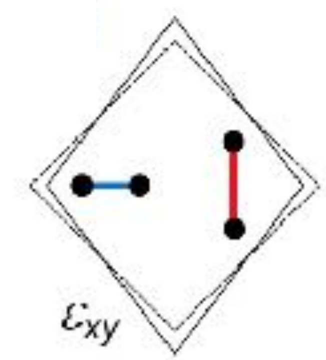


Anomalies H_{c6}, H_{c8}, and H_{c9} compatible with iPEPS results

Reduction of ultrasound velocity in 1/2 plateau?

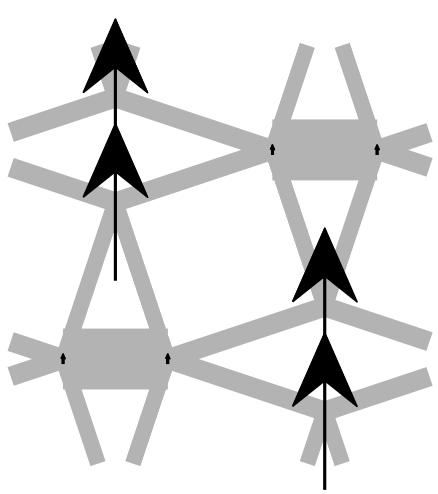


Strain of c66 mode:

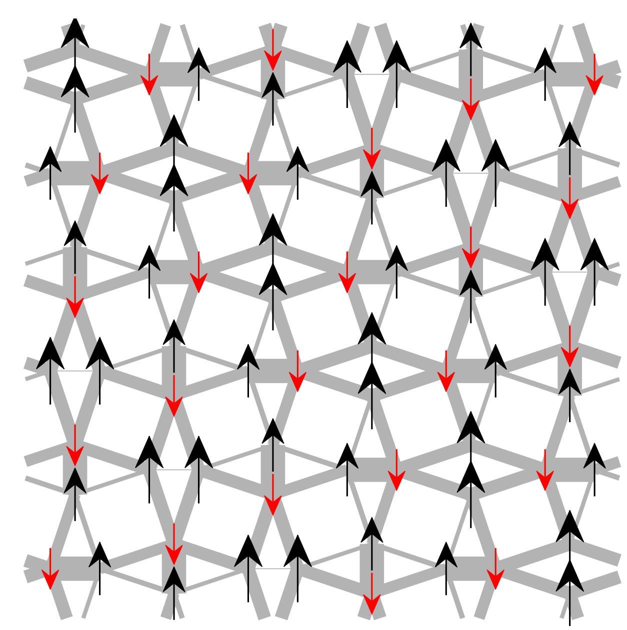


- Strong reduction in 1/2 plateau
- Tiny reduction in 1/3 plateau

- Both E' and E'' of the magnetic energy contribute to the elastic constant
- E' has large magnitude in 1/2, but vanishing for 1/3 plateau

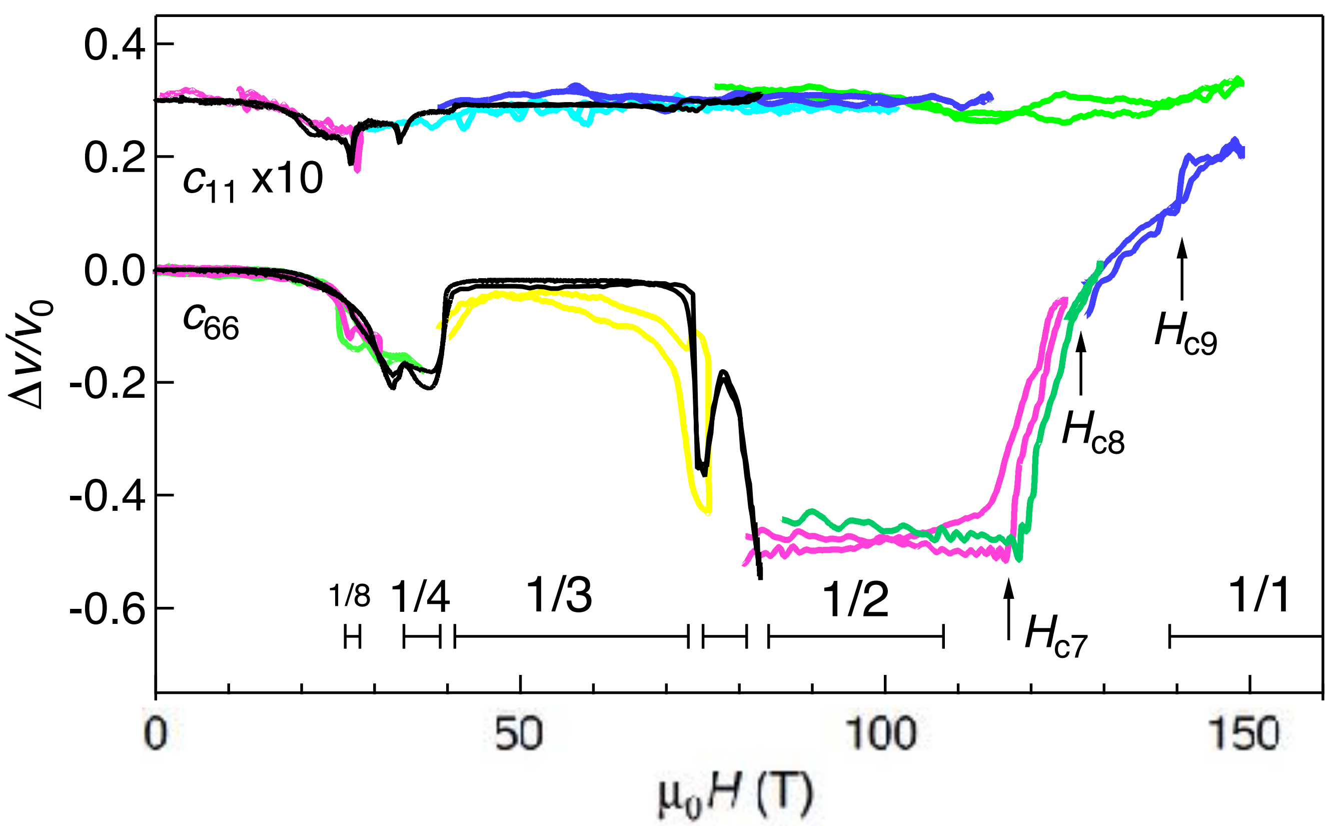


Checkerboard structure with positive (triplet) and negative (singlet) bonds → contributions to E' add up → large magnitude

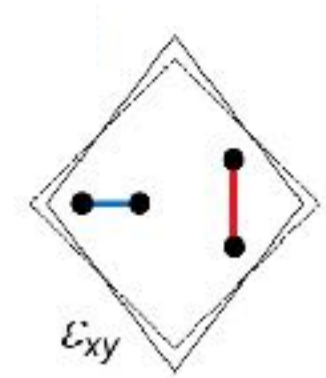


odd periodicity → cancellation

Reduction of ultrasound velocity in 1/2 plateau?



Strain of c66 mode:



- Strong reduction in 1/2 plateau
- Tiny reduction in 1/3 plateau

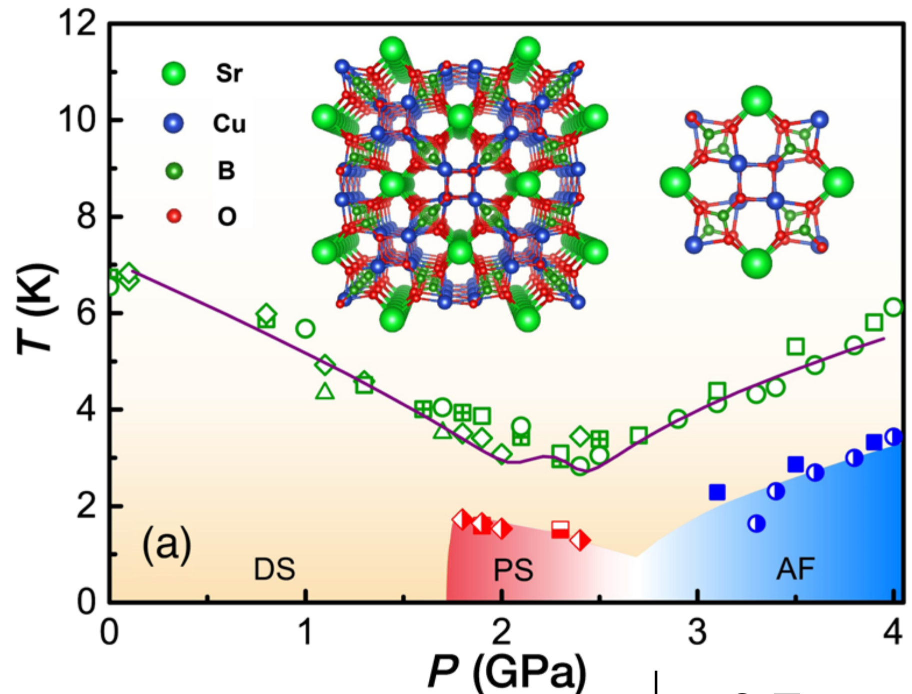
- Both E' and E'' of the magnetic energy contribute to the elastic constant
- Fit: $\lambda_1 E' + \lambda_2 E'' \sim \Delta c/c, \quad c = \rho v^2$

Plateau	E'	E''	$\Delta v/v_0$ iPEPS	$\Delta v/v_0$ Exp.
1/8	-0.014	-0.44	-0.13	-0.11(4)
1/4	-0.051	-0.31	-0.16	-0.19(3)
1/3	0	-0.18	-0.04	-0.03(2)
1/2	-0.23	-0.034	-0.49	-0.48(7)

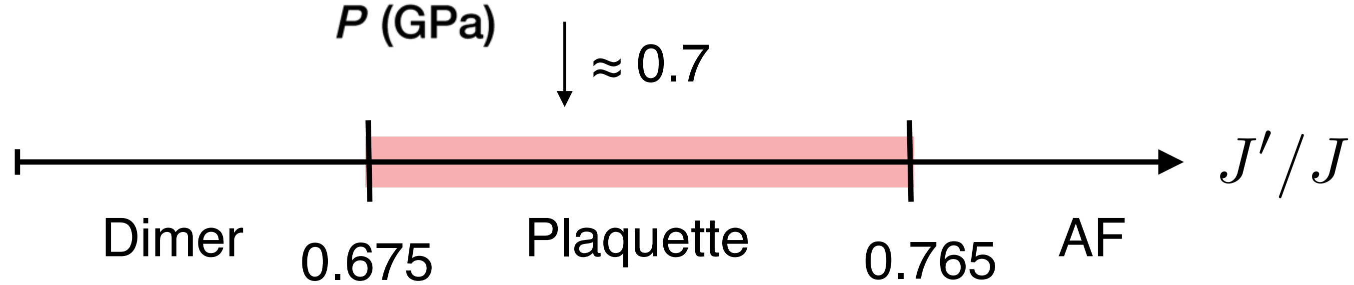
Estimates in good agreement with experiment

Part IV: SSM with interlayer coupling

- Extent of the plaquette phase is smaller in experiments than in theory



Guo, et al (2020)



- **Pressure model:** Shi, et al. (2022)

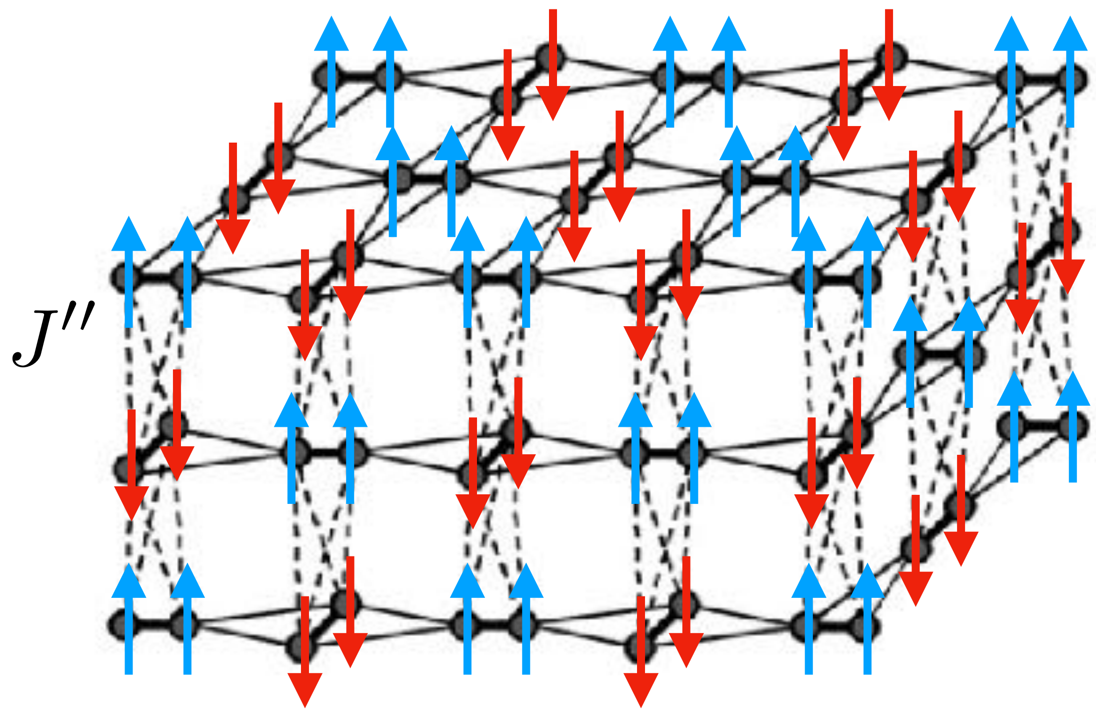
$$p_0 \leftrightarrow J'/J = 0.63 \qquad p_c = 1.8GPa \leftrightarrow J'/J = 0.675 \qquad J = 81.5K$$

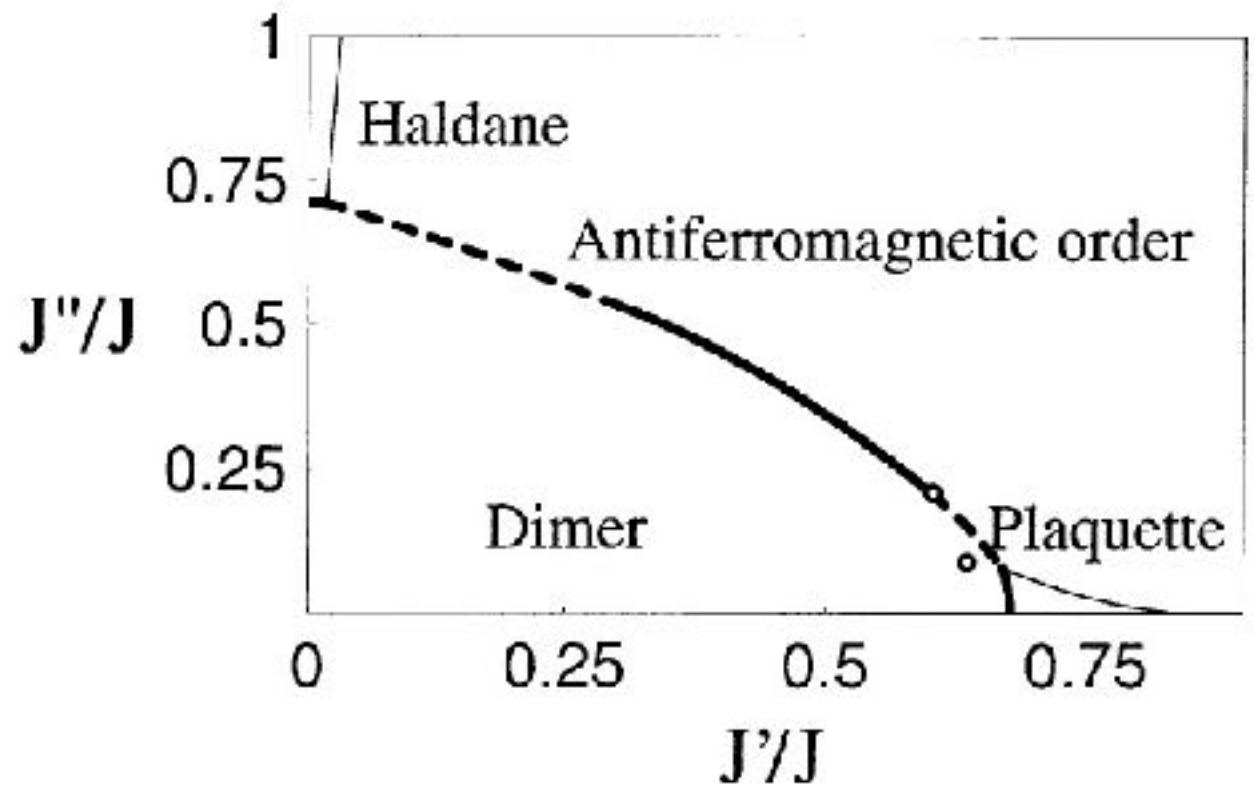
J'(p), J(p): linear functions. *J'(p)* changes by 5% between p_0 and p_c (ESR)

Sakurai, et al., J. Phys. Soc. Jpn. 87, 033701 (2018)

SSM with interlayer coupling

- Series expansion results Koga, J. Phys. Soc. Japan 69 (2000)



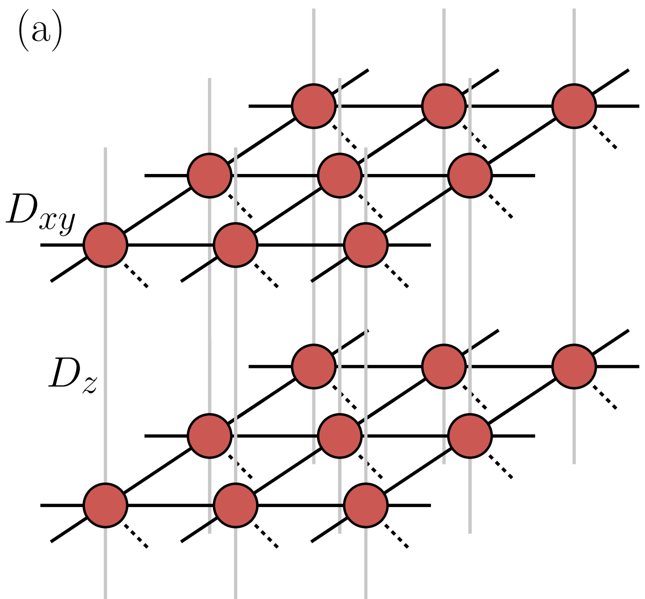


AF phase becomes favored over plaquette phase with increasing J"

- Predicted values for *J" (no consensus yet)*
  - ✦ *J"/J = 0.09 … 0.21* from fits to susceptibility [Miyahara & Ueda (2000), Knetter et al (2000)]
  - ✦ J"/J < 0.03 from ab-initio calculations [Radtke et al., PNAS 112 (2015)]

iPEPS for layered systems

Vlaar, PC, PRL 130 (2023)



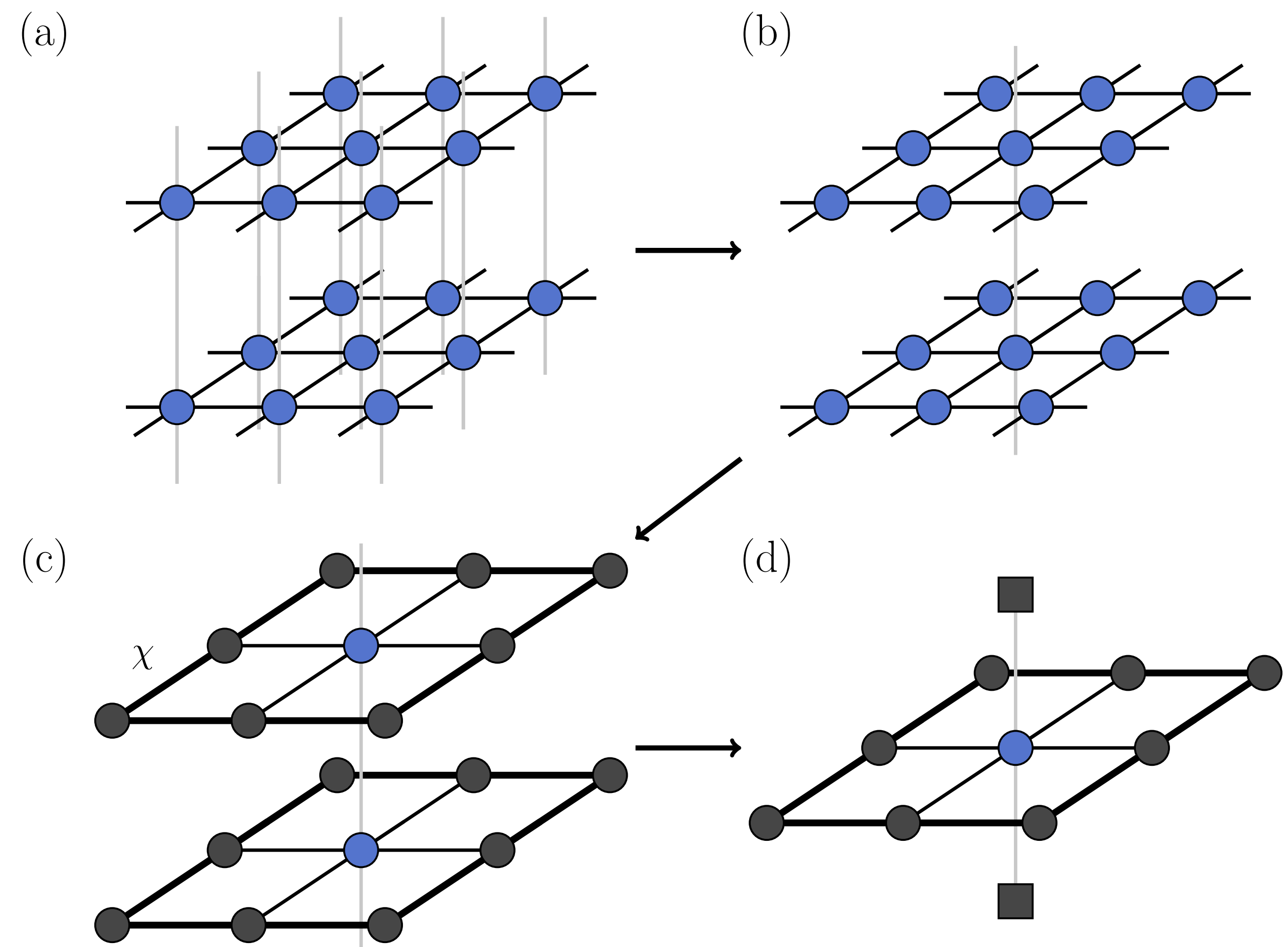
Ansatz:

- 3D tensor network ansatz (coupled iPEPS)
- $D_{xy} > D_z$ for weak interlayer coupling
- $D_z = 1$ → product state of iPEPSs

Patrick Vlaar

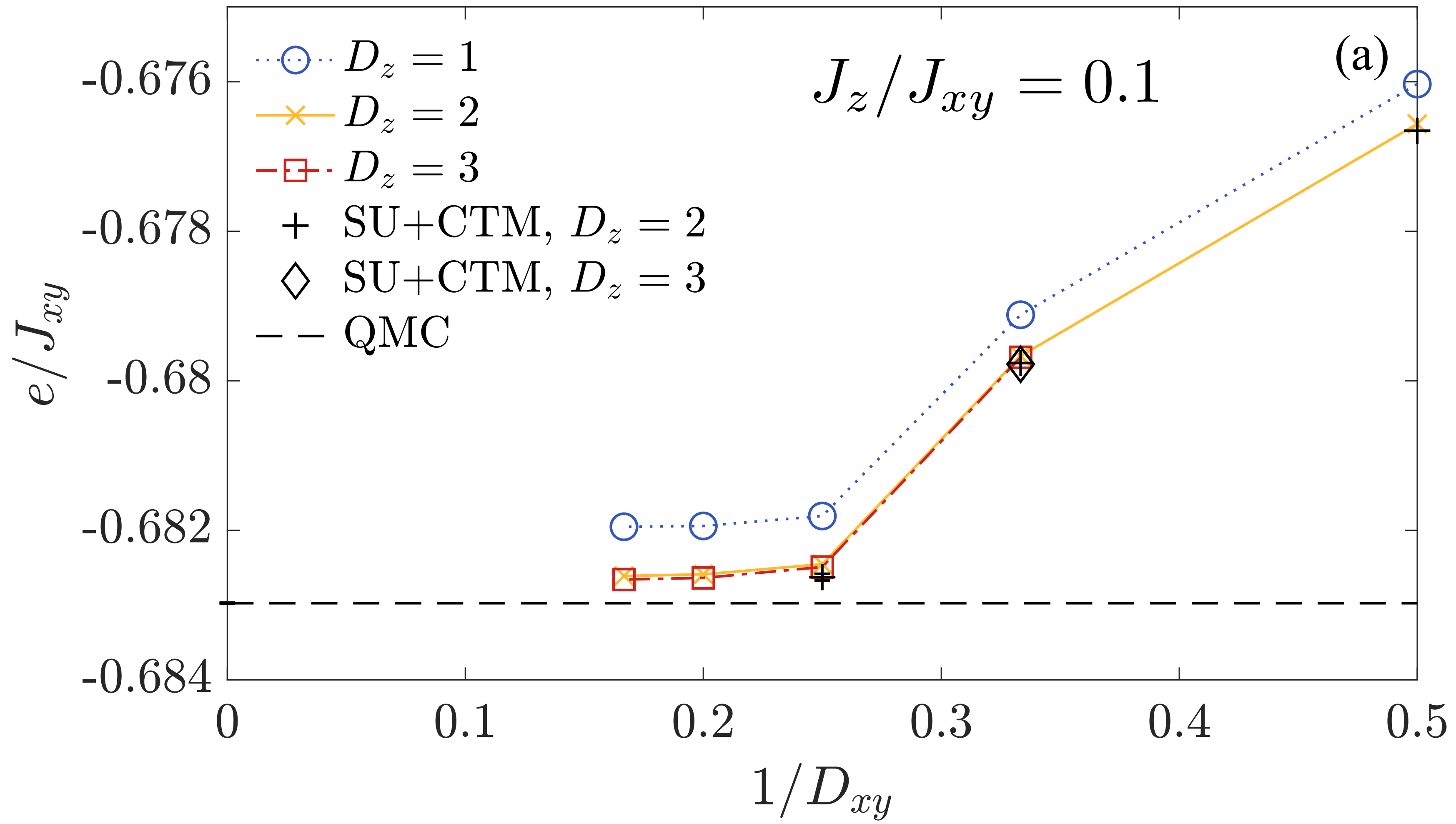
Contraction:

- $D_z = 1$: contract individual layers (2D)
- $D_z > 1$: perform effective decoupling away from center → 2D contraction
- Interlayer correlations beyond mean-field level are included by the $D_z > 1$ bonds in the center
- Layered corner transfer matrix (LCTM) method



Benchmarks for 3D anisotropic Heisenberg model

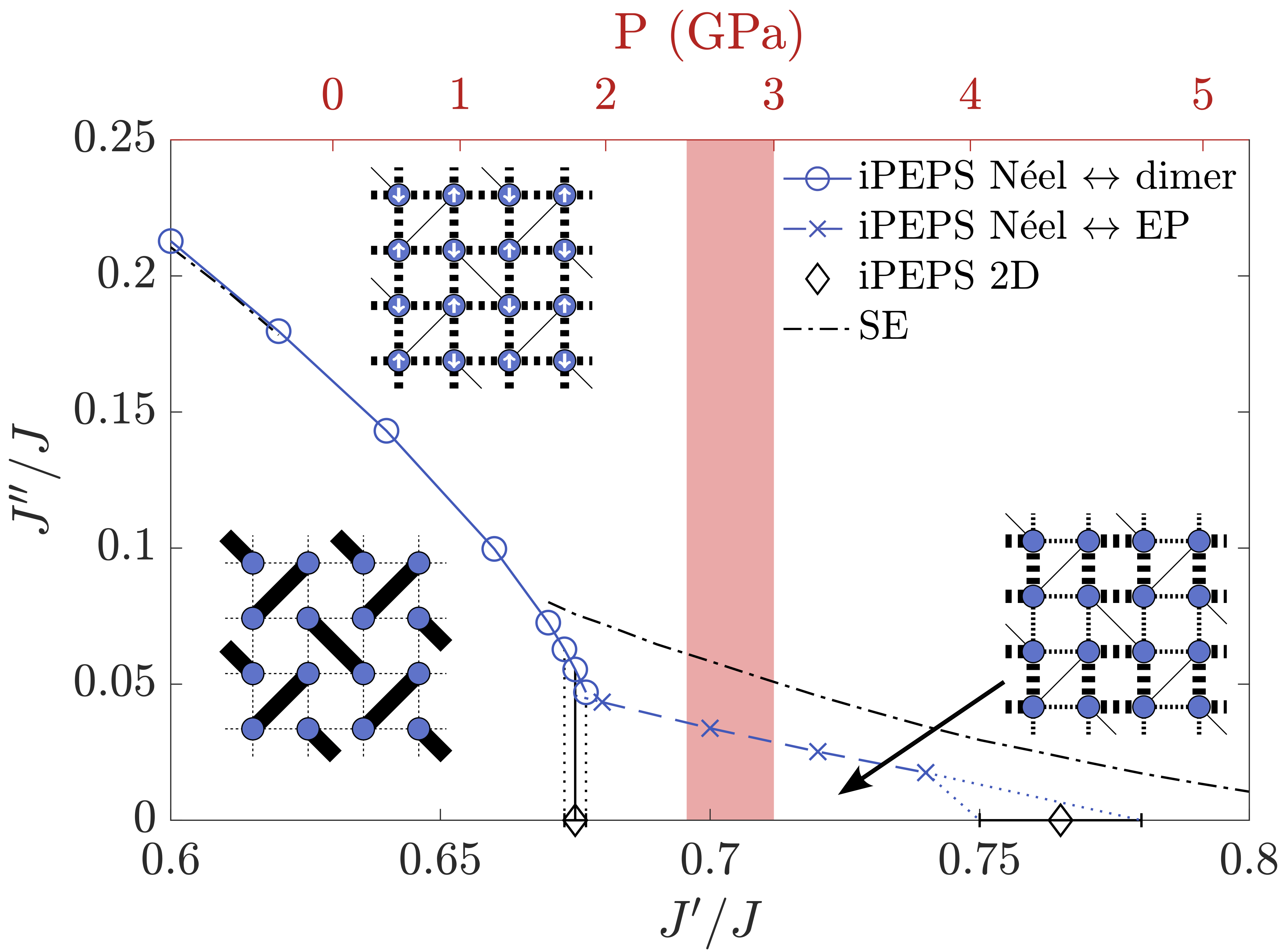
Vlaar, PC, PRL 130 (2023)



- Substantial improvement from $D_z = 1$ to $D_z = 2$
- Values close to the extrapolated QMC result
- In agreement with more expensive full 3D contractions

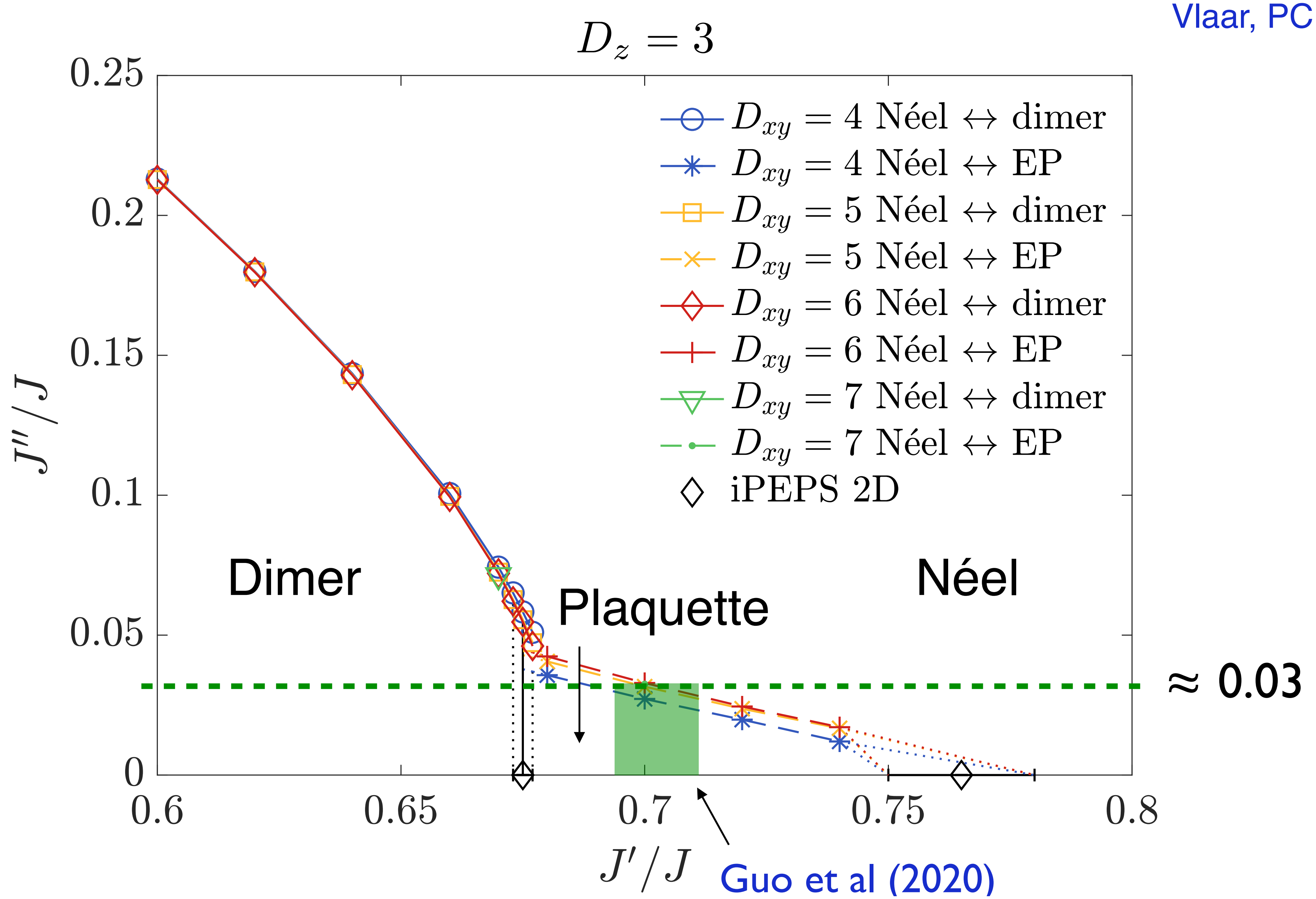
Vlaar & PC, PRB 103, 205137 (2021)

Phase diagram: SSM with interlayer coupling



Phase diagram: SSM with interlayer coupling

Vlaar, PC, arxiv:2302.07894



Estimate for the strength of interlayer coupling: J''/J ≈ 0.03

LCTM: promising approach also for other layered systems

Conclusion

- ✓ $SrCu_2(BO_3)_2$ under pressure / in a magnetic field exhibits very rich physics!
- ✓ Finite temperature Ising critical point, analogous to critical point of water
- ✓ New type of 1/5 plateau and supersolid phases at high pressure & field
- ✓ Results up to saturation in good agreement with experiments & understanding of the reduction of ultrasound velocity in the 1/2 plateau
- ✓ Reduction of plaquette phase due to interlayer coupling

- Progress with iPEPS: versatile tool for ground state and finite temperature calculations + extensions to layered systems

Thank you for your attention!

Acknowledgements:

F. Mila, S. Crone, P. Vlaar, P. Czarnik, J. Dziarmaga, L. Weber, A. Wietek, S. Wessel, B. Normand, A. Honecker, A. Läuchli, J. Larrea Jimenez, E. Fogh, R. Lortz, M. E. Zayed, K. Conder, E. Pomjakushina, Ch. Rüegg, H. M. Rønnow, T. Nomura, A. Miyata, S. Zherlitsyn, Y. Ishii, Y. Kohama, Y. Matsuda, A. Ikeda, C. Zhong, H. Kageyama, Z. Shi, S. Dissanayake, W. Steinhardt, D. Graf, D. M. Silevitch, H. A. Dabkowska, T. F. Rosenbaum, S. Haravifard

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