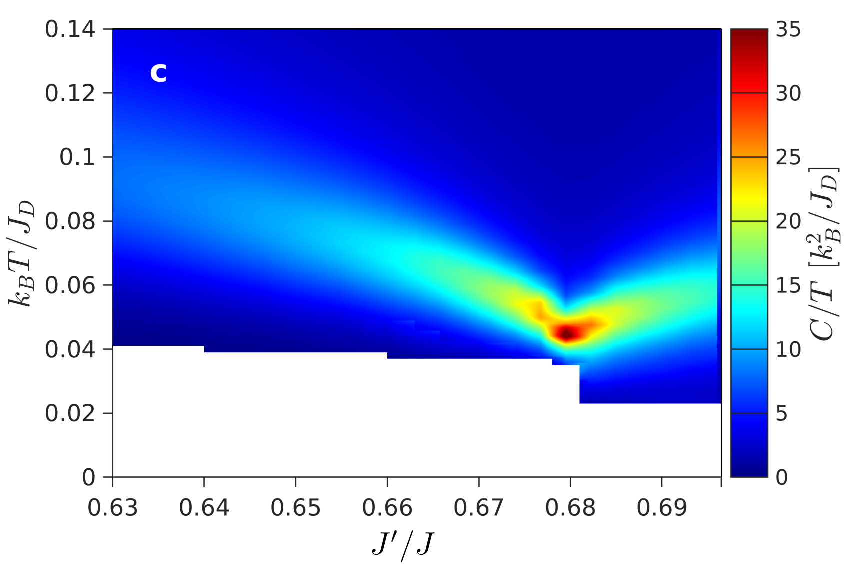
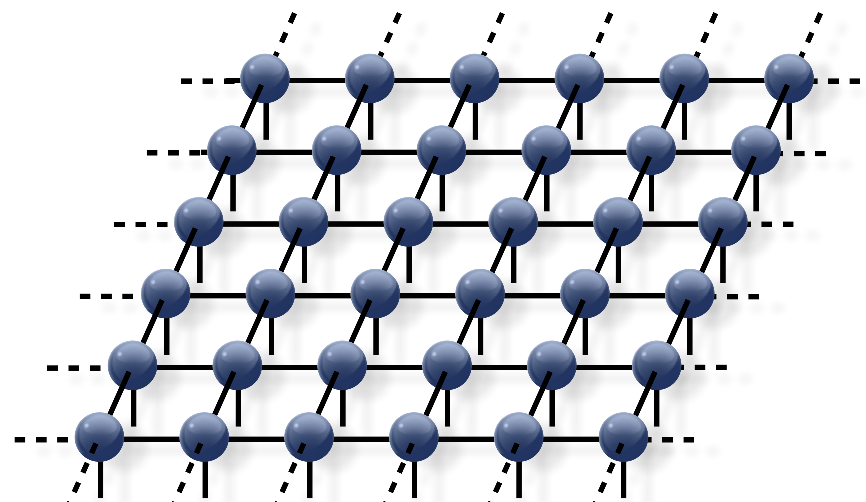
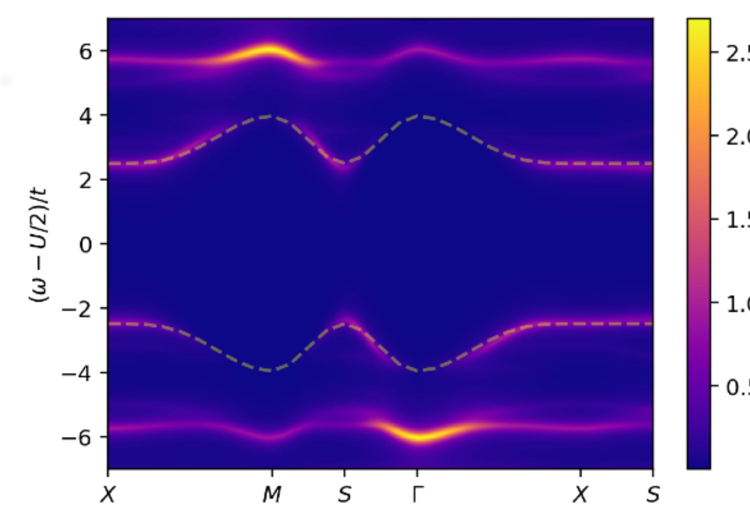
Infinite projected entangled-pair states: *ground states, finite temperature, excitations and extensions to 3D*

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam







Delta Institute for Theoretical Physics
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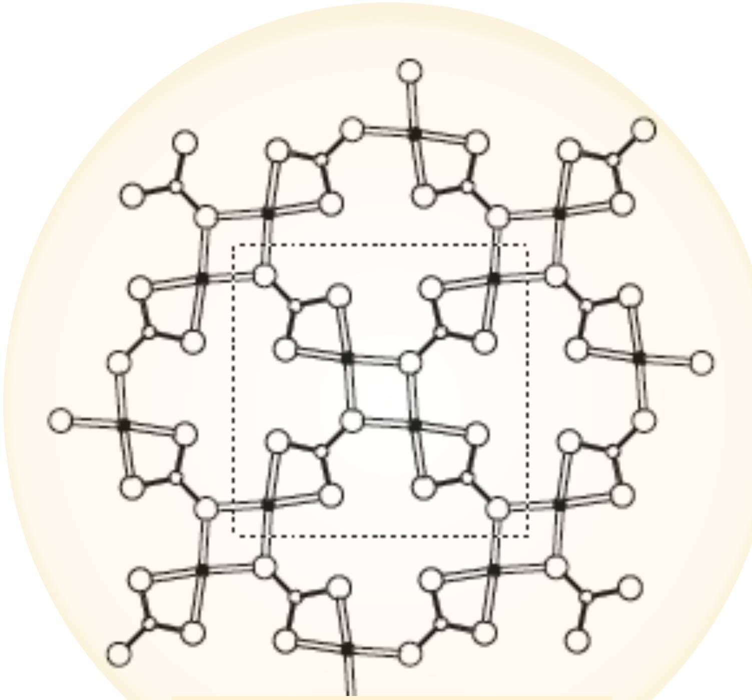
QuSoft

Outline

- Introduction to iPEPS & corner transfer matrix (CTM) method & imaginary time evolution (simple & full update)

- Ground state simulations with iPEPS:
  the Shastry-Sutherland model ($SrCu_2(BO_3)_2$)



$SrCu_2(BO_3)_2$

- iPEPS at finite temperature

  P. Czarnik & PC, PRB 99, 245107 (2019)
  Wietek, PC, Wessel, Normand, Mila, and Honecker, PRR 1 (2019)
  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 & F. Mila, Nature 592, 370 (2021)

- iPEPS for 3D & layered systems

  P. Vlaar & PC, PRB 103, 205137 (2021); arxiv:2208.06423; arxiv:2302.07894

- Excitations with iPEPS

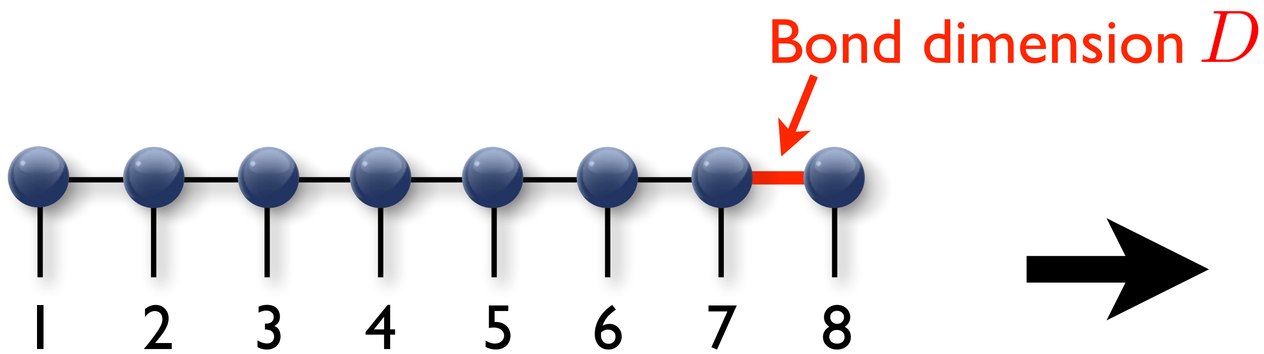
  B. Ponsioen and PC, PRB 101, 195109 (2020)
  B. Ponsioen, F. F. Assaad, PC, SciPost Physics, 12, 006 (2022)

MPS & PEPS

1D

MPS

Matrix-product state



Physical indices (lattices sites)

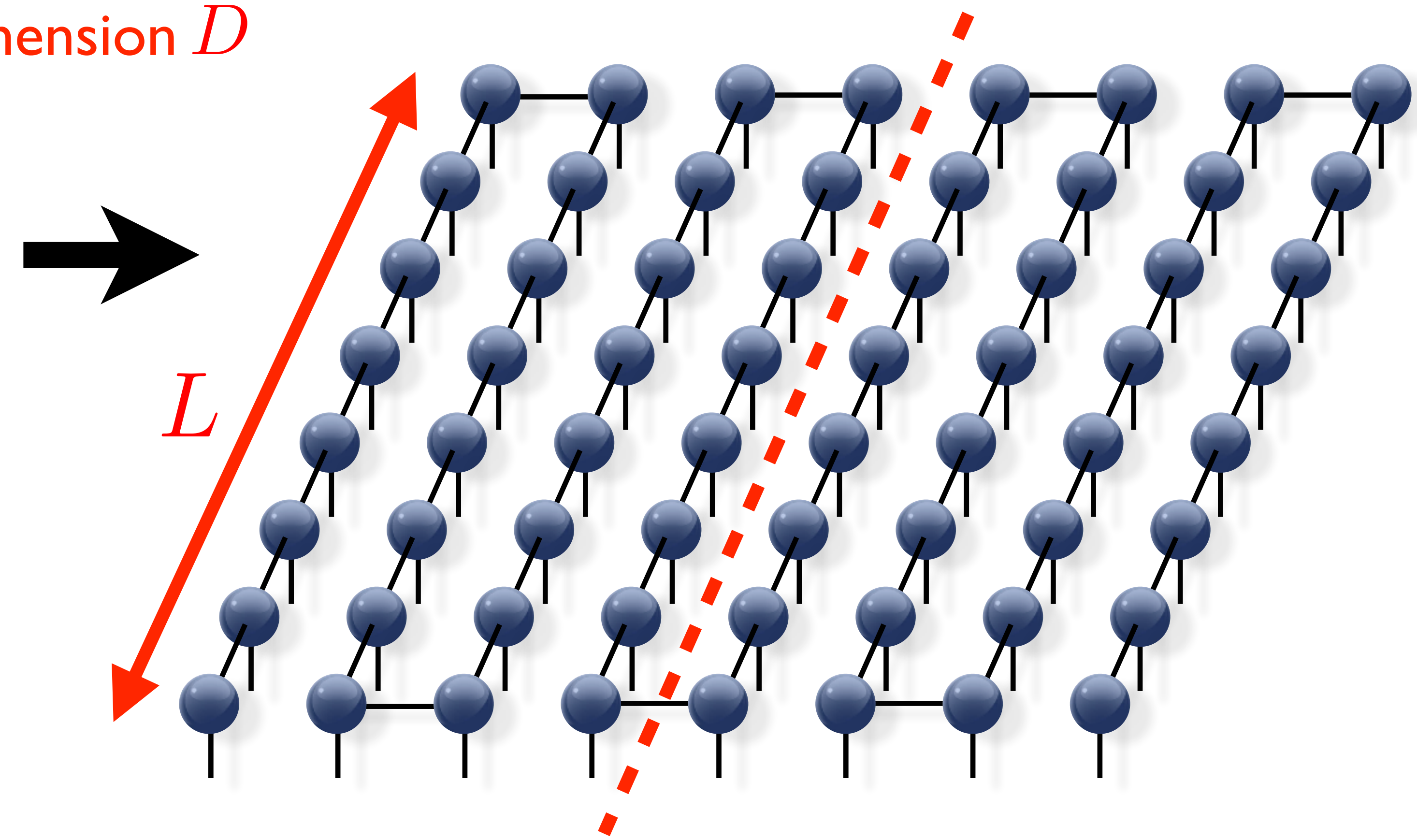
S. R. White, PRL 69, 2863 (1992)

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

Östlund, Rommer, PRL 75, 3537 (1995)

2D

Snake MPS (2D DMRG)



Computational cost:

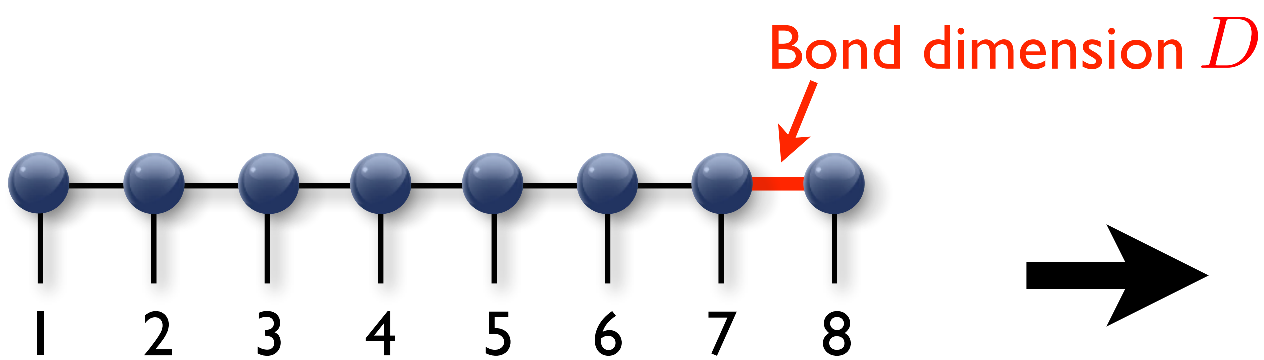
$$\propto \exp(L)$$

MPS & PEPS

1D

MPS

Matrix-product state



Physical indices (lattices sites)

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

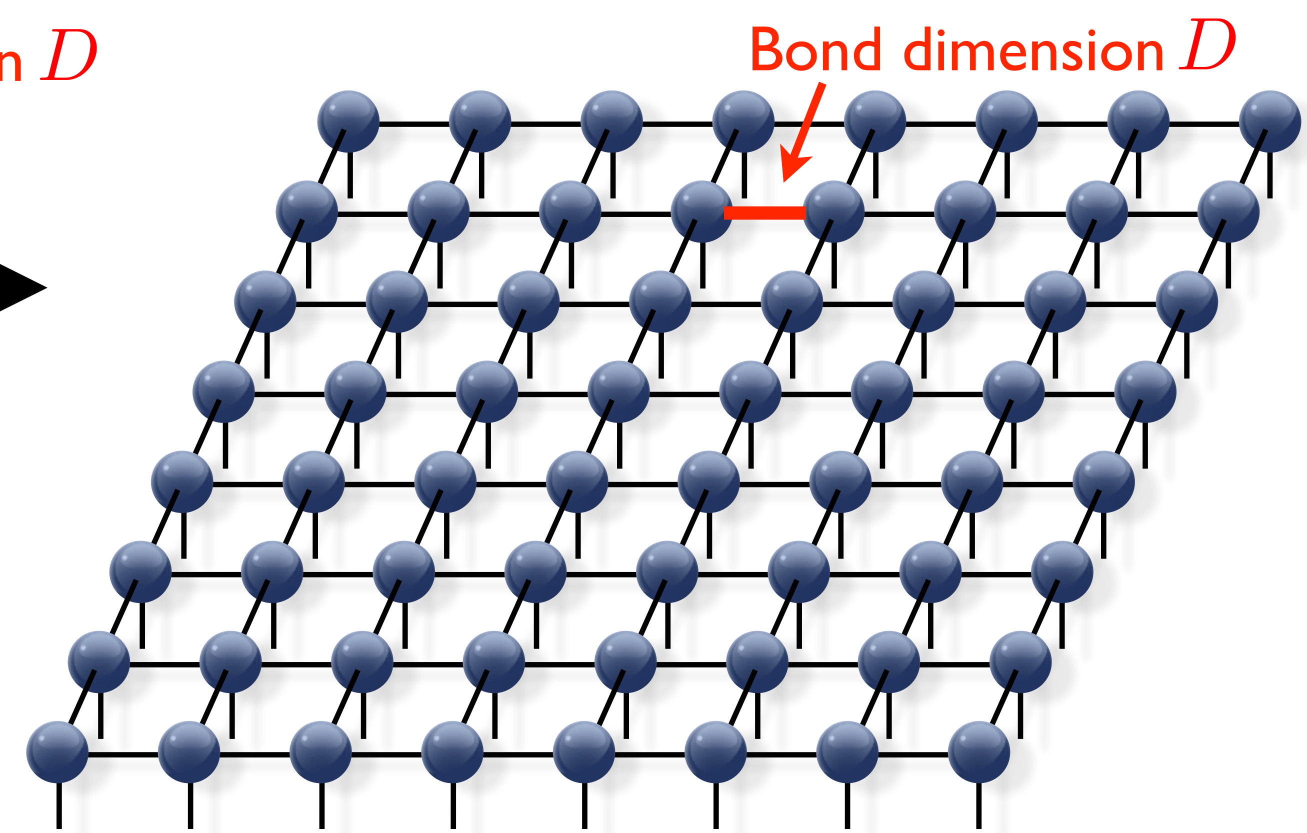
Fannes et al., CMP 144, 443 (1992)

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

Computational cost:

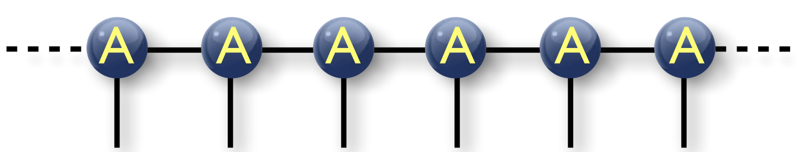
$$\propto poly(L, D)$$

Infinite PEPS (iPEPS)

1D

iMPS

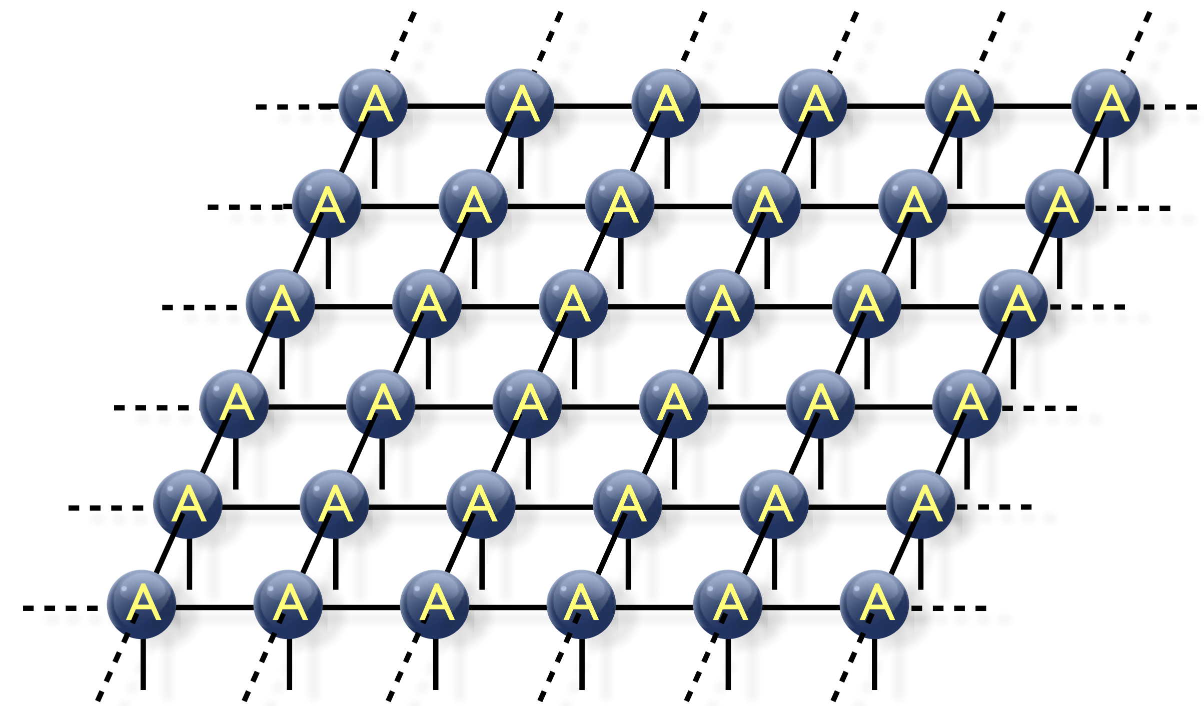
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



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

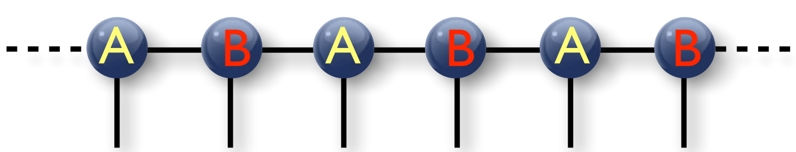
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

Infinite PEPS (iPEPS)

1D

iMPS

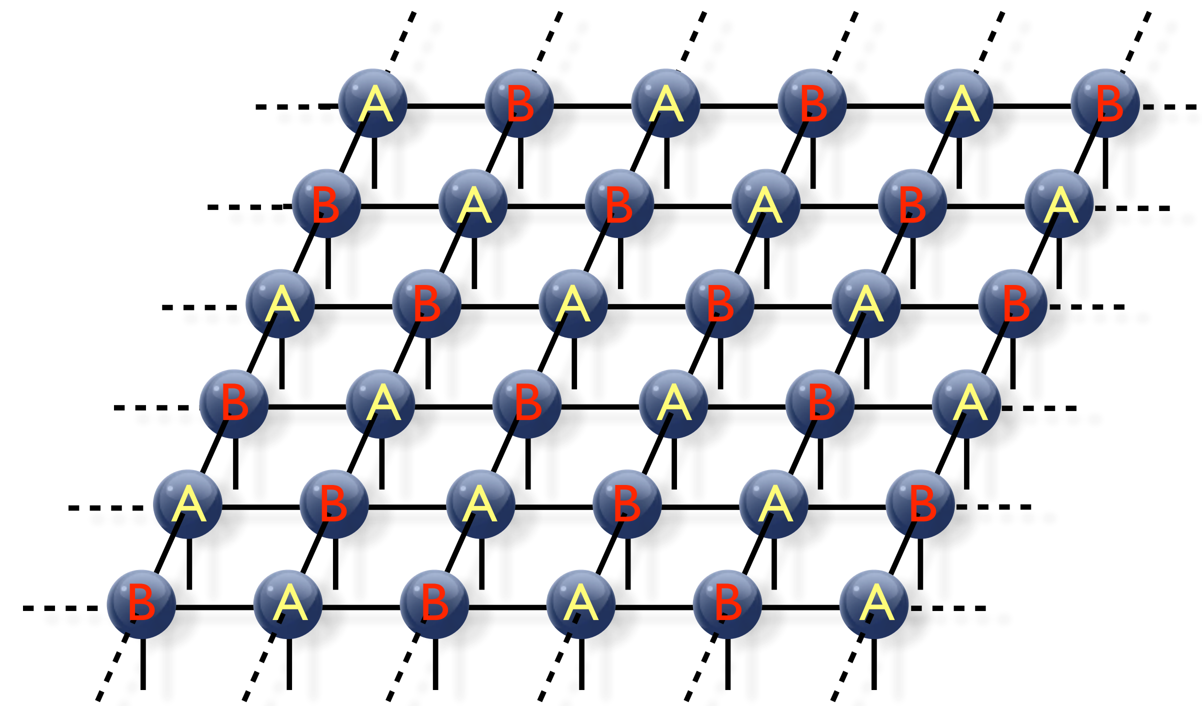
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



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

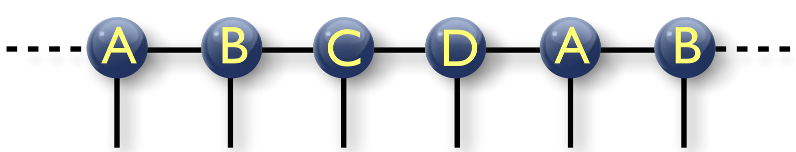
★ Work directly in the thermodynamic limit:
No finite size and boundary effects!

iPEPS with arbitrary unit cells

1D

iMPS

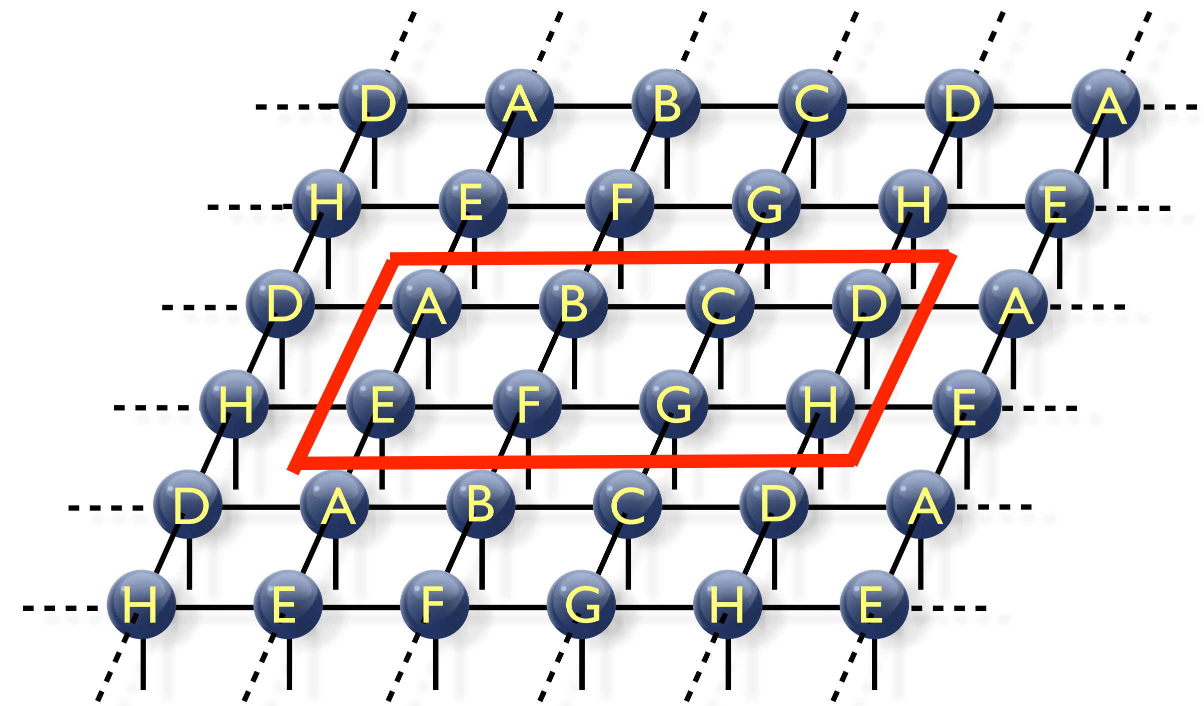
infinite matrix-product state



2D

iPEPS

with arbitrary unit cell of tensors



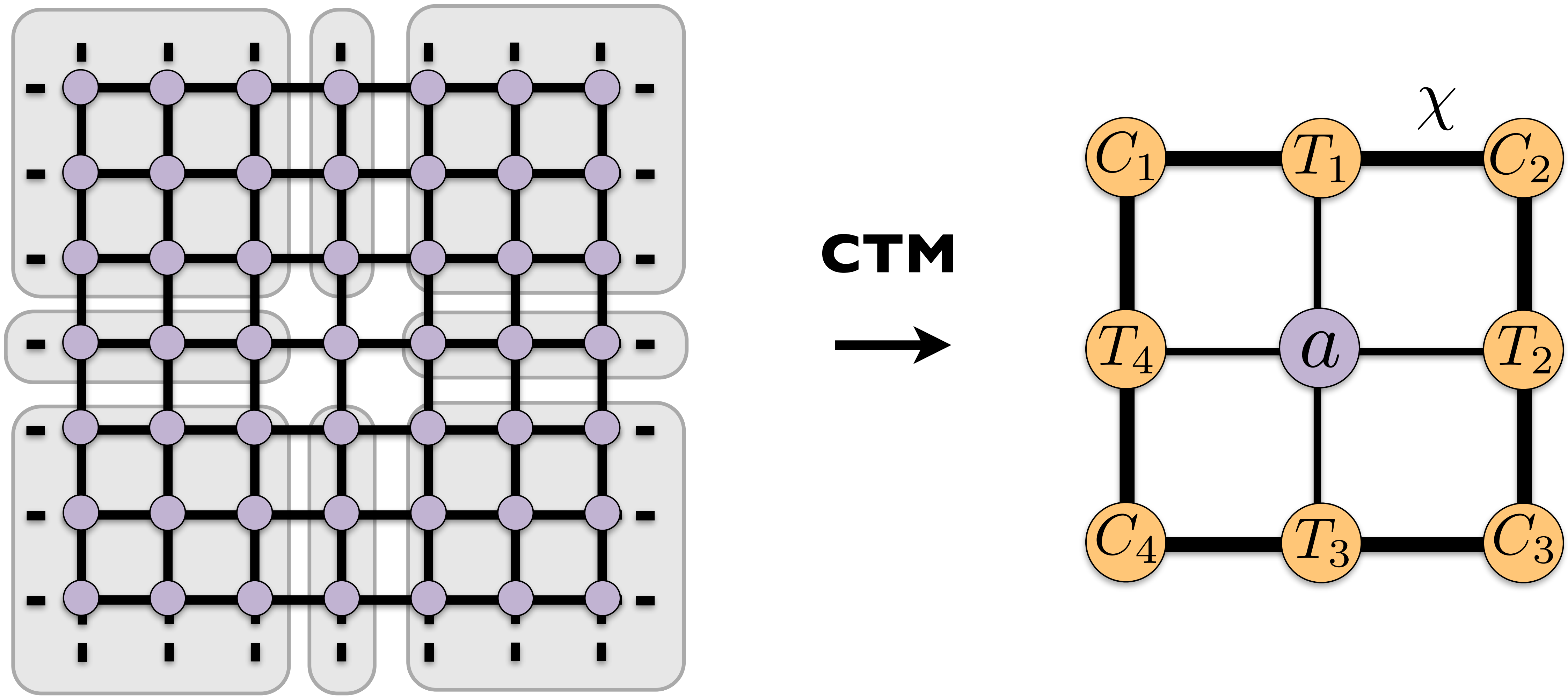
here: 4x2 unit cell

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

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

Contracting the iPEPS using the corner transfer matrix method

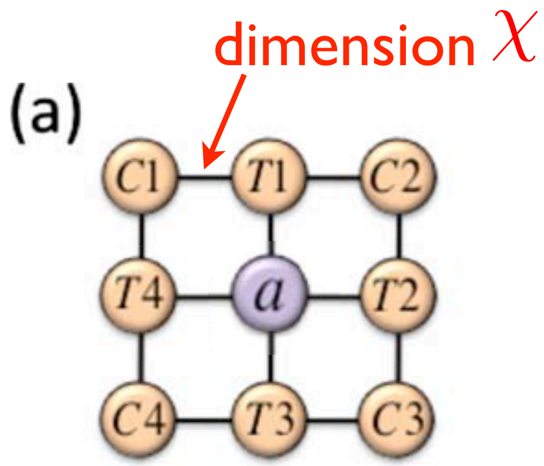
Nishino, Okunishi, JPSJ65 (1996)



- Environment tensors account for infinite system around a bulk site
- CTM: Compute environment in an iterative way
- Accuracy can be systematically controlled with χ

Contracting the iPEPS using the corner transfer matrix method

Nishino, Okunishi, JPSJ65 (1996)
Orus, Vidal, PRB 80 (2009)



- ★ Let the system grow in all directions.
- ★ Repeat until convergence is reached
- ★ The boundary tensors form the **environment**
- ★ Can be generalized to arbitrary unit cell sizes

  PC, et al., PRB 84 (2011)
  PC, et al., PRL 113 (2014)

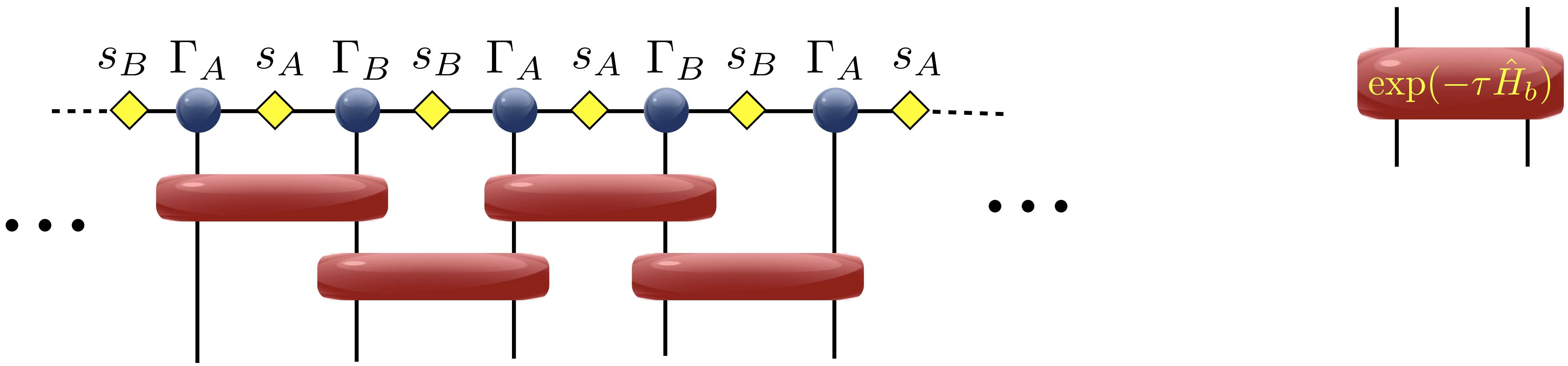
Optimization via imaginary time evolution

- **Idea:** $\exp(-\beta \hat{H})|\Psi_i\rangle \xrightarrow{\beta \to \infty} |\Psi_{GS}\rangle$

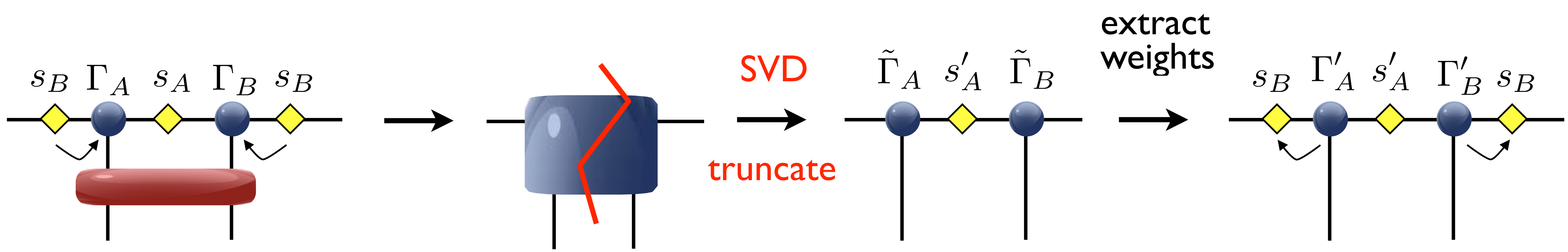
Trotter-Suzuki decomposition:

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

- 1D:

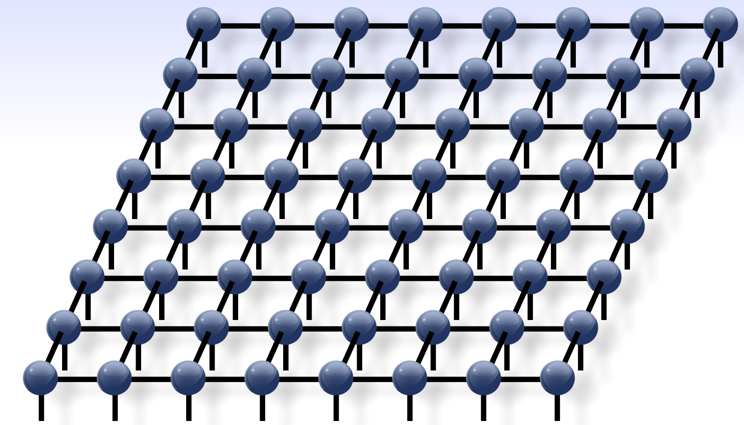


- At each step: apply a two-site operator to a bond and truncate bond back to *D*



infinite **T**ime **E**volving **B**lock **D**ecimation (iTEBD)

Optimization via imaginary time evolution



- **2D: same idea:** apply $\exp(-\tau \hat{H}_b)$ to a bond and truncate bond back to *D*

- **However**, SVD update is not optimal (because of loops in PEPS)!

simple update (SU)

Jiang et al, PRL 101 (2008)

★ "local" update like in TEBD

★ Cheap, but not optimal (e.g. overestimates magnetization in S=1/2 Heisenberg model)

full update (FU)

Jordan et al, PRL 101 (2008)

★ Take the full wave function into account for truncation

★ optimal, but more expensive

★ Fast-full update [Phien et al, PRB 92 (2015)]

Cluster update

Wang, Verstraete, arXiv:1110.4362 (2011)

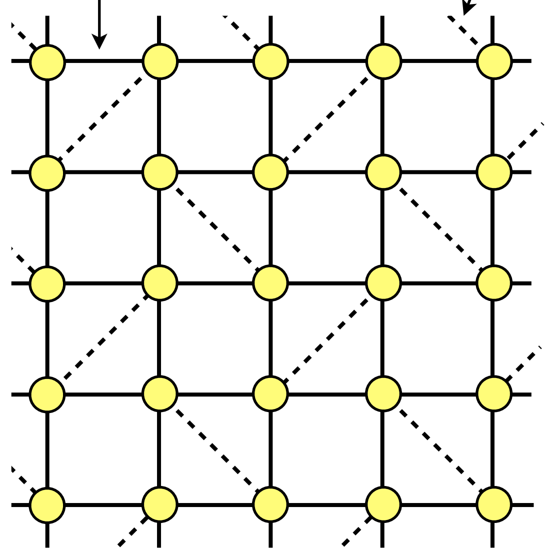
iPEPS ground state simulations

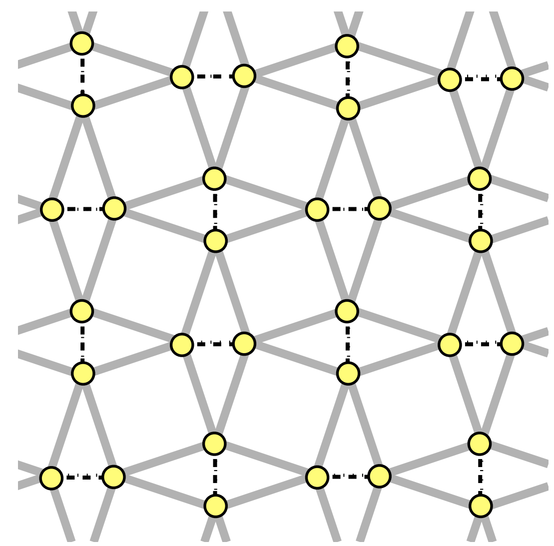
- Many applications to challenging problems, including frustrated spin, SU(N), bosonic systems, t-J / Hubbard models, and more, see e.g.:

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 …

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

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

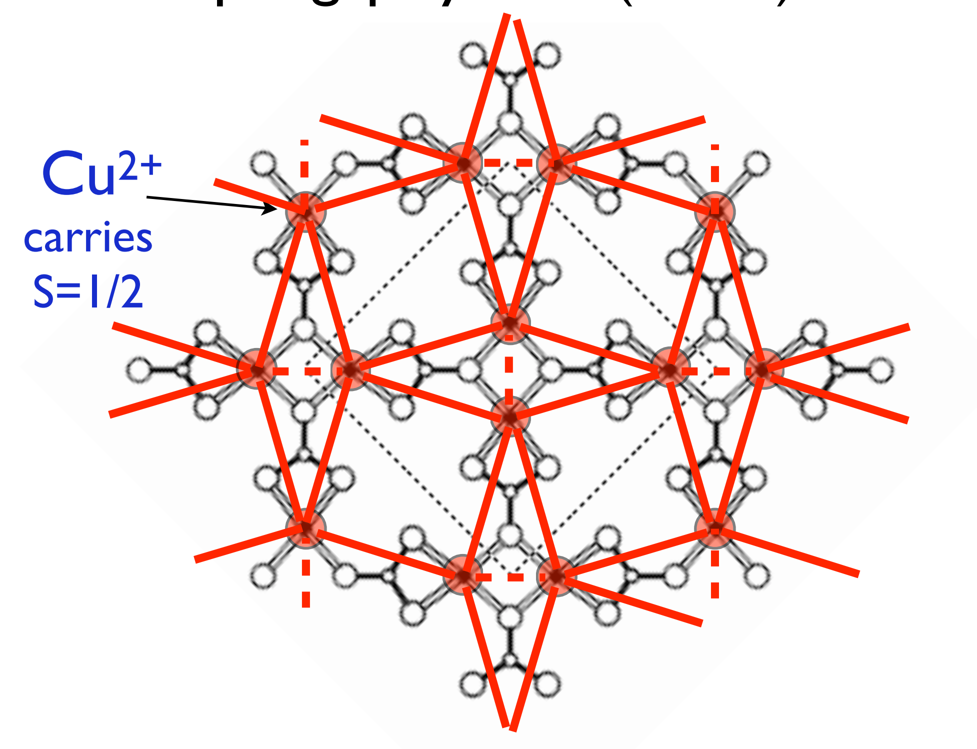




Shastry & Sutherland, Physica B+C **108** (1981).

$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



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

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

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

$SrCu_2(BO_3)_2$

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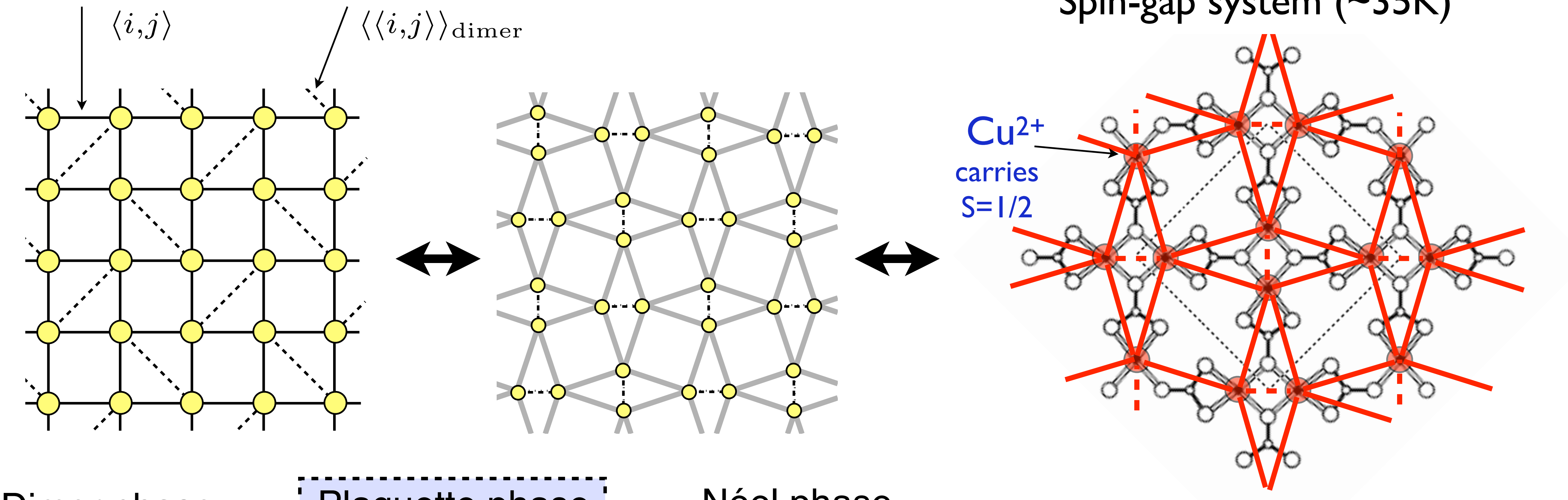
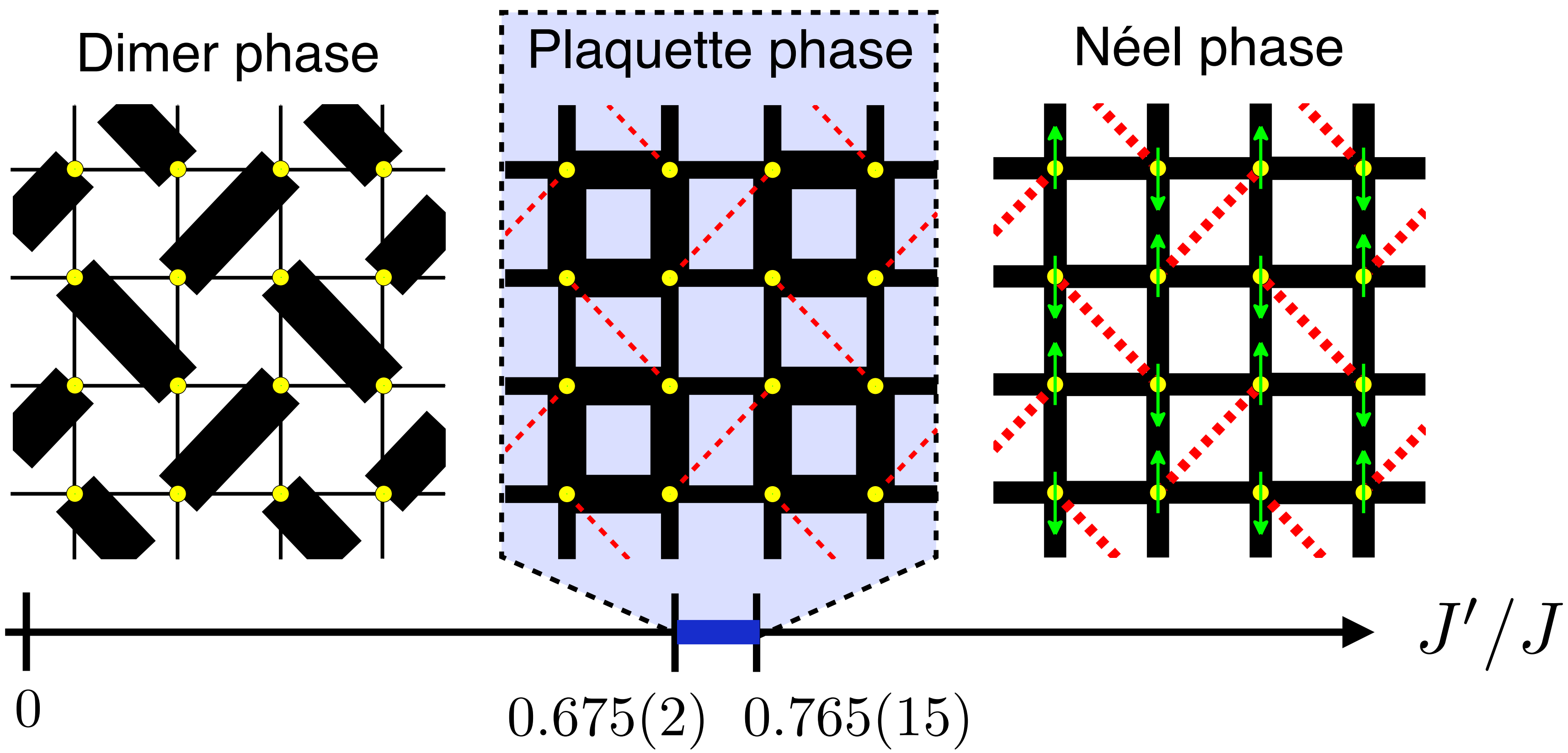


Kageyama et al. PRL **82** (1999)



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

previously found in:

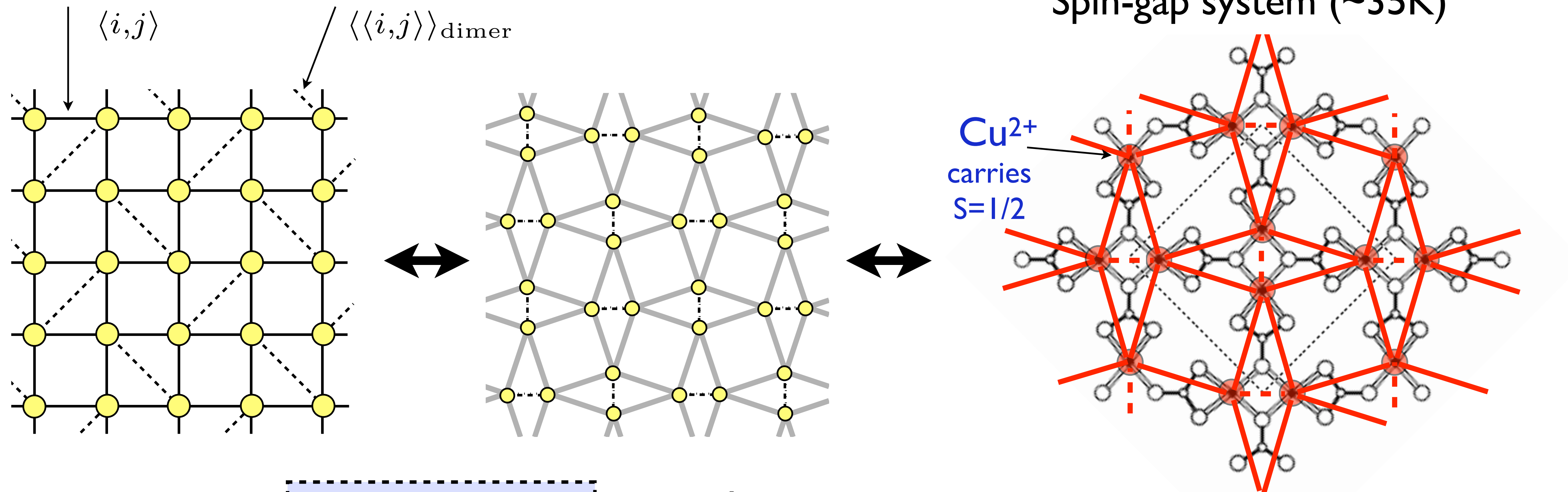
Koga and Kawakami, PRL **84** (2000)
Takushima et al., JPSJ **70** (2001)
Chung et al, PRB **64** (2001)
Läuchli et al, PRB **66** (2002)

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

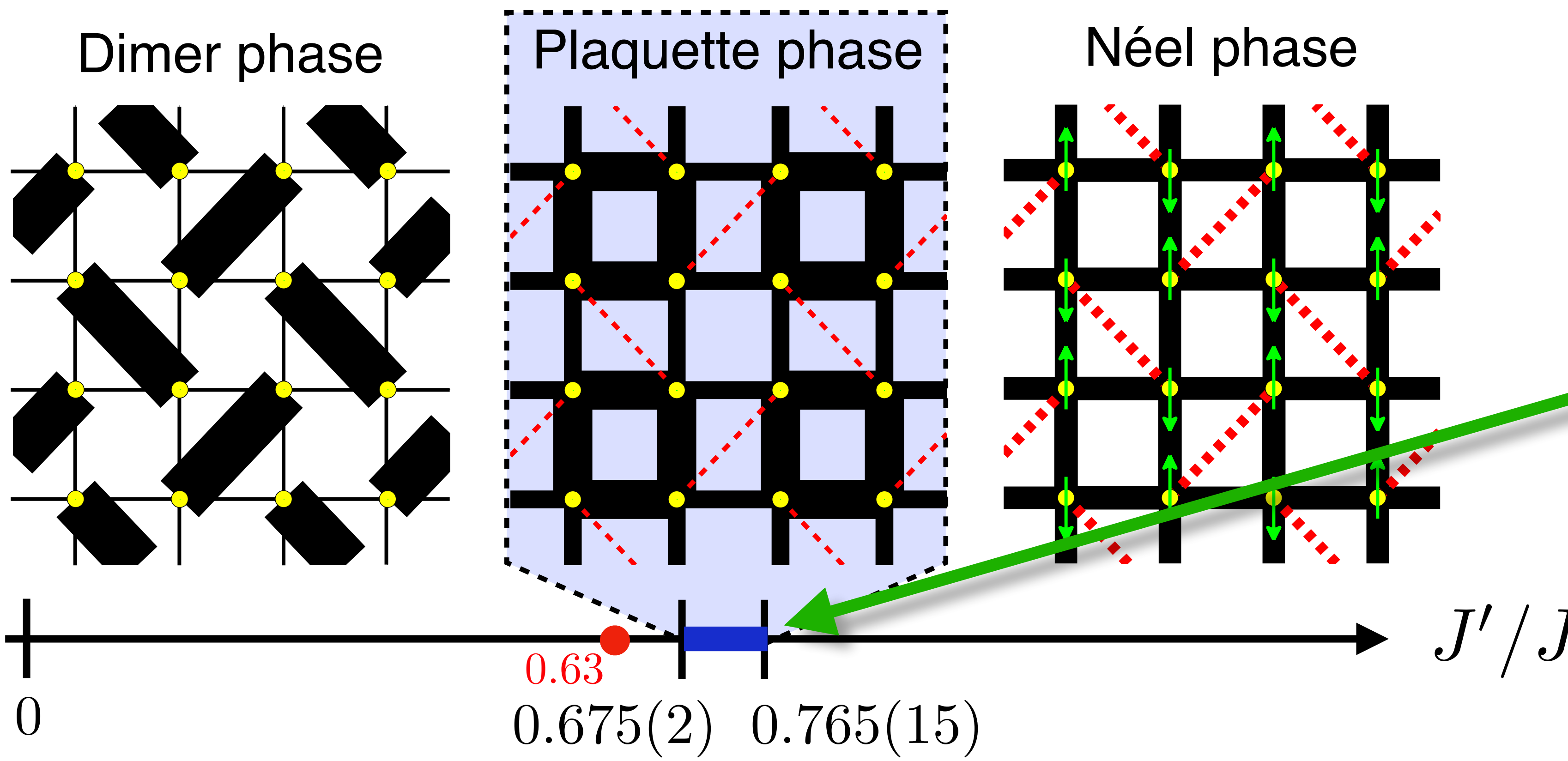
$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\text{dimer}}} S_i \cdot S_j$$

$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



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



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

Deconfined QCP?

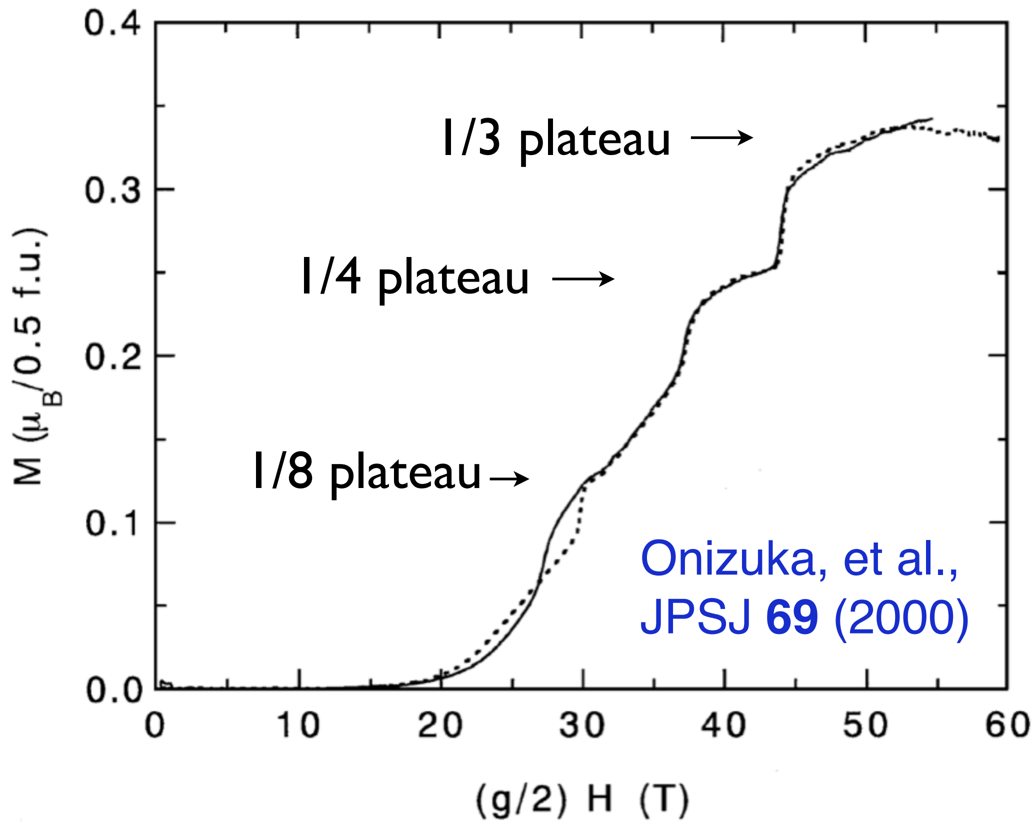
Lee, You, Sachdev & Vishwanath, PRX 9 (2019)

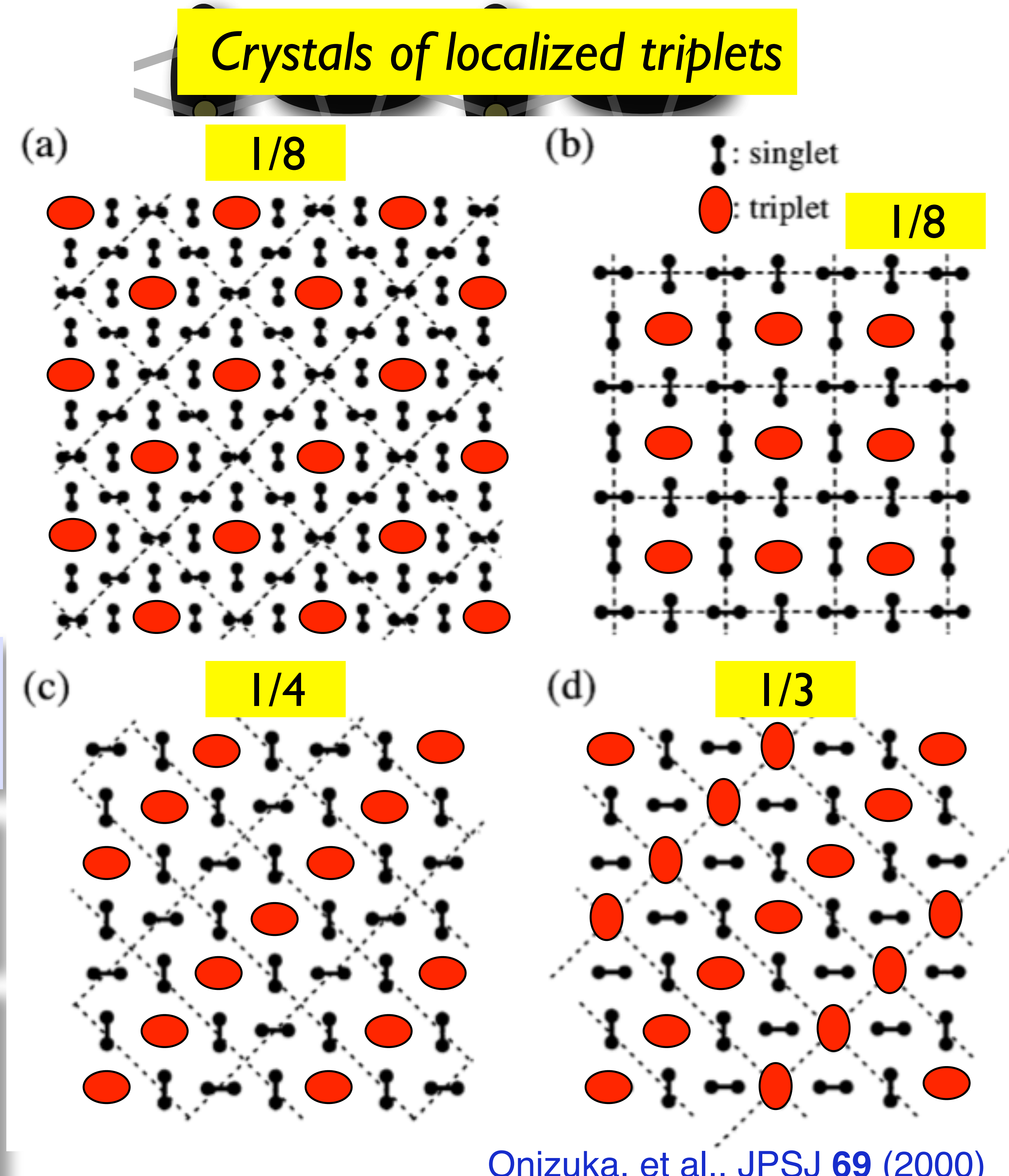
Intermediate QSL phase?

Yang, Sandvik & Wang, PRB 105 (2022)

Magnetization plateaus

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



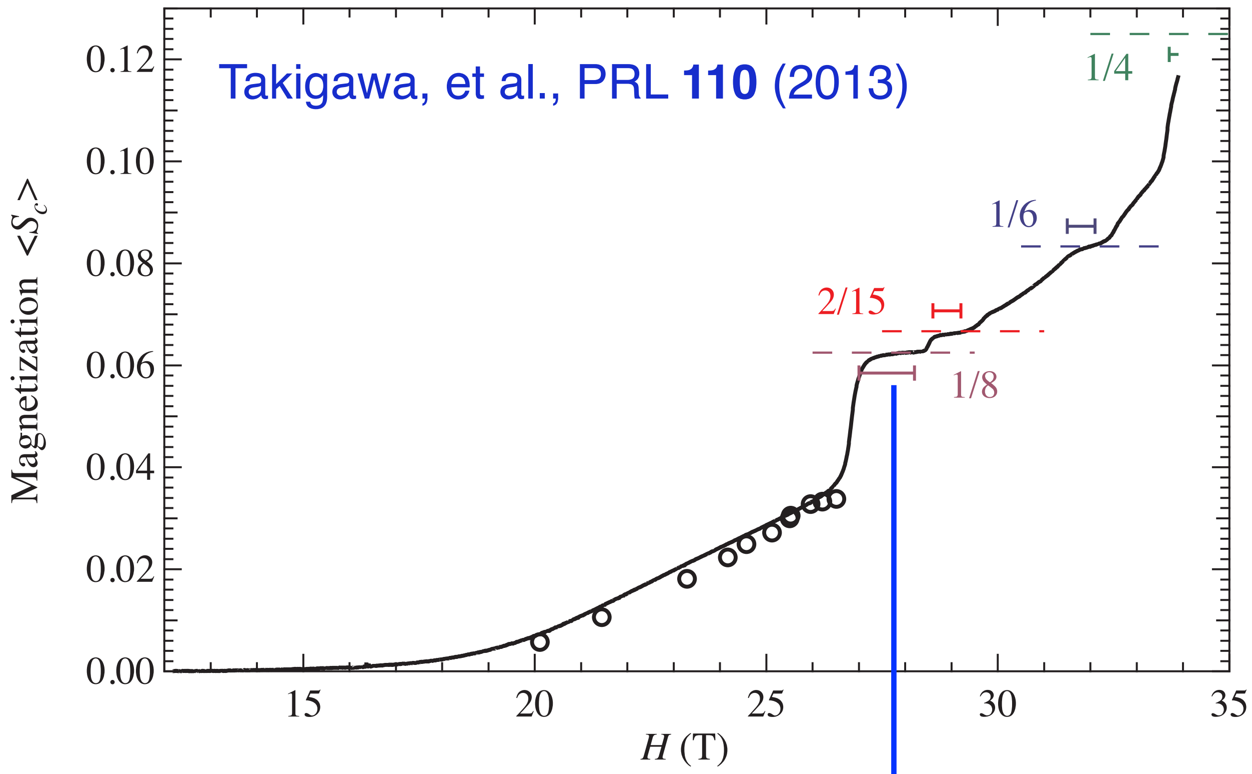


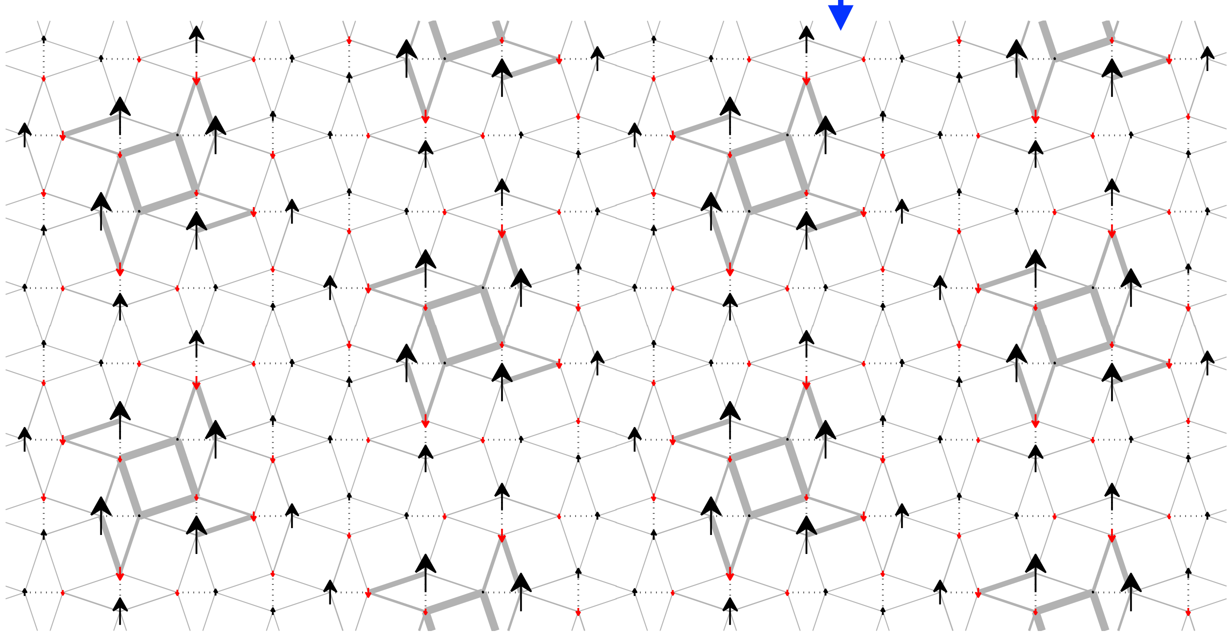
The SSM has almost localized triplet excitations [Miyahara&Ueda'99, Kageyama et al. '00]

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





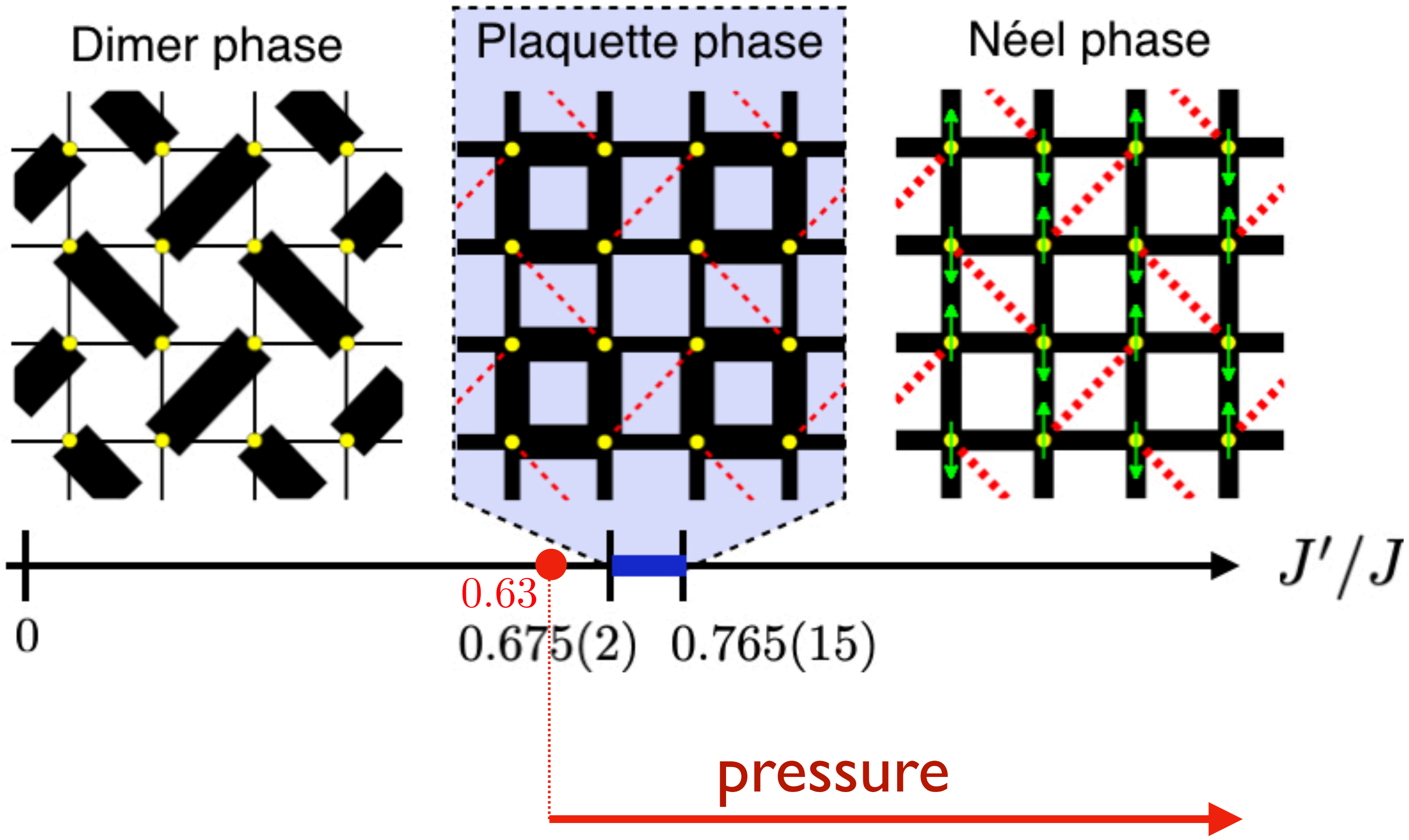
★ Crystals of triplet-bound states

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

Many experimental / theoretical studies

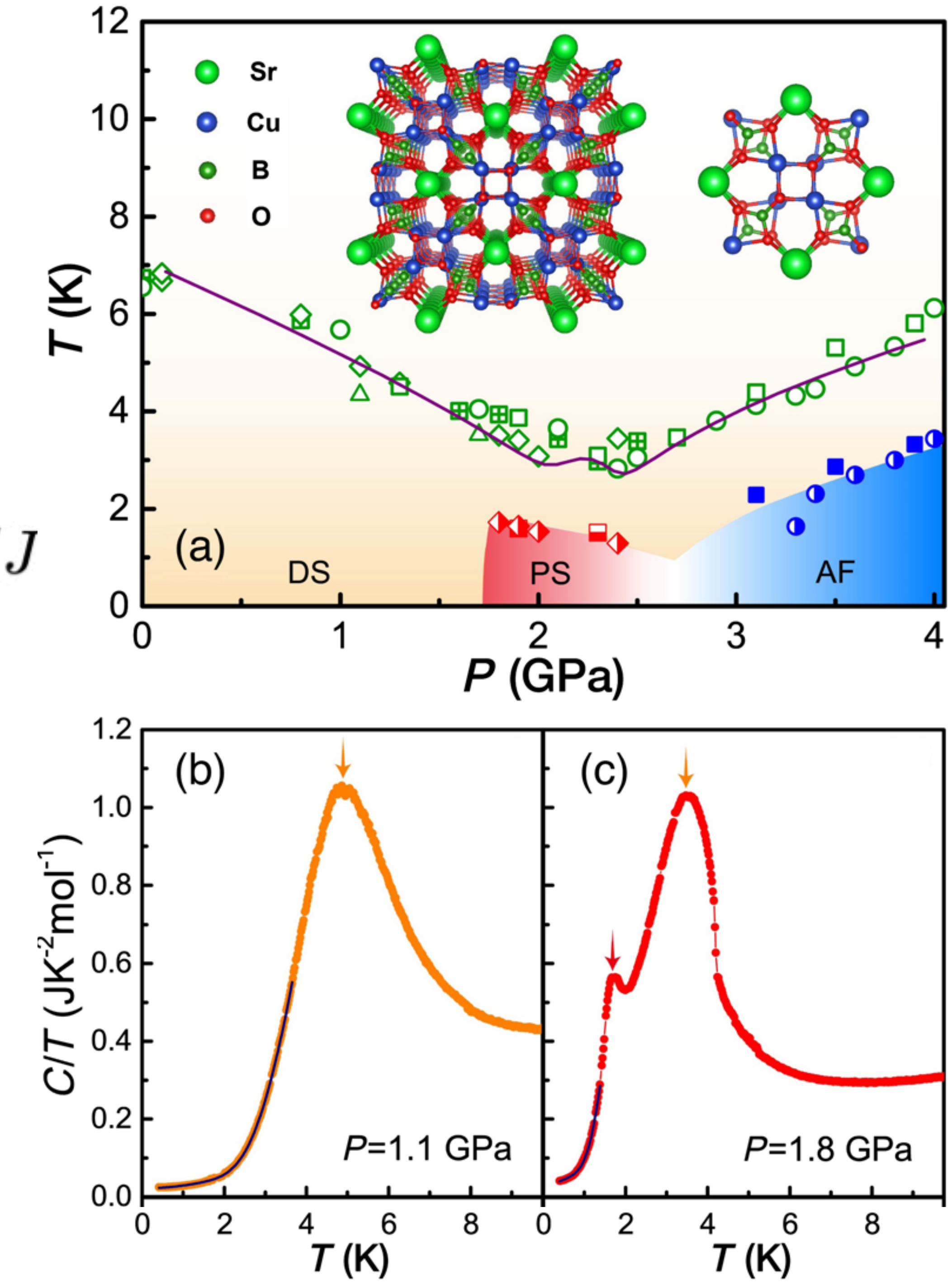
Kageyama et al, PRL **82** (1999)
Onizuka et al, JPSJ **69** (2000)
Kageyama et al, PRL **84** (2000)
Kodama et al, Science **298** (2002)
Takigawa et al, Physica **27** (2004)
Levy et al, EPL **81** (2008)
Sebastian et al, PNAS **105** (2008)
Isaev et al, PRL **103** (2009)
Jaime et al, PNAS **109** (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



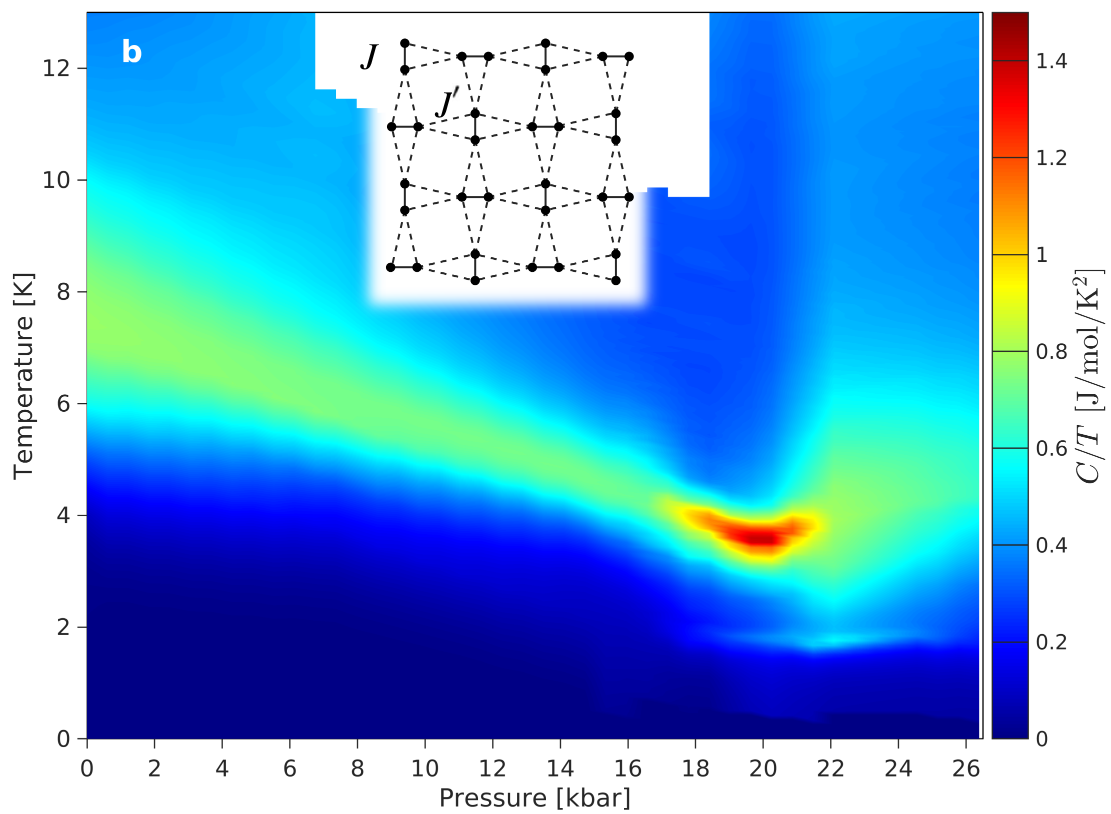
Drive system across the phase transitions!

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)
…

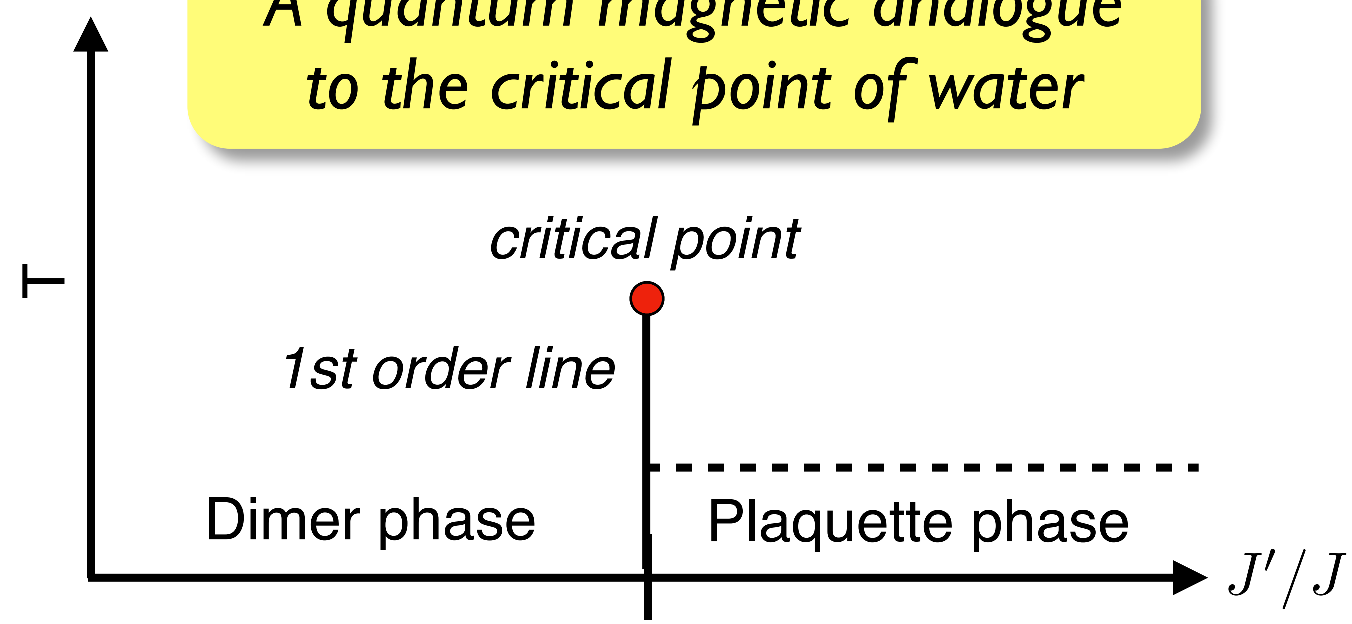


Guo, et al., PRL 124, 206602 (2020)

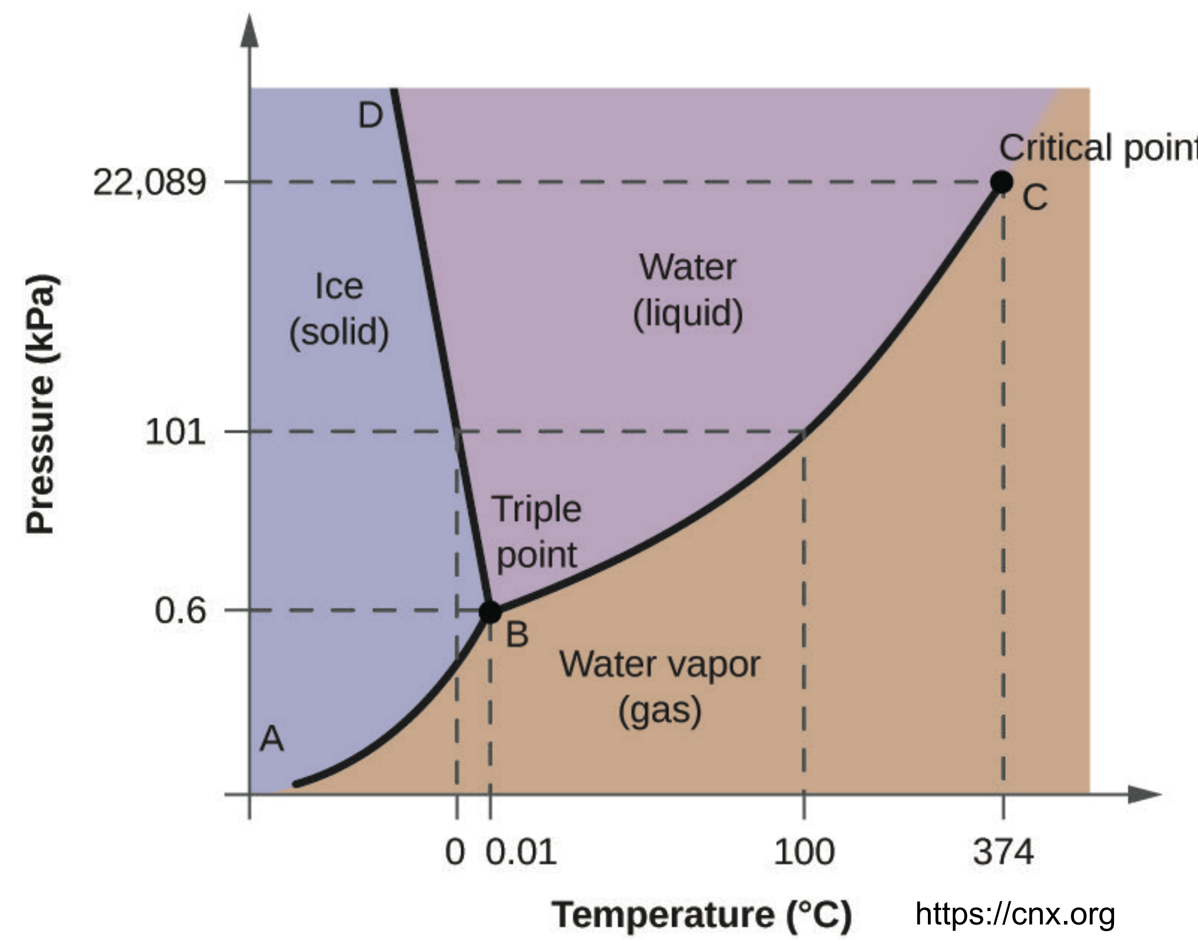
Specific heat data (group of H. M. Rønnow)



A quantum magnetic analogue to the critical point of water



Can we reproduce this with iPEPS?

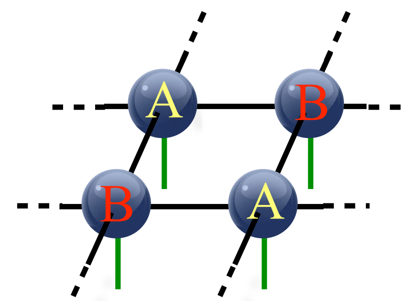


Finite temperature simulations with iPEPS

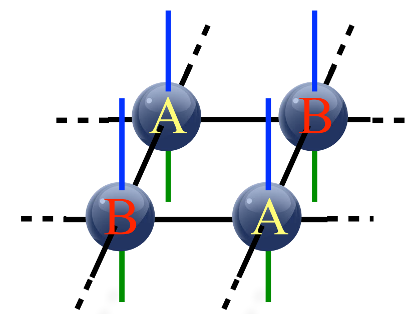
- Methodological developments (2D):

  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), …

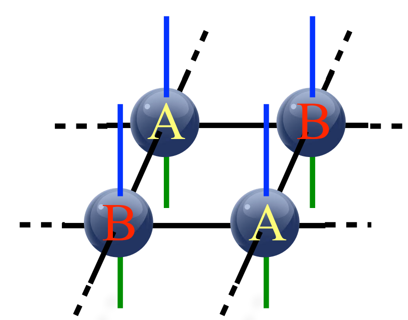
- Wave-function: $|\Psi\rangle \approx$



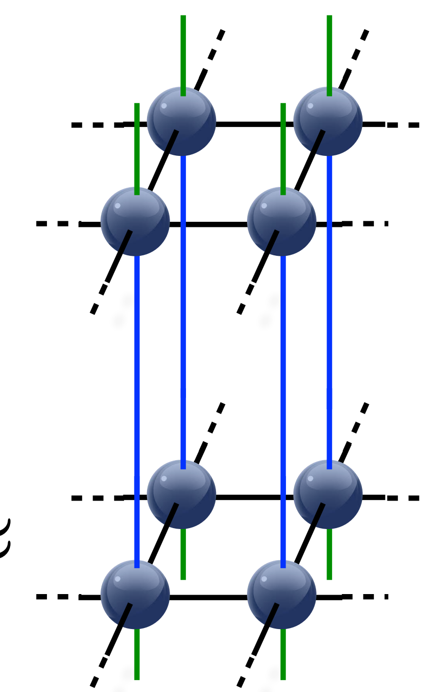
- Density-operator: $\hat{\rho} = e^{-\beta \hat{H}} \approx$



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



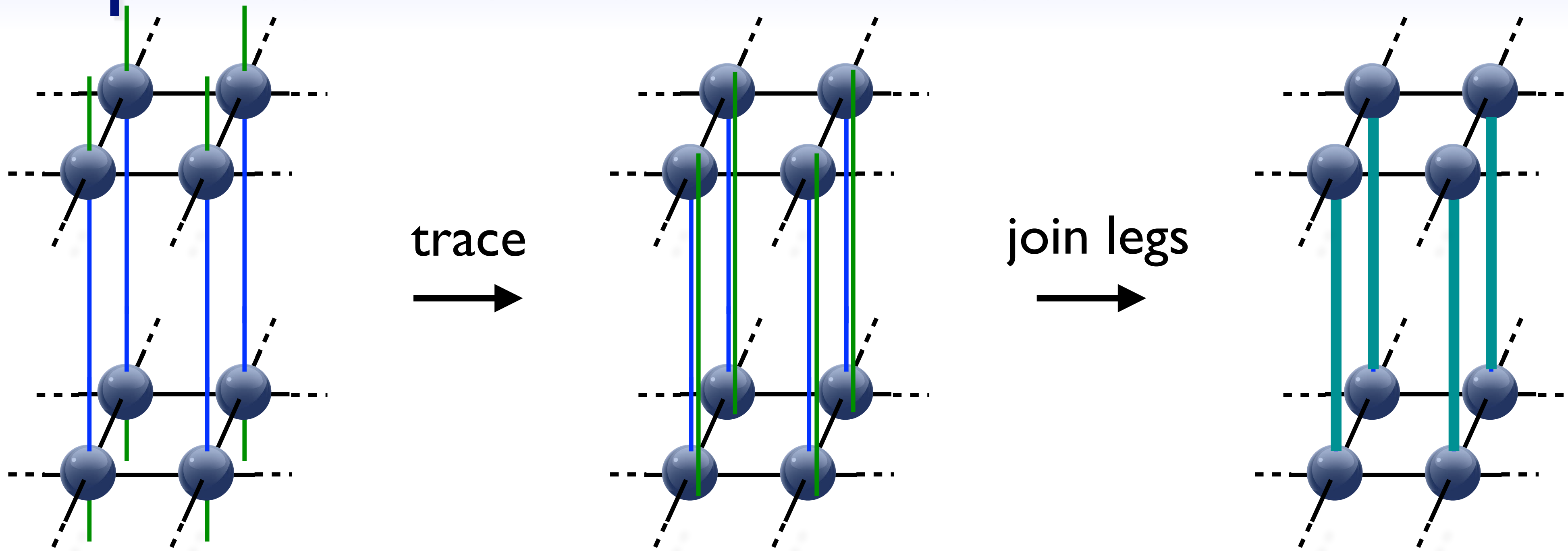
$\hat{\rho}(\beta) \approx$



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

Finite temperature simulations with iPEPS

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



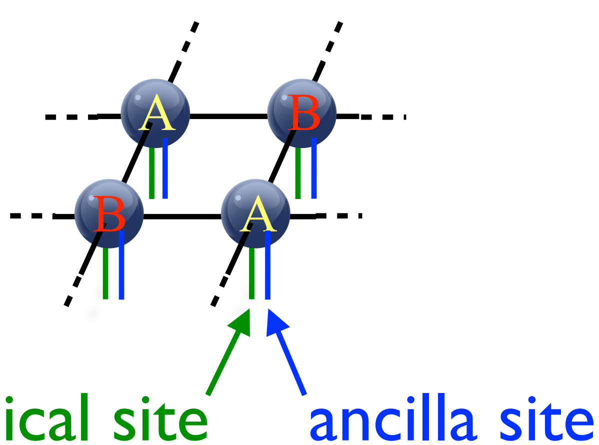
$\langle \tilde{\Psi} | \tilde{\Psi} \rangle$

same structure as for wave functions

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

Other (equivalent) formulation using purification:

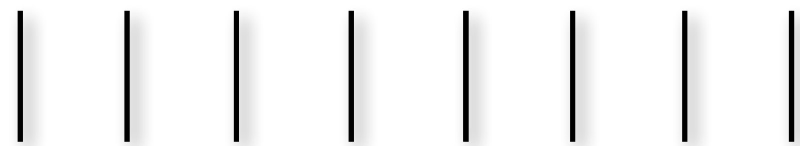
$|\tilde{\Psi}\rangle \approx$



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

Imaginary time evolution

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

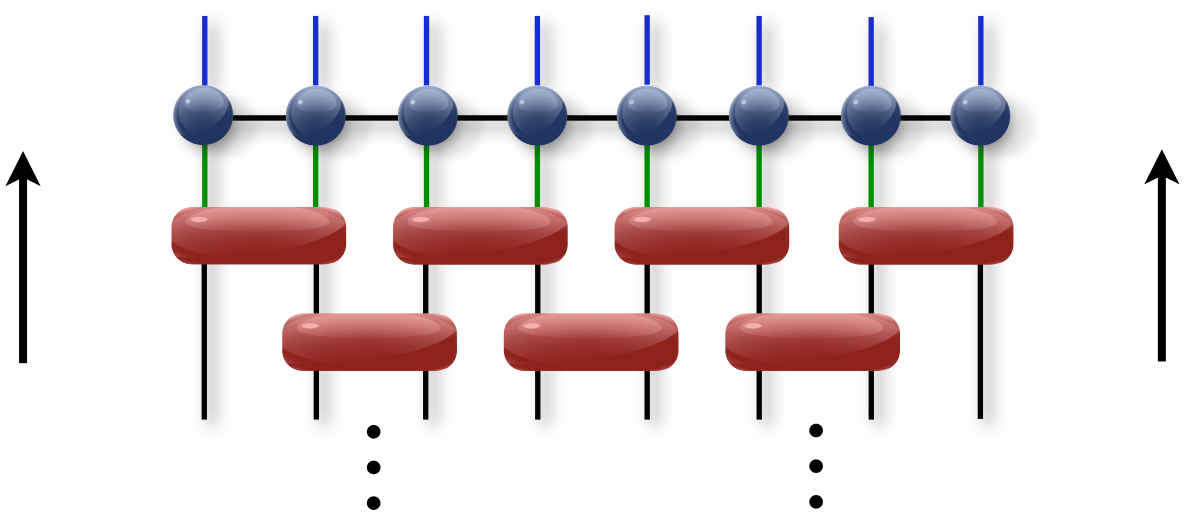
- Initial state:  exact!

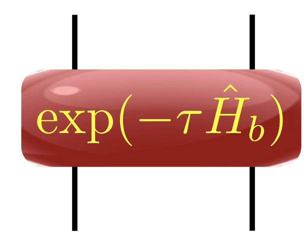
- Evolve in imaginary time: $\hat{\rho}(\beta) = e^{-\beta \hat{H}/2} \hat{\rho}(0) e^{-\beta \hat{H}/2}$

Trotter-Suzuki decomposition:

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

$\tau = \beta / n$





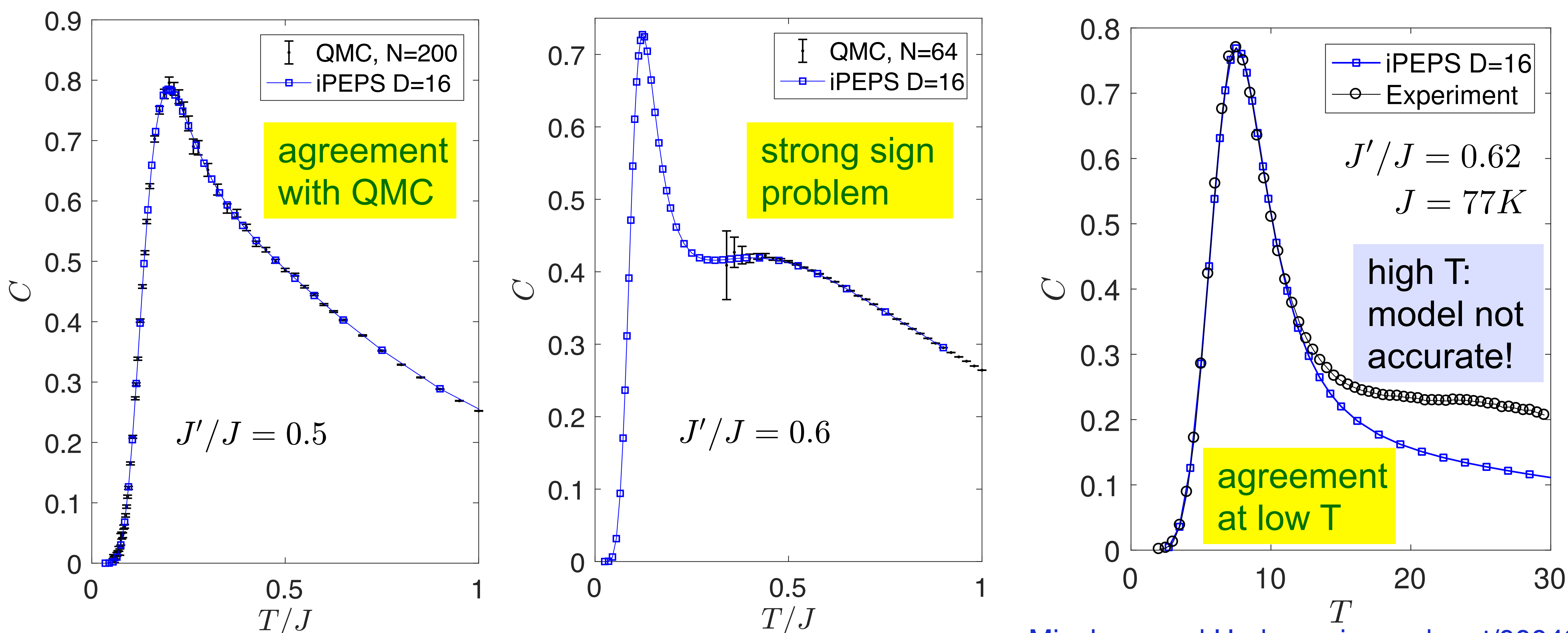
- Truncate after each step (using simple update (SU) or full update (FU))

- Evolve up to target $\beta/2$

Finite temperature simulations with iPEPS

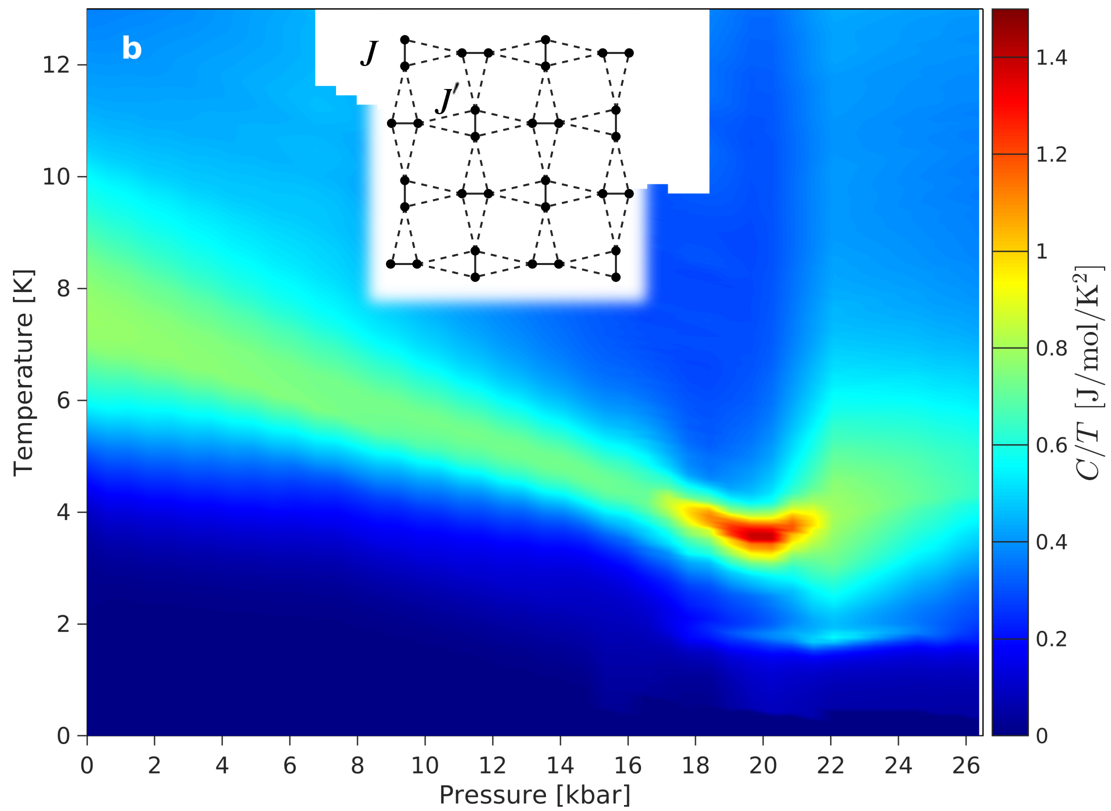
Wietek, PC, Wessel, Normand, Mila, and Honecker, PRR 1 (2019)

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

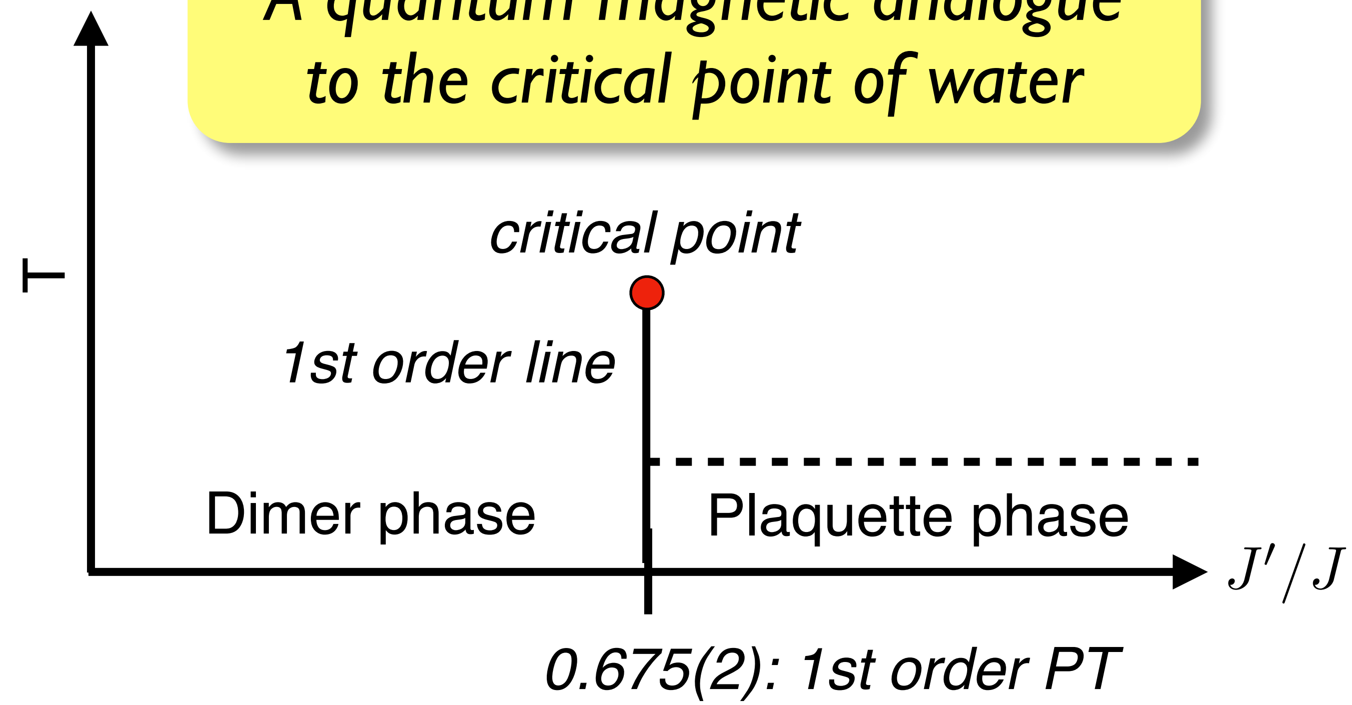


Miyahara and Ueda, arxiv:cond-mat/0004260

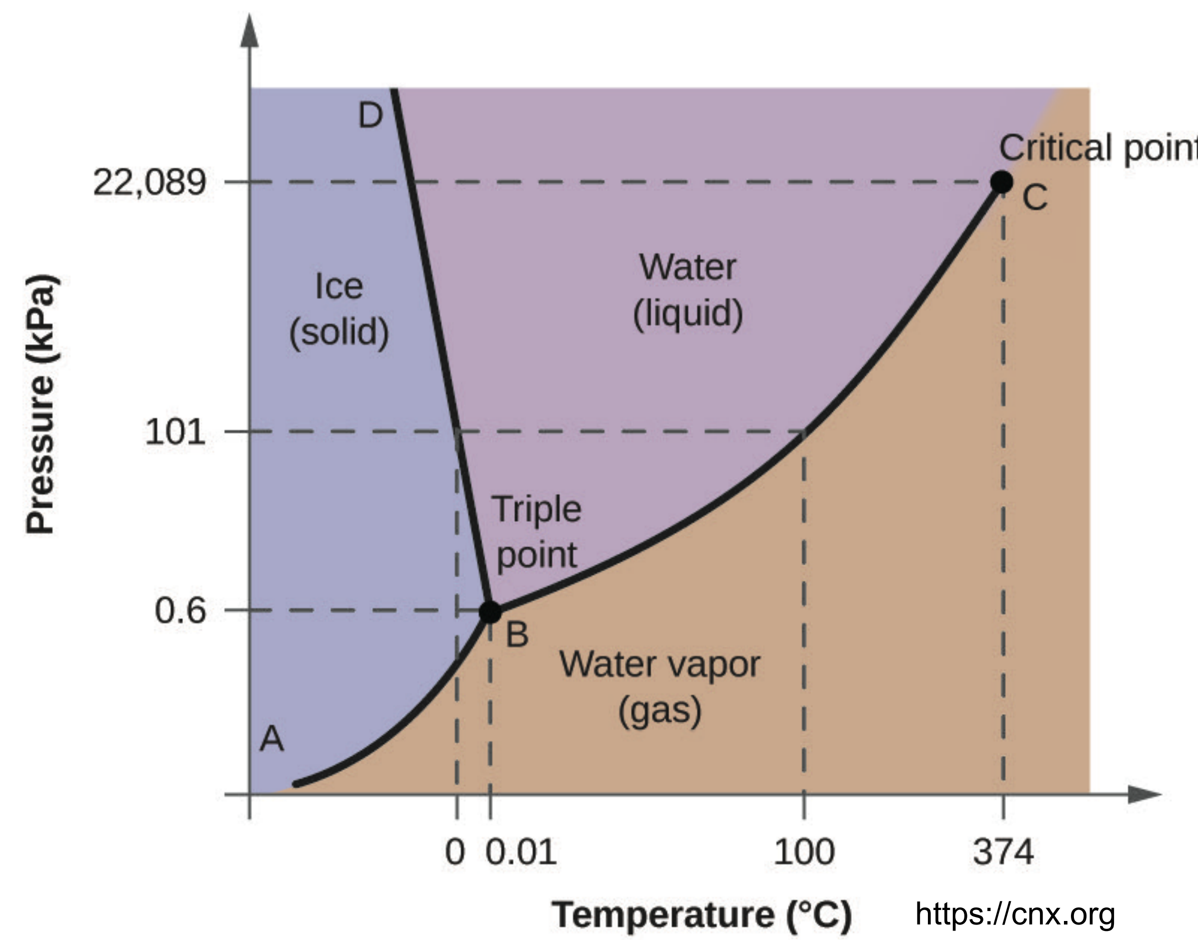
Specific heat data (group of H. M. Rønnow)



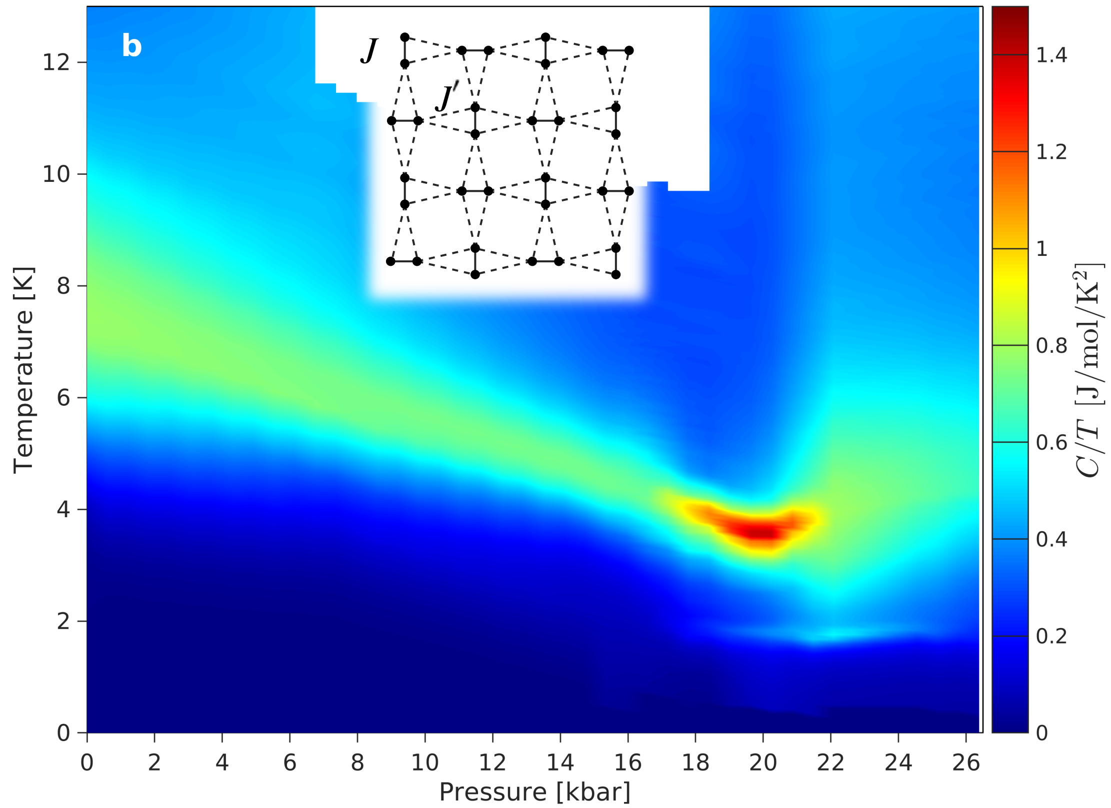
A quantum magnetic analogue to the critical point of water

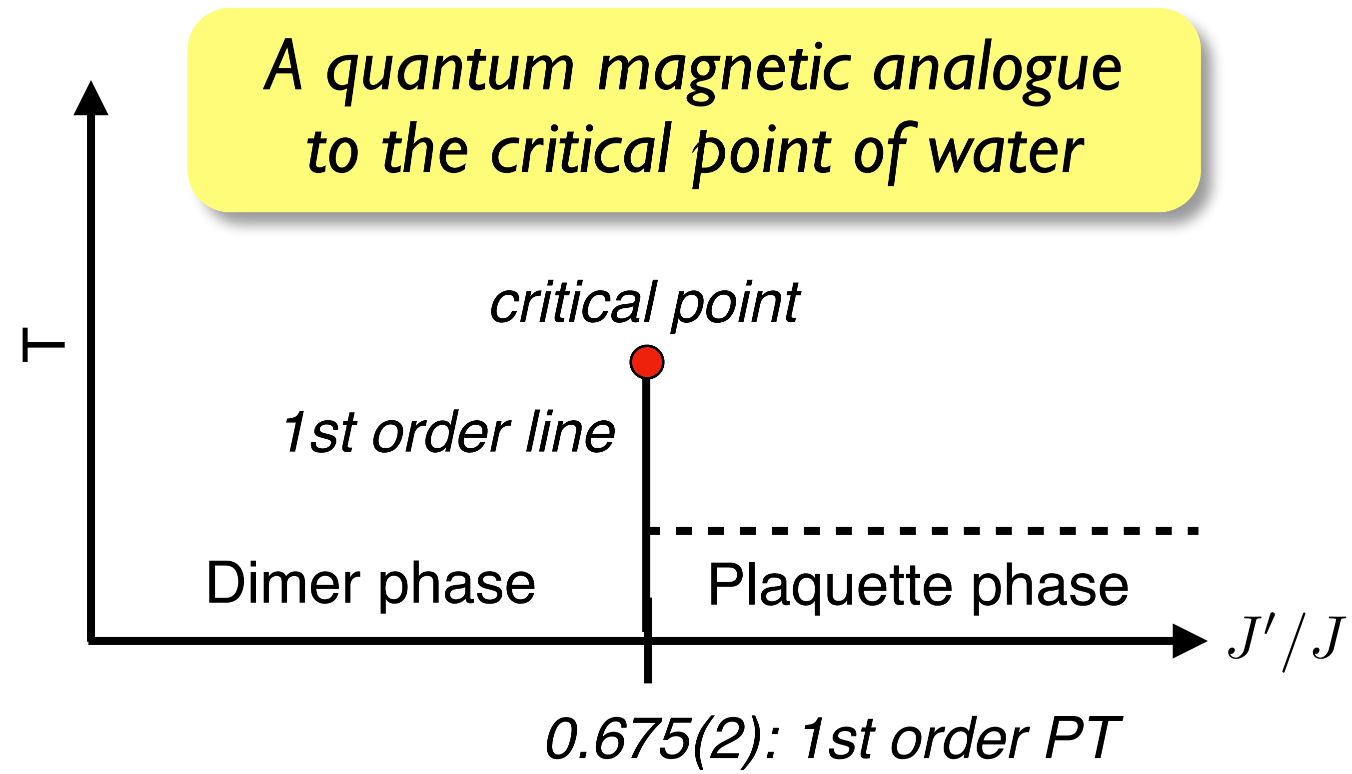


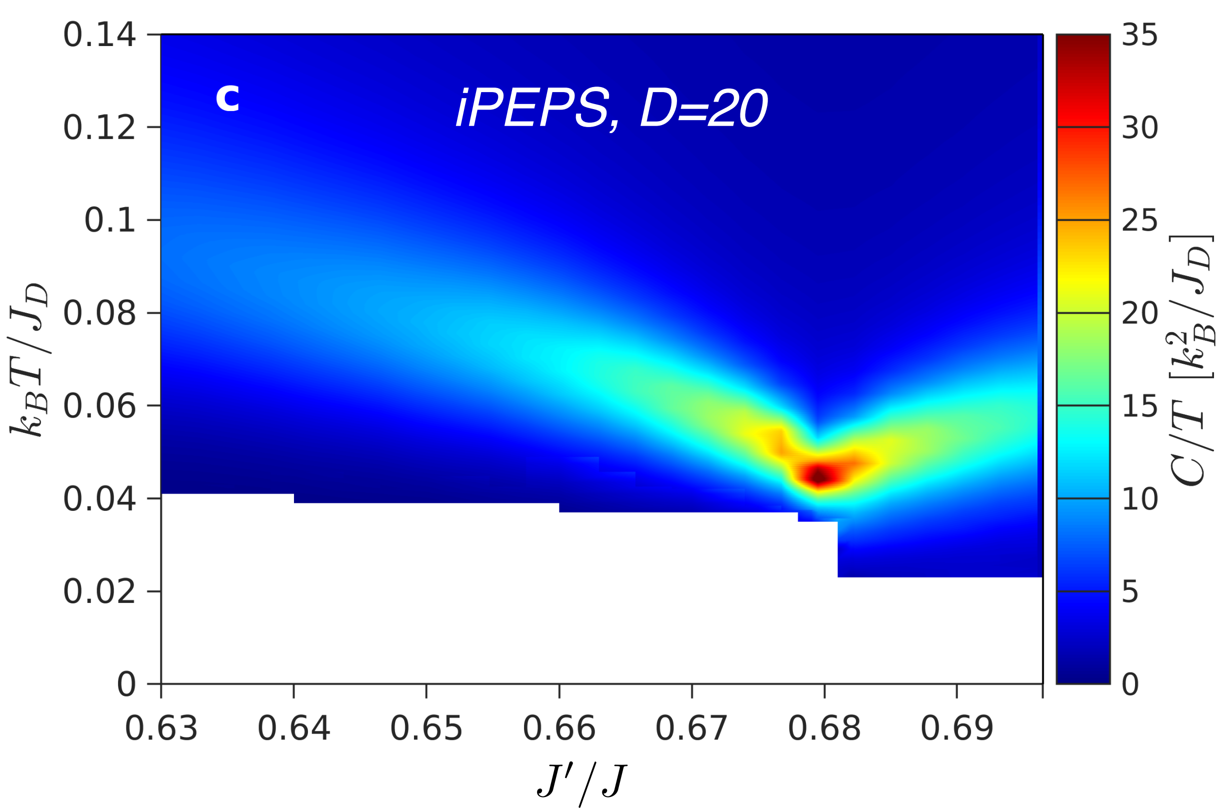
Can we reproduce this with iPEPS?

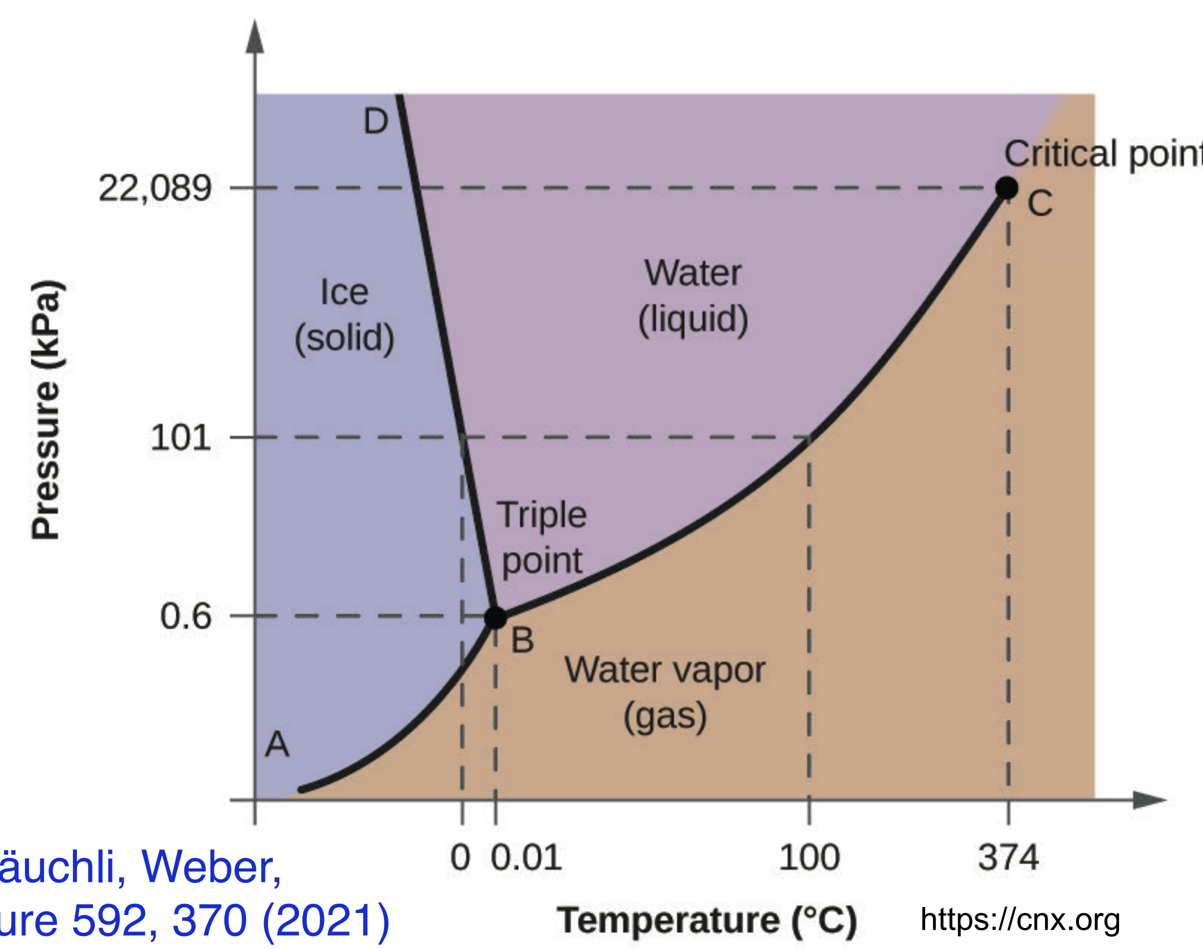


Specific heat data (group of H. M. Rønnow)



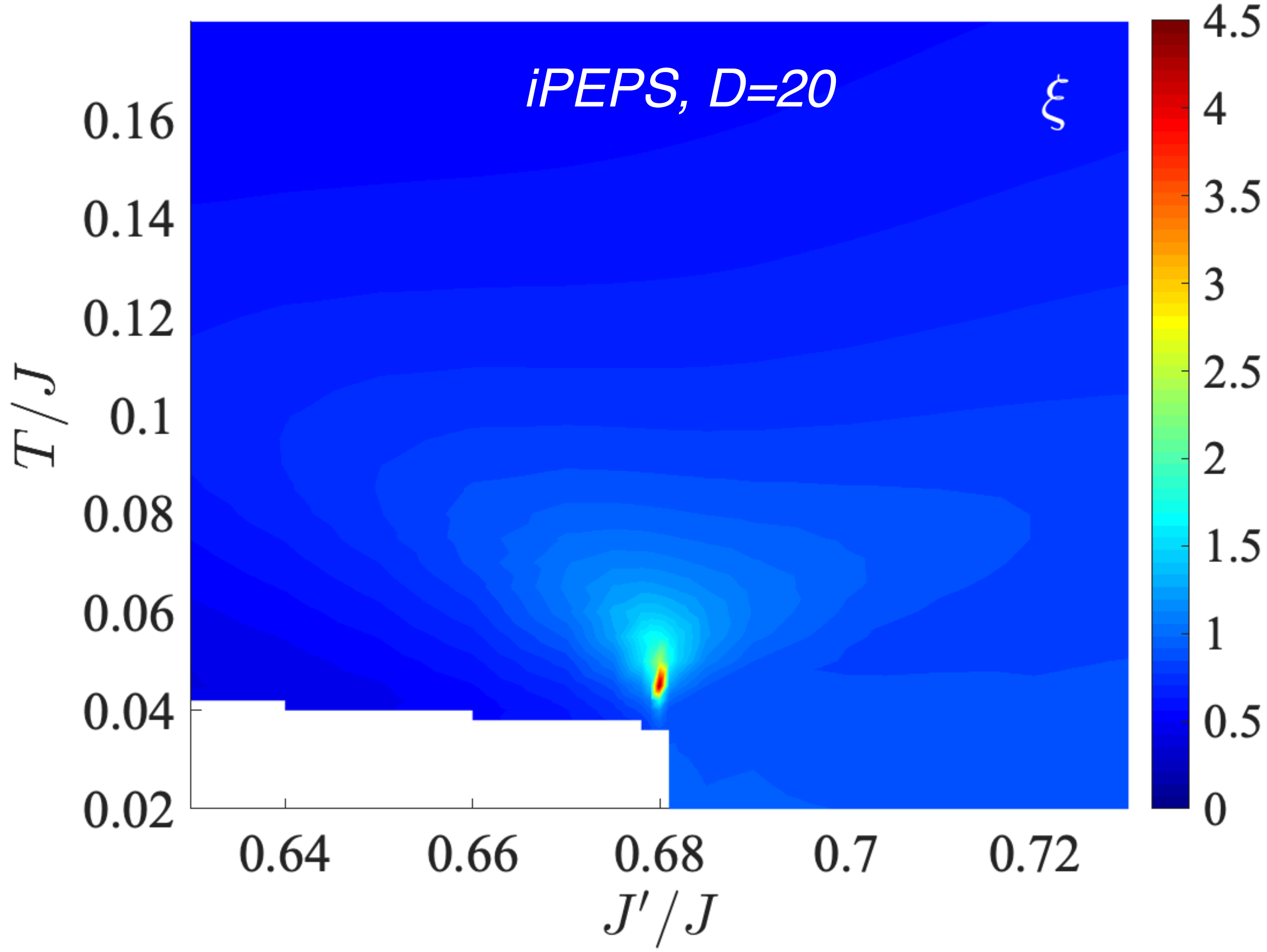




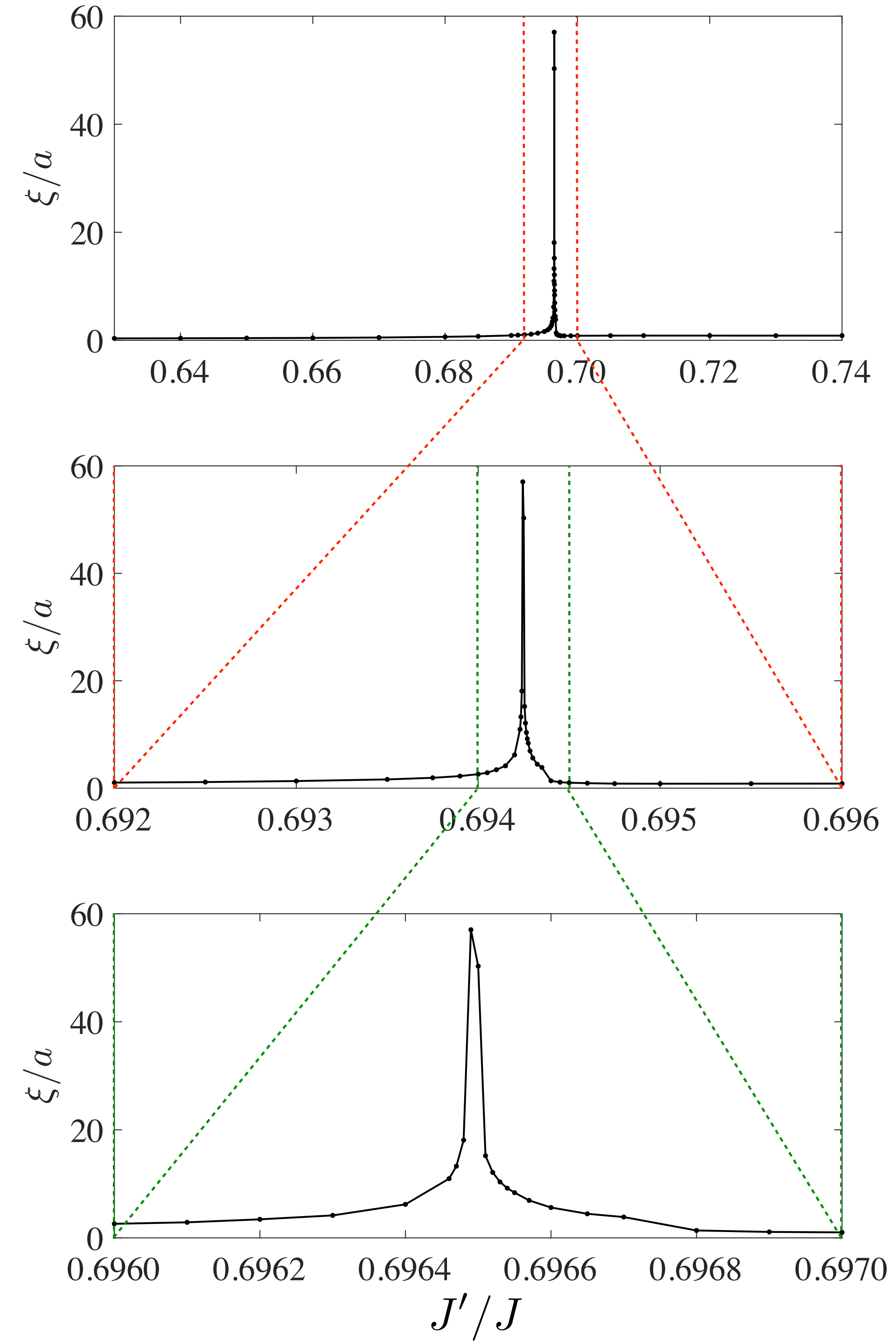


Jiménez, Crone, Fogh, Zayed, Lortz, Pomjakushina, Conder, Läuchli, Weber, Wessel, Honecker, Normand, Rüegg, PC, Rønnow & Mila, Nature 592, 370 (2021)

Correlation length



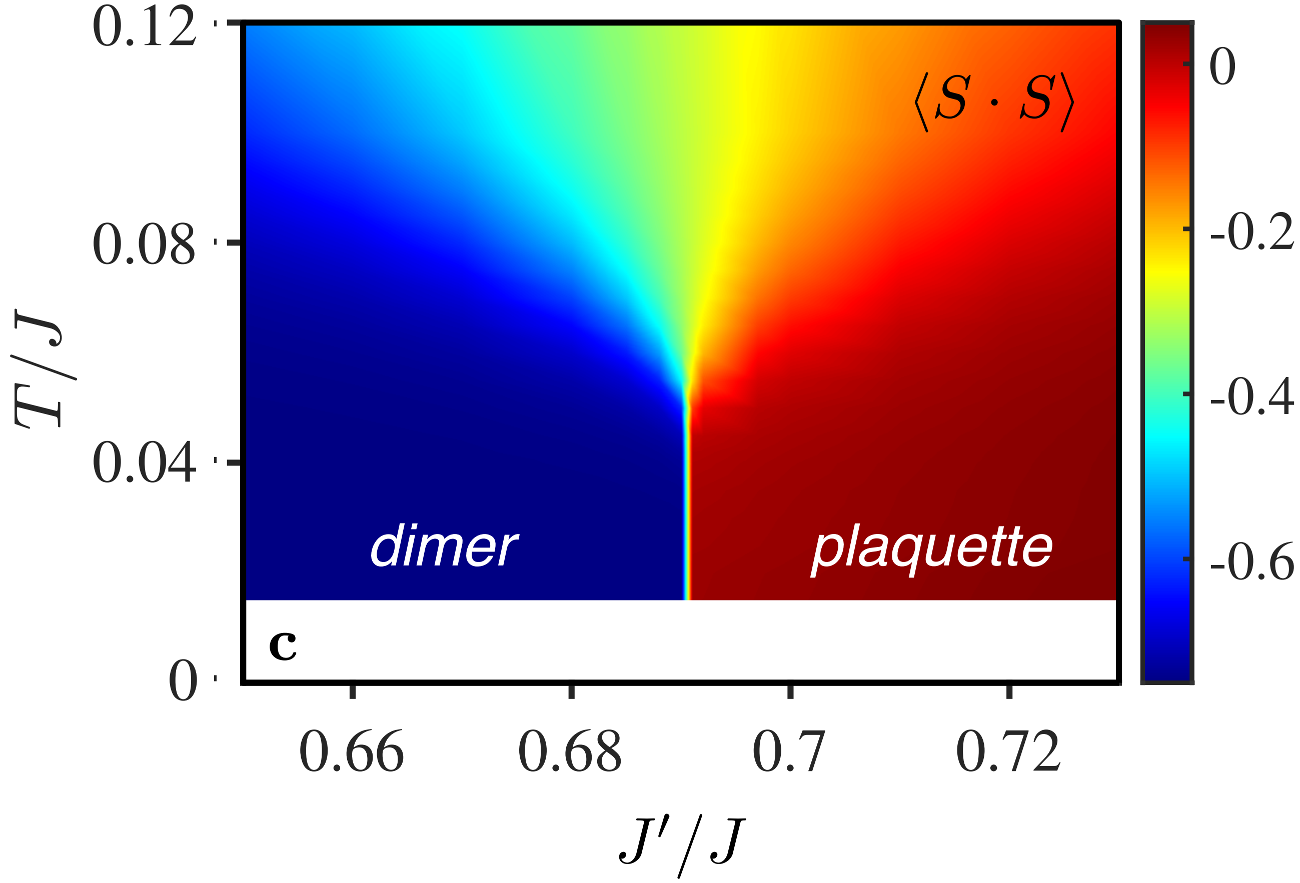
Zooming-in (D=8)



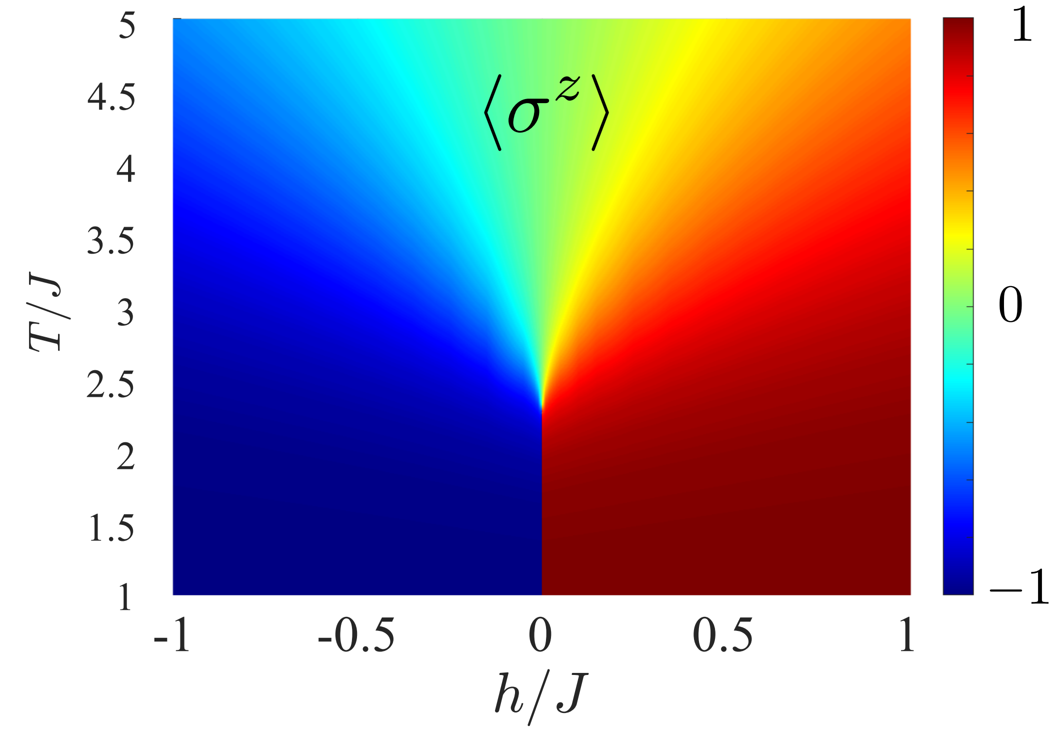
Diverging correlation length compatible with a critical point

Jump in <S · S> on dimer

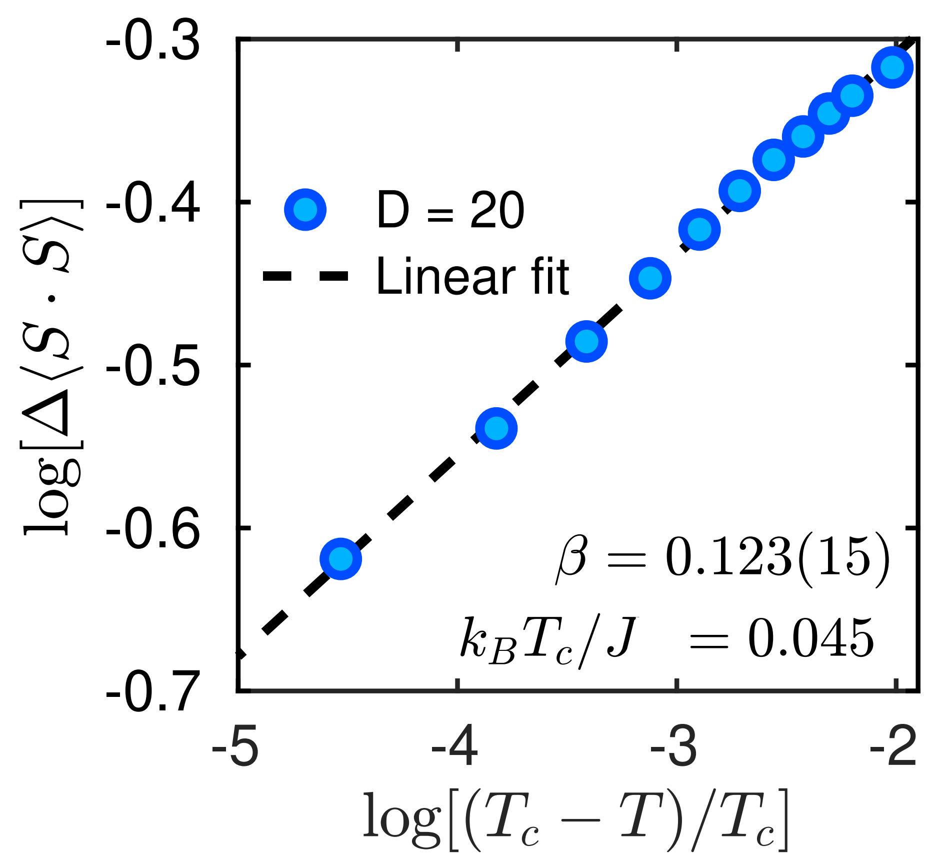
iPEPS D=10 (with DM)



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

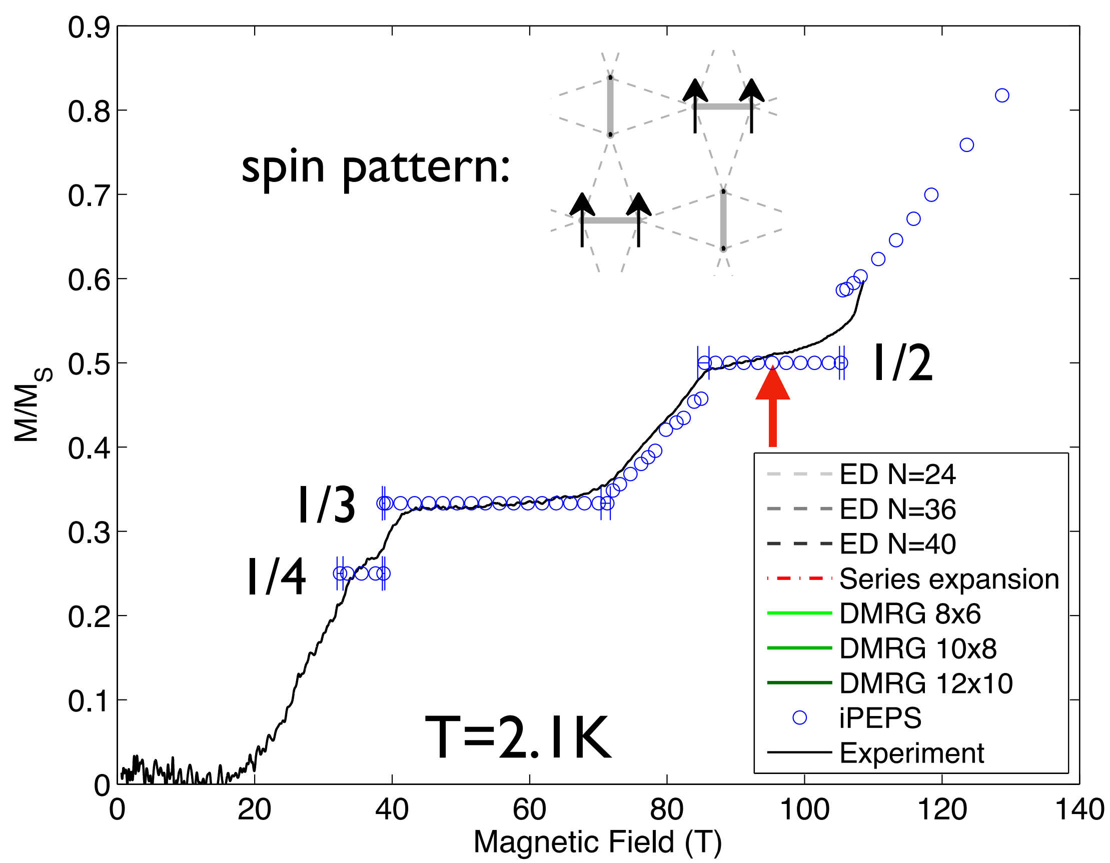


exact value:
$\beta = 0.125$

Finite T iPEPS study of the m=1/2 plateau in SCBO

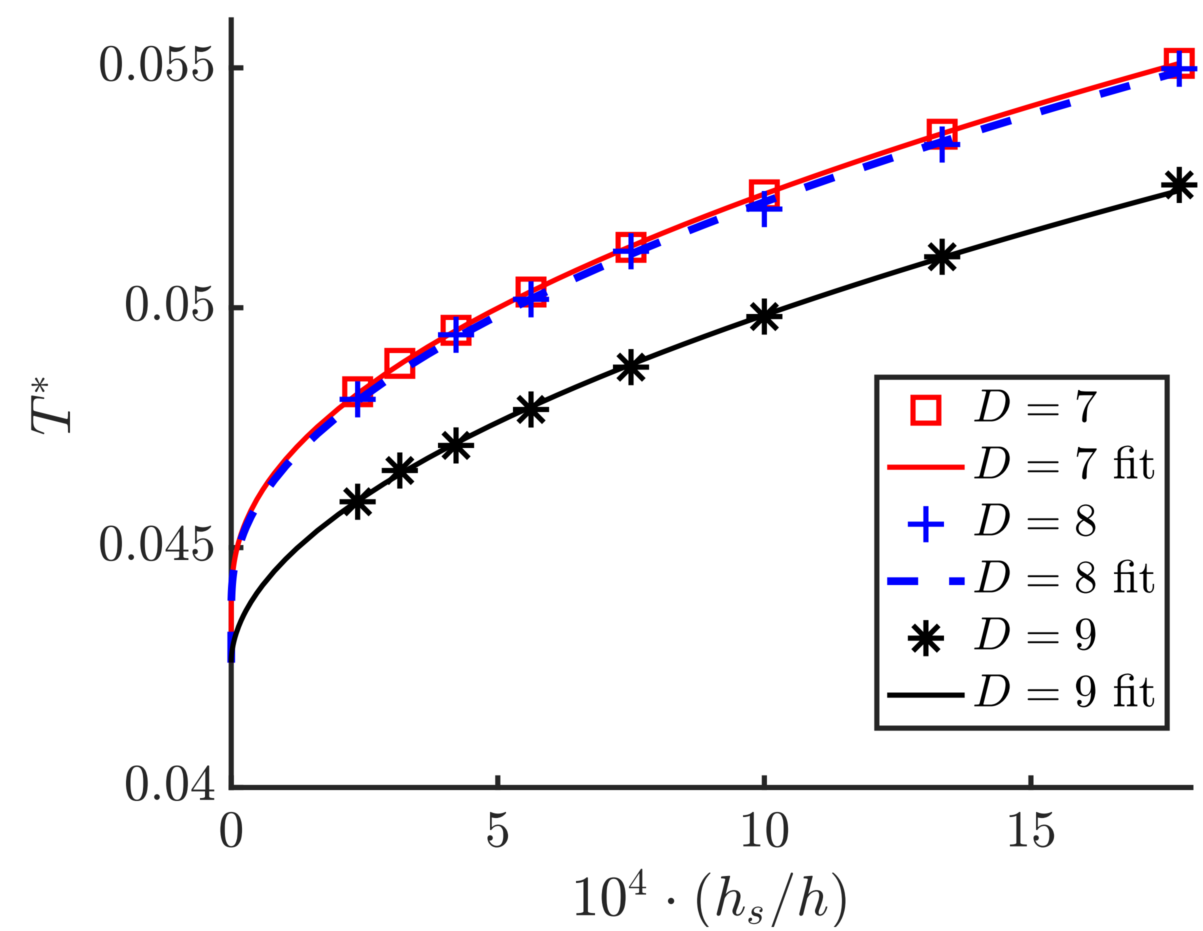
P. Czarnik, M. M. Rams, PC, and J. Dziarmaga, PRB 103, 075113 (2021)

High-field magnetization data



Matsuda et al. PRL 111 (2013)

Systematic scaling analysis



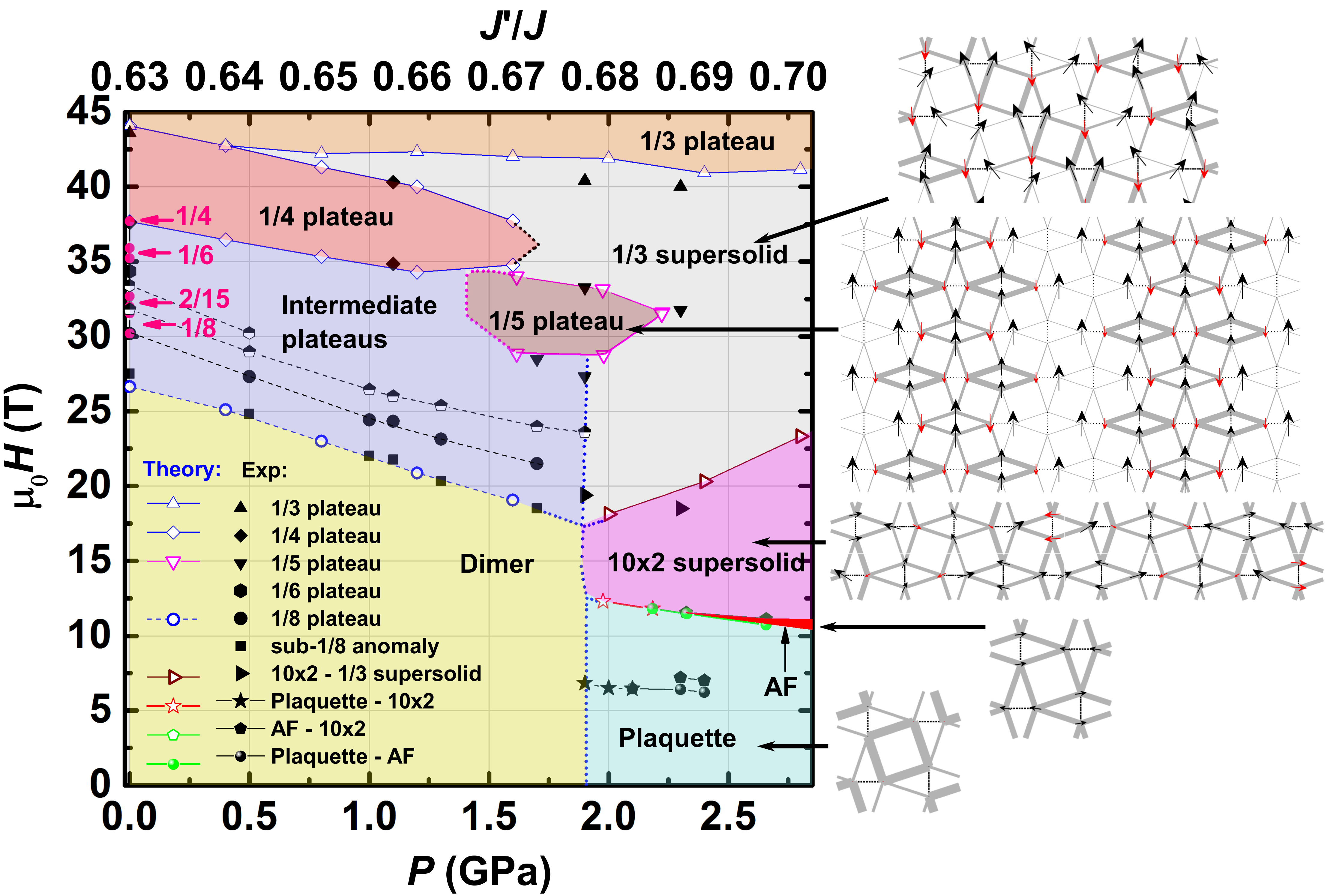
$$T^*(h_s, \xi_D) = T_c + a h_s^{1/\tilde{\beta}\delta} + \frac{b}{\xi_D^c} h_s^{(1-c\nu)/\tilde{\beta}\delta}$$

Critical exponents compatible with 2D Ising universality class

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

$SrCu_2(BO_3)_2$ under pressure in a magnetic field

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

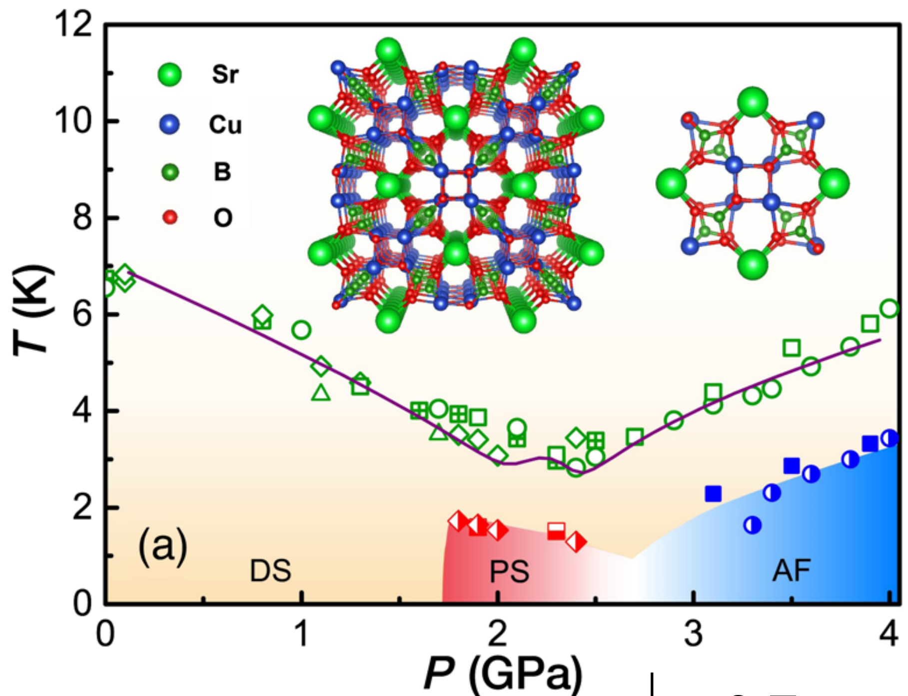


new 1/5 plateau

new supersolid

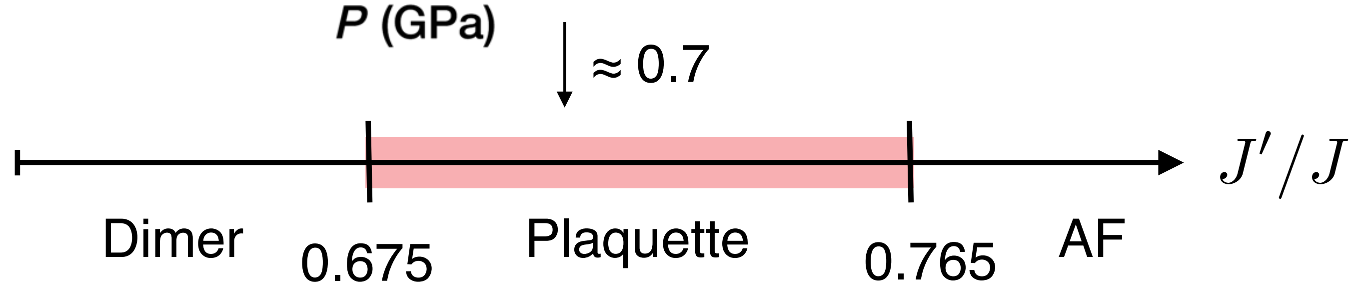
Limitations of the Shastry-Sutherland model

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

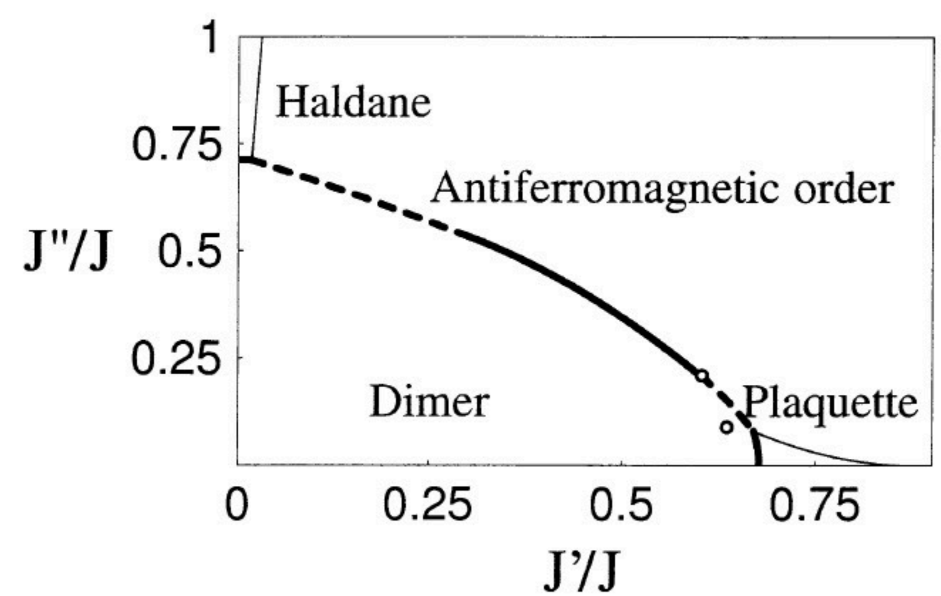


Guo, et al (2020)

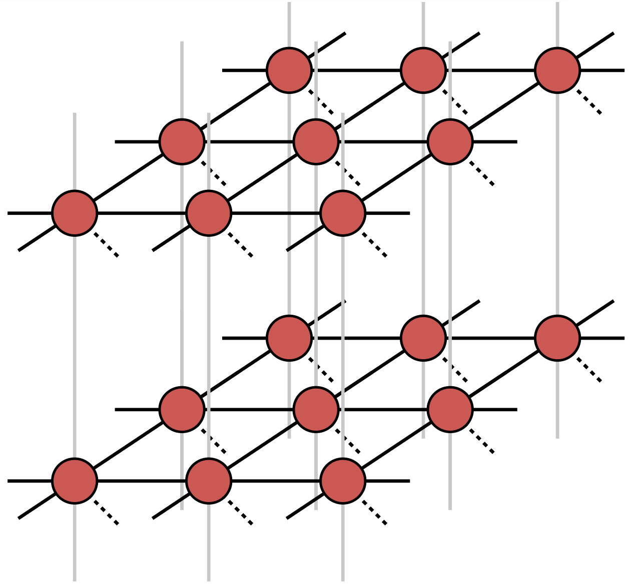
How about iPEPS in 3D?



- Series expansion results Koga, JPSJ 69 (2000)
  - ✦ A interlayer coupling reduces the extent of the plaquette phase



Tensor networks for 3D quantum systems

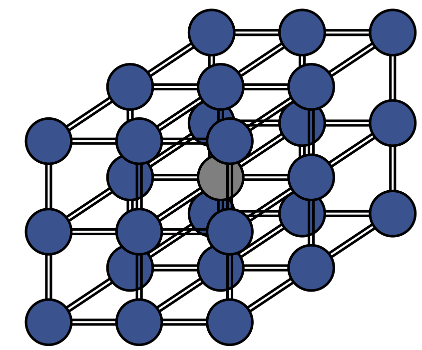


- **Main challenge: how to contract it??**
- Several works in the context of 3D classical or 2+1D:
  - ✦ **3D HOTRG:**
    Xie, Chen, Qin, Zhu, Yang, Xiang, PRB 86, 045139 (2012)
  - ✦ **Corner-transfer matrix (CTM) in 3D:**
    Nishino and Okunishi, J. Phys. Soc. Jpn. 67, 3066 (1998)
    Orús, Phys. Rev. B 85, 205117 (2012)
  - ✦ **Approaches based on a boundary iPEPS:**
    Nishino, Okunishi, Hieida, Maeshima, and Akutsu, Nucl. Phys. B 575, 504 (2000)
    Nishino, Hieida, Okunishi, Maeshima, Akutsu, Gendiar, Prog. Theor. Phys. 105 (2001)
    Gendiar, Nishino, Phys. Rev. E 65, 046702 (2002)
    Gendiar, Maeshima, and Nishino, Prog. Theor. Phys. 110, 691 (2003)
    Gendiar and Nishino, Phys. Rev. B 71, 024404 (2005)
    Vanderstraeten, Vanhecke, and Verstraete, Phys. Rev. E 98, 042145 (2018)
  - ✦ **Other approaches:**
    Ran, Piga, Peng, Su, and Lewenstein, Phys. Rev. B 96, 155120 (2017)
    Jahromi and Orús, Phys. Rev. B 99, 195105 (2019); Sci. Rep. 10, 19051 (2020)
    Tepaske and Luitz, arXiv:2005.13592
    Magnifico, Felser, Silvi, and Montangero, arXiv:2011.10658

Overview

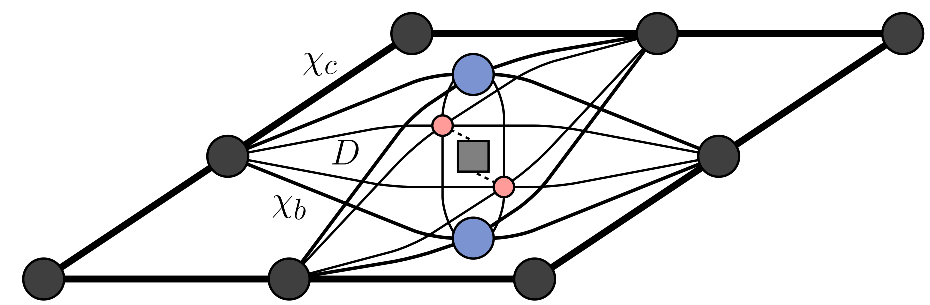
Vlaar & PC, PRB 103, 205137 (2021); arxiv:2208.06423

- **Cluster contractions:**
  - ✦ Contract finite clusters instead of full network
  - ✦ cheap & simple
  - ✦ Not very accurate, but useful for quick results

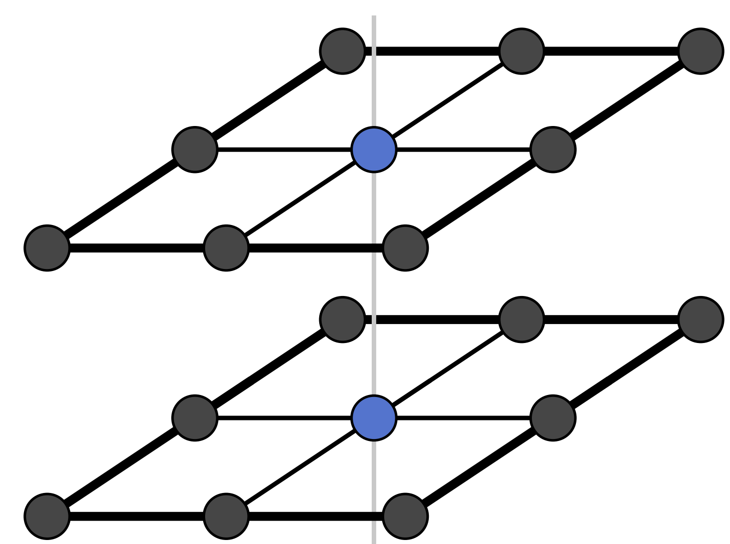


Patrick Vlaar

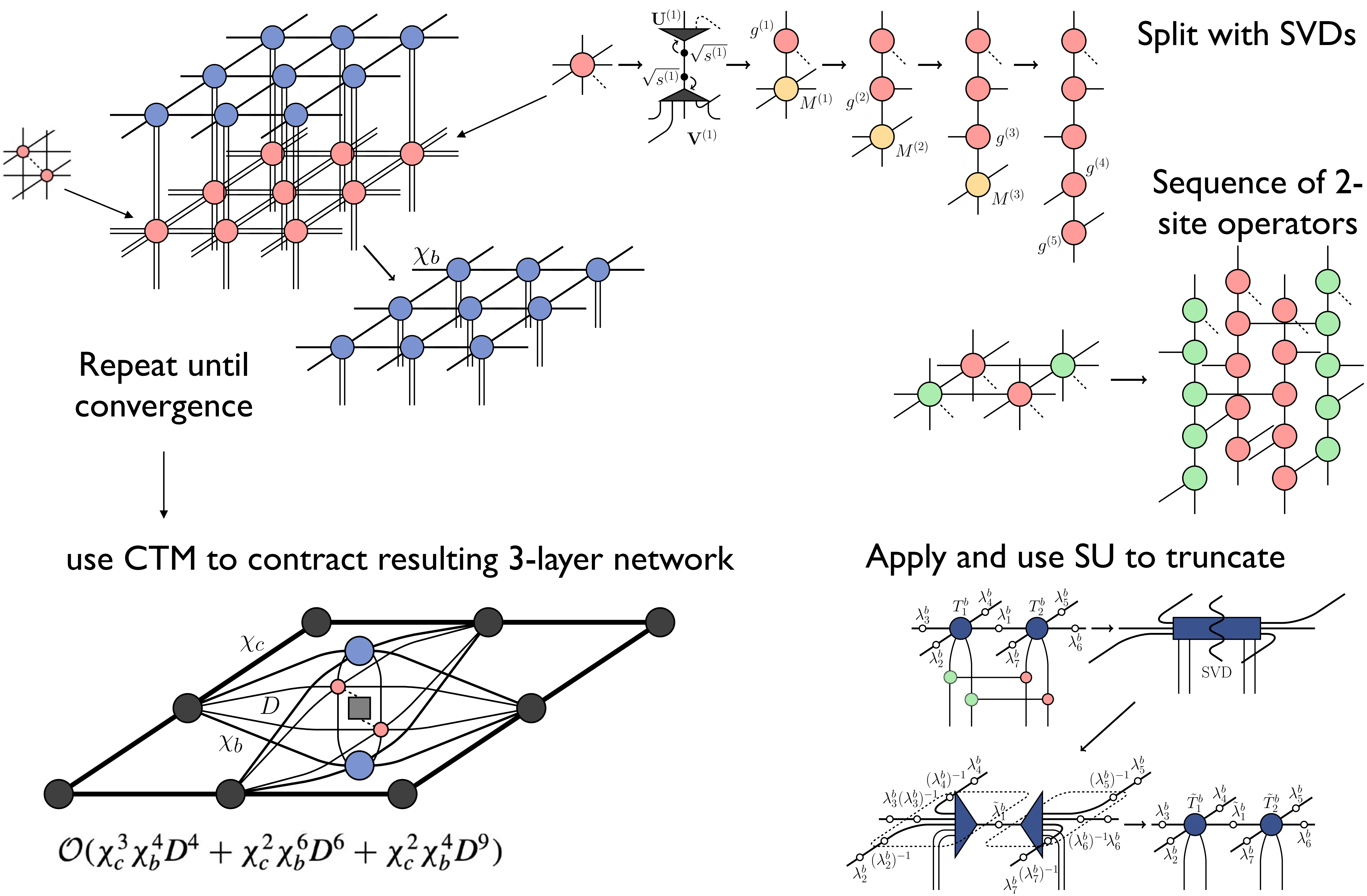
- **Full 3D contraction: the SU + CTM approach**
  - ✦ Boundary iPEPS approach
  - ✦ Combination of simple update (SU) truncation + CTM method
  - ✦ Good accuracy & convergence & tractable cost



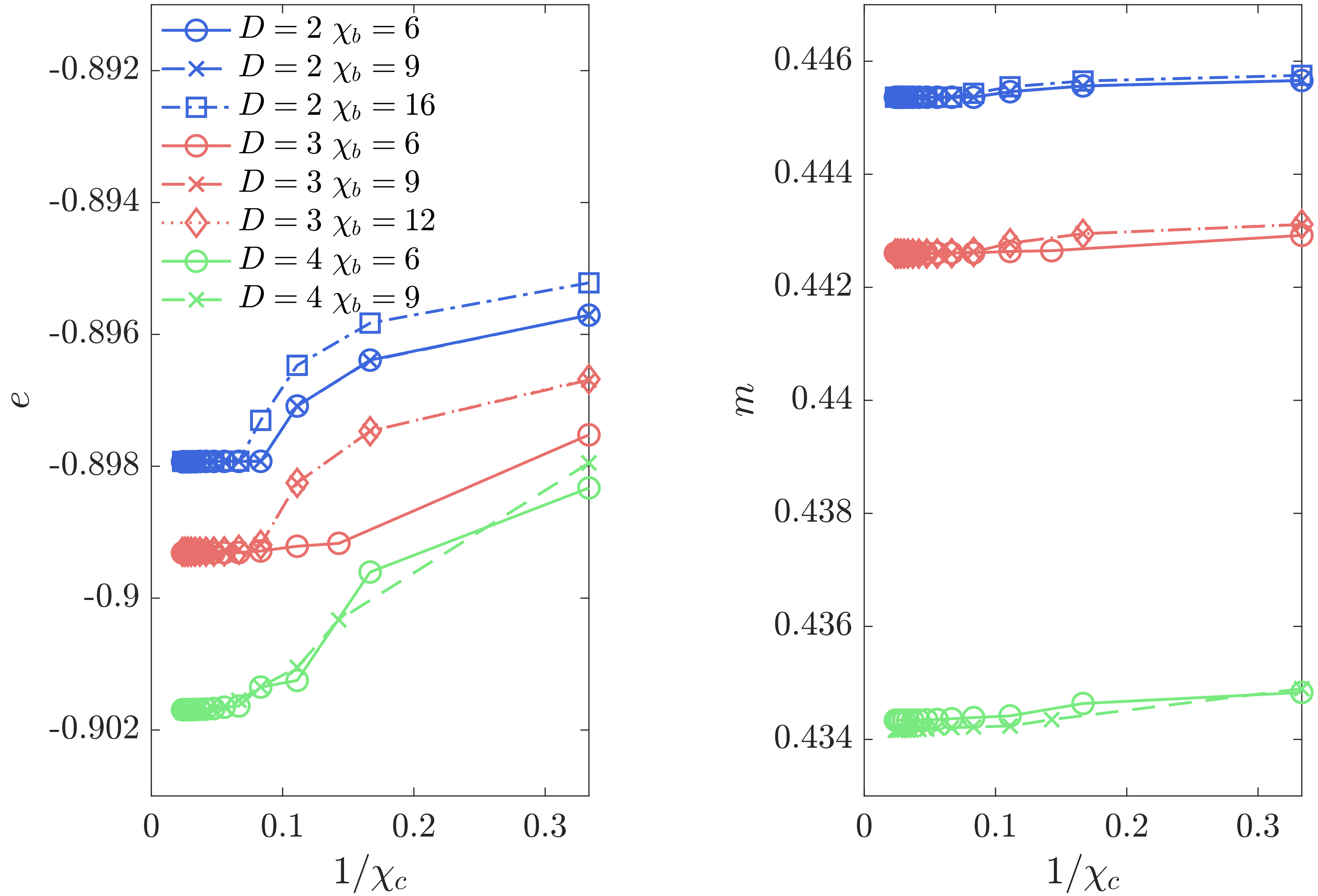
- **Contraction of layered systems: LCTM**
  - ✦ Decouple layers away from the center → use CTM to contract 2D layers
  - ✦ Good accuracy for anisotropic systems
  - ✦ Lower cost than full 3D algorithm



Full 3D contraction: SU + CTM approach

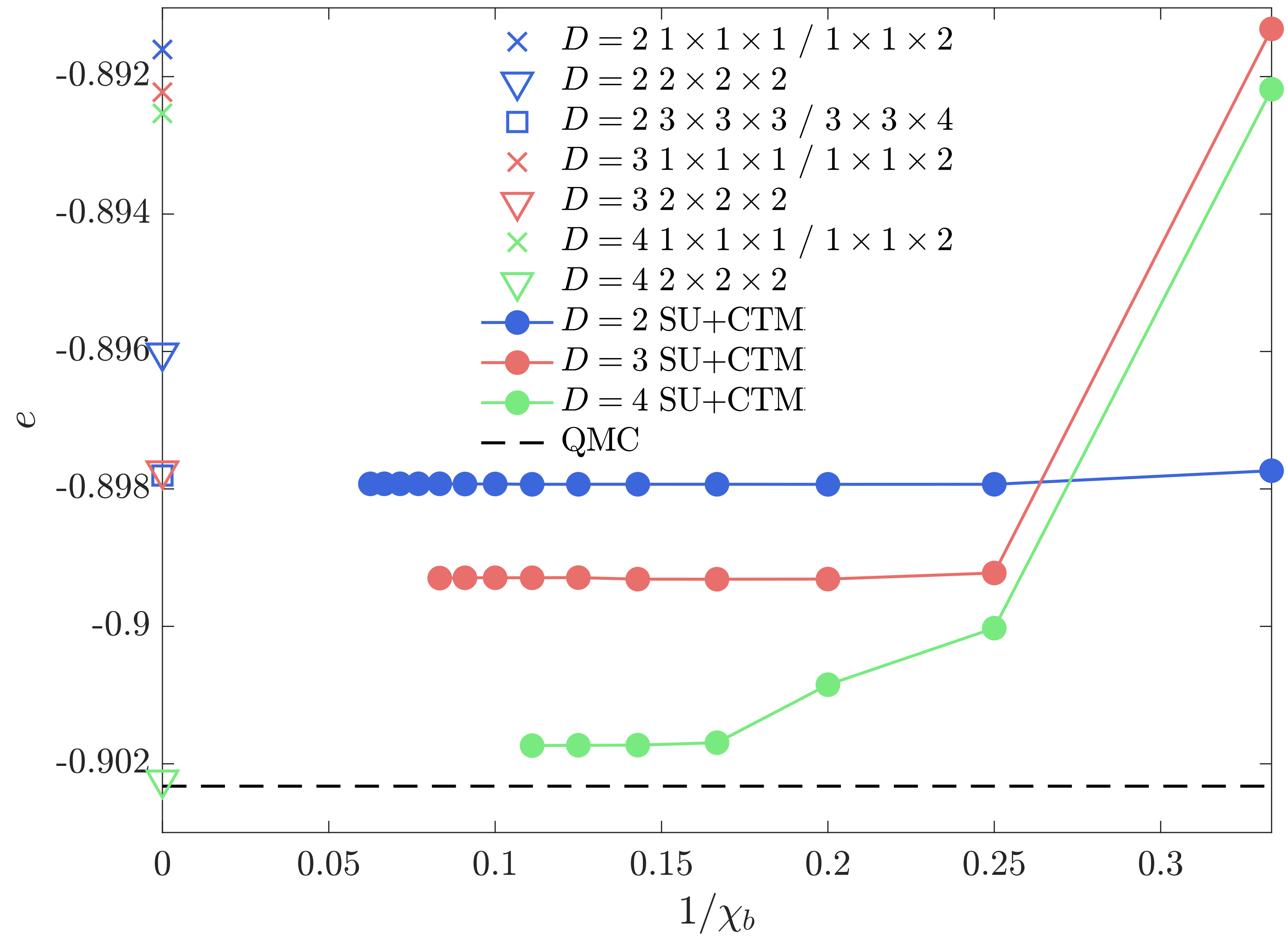


Convergence in χc (3D Heisenberg model)



★ Systematic convergence in χc

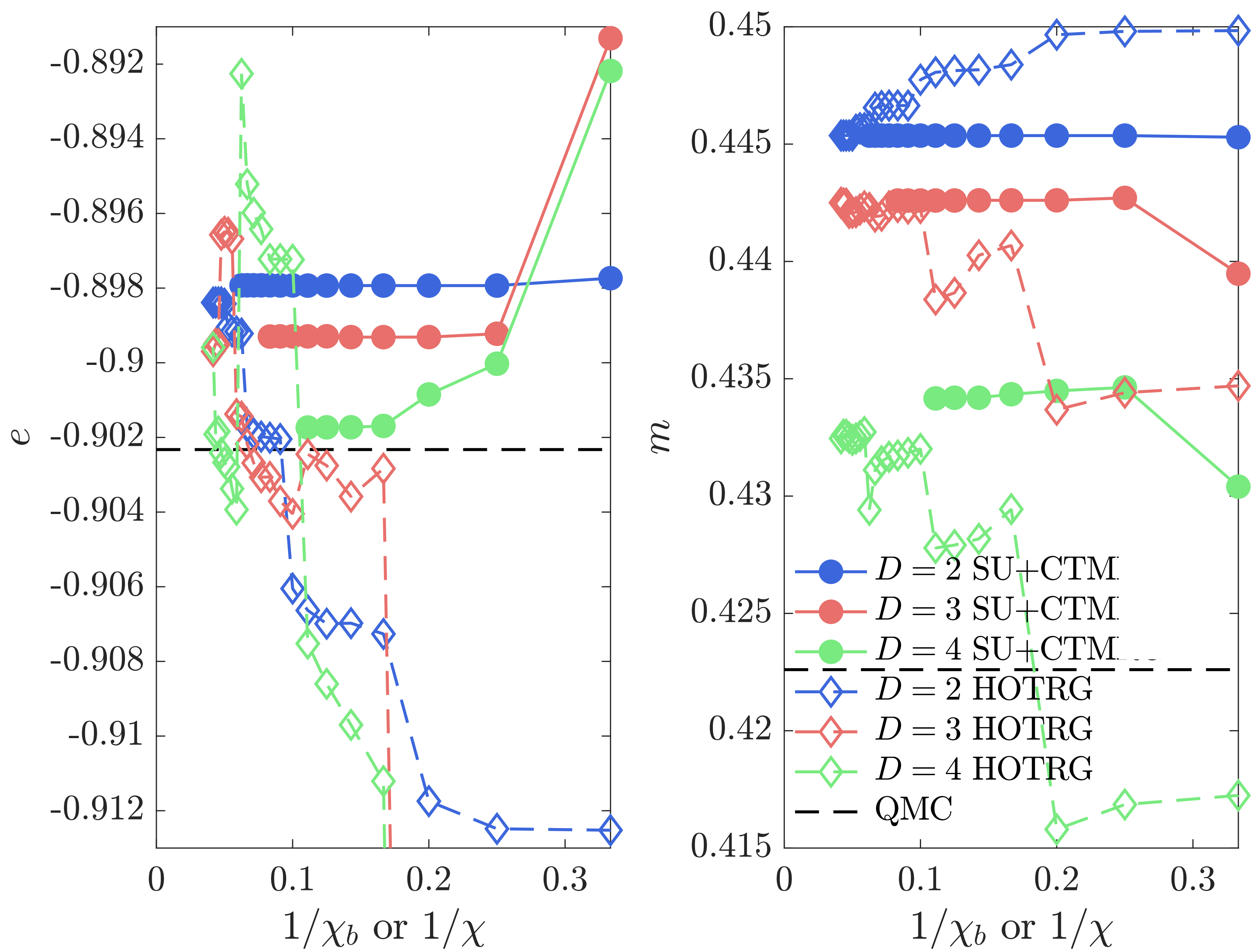
Convergence in χ_b (3D Heisenberg model)



- ★ Systematic convergence in χ_b
- ★ Small clusters inaccurate
- ★ Good accuracy for 3x3x4
- ★ Rough estimate for 2x2x2

Comparison with HOTRG

Xie, Chen, Qin, Zhu, Yang, Xiang, PRB 86, 045139 (2012)

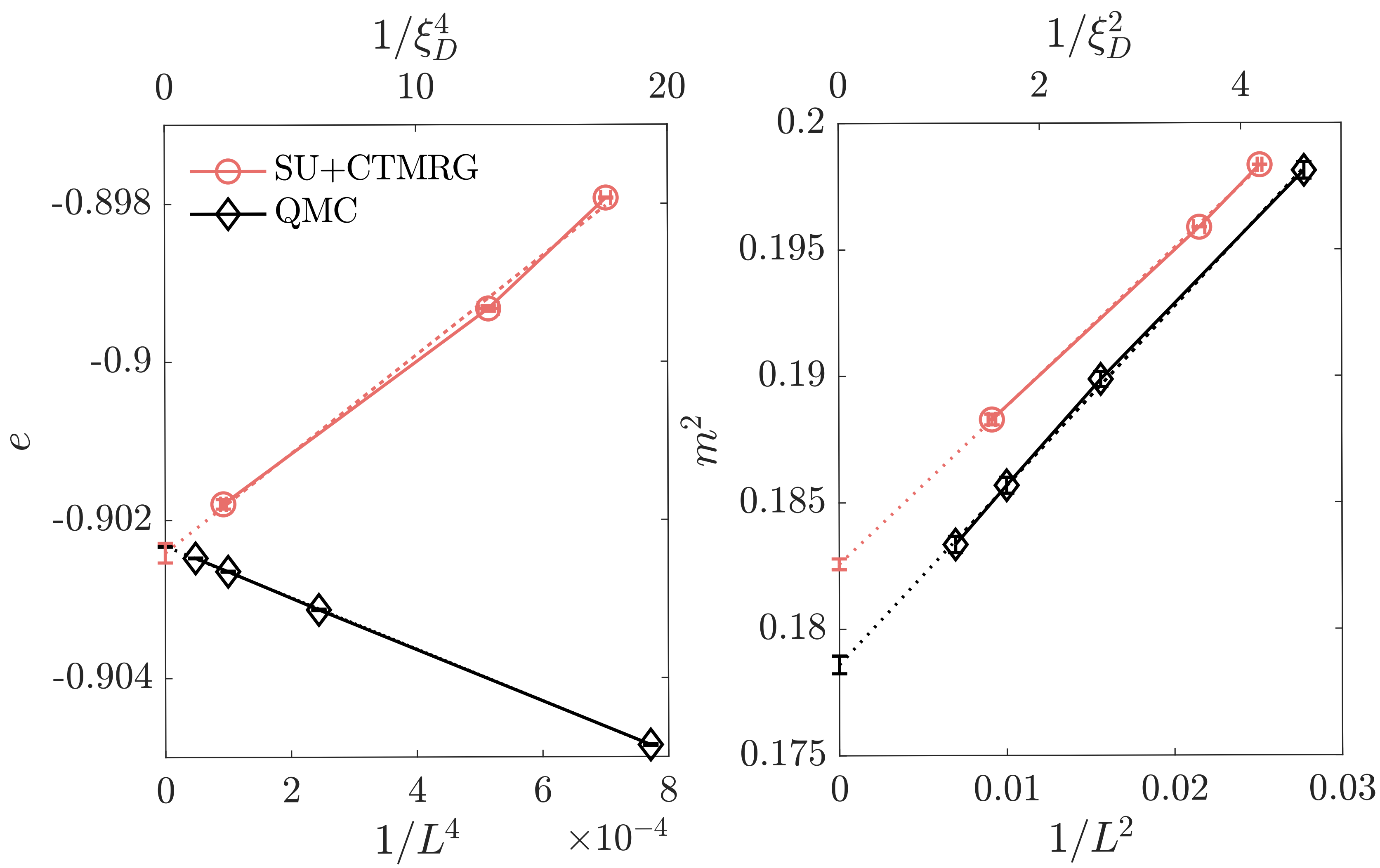


★ Very irregular convergence with HOTRG, in contrast to SU+CTM

3D Heisenberg model: finite correlation length scaling

- Idea: extrapolate in effective correlation length ξ_D

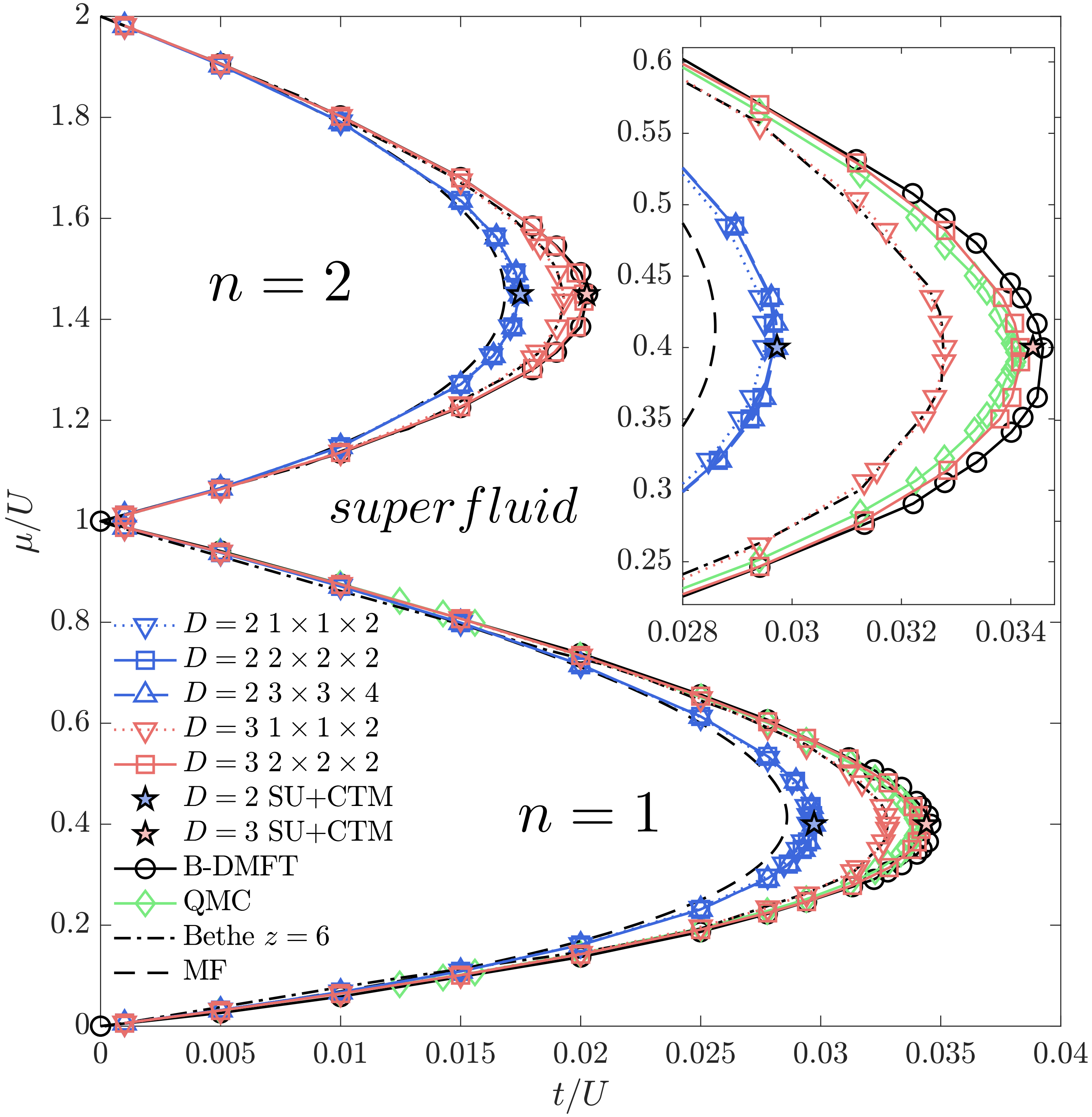
Tagliacozzo, et al (2008); Pollmann et al (2009); Pirvu et al (2012)
PC, Czarnik, Kapteijns & Tagliacozzo, PRX 8 (2018); Rader & Läuchli, PRX 8 (2018)



★ Energy in agreement
★ Magnetization 2% off (→ SU optimization)

3D Bose-Hubbard model

$$\hat{H} = -t \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i \hat{n}_i(\hat{n}_i - 1) - \mu \sum_i \hat{n}_i$$



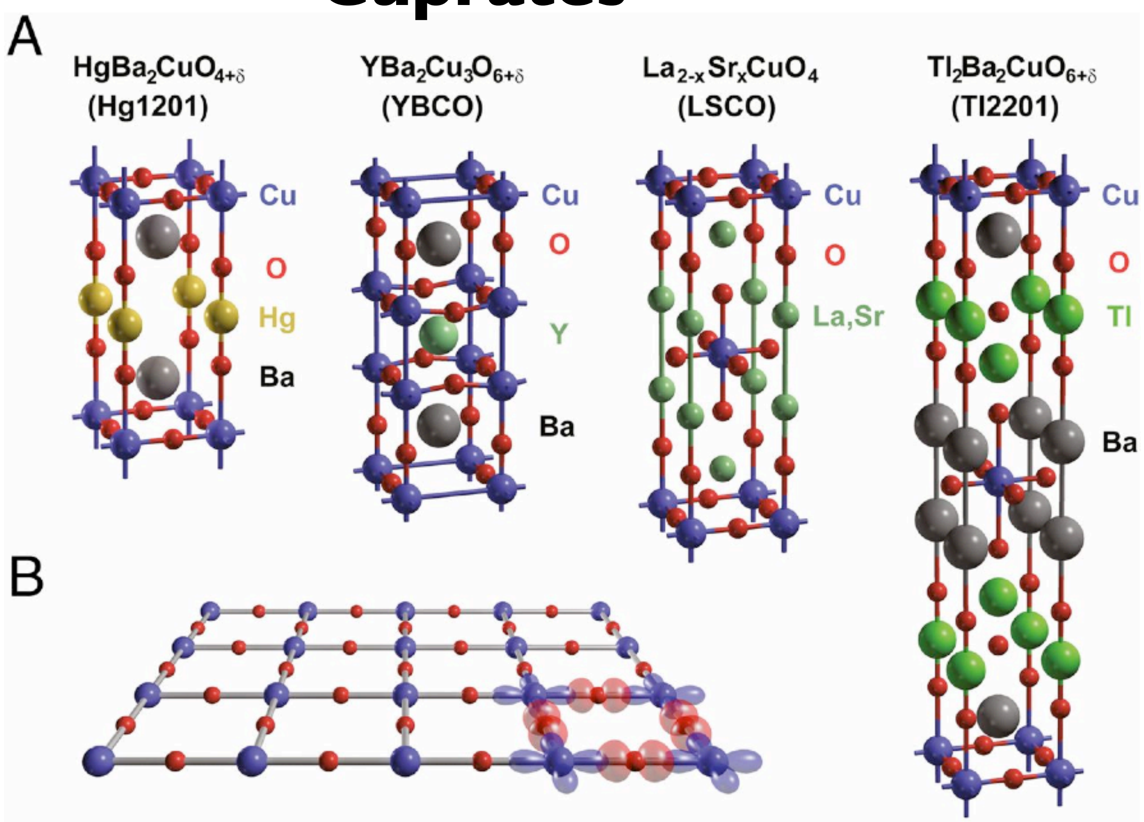
★ D=2: improvement over MF result

★ D=3: close to QMC result, better than B-DMFT

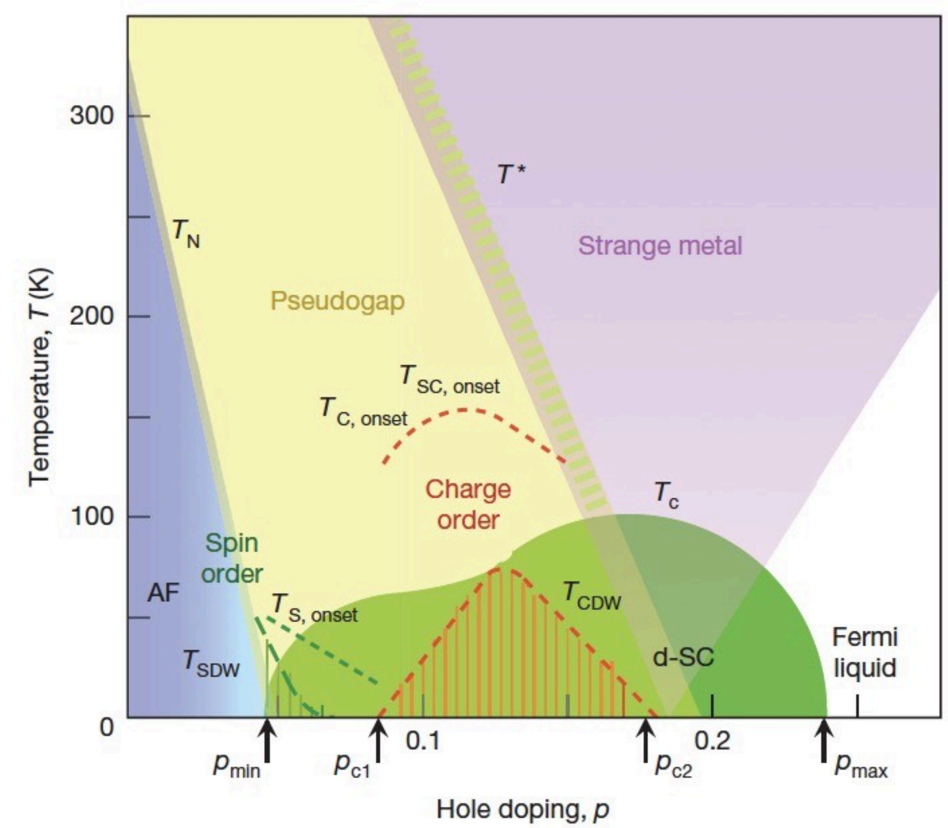
★ 2x2x2 close to SU+CTM → useful to get quick results

iPEPS for layered systems (anisotropic 3D)

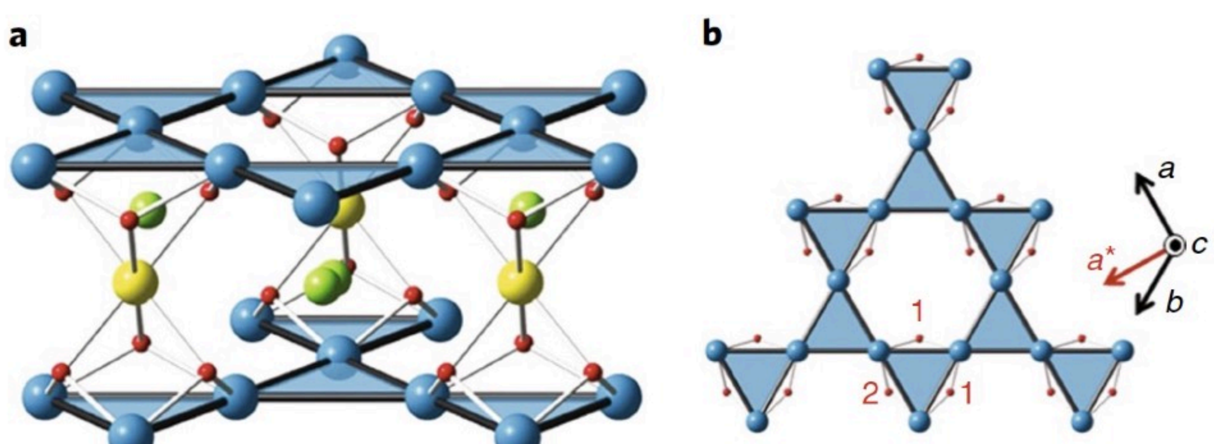
Cuprates



Barišić, et al., PNAS 110, 12235 (2013)

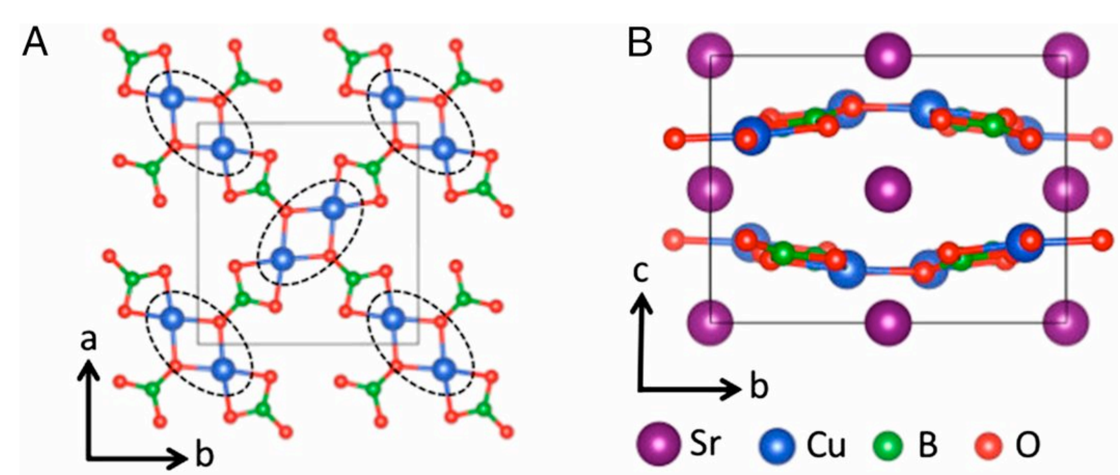


Herbertsmithite



Khuntia et al., Nature Physics 16, 469 (2020)

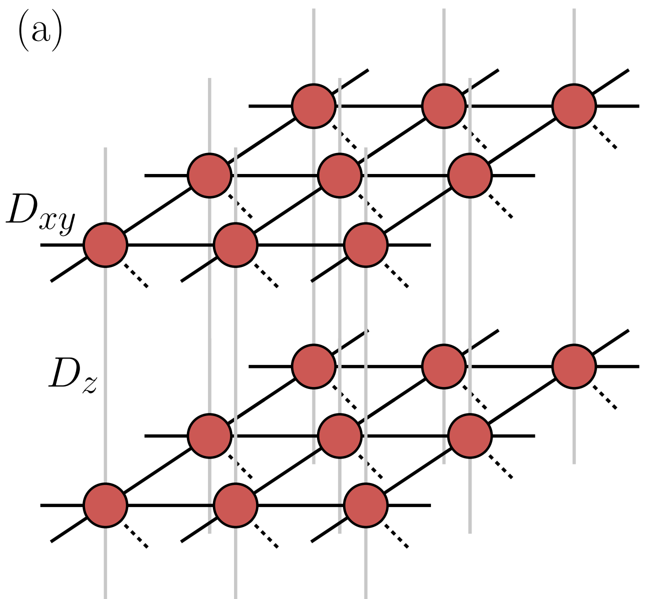
$SrCu_2(BO_3)_2$



Radtke et al., PNAS 112 (2015)

iPEPS for layered systems (anisotropic 3D)

Vlaar, PC, arxiv:2208.06423

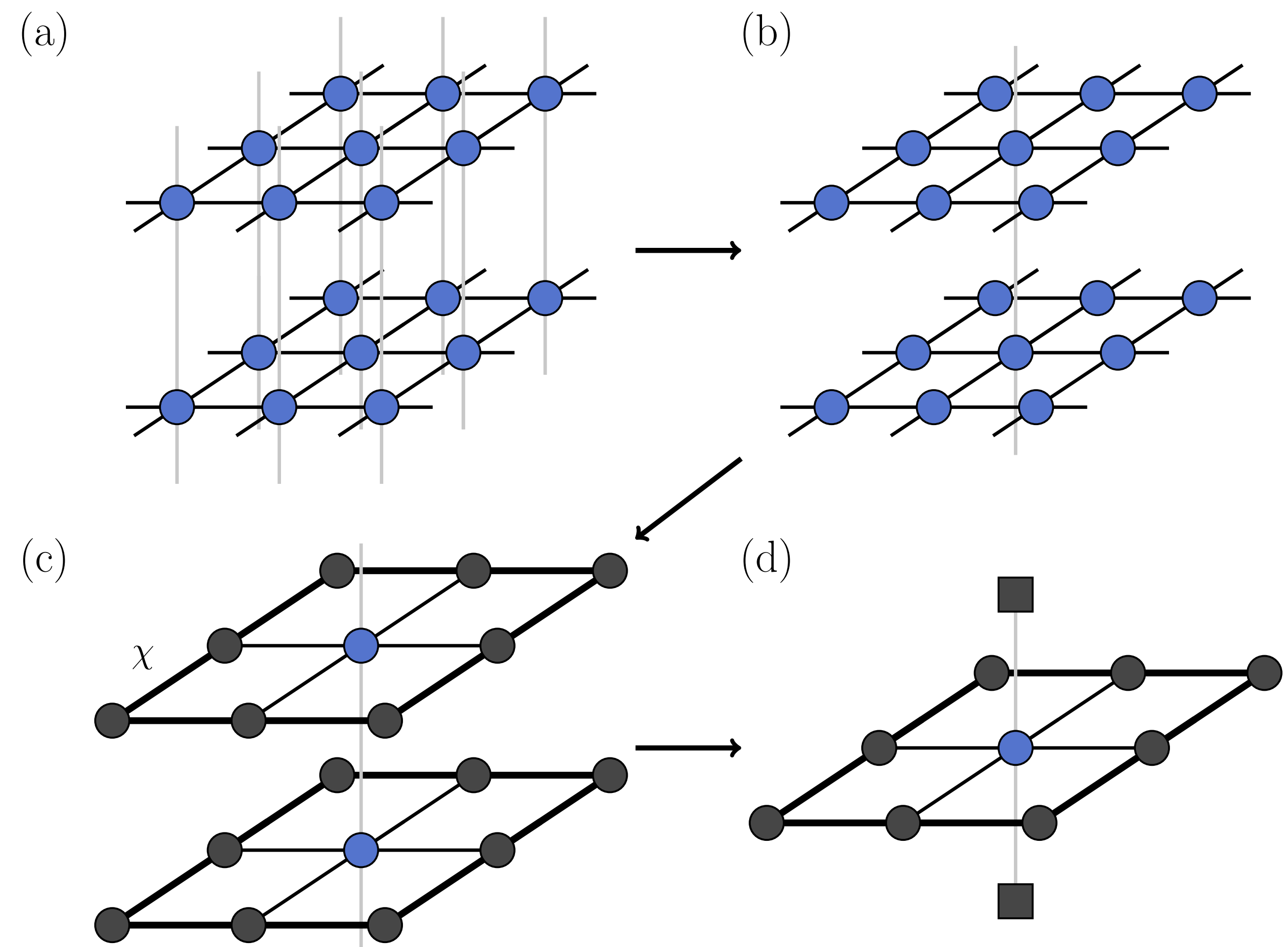


Ansatz:

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

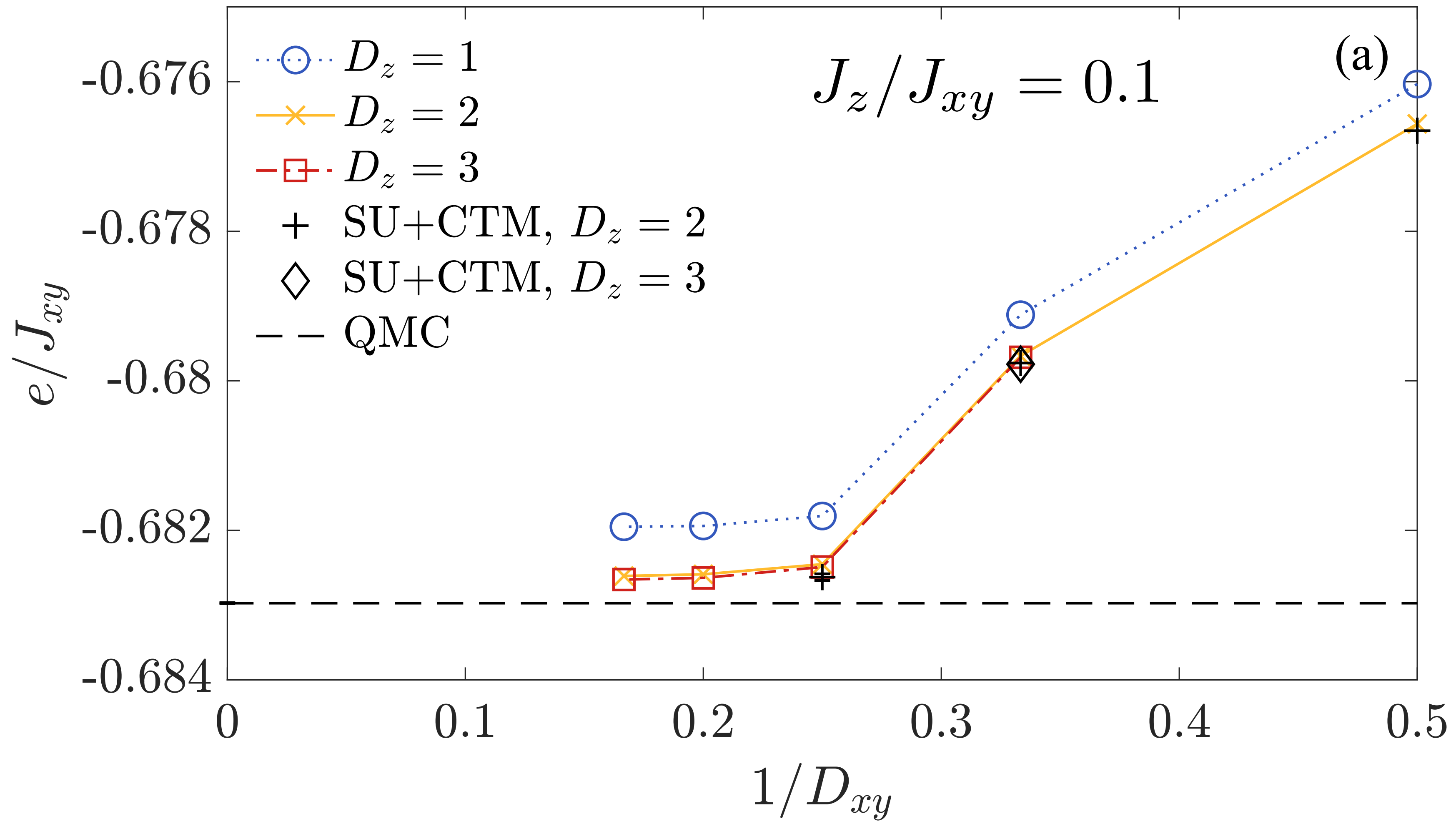
Contraction:

- $D_z = 1$: 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, arxiv:2208.06423

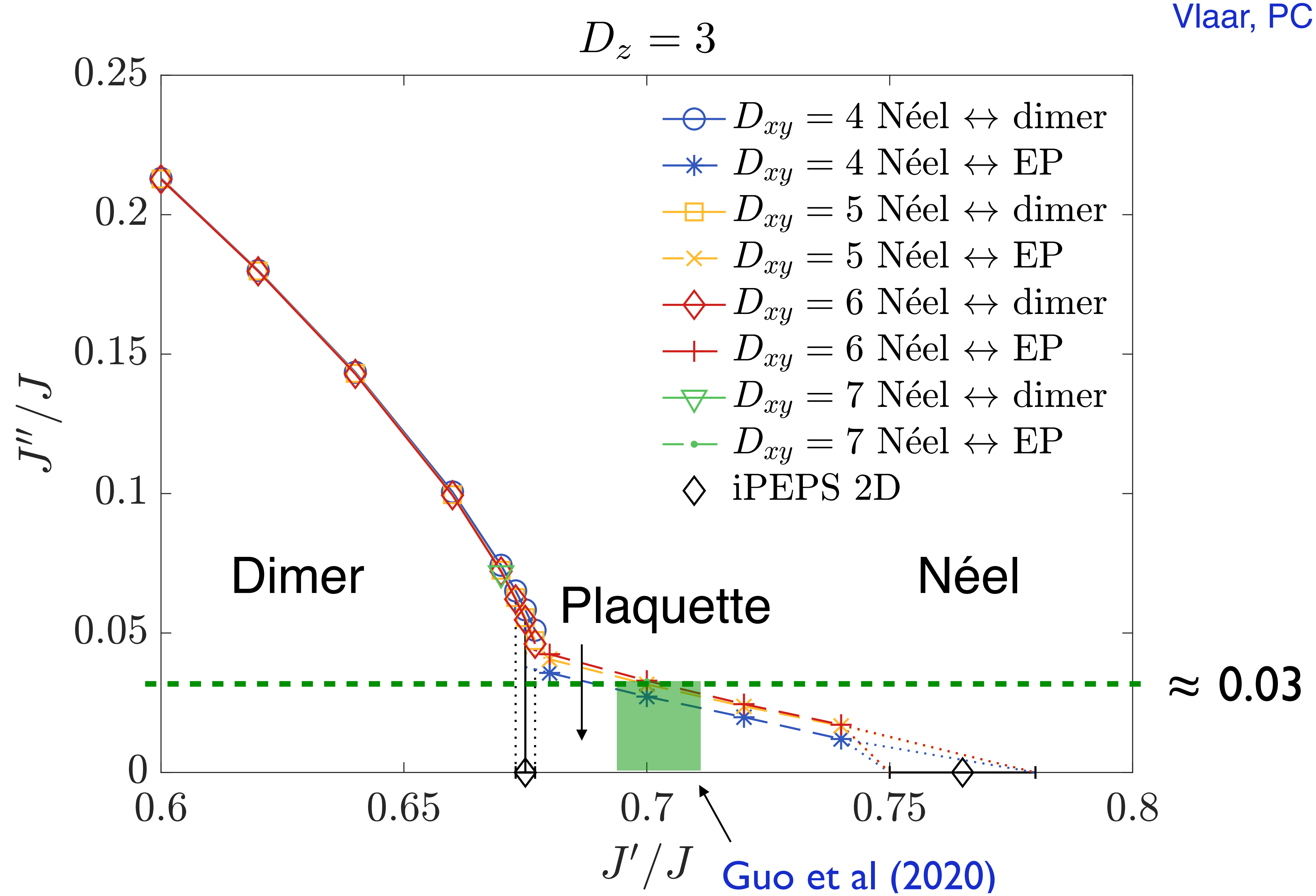


- Substantial improvement from $D_z = 1$ to $D_z = 2$
- Values close to the extrapolated QMC result
- In agreement with more expensive full 3D contraction

Vlaar & PC, PRB 103, 205137 (2021)

Shastry-Sutherland model with interlayer coupling

Vlaar, PC, arxiv:2302.07894



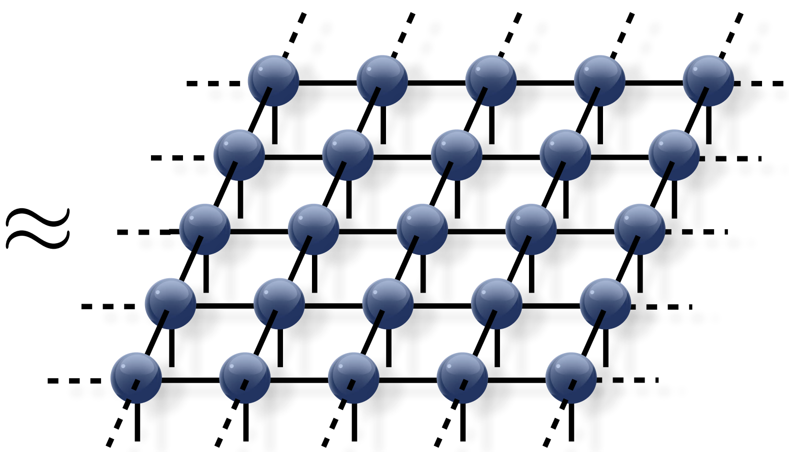
Estimate for the strength of interlayer coupling: J''/J

LCTM: Powerful approach also for other layered systems

Excitations with iPEPS

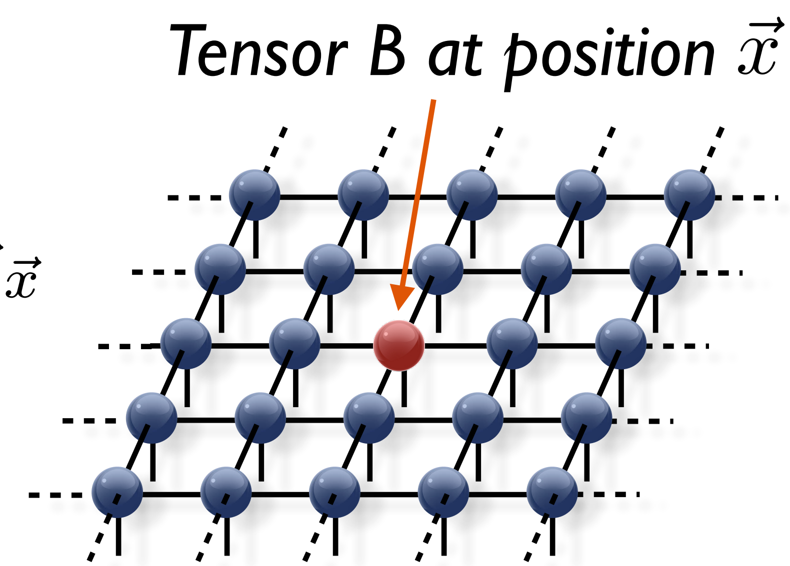
iPEPS excitation ansatz

- Ground state: $|\Psi\rangle \approx$



- Excitation on top of ground state with momentum k

$$|\Phi_{\vec{k}}(B)\rangle \approx \sum_{\vec{x}} e^{i\vec{k}\vec{x}}$$

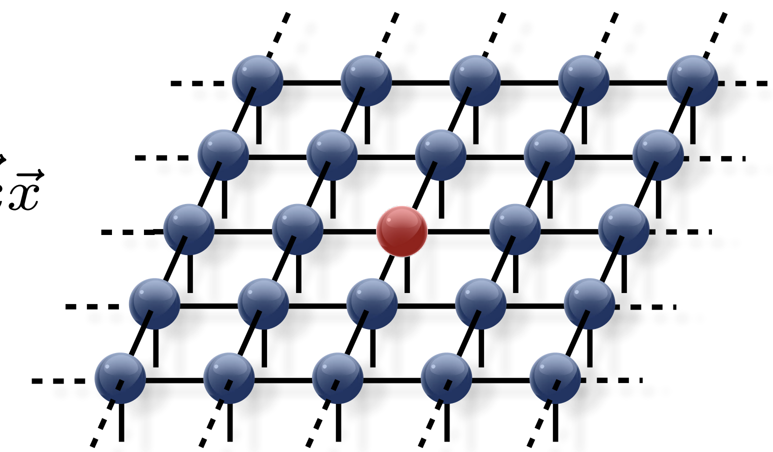


Haegeman, Pirvu, Weir, Cirac, Osborne, Verschelde, and Verstraete, PRB 85, 100408(R) (2012).
Haegeman, Michalakis, Nachtergaele, Osborne, Schuch, and Verstraete, PRL 111, 080401 (2013).
Haegeman, Osborne, and Verstraete, PRB 88, 075133 (2013).
Zauner, Draxler, Vanderstraeten, Degroote, Haegeman, Rams, Stojevic, Schuch, and Verstraete, New J. Phys. 17, 053002 (2015).
Vanderstraeten, Marien, Verstraete, and Haegeman, PRB 92, 201111 (2015)
Vanderstraeten, Haegeman, and Verstraete, PRB 99, 165121 (2019)

iPEPS excitation ansatz: the challenge

- Excitation on top of ground state with momentum k

$$|\Phi_{\vec{k}}(B)\rangle \approx \sum_{\vec{x}} e^{i\vec{k}\vec{x}}$$



Ansatz consists of an infinite sum!

- Minimizing: $\langle \Phi_{\vec{k}}(B)|\hat{H}|\Phi_{\vec{k}}(B)\rangle$

Triple infinite sum!

Translational invariance
→ Double infinite sum

Boris Ponsioen

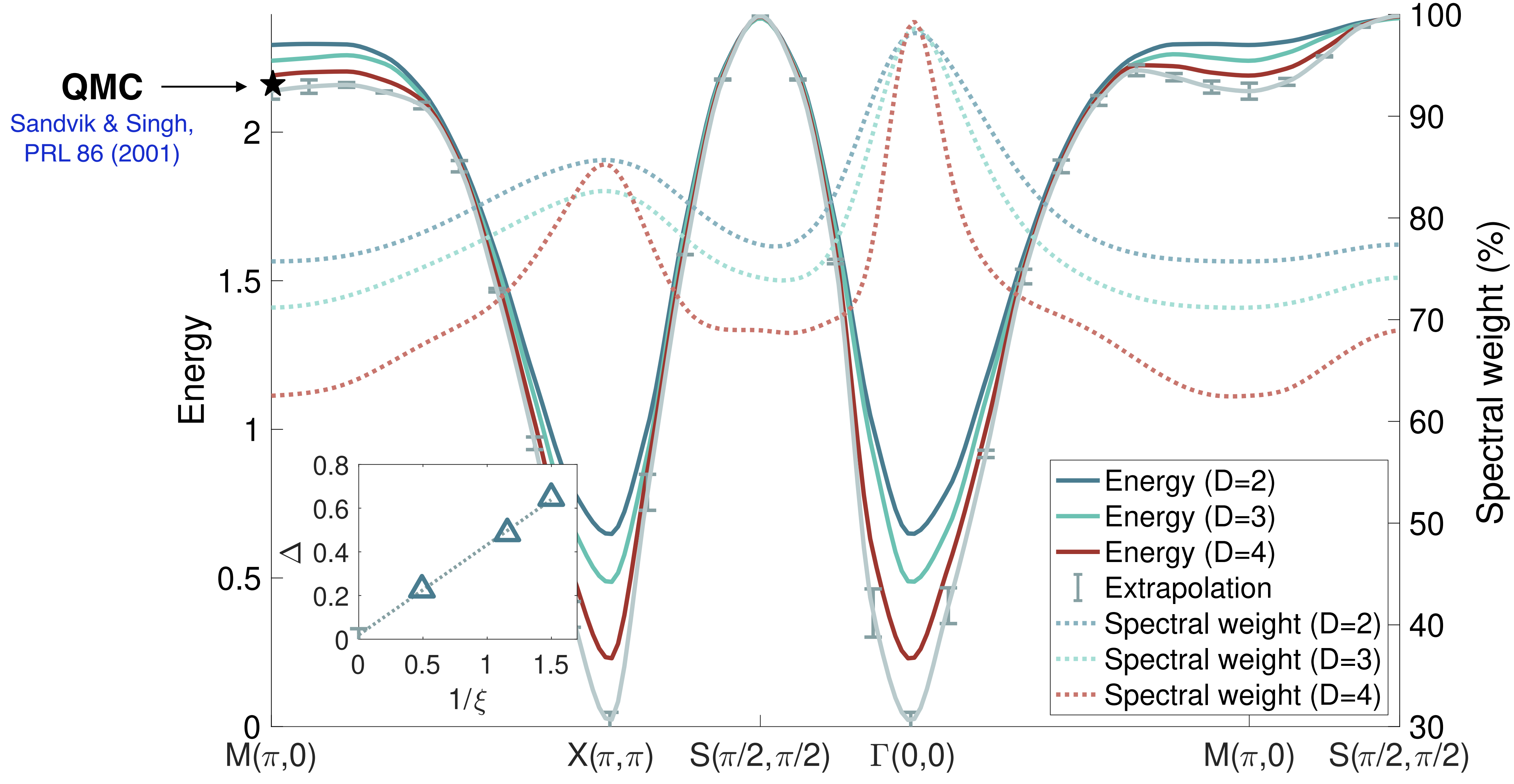
- Use systematic summation:

Channel environments Vanderstraeten, Marien, Verstraete, and Haegeman, PRB 92 (2015)
Vanderstraeten, Haegeman, and Verstraete, PRB 99 (2019)

CTM approach Ponsioen and PC, PRB 101, 195109 (2020)

CTM + AD approach Ponsioen, Assaad, PC, SciPost Physics, 12, 006 (2022)

Benchmark: square lattice Heisenberg model

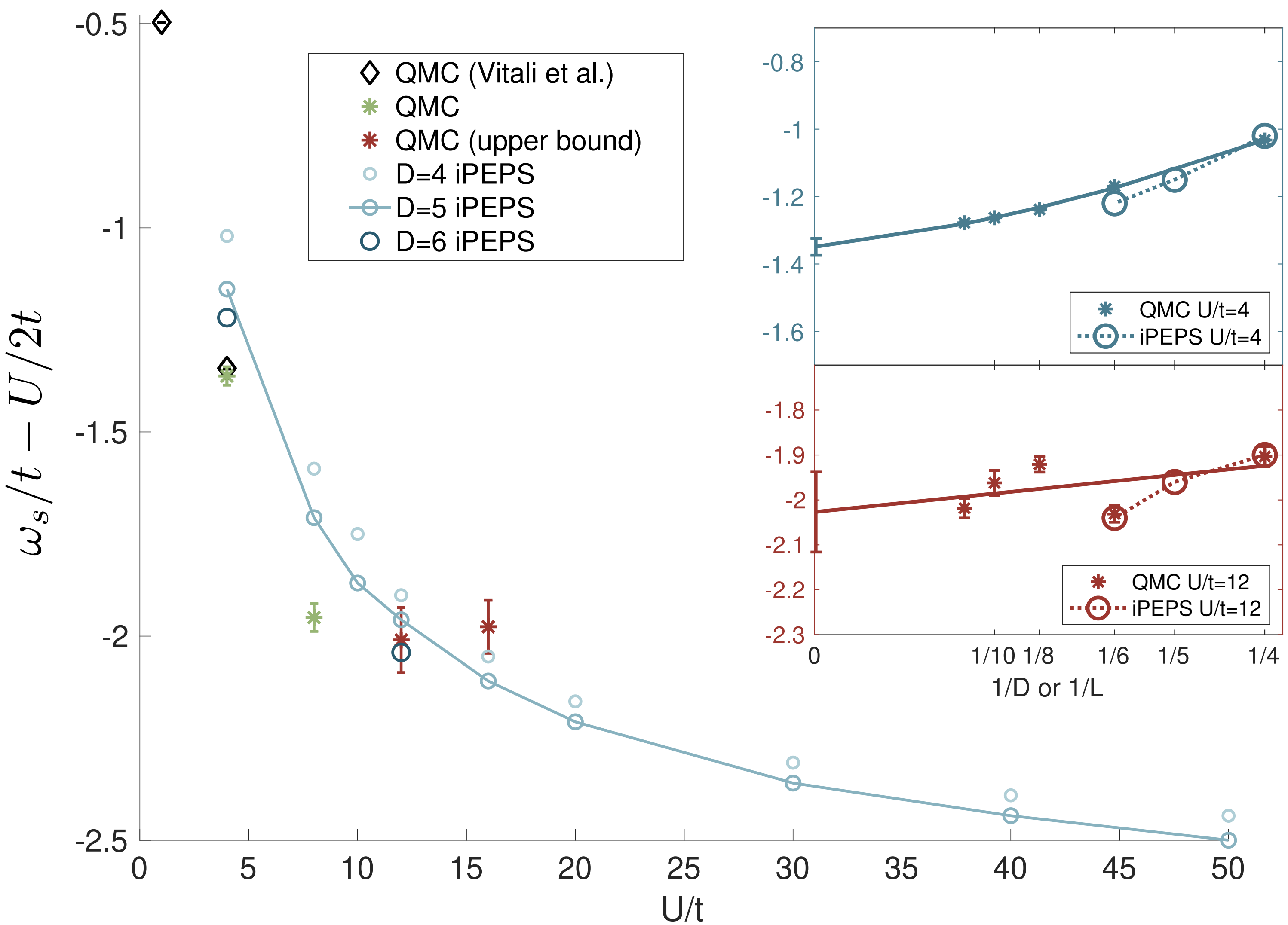


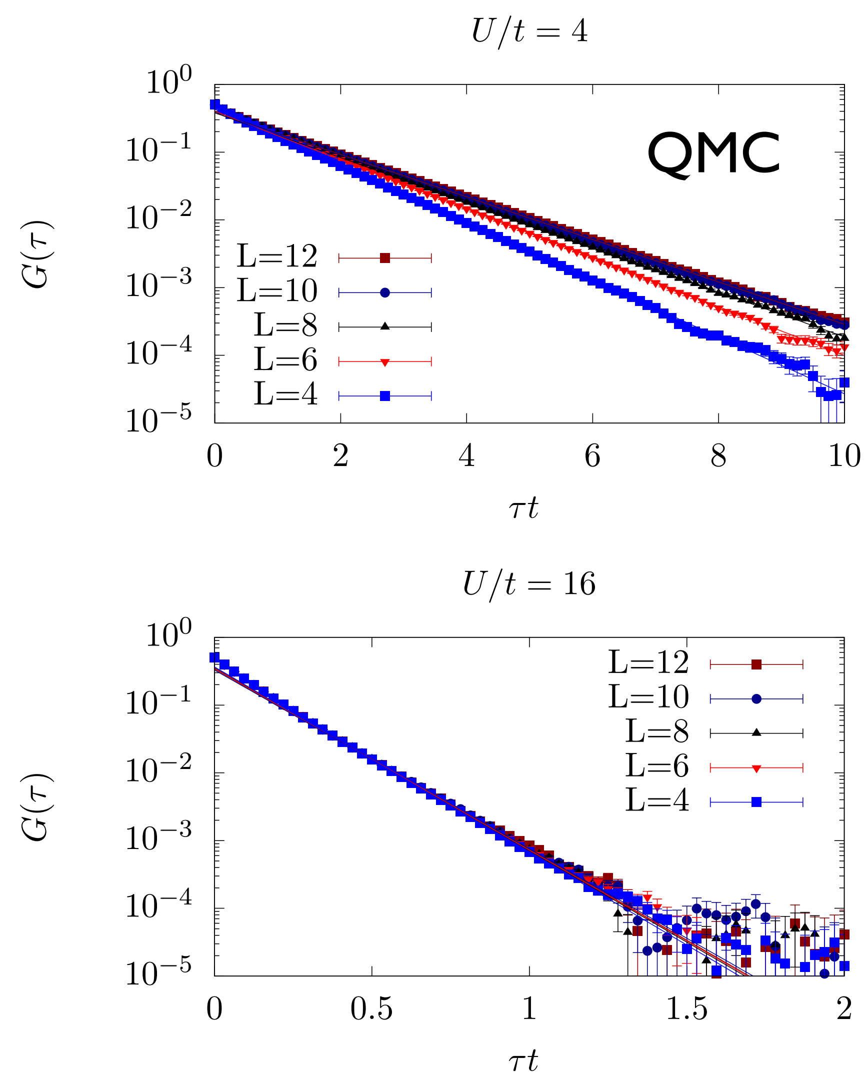
Ponsioen and PC, PRB 101, 195109 (2020)

similar results in: Vanderstraeten, Haegeman, Verstraete, PRB 99 (2019)

Charge gap in the half-filled Hubbard model

Ponsioen, Assaad, PC, SciPost Physics, 12, 006 (2022)

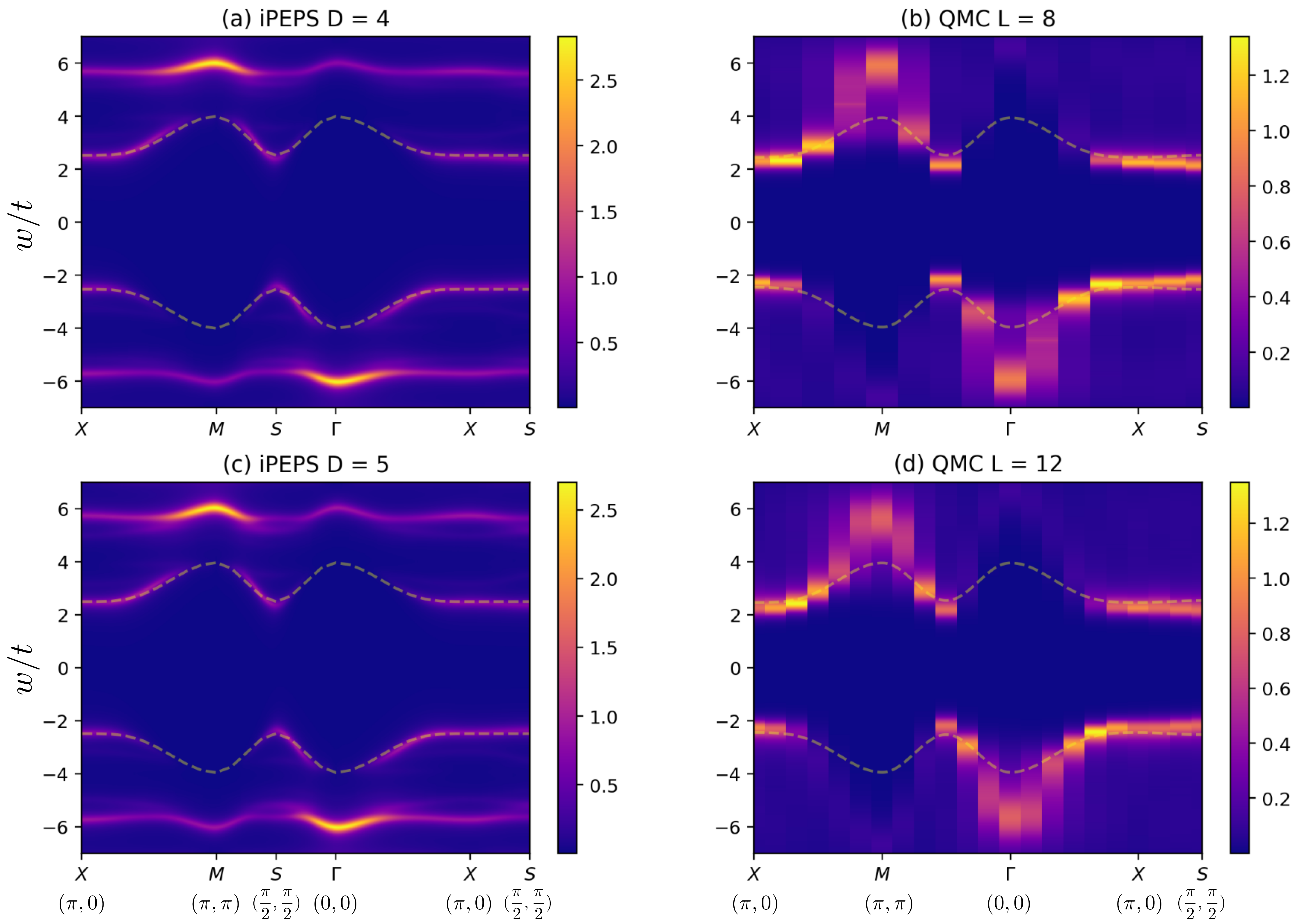




★ Systematic improvement with D, approaching QMC for U/t=4 and U/t=8

★ QMC: extracting gap at large U/t is exponentially hard, in contrast to iPEPS

Spectral function A(ω, k) for U/t=8



Summary

- ✓ iPEPS: powerful and versatile tool for strongly correlated systems
- ✓ Various applications & new methodological developments:
  - ★ 2D ground state calculations
  - ★ Extension to finite temperature ➔ $SrCu_2(BO_3)_2$
  - ★ iPEPS for 3D and layered systems
  - ★ iPEPS excitation ansatz
- ✓ Still room for improvement

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