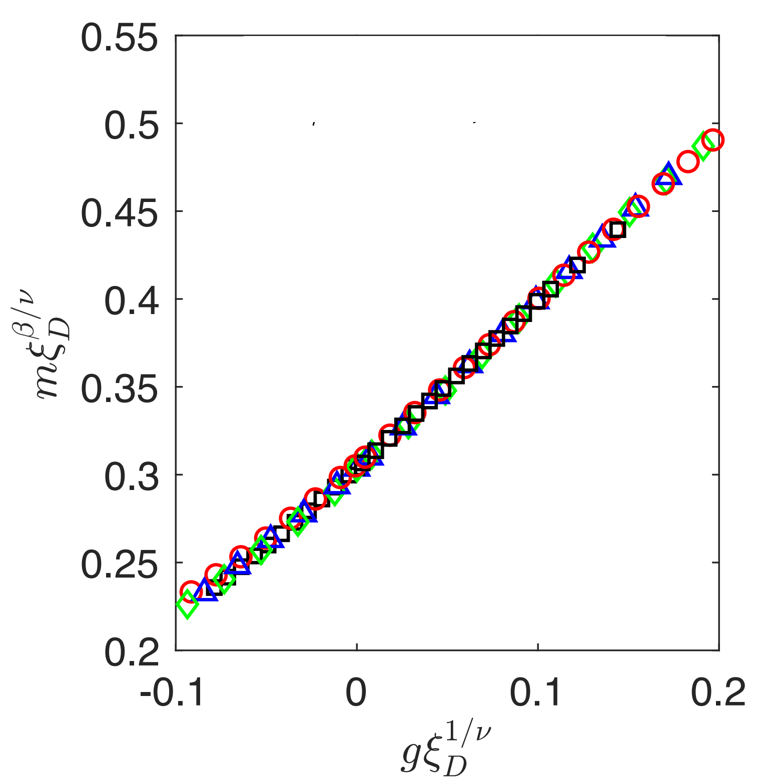
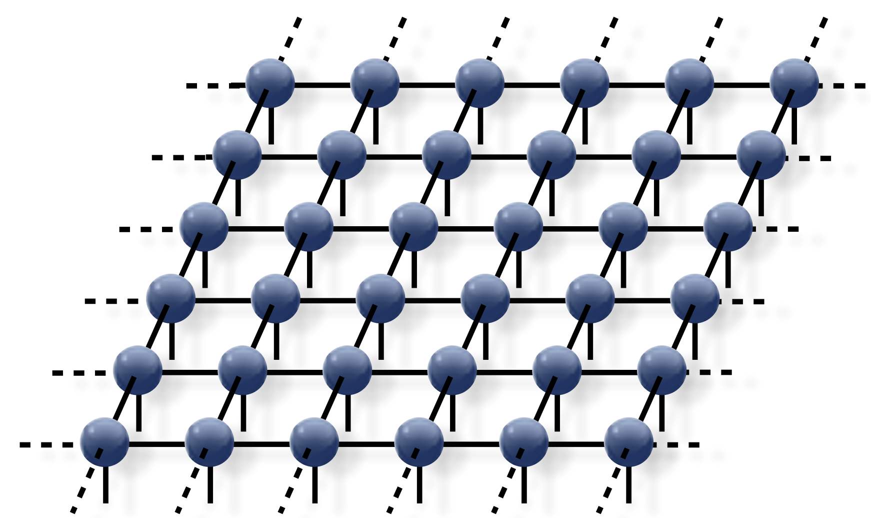
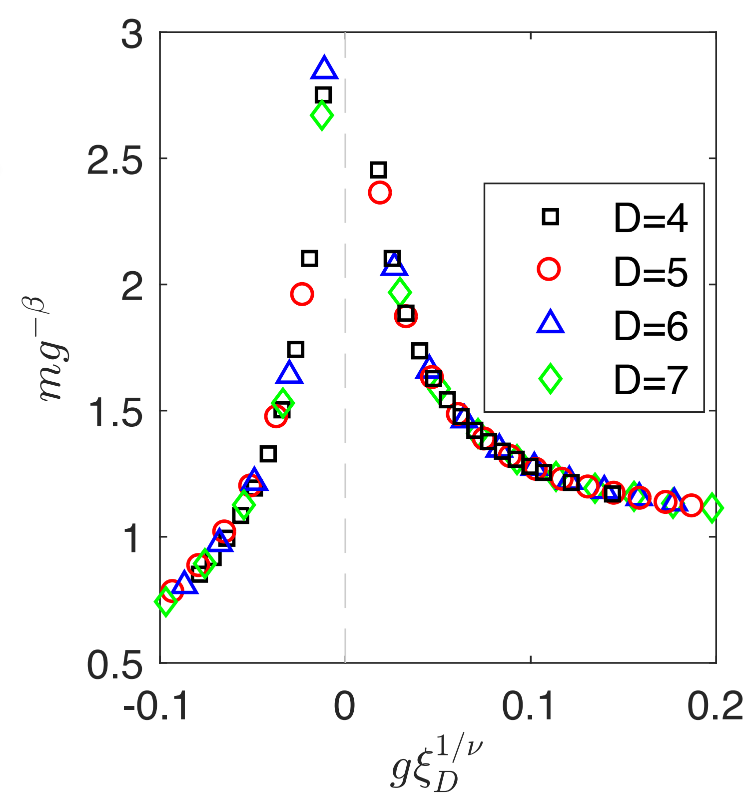
Applications of finite correlation length scaling with iPEPS

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam







Outline

- Introduction to iPEPS & corner transfer matrix (CTM) method
- Part I: Finite correlation length scaling for iPEPS ground states

  PC, P. Czarnik, G. Kapteijns, L. Tagliacozzo, PRX 8 (2018)

  M. Rader and A. M. Läuchli, PRX 8 (2018)
- Part II: FCL scaling at finite temperature

  P. Czarnik & PC, PRB 99, 245107 (2019); P. Czarnik, M. M. Rams, PC & J. Dziarmaga, PRB 103 (2021)

  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)
- Part III: FCL scaling with 3D iPEPS

  P. Vlaar & PC, PRB 103, 205137 (2021)
- Part IV: FCL scaling with the iPEPS excitation ansatz

  Ponsioen and PC, PRB 101, 195109 (2020)

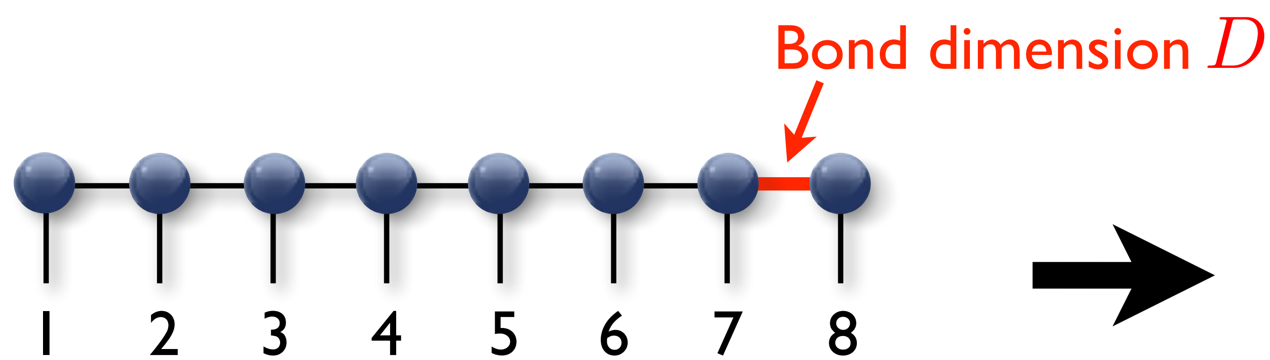
  B. Ponsioen, F. F. Assaad, PC, SciPost Physics, 12, 006 (2022)

MPS & PEPS

1D

MPS

Matrix-product state



Physical indices (lattices sites)

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

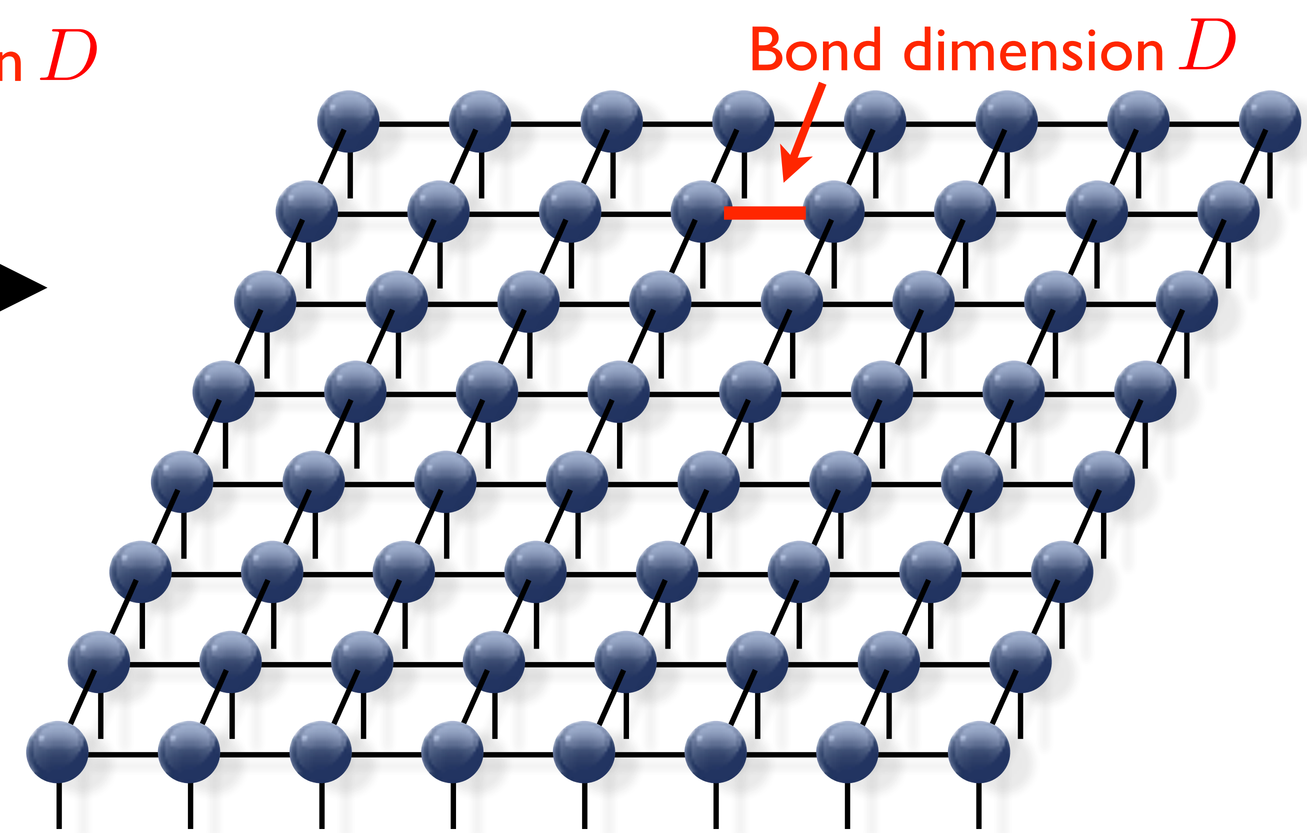
Fannes et al., CMP 144, 443 (1992)

Östlund, Rommer, PRL 75, 3537 (1995)

2D

PEPS (TPS)

projected entangled-pair state
(tensor product state)



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

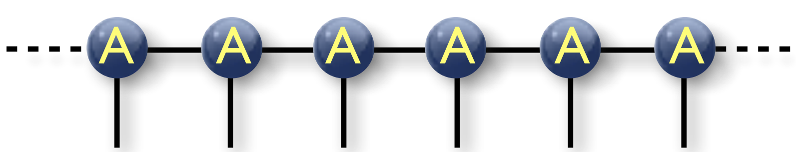
Nishio, Maeshima, Gendiar, Nishino, cond-mat/0401115

Infinite PEPS (iPEPS)

1D

iMPS

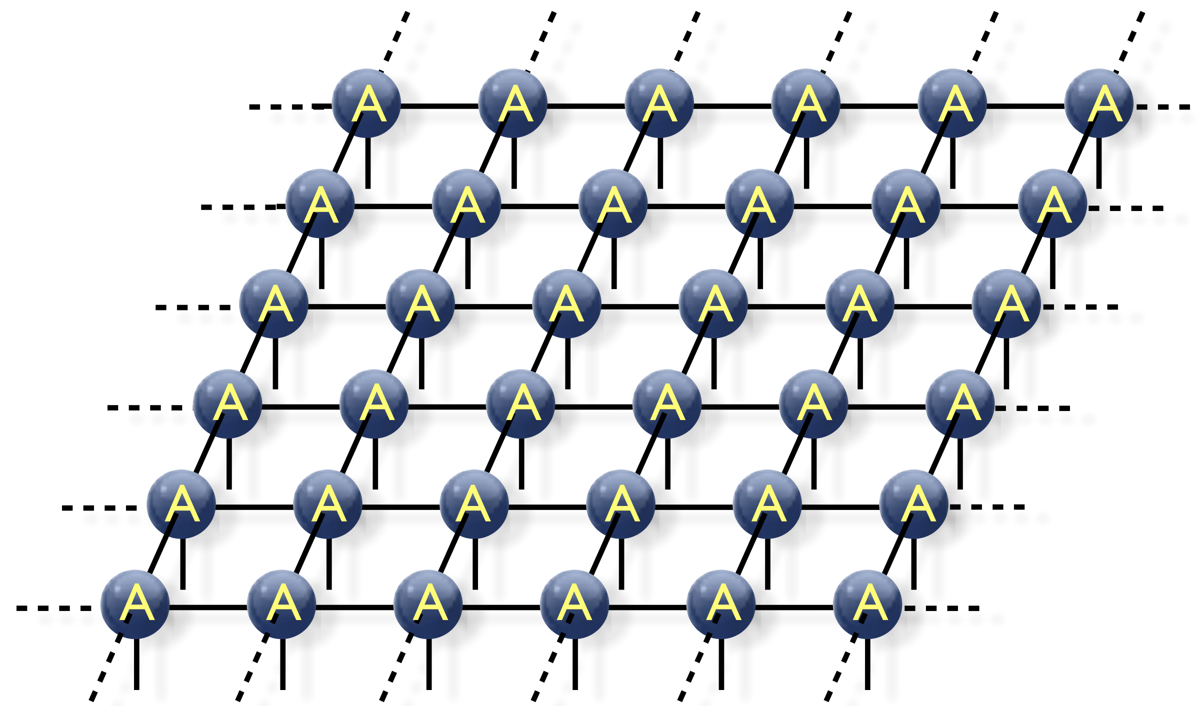
infinite matrix-product state



2D

iPEPS

infinite projected entangled-pair state



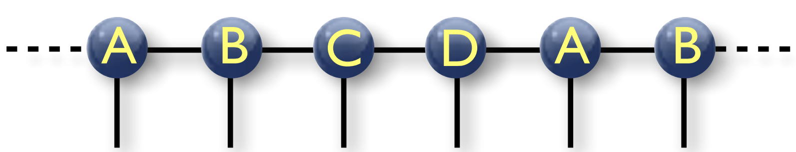
Jordan, Orus, Vidal, Verstraete, Cirac, PRL (2008)

iPEPS with arbitrary unit cells

1D

iMPS

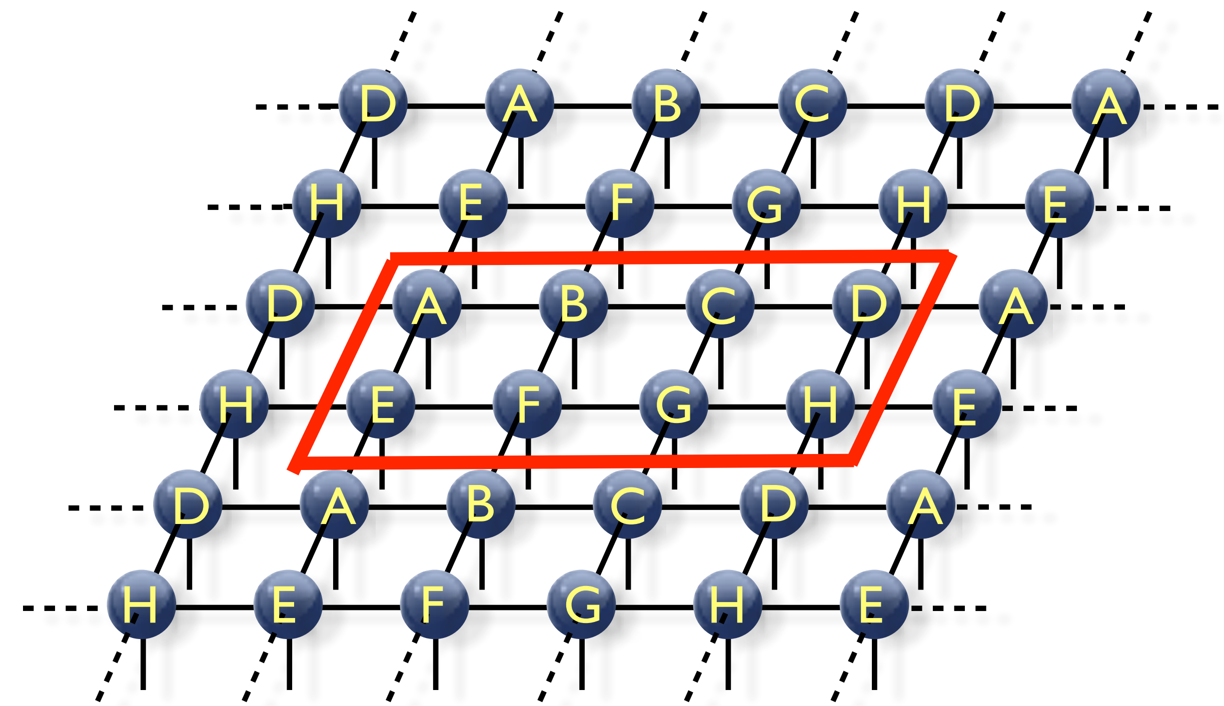
infinite matrix-product state



2D

iPEPS

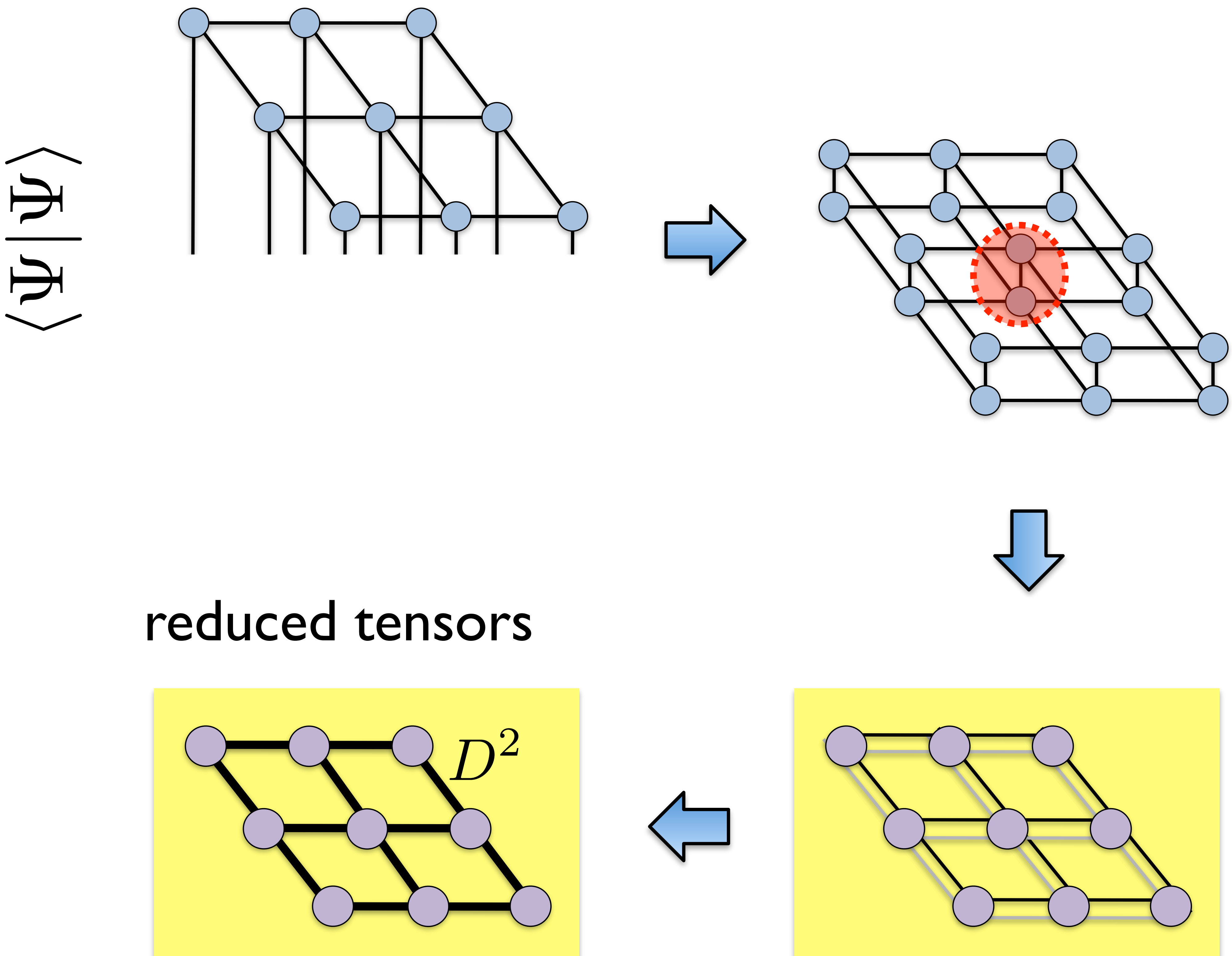
with arbitrary unit cell of tensors



here: 4x2 unit cell

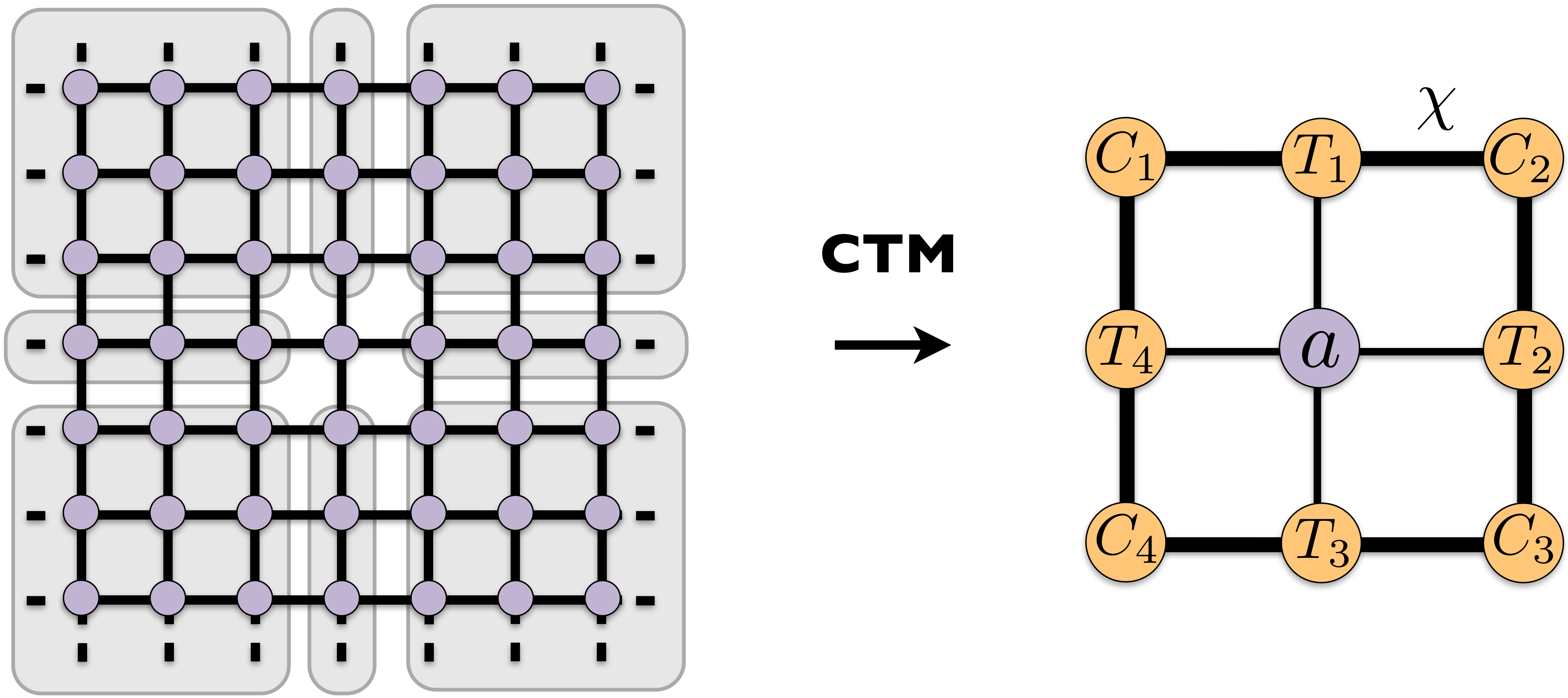
PC, White, Vidal, Troyer, PRB **84** (2011)

Contracting a PEPS



Contracting the iPEPS using the corner transfer matrix method

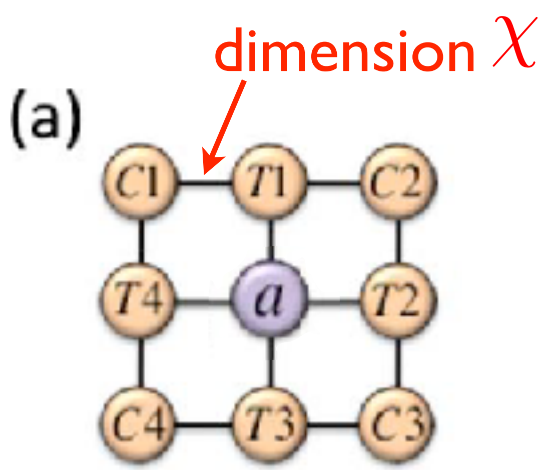
Nishino, Okunishi, JPSJ65 (1996)



- 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)

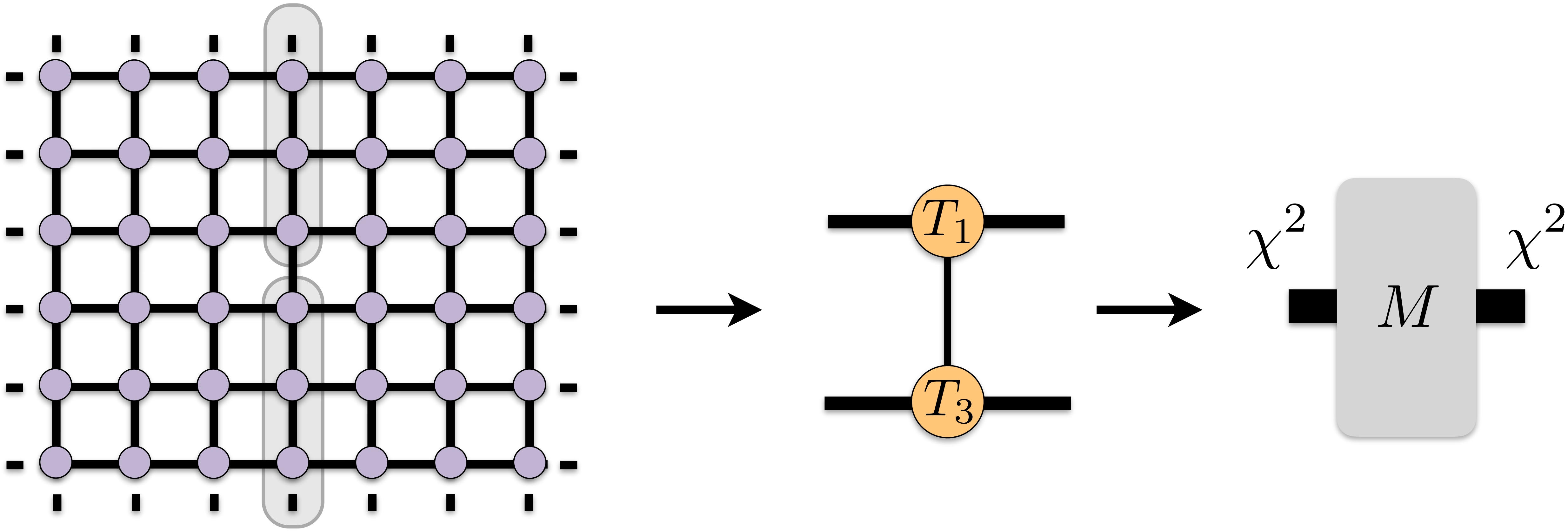


- ★ Let the system grow in all directions.
- ★ Repeat until convergence is reached
- ★ The boundary tensors form the **environment**
- ★ Can be generalized to arbitrary unit cell sizes

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

Computing the correlation length with CTM

Nishino, Okunishi, Kikuchi, Physics Lett. A 213, 69 (1996)



$$\xi(\chi) = \frac{1}{\log\left(\frac{\lambda_0}{\lambda_1}\right)}$$

1st and 2nd lowest eigenvalue of M

Finite correlation length scaling with iPEPS

PHYSICAL REVIEW X 8, 031030 (2018)

Finite Correlation Length Scaling in Lorentz-Invariant Gapless iPEPS Wave Functions

Michael Rader and Andreas M. Läuchli
Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Austria

(Received 28 March 2018; published 30 July 2018)

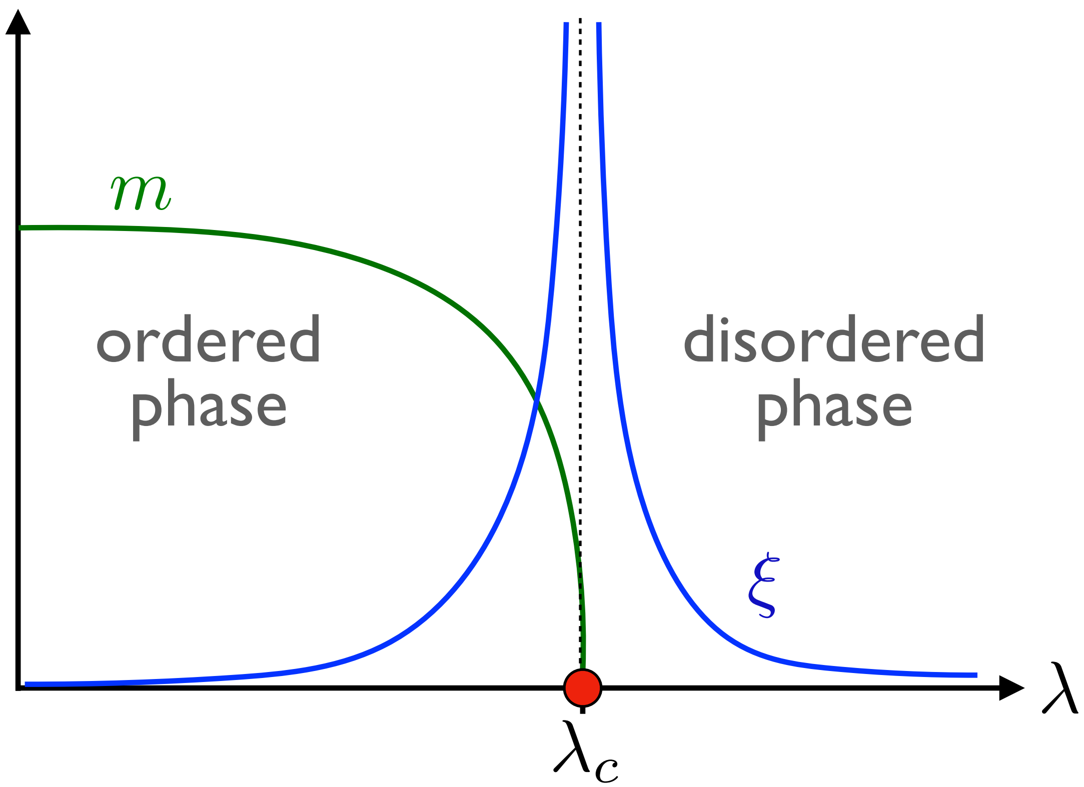
PHYSICAL REVIEW X 8, 031031 (2018)

Finite Correlation Length Scaling with Infinite Projected Entangled-Pair States

Philippe Corboz,[1] Piotr Czarnik,[2] Geert Kapteijns,[1] and Luca Tagliacozzo[3]
[1]*Institute for Theoretical Physics and Delta Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, Netherlands*
[2]*Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, PL-31342 Kraków, Poland*
[3]*Department of Physics and SUPA, University of Strathclyde, Glasgow G4 0NG, United Kingdom and Departament de Física Quàntica i Astrofísica, Universitat de Barcelona, Barcelona 08028, Spain*

(Received 28 March 2018; revised manuscript received 12 June 2018; published 30 July 2018)

Motivation: study of continuous quantum phase transitions



$$m \sim |g|^{\beta}$$

$$\xi \sim |g|^{-\nu}$$

$$g = \frac{\lambda - \lambda_c}{\lambda_c}$$

Critical coupling?

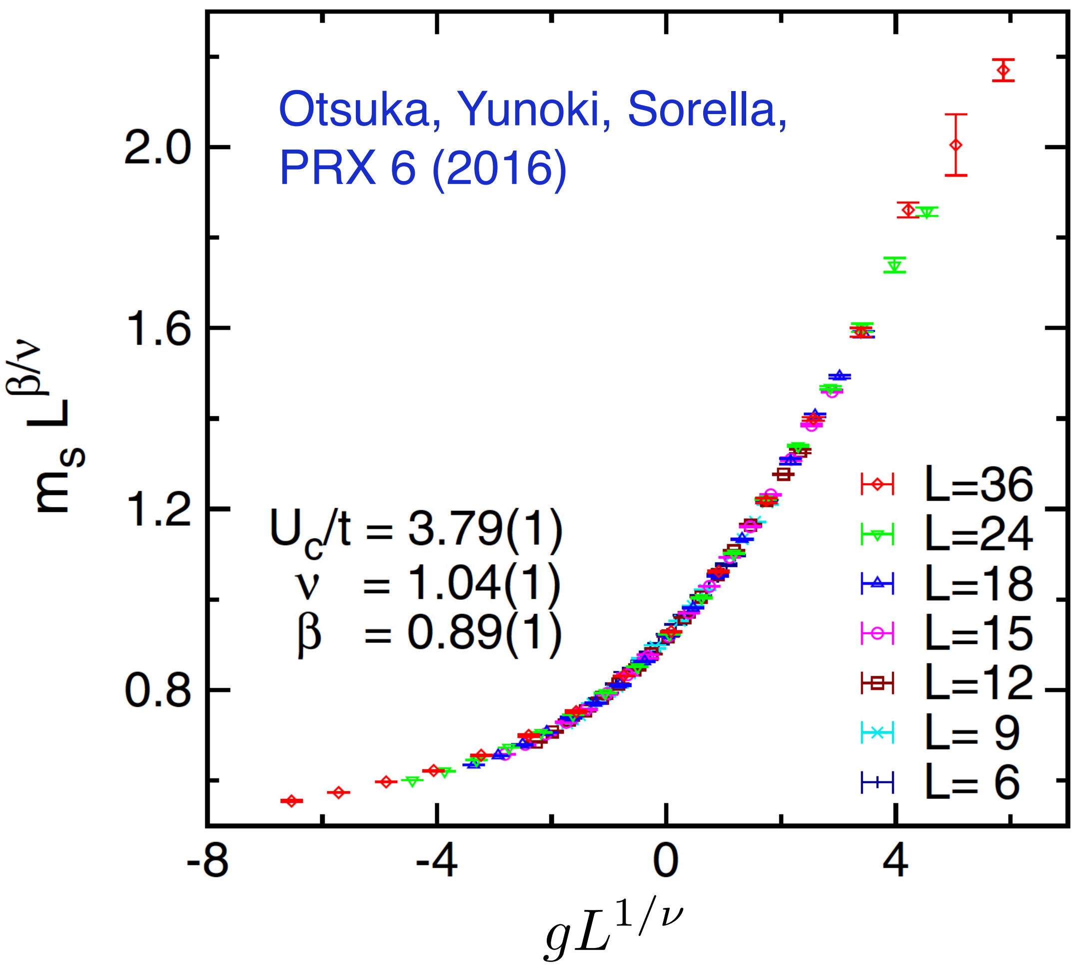
Universal critical exponents?

Challenging!

- Strong finite size effects in the vicinity of the critical point

- Powerful approach: *finite size scaling:* $m(g, L) = L^{-\beta/\nu} \mathcal{F}(g L^{1/\nu})$

Motivation: study of quantum phase transitions



$$m \sim |g|^{\beta}$$

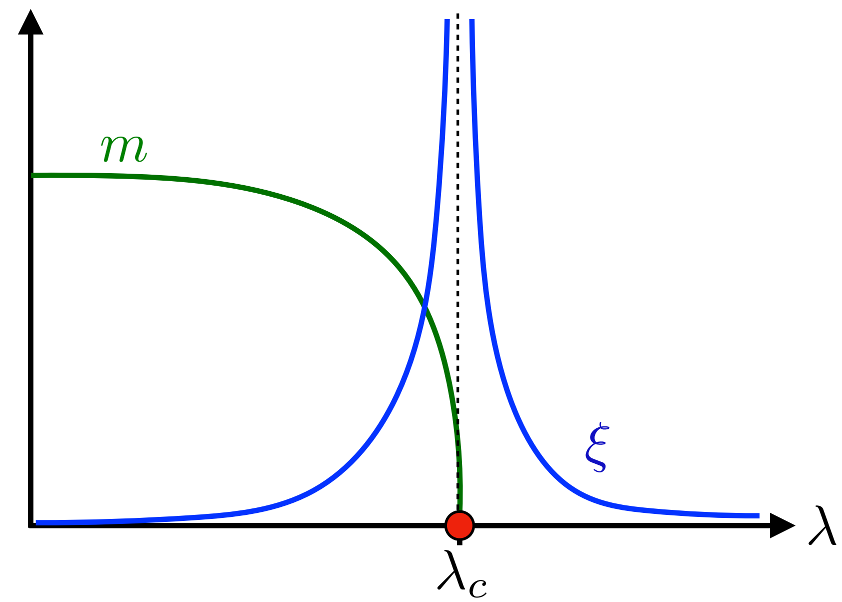
$$\xi \sim |g|^{-\nu}$$

$$g = \frac{\lambda - \lambda_c}{\lambda_c}$$

- Strong finite size effects in the vicinity of the critical point
- Powerful approach: *finite size scaling:* $m(g,L) = L^{-\beta/\nu}\mathcal{F}(gL^{1/\nu})$
- **Can we do something similar with infinite tensor networks?**

Finite correlation length scaling in 1D (iMPS)

- iMPS with finite D can only represent states with a finite correlation length
- Correlation length at the critical point: ξ_D
- ξ_D acts as a cut-off on the diverging correlation length, similarly to a finite L



$$m(g, L) = L^{-\beta/\nu}\mathcal{F}(gL^{1/\nu}) \quad \longleftrightarrow \quad m(g, D) = \xi_D^{-\beta/\nu}\mathcal{M}(g\xi_D^{1/\nu})$$

Finite size scaling ansatz

Finite correlation length scaling ansatz

Tagliacozzo, de Oliveira, Iblisdir & Latorre, PRB 78 (2008)
Pollmann, Mukerjee, Turner & Moore, PRL 102 (2009)
Pirvu, Vidal, Verstraete & Tagliacozzo, PRB 86 (2012)

- Similar idea for 2D tensor networks for 2D classical partition functions

Nishino, Okunishi, Kikuchi, Phys. Lett. A 213 (1996)

$$m(g, \chi) = \xi_\chi^{-\beta/\nu}\mathcal{M}(g\xi_\chi^{1/\nu})$$

χ: *bond dimension for contraction*

How about in (2+1)D with iPEPS?

- iPEPS: There exist critical states with a finite D

see e.g. Kraus et al. PRA 81 (2010), Verstraete et al. PRL 96 (2006)

- However, these are 2D classical states or ground states of generalized Rokhsar-Kivelson Hamiltonians at the critical point which can effectively be described by a (2+0)D CFT

see e.g. Henley, JPCM 16 (2004); Ardonne, Fendley & Fradkin, Ann. Phys. 310 (2004); Castelnovo, Chamon, Mudry & Pujol, Ann. Phys. 318 (2005); Isakov, et al. PRB 83 (2011)

- For Lorentz-invariant critical points (2+1D): no example of a critical iPEPS is known

Dynamical critical exponent: $z = 1$ $\qquad \xi_{time} \sim \xi_{space}^{z} \sim \xi_{space}$

- All simulations suggest: $D \rightarrow \xi_D$ *despite that these states obey an area law!*

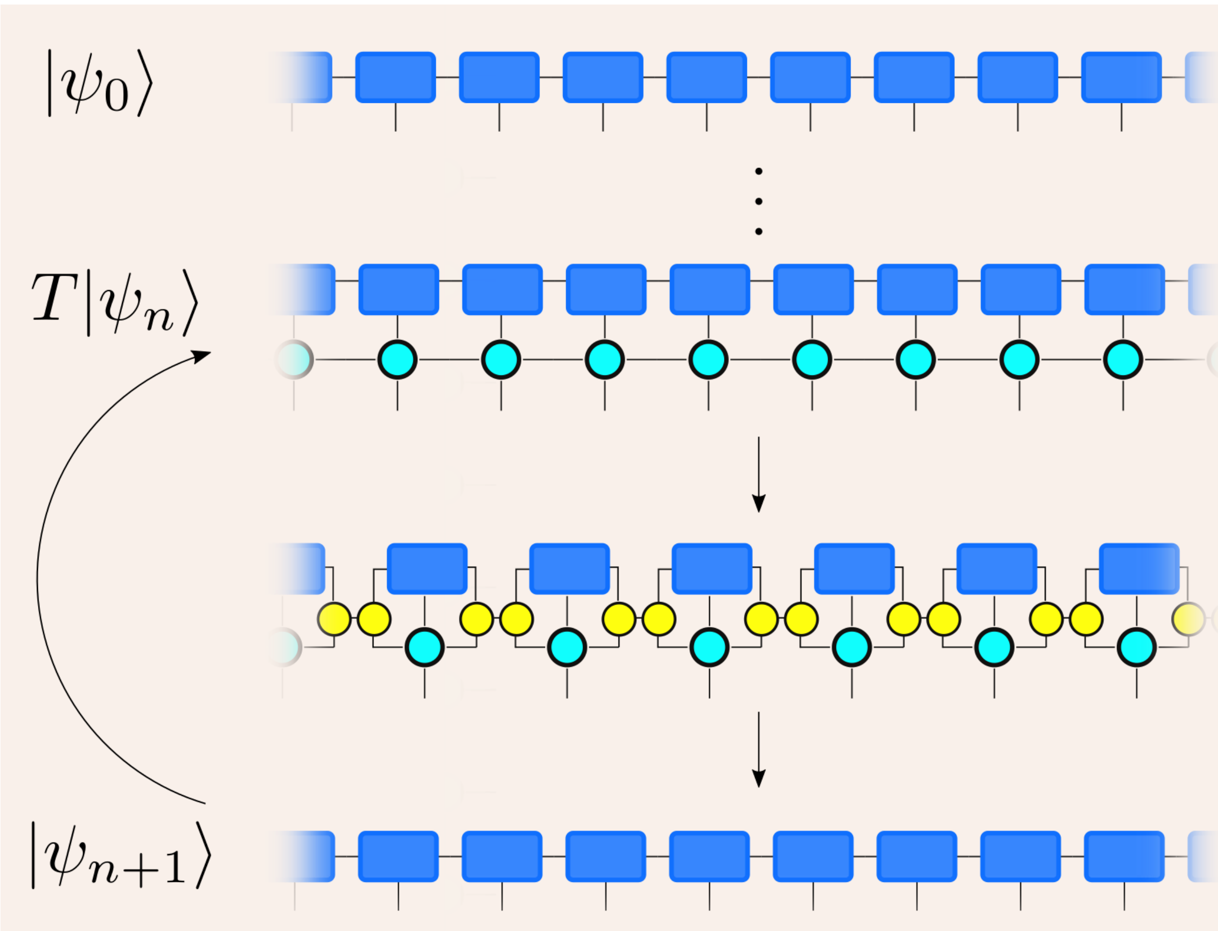
- *Example of a state with an area law which cannot be represented with finite D*

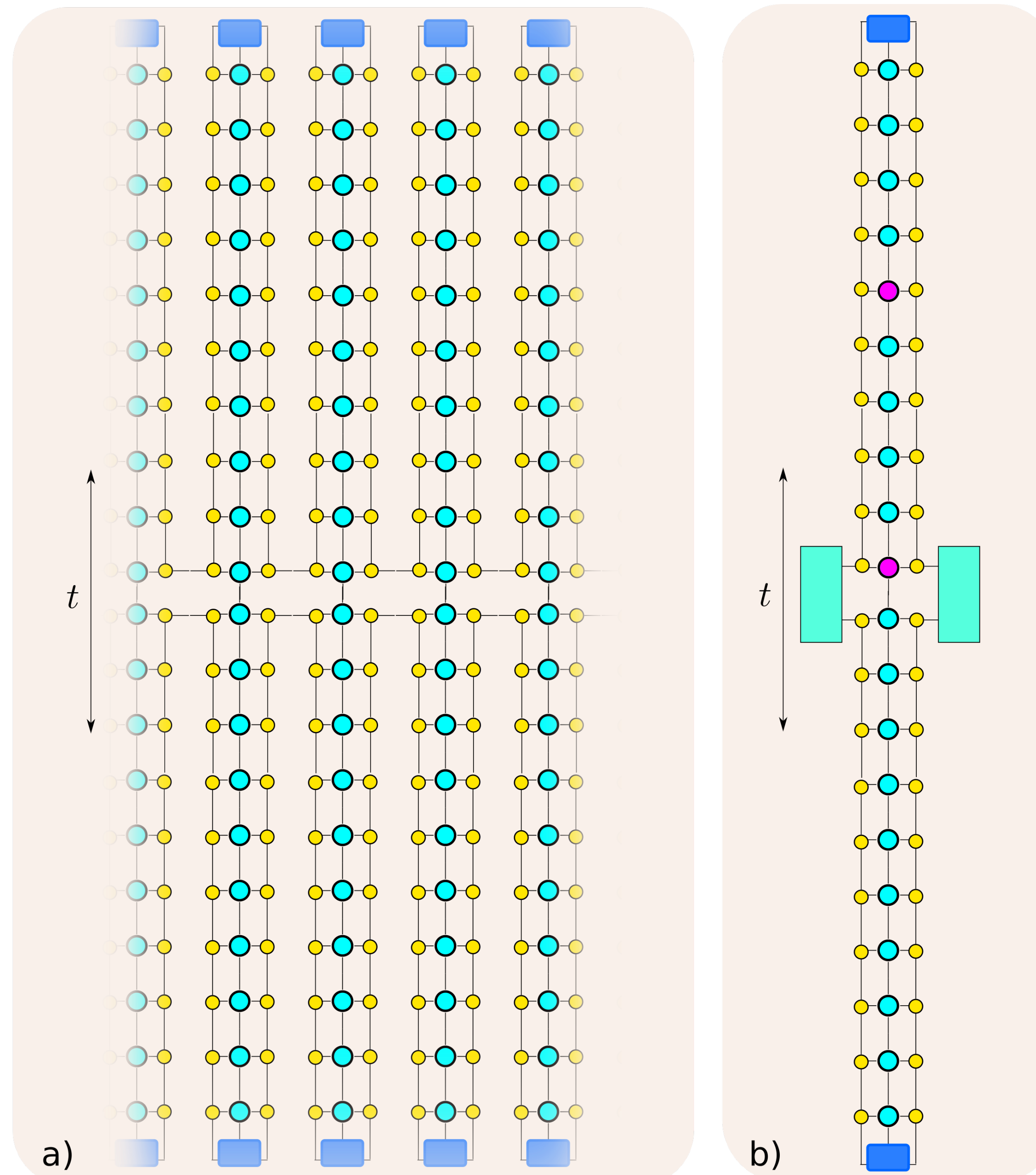
★ We can apply finite correlation length scaling also in 2D

Intuitive argument why $D \to \xi_D$

$\langle \Omega | \mathcal{O}(t_0) \mathcal{O}(t_1) | \Omega \rangle$

Consider imaginary time evolution:





Channel in the time-direction has an MPS structure: $D \to \xi_{time}$

Lorentz invariance: $\xi_{space} \sim \xi_{time}$

$D \to \xi_{space}$

The best finite D state tries to reproduce Lorentz invariance

Finite correlation length scaling with iPEPS

- Complication: there are two bond dimensions:

Bond dimension of the TN ansatz:

$$D \to \xi_D$$

Boundary dimension in contraction:

$$\chi \to \xi_\chi$$

- Scaling ansatz: $m(g, D, \chi) = \xi_D^{-\beta/\nu} \mathcal{M}(g\xi_D^{1/\nu}, \xi_D/\xi_\chi)$

- Simplify: eliminate χ dependence by taking $\chi \to \infty$ limit

- Now same as in iMPS (1D) case:

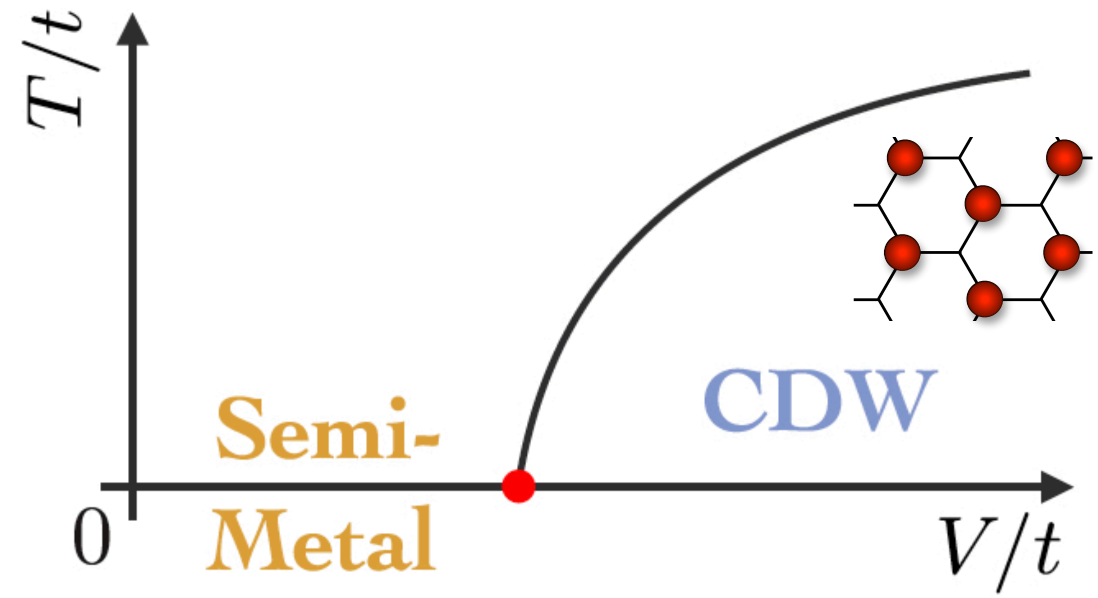
$$\boxed{m(g, D) = \xi_D^{-\beta/\nu} \mathcal{M}(g\xi_D^{1/\nu})}$$

Benchmark example: spinless fermions on honeycomb lattice

- Model:

$$\hat{H} = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \left[\hat{c}_{\mathbf{i}}^{\dagger} \hat{c}_{\mathbf{j}} + h.c. \right] + V \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \hat{n}_{\mathbf{i}} \hat{n}_{\mathbf{j}}$$

at half filling



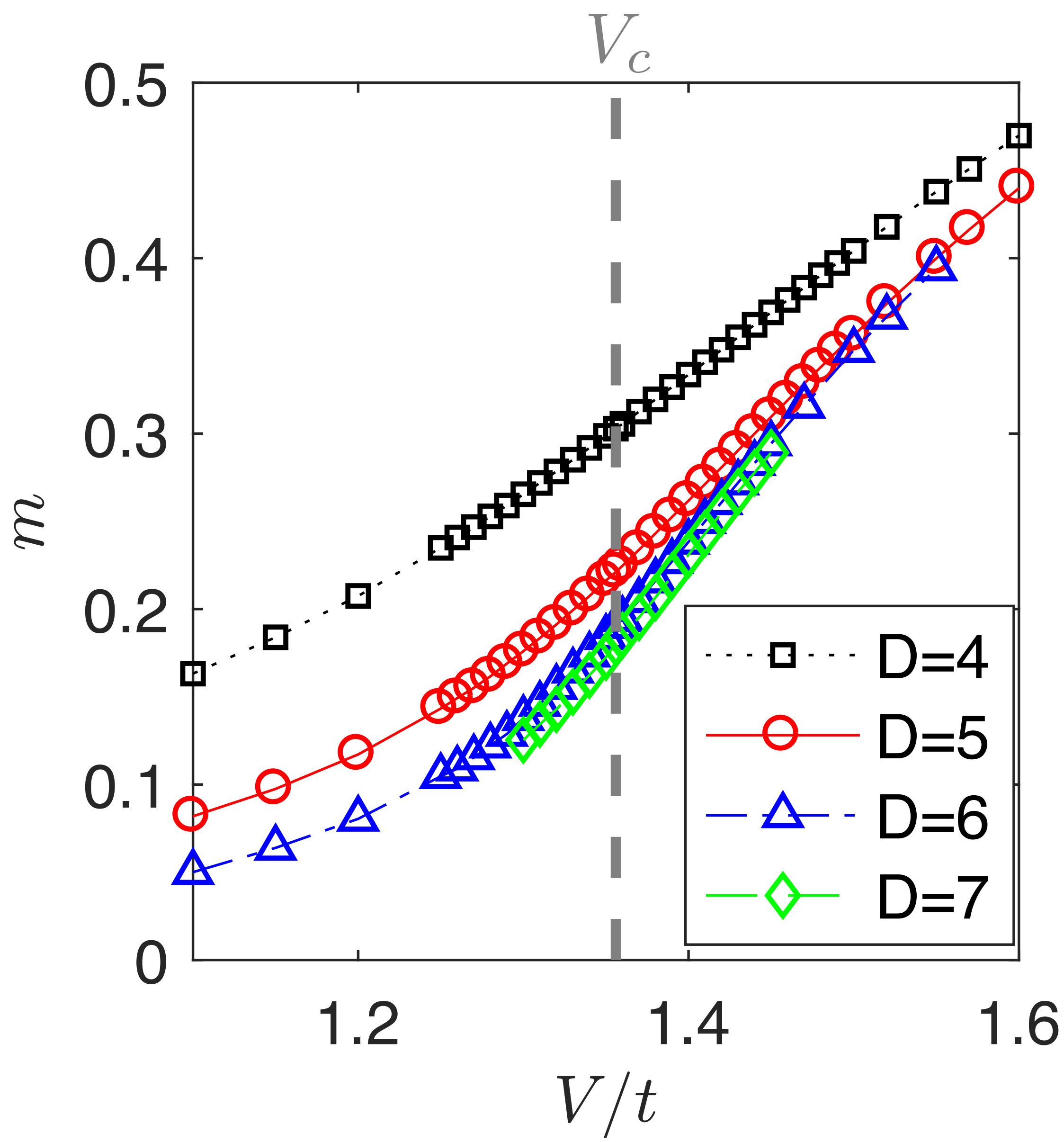
Wang, PC, Troyer, NJP 16 (2014)

- Continuous PT between a semi-metal phase and charge-density wave phase (CDW) *(Chiral Ising Gross-Neveu universality class with z=1)*

- No sign problem in Quantum Monte Carlo

Huffman, Chandrasekharan, PRB 89 (2014); Wang, PC, Troyer, NJP 16 (2014); Li, Jiang, Yao, NJP 17 (2015); Wang, Iazzi, PC & Troyer, PRB 91 (2015); Wang, Liu, Troyer PRB 93 155117 (2016); Hesselmann & Wessel, PRB 93 (2016)

Benchmark example: spinless fermions on honeycomb lattice



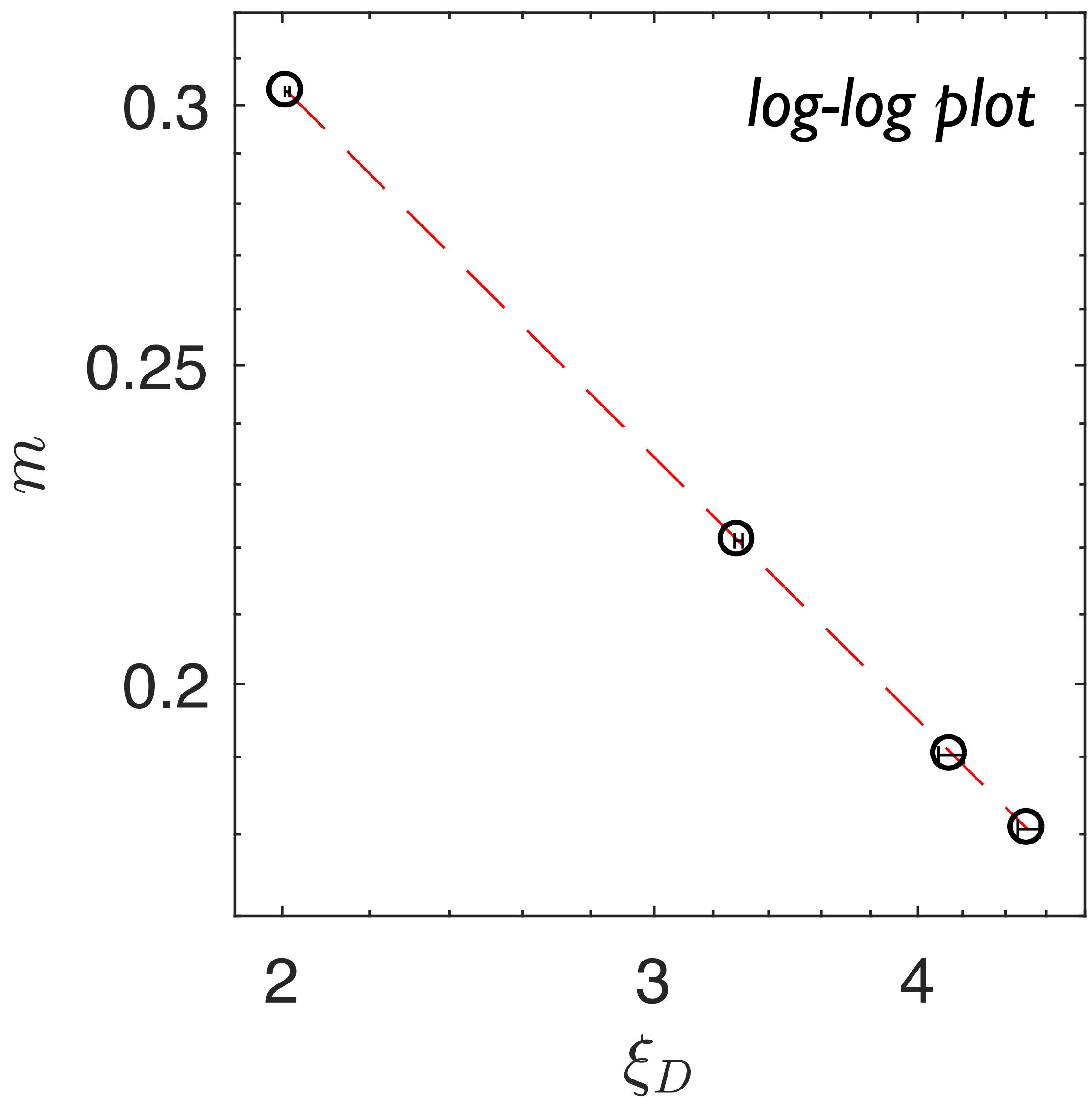
CDW order parameter:

$$m = |n_A - n_B|$$

- Finite D effects get weaker with increasing D

Scaling ansatz at the critical point, $V_c/t = 1.356$

$$m(g=0, D) = \xi_D^{-\beta/\nu}\mathcal{M}(0\cdot\xi_D^{1/\nu}) \sim \xi_D^{-\beta/\nu} \qquad g = (V - V_c)/V_c$$



- Linear fit to log-log plot yields

  $\beta/\nu = 0.64(2)$

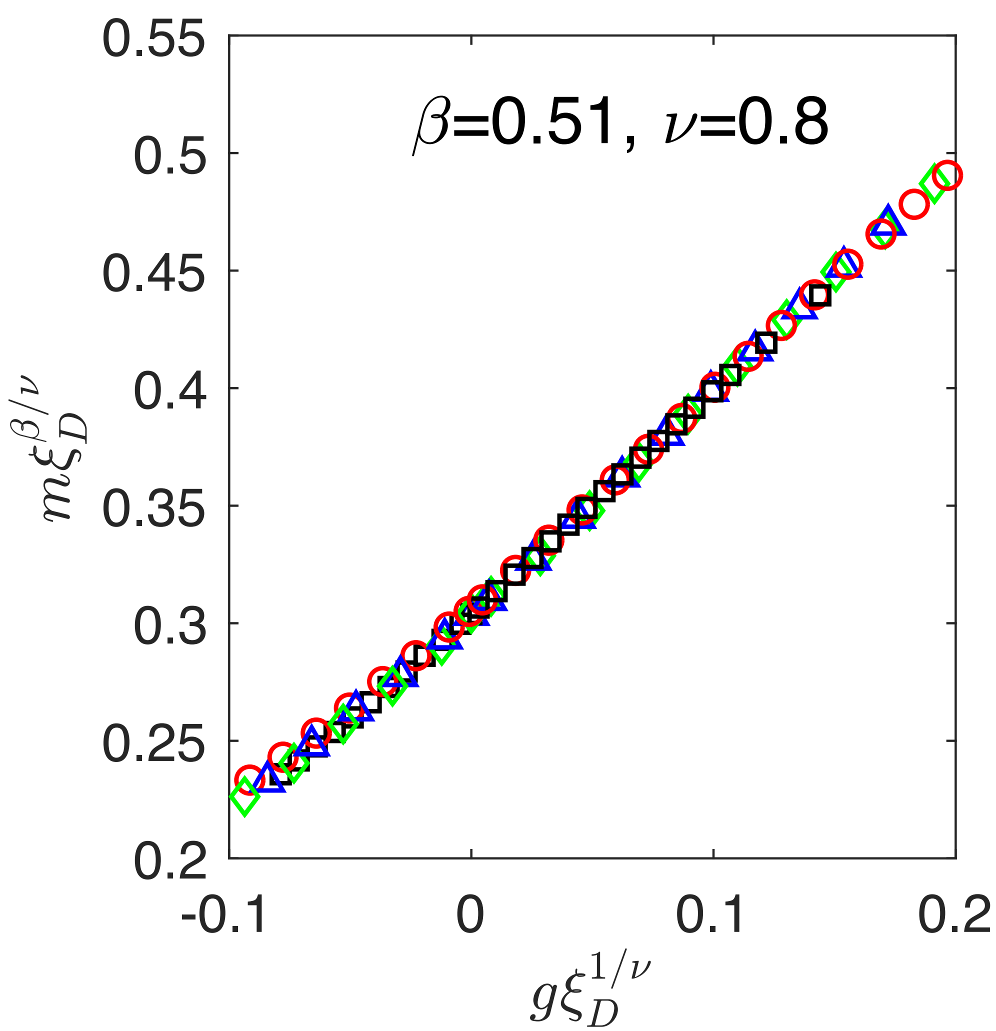
- In agreement with QMC:

  $\beta/\nu = 0.65(4)$

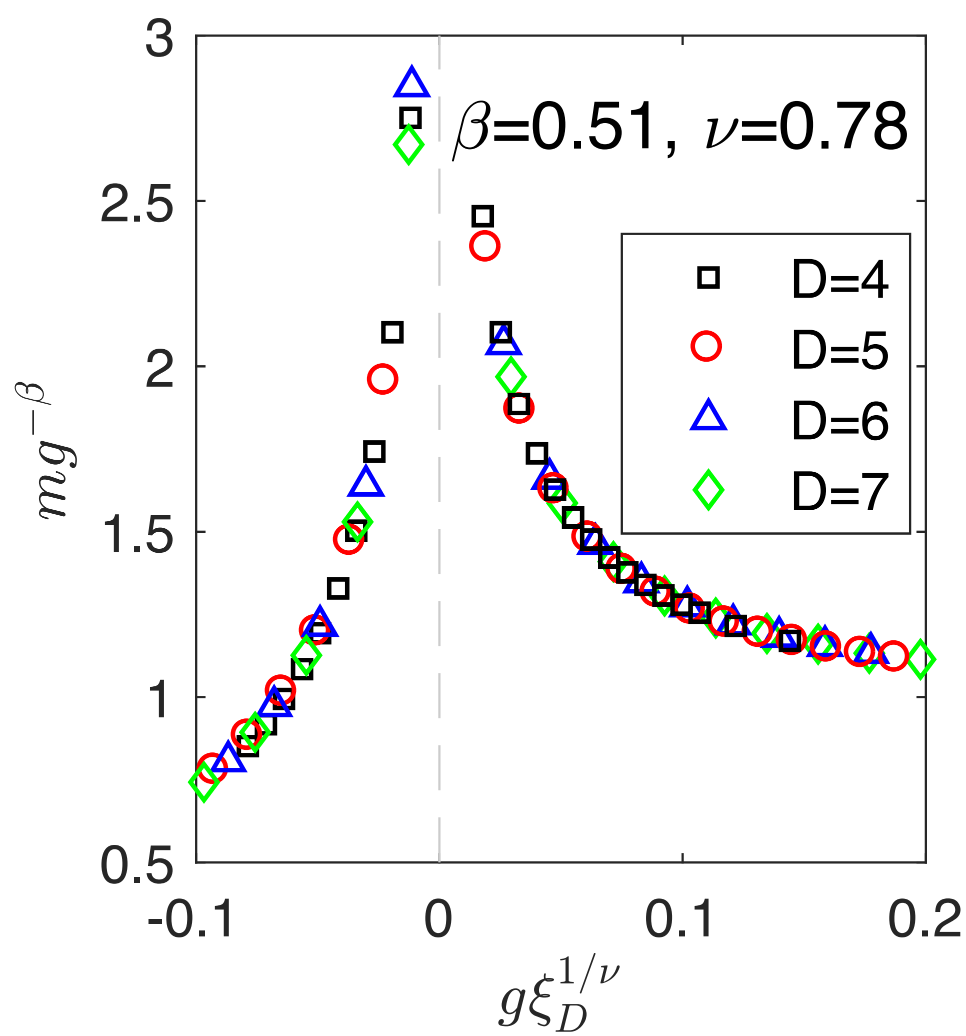
  Wang, PC, Troyer, NJP16 (2014)

Data collapse

$$m(g, D)\, \xi_D^{\beta/\nu} = \mathcal{M}(g\xi_D^{1/\nu})$$



$$m(g, D)\, g^{-\beta} = \tilde{\mathcal{M}}(g\xi_D^{1/\nu})$$



iPEPS: $\beta = 0.51(1) \quad \nu = 0.79(2)$

QMC: $\beta = 0.52(3) \quad \nu = 0.80(3)$

Wang, PC, Troyer, NJP16 (2014)

How to determine V_c?

- Derive ansatz including derivative of m:

$$m(g,D) = \xi_D^{-\beta/\nu}\mathcal{M}(g\xi_D^{1/\nu})$$

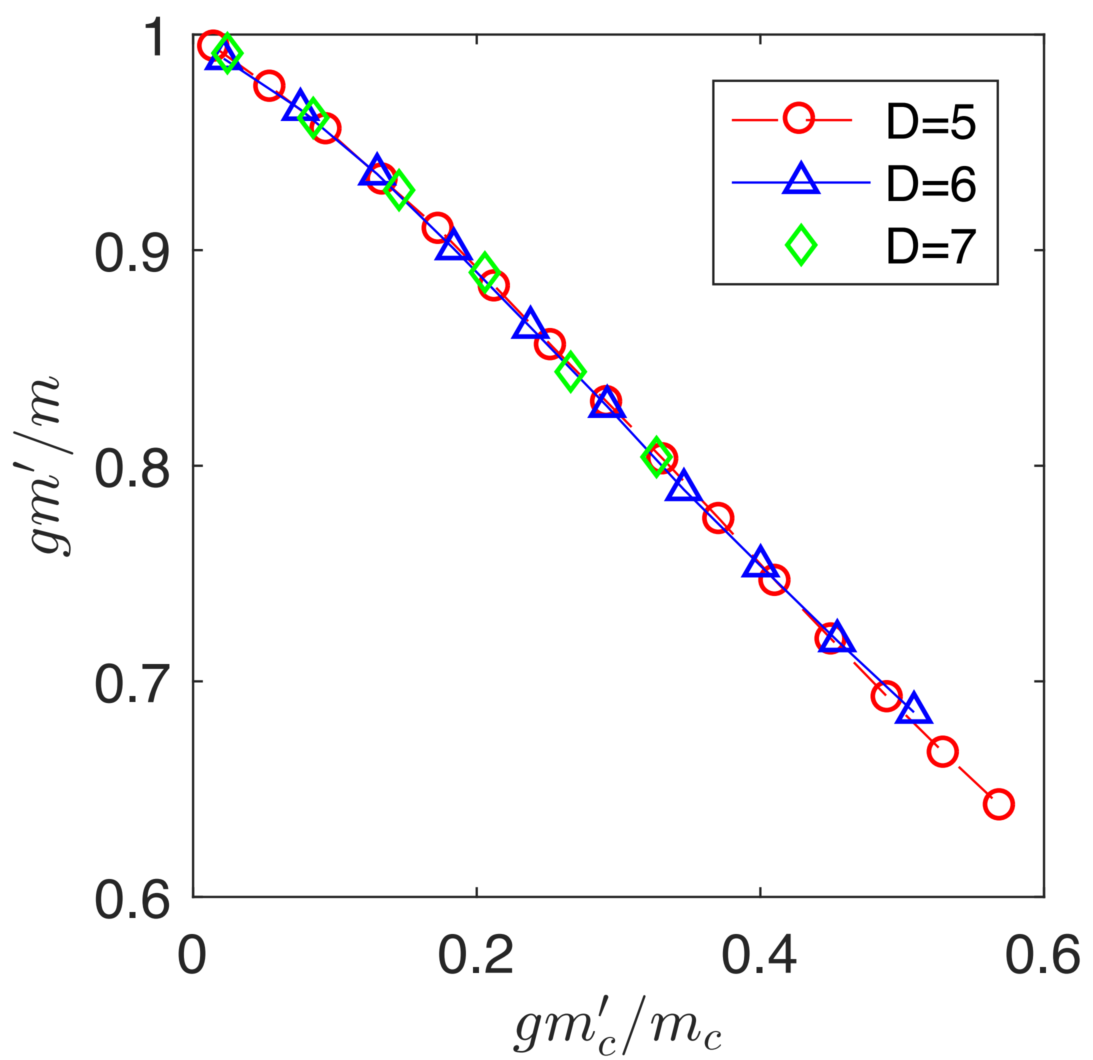
$$m'(g,D) = \xi_D^{-(\beta-1)/\nu}\mathcal{M}'(g\xi_D^{1/\nu})$$

$$\frac{m_c'(D)}{m_c(D)} := \frac{m'(g=0,D)}{m(g=0,D)} \sim \xi_D^{1/\nu}$$

$$\mathcal{M}(g\xi_D^{1/\nu}) \sim \mathcal{P}\left(g\frac{m_c'(D)}{m_c(D)}\right)$$

$$g\frac{m'(g,D)}{m(g,D)} = \mathcal{P}\left(g\frac{m_c'(D)}{m_c(D)}\right)$$

m'/m - approach



iPEPS: $V_c/t = 1.356(2)$

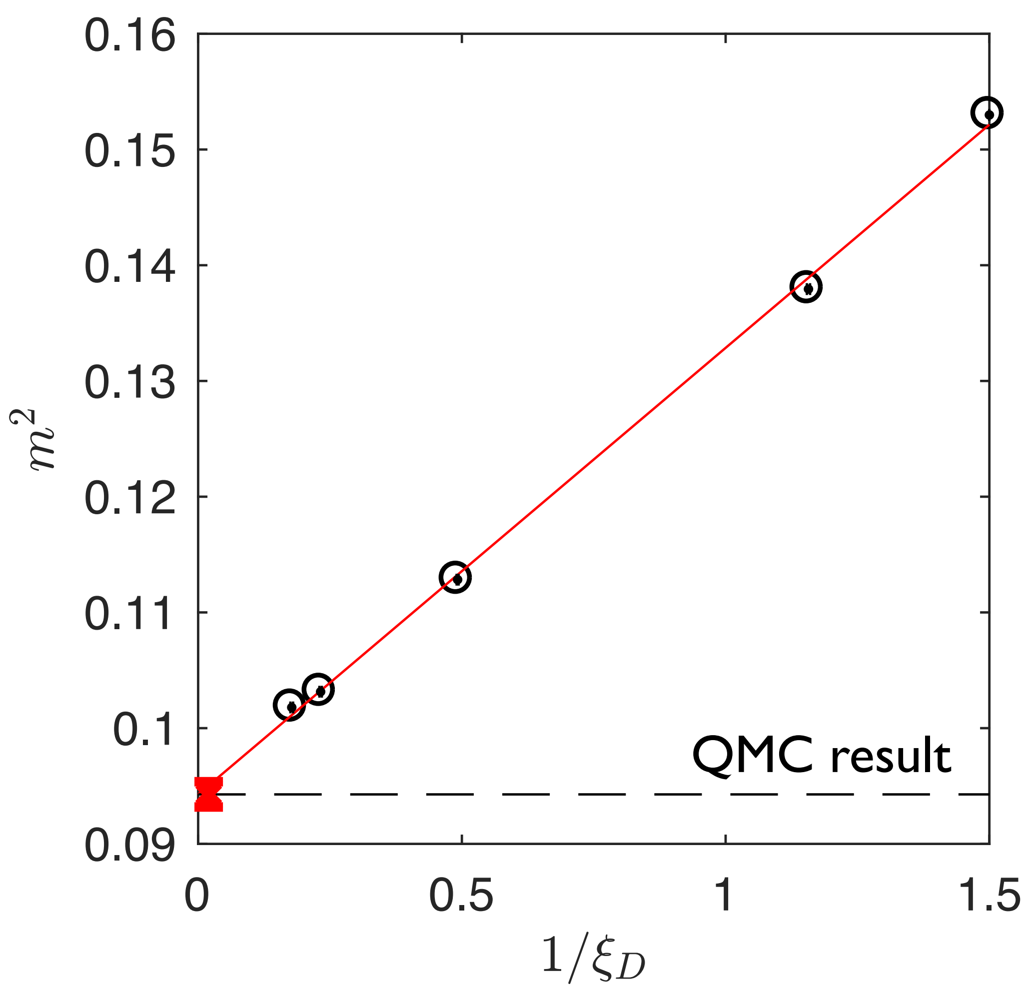
QMC: $V_c/t = 1.356(1)$

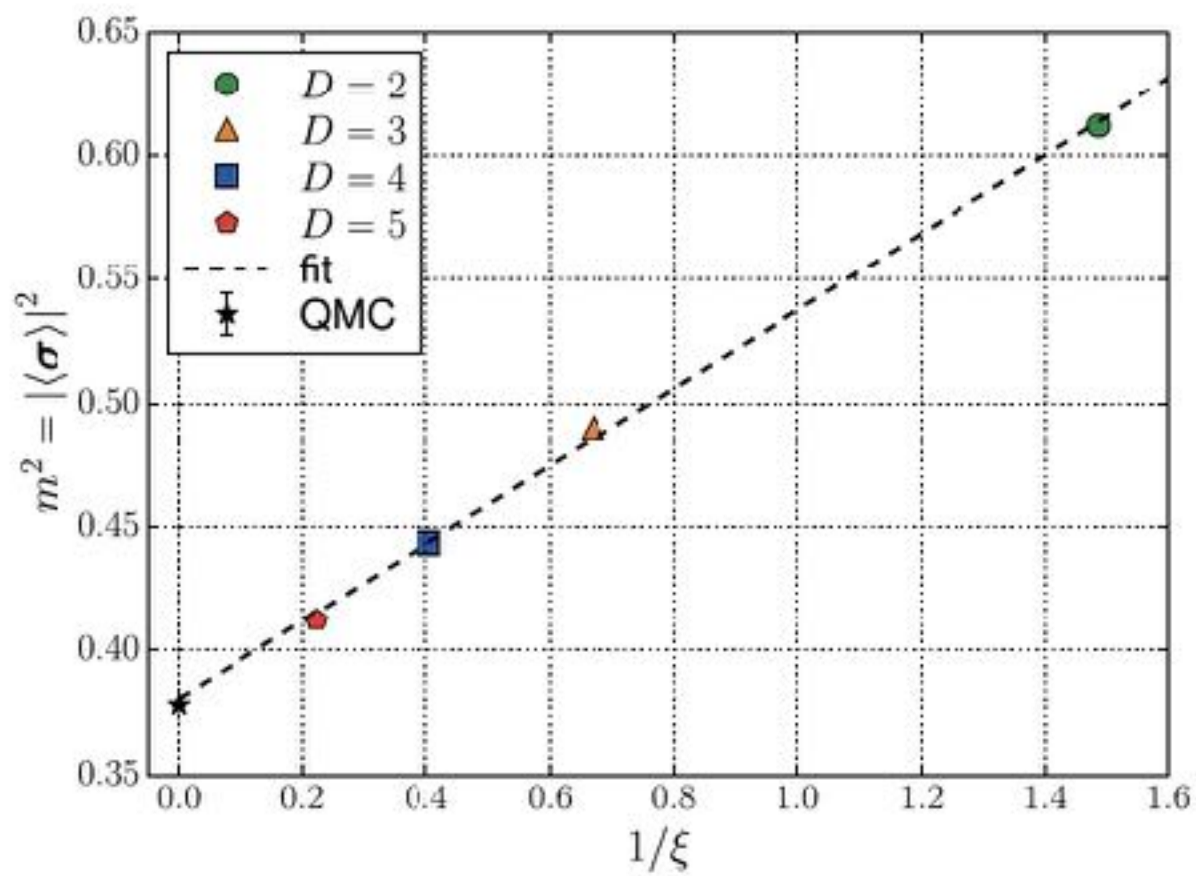
Wang, PC, Troyer, NJP16 (2014)

Extrapolation of order parameter: 2D Heisenberg model

- Use FCL scaling to extrapolate the order parameter in gapless system

Extrapolation in $1/\xi_D$





M. Rader and A. M. Läuchli, PRX 8 (2018)

iPEPS: $m = 0.307 \pm 0.002$

QMC: $m = 0.30743(1)$

Sandvik & Evertz (2010)

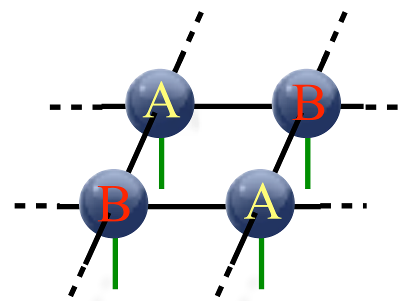
Finite correlation length scaling at finite temperature

Finite temperature simulations with iPEPS

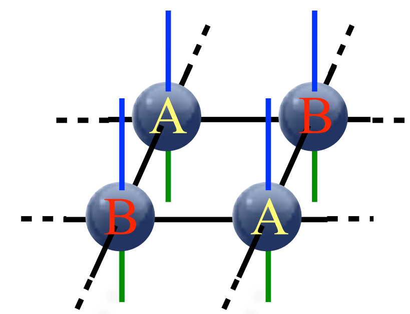
- Methodological developments (2D):

  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), …

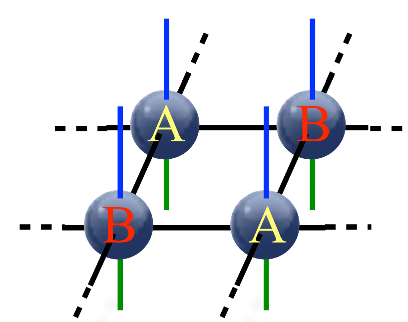
- Wave-function: $|\Psi\rangle \approx$



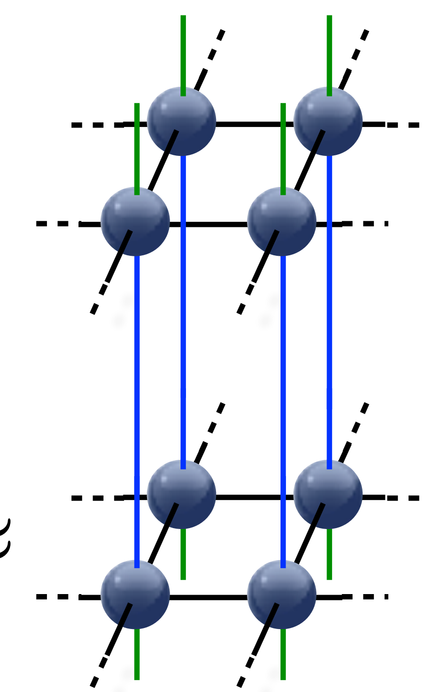
- Density-operator: $\hat{\rho} = e^{-\beta \hat{H}} \approx$



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



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



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

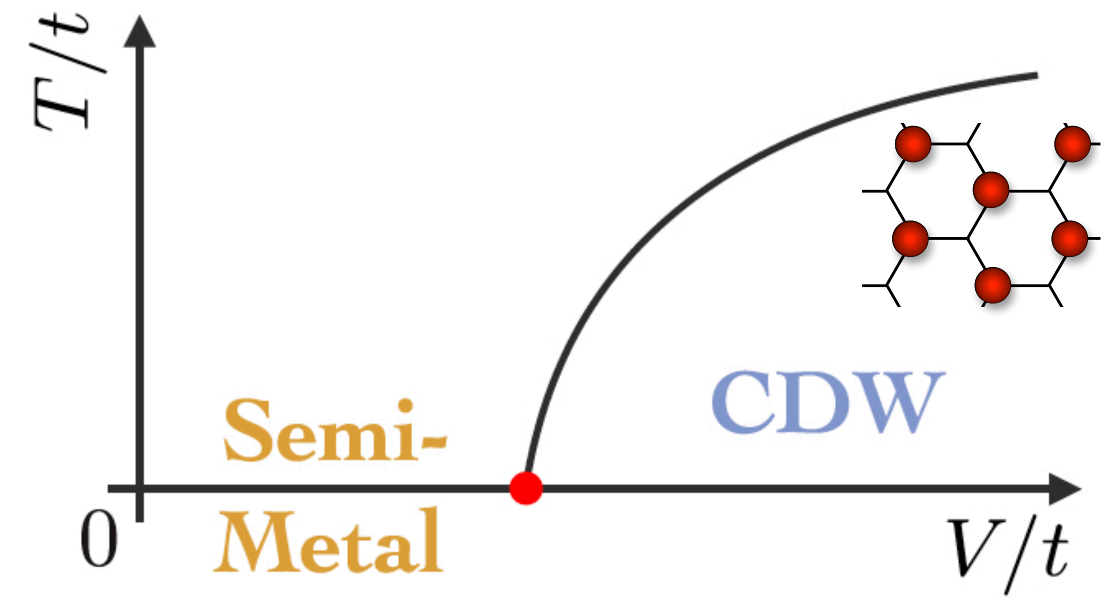
by construction

Finite correlation length scaling at finite T

- Spinless fermions on the honeycomb lattice at finite T (half filling)

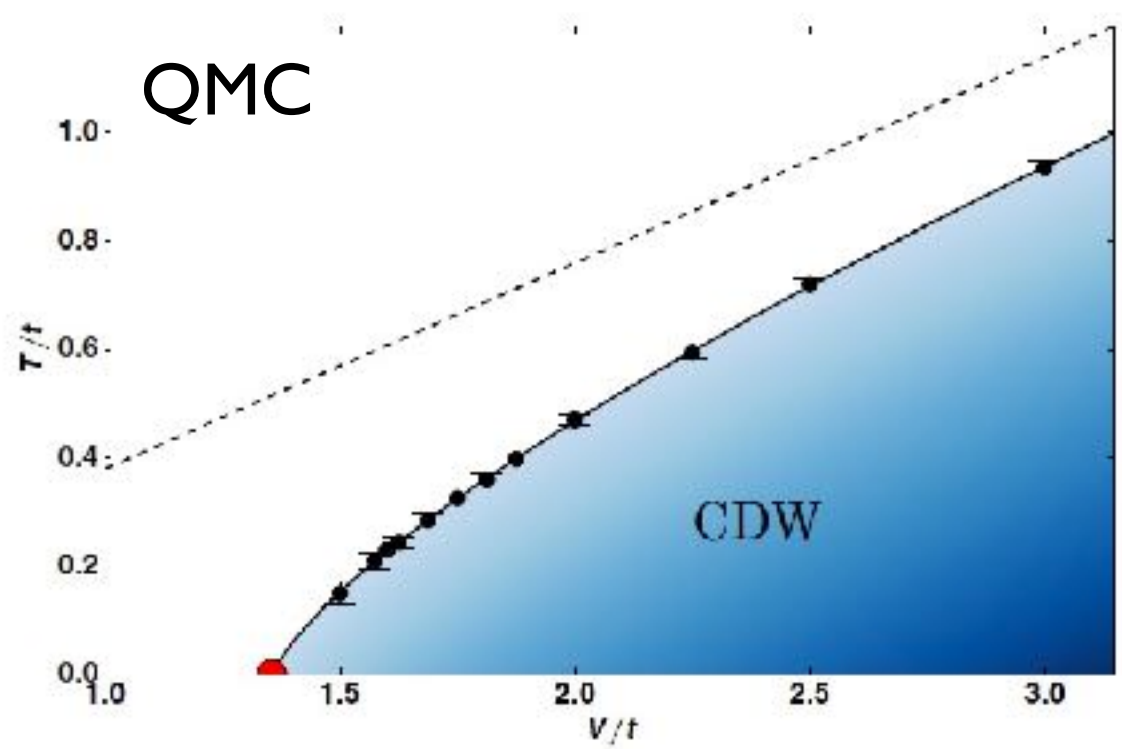
  P. Czarnik & PC, PRB 99, 245107 (2019)

$$\hat{H} = -t \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \left[\hat{c}_{\mathbf{i}}^{\dagger} \hat{c}_{\mathbf{j}} + h.c. \right] + V \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \hat{n}_{\mathbf{i}} \hat{n}_{\mathbf{j}}$$



- Regime: D < D_{exact} $\rightarrow$ finite ξ_D

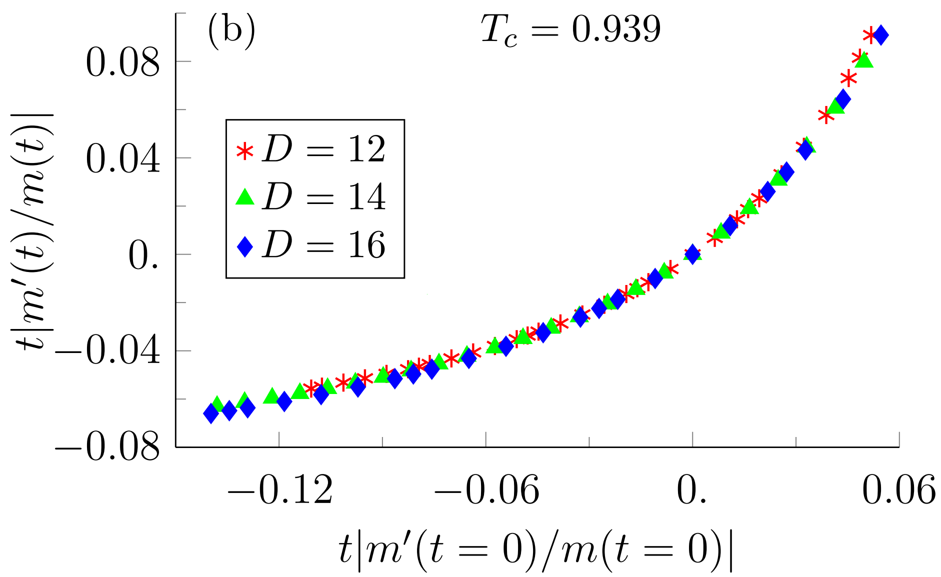
- Consider cuts at V/t=3 and V/t=2

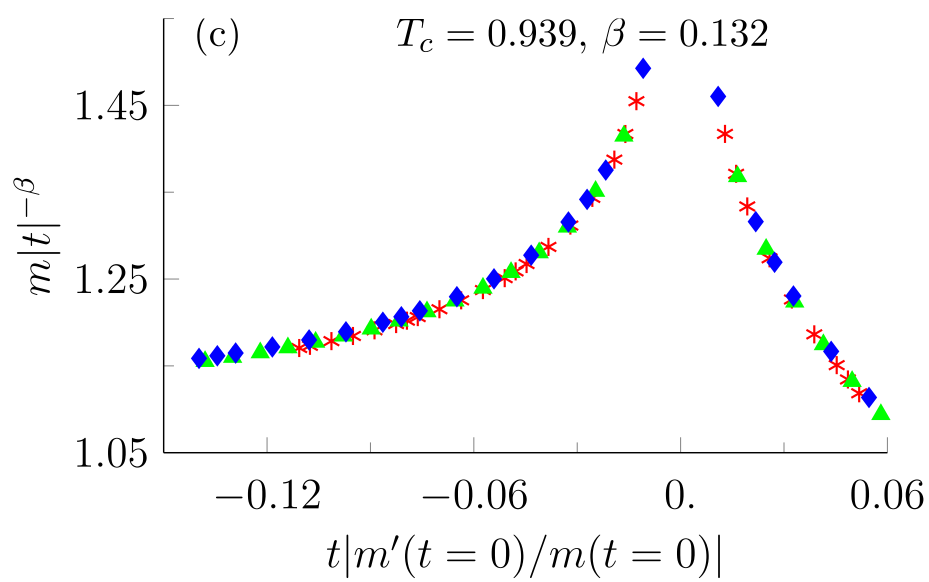


Hesselmann & Wessel, PRB 93 (2016)

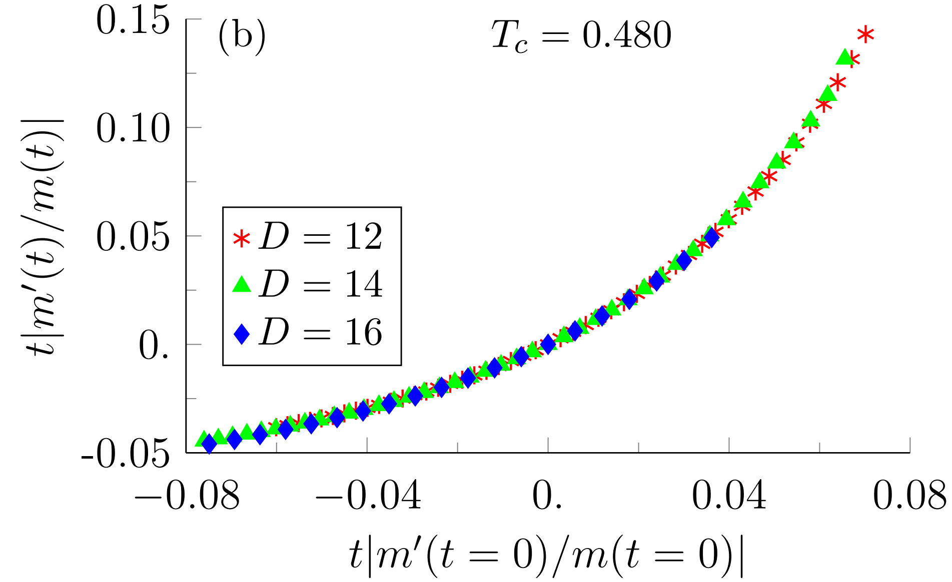
Finite correlation length scaling at finite T

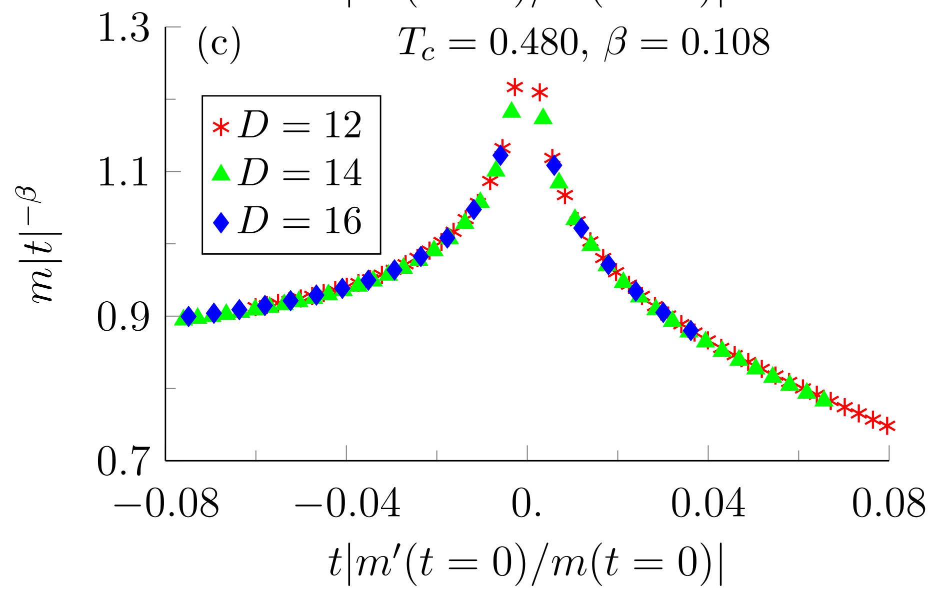
$V/t = 3$





$V/t = 2$





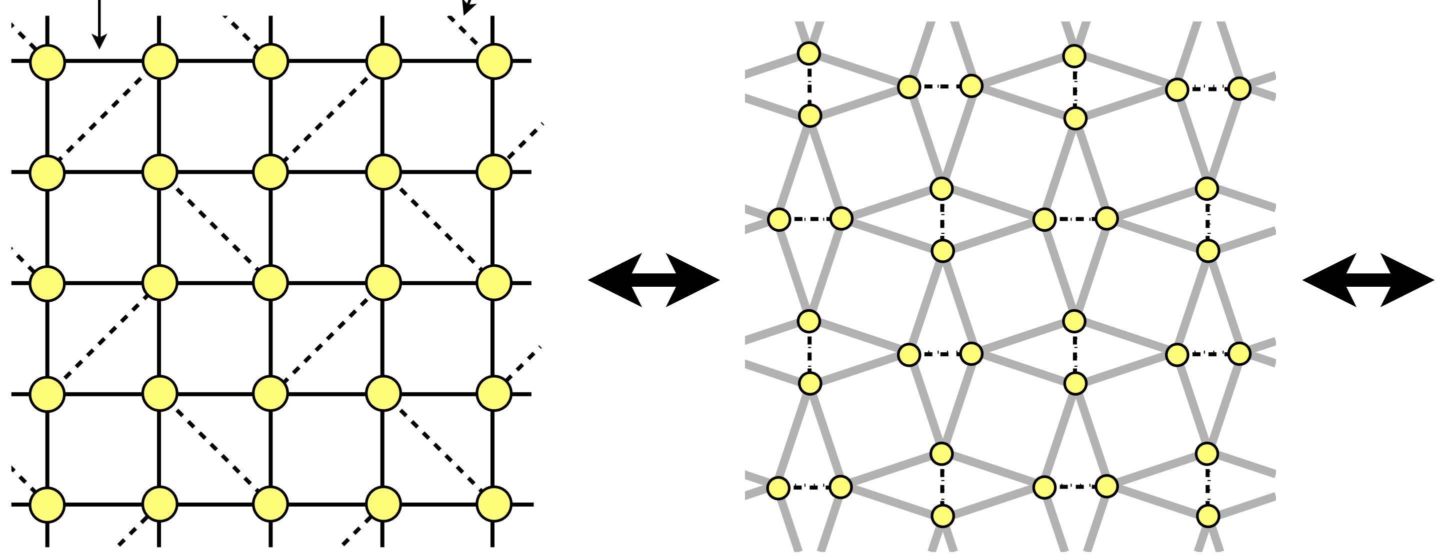
iPEPS: $T_c = 0.939(4)$ $\beta = 0.132(8)$ $T_c = 0.480(5)$ $\beta = 0.108(4)$

QMC: $T_c = 0.936(10)$ $\beta_{exact} = 1/8$ $T_c = 0.47(1)$ $\beta_{exact} = 1/8$

Hesselmann & Wessel, PRB 93 (2016)

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

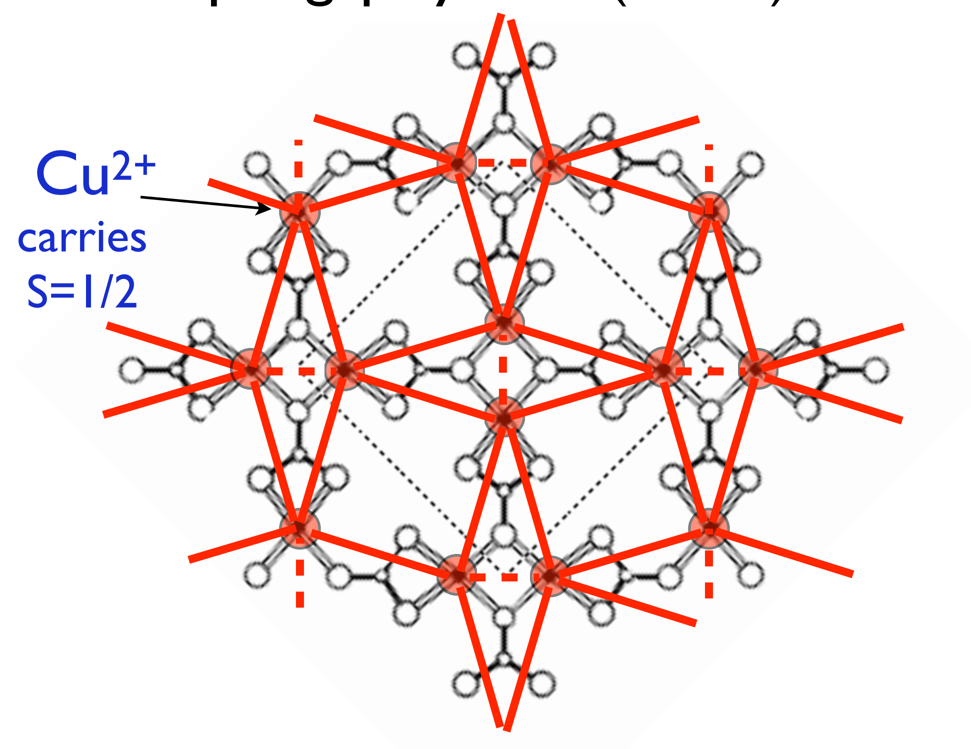
$$\hat{H} = J' \sum_{\langle i,j \rangle} S_i \cdot S_j + J \sum_{\langle\langle i,j \rangle\rangle_{\rm dimer}} S_i \cdot S_j$$



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

$SrCu_2(BO_3)_2$

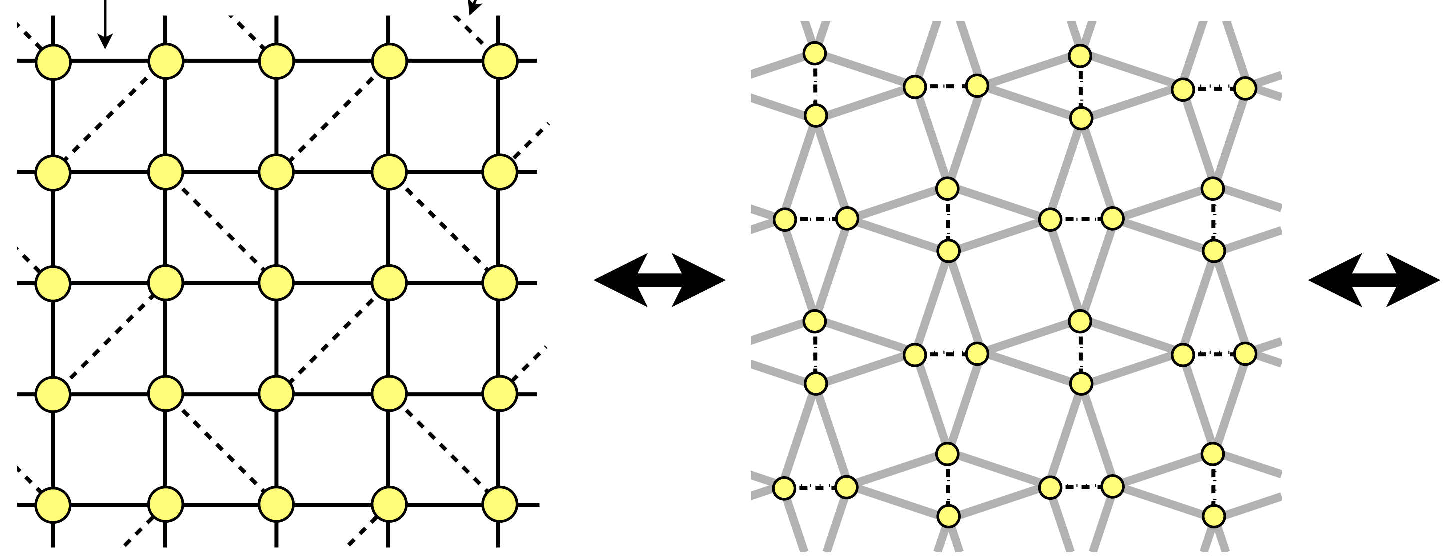
Spin-gap system (~35K)



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

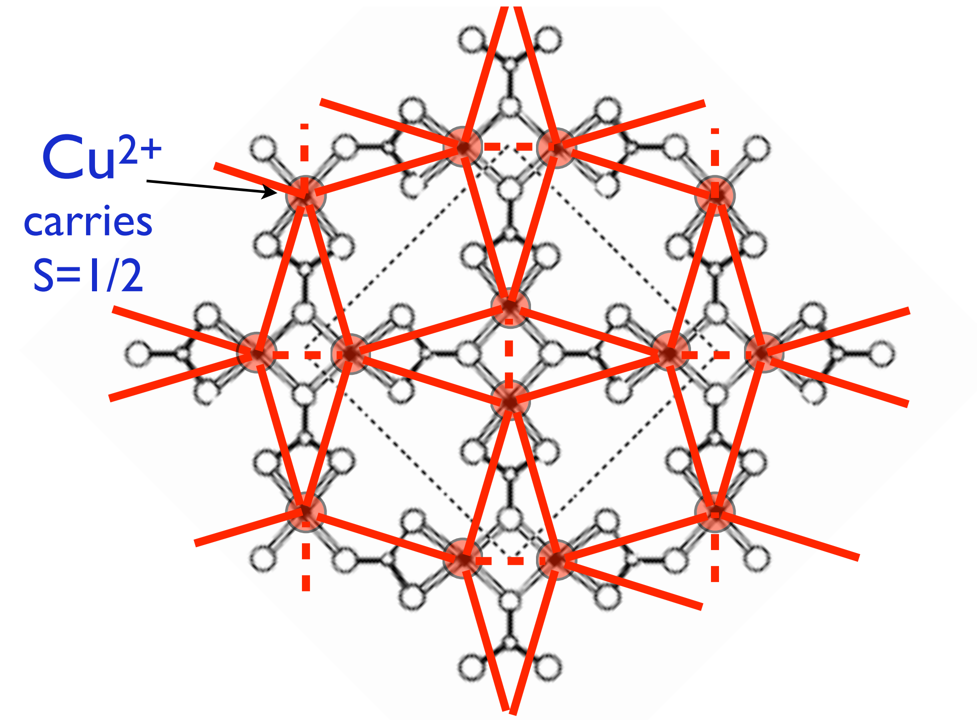
The Shastry-Sutherland model and $SrCu_2(BO_3)_2$

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

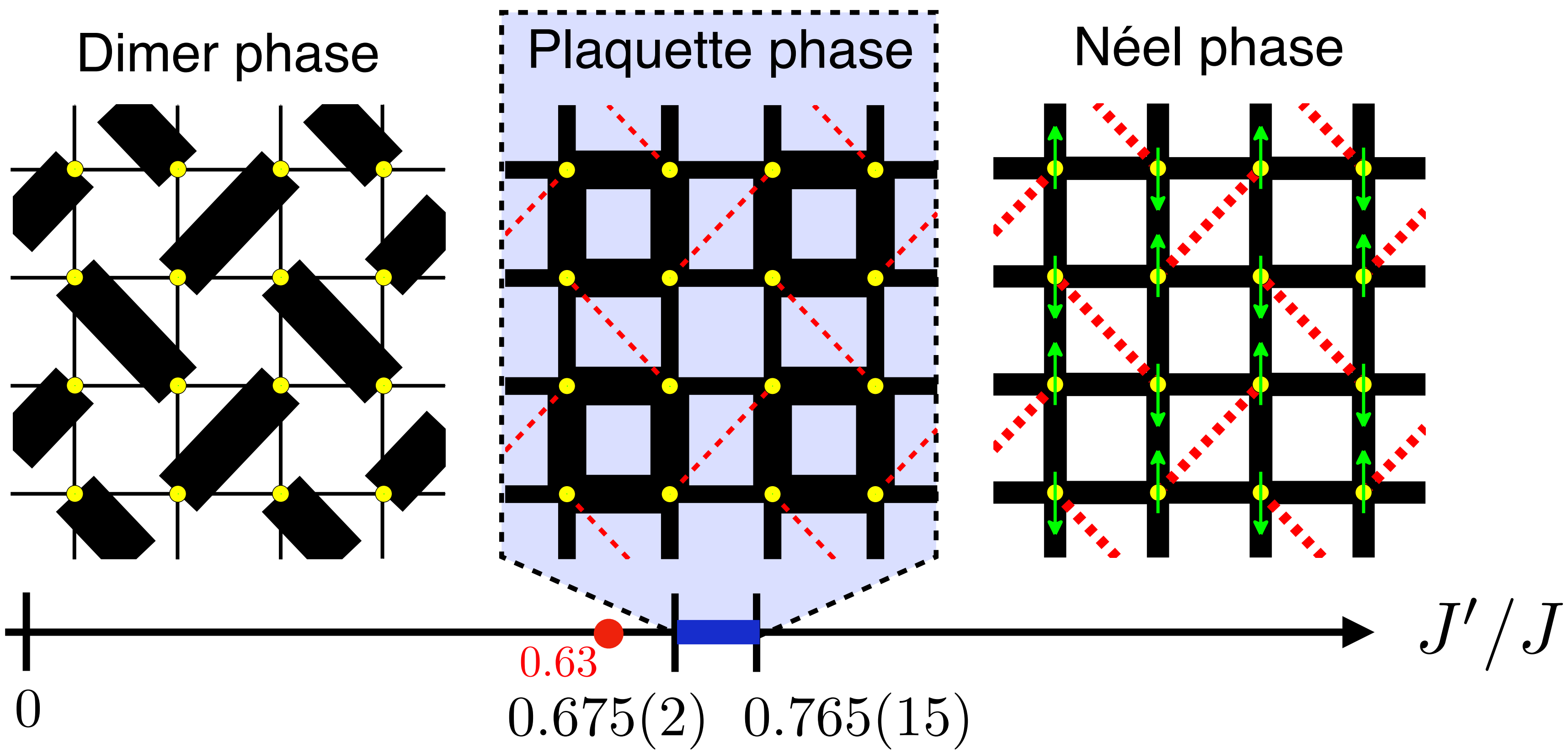


$SrCu_2(BO_3)_2$

Spin-gap system (~35K)



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

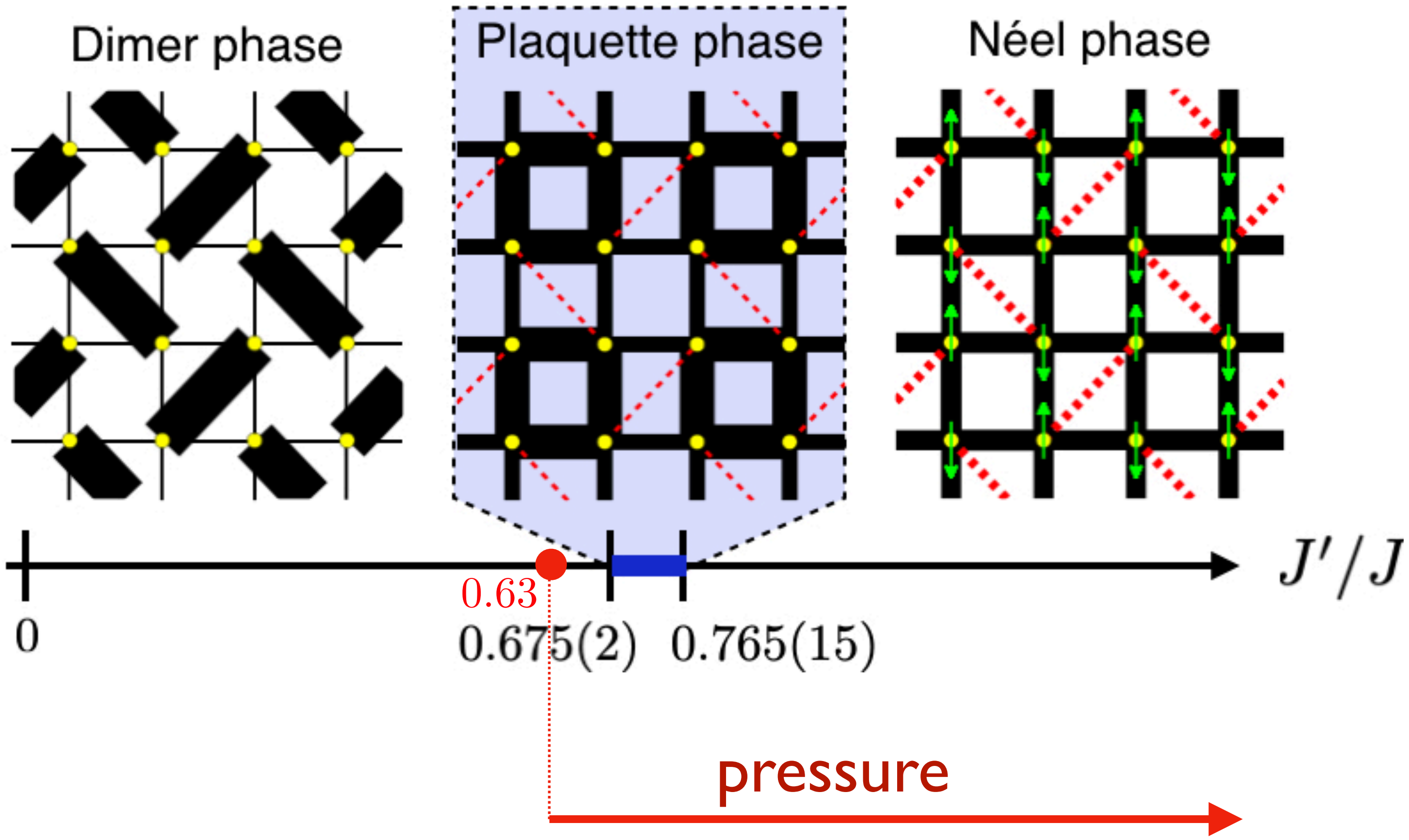


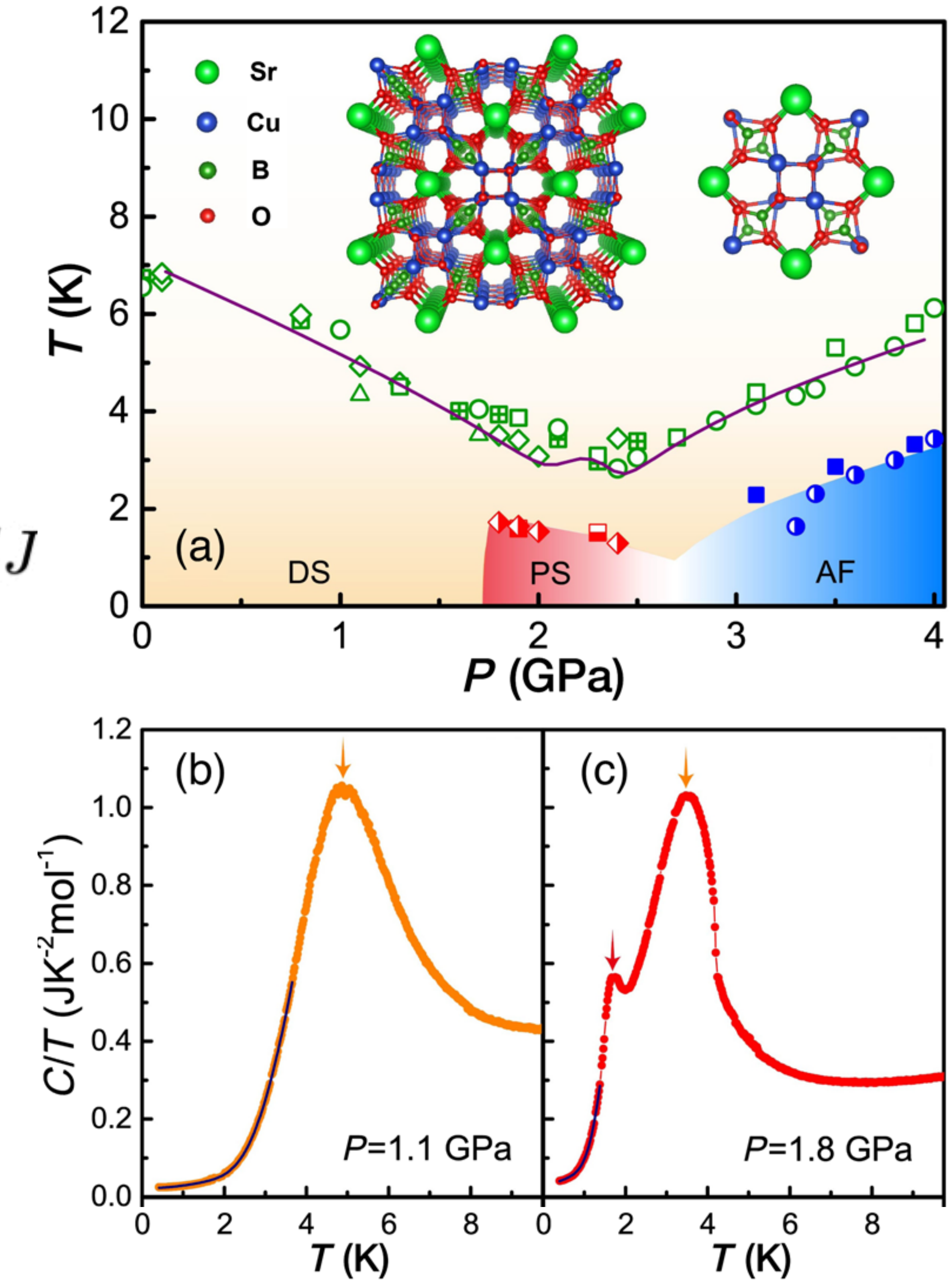
Corboz and Mila, PRB **87** (2013)

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



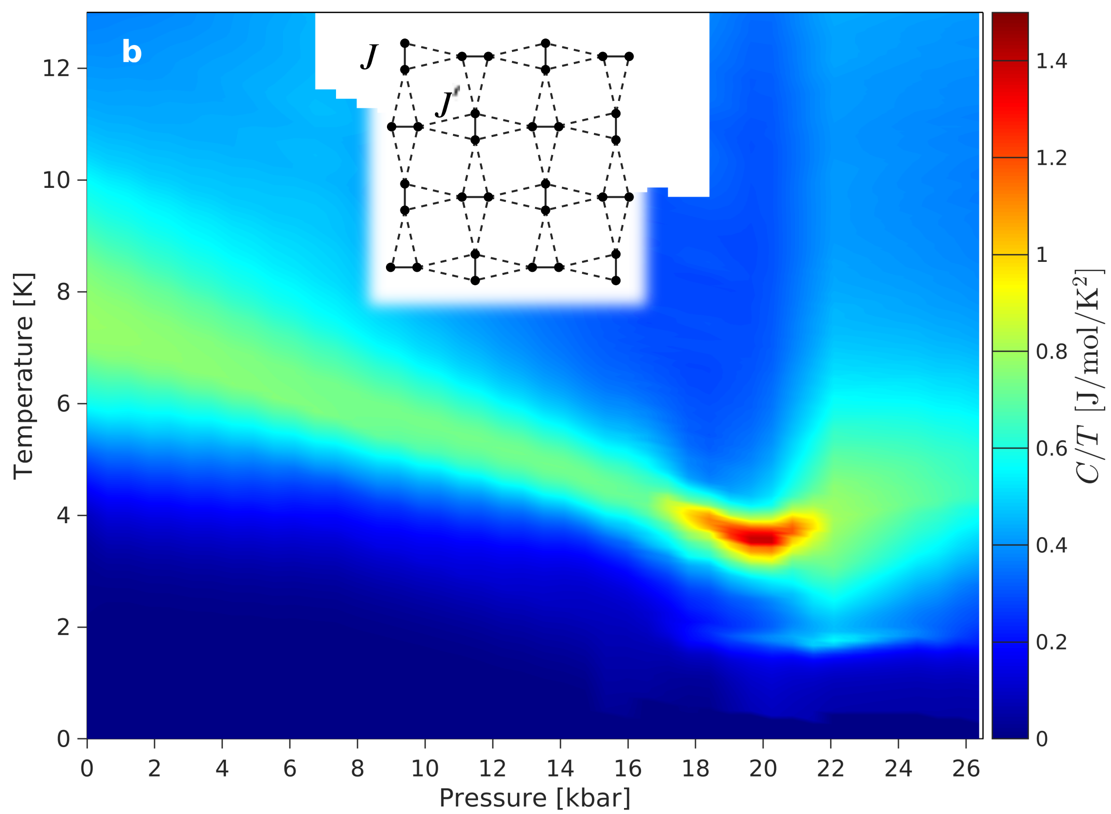


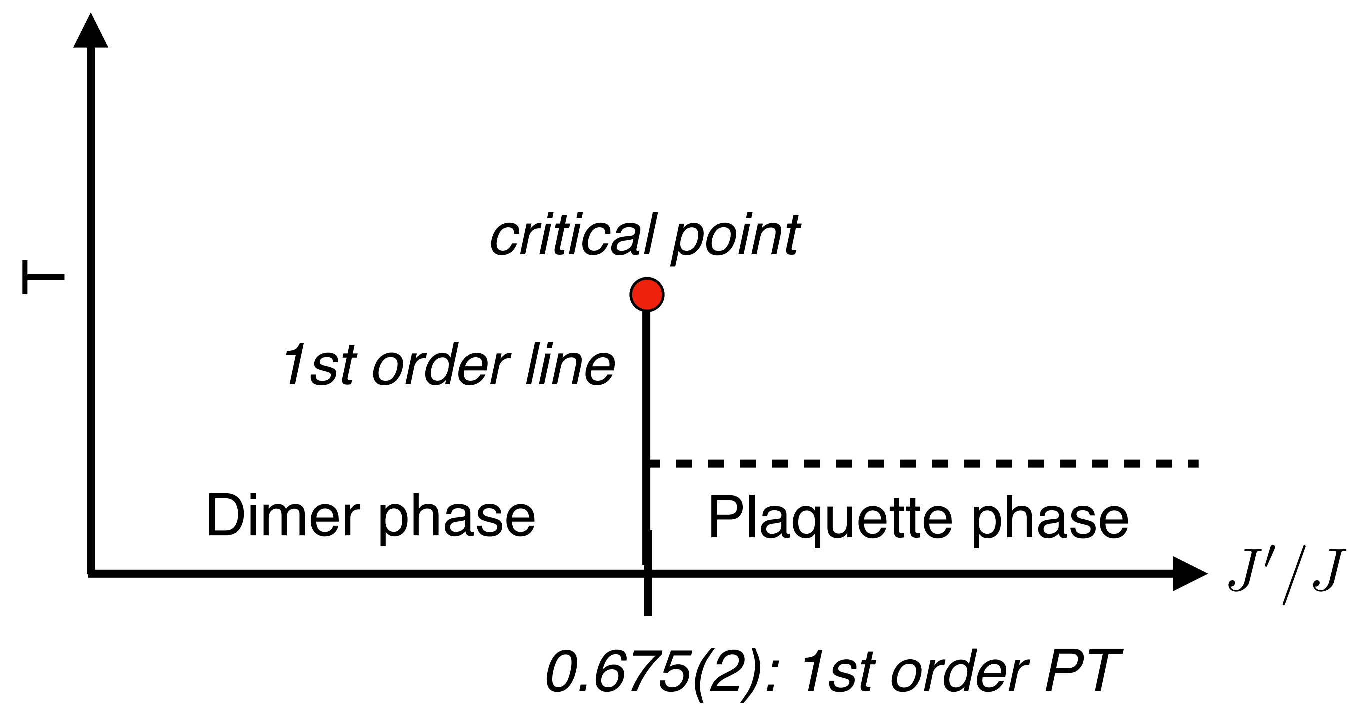
Guo, et al., PRL 124, 206602 (2020)

Drive system across the phase transitions!

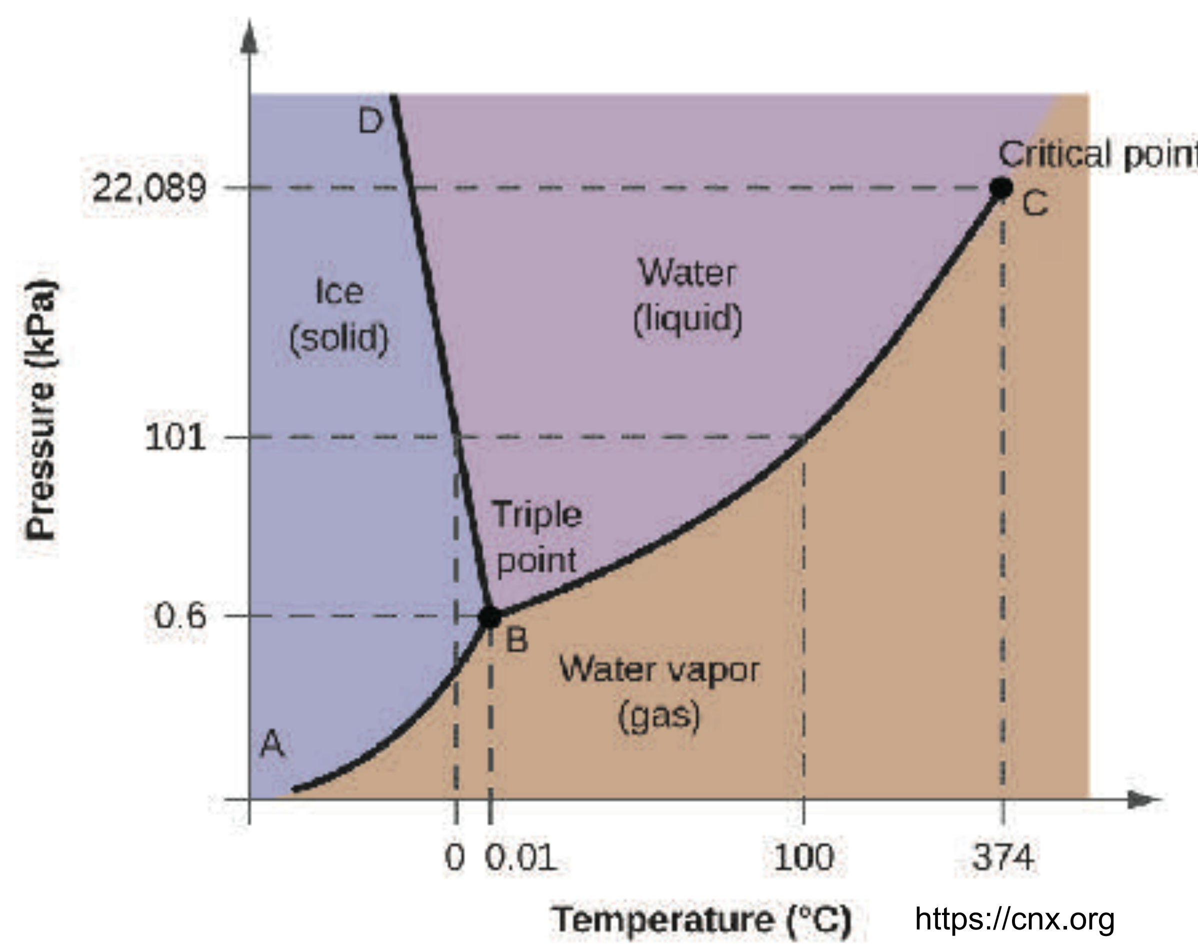
Waki, et al. J. Phys. Soc. Jpn. 76, 073710 (2007)
Haravifard, et al. Nat. Commun. 7, 11956 (2016)
Zayed, et al., Nat. Phys. 13, 962 (2017)
Sakurai, et al., J. Phys. Soc. Jpn. 87, 033701 (2018)
Guo, et al., PRL 124, 206602 (2020)
Bettler, et al,. Phys. Rev. Research 2, 012010 (2020)
…

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

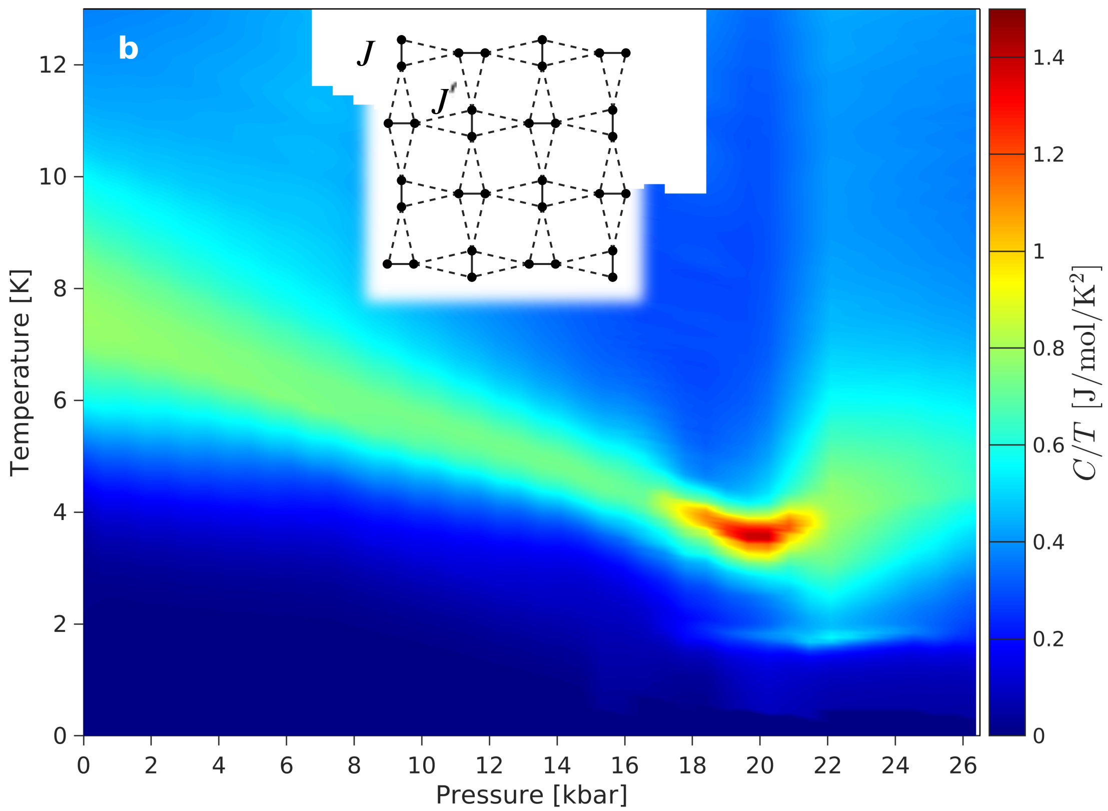


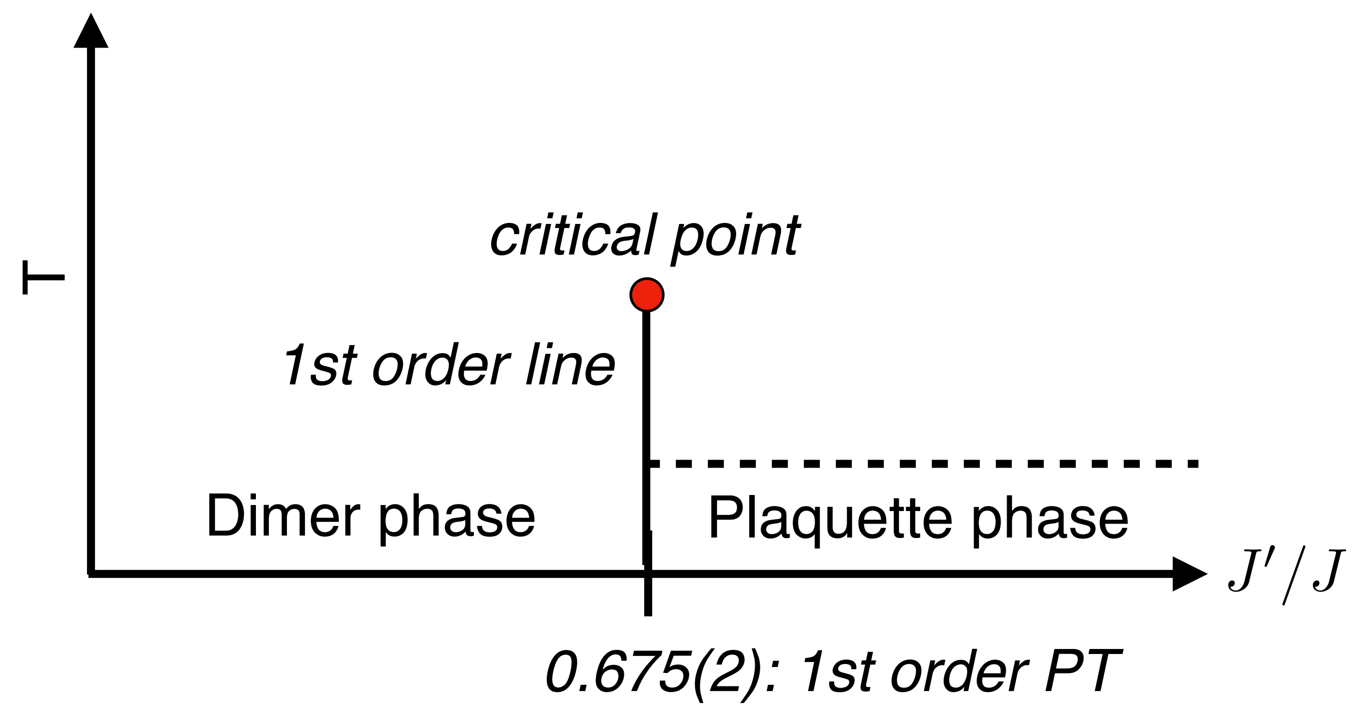


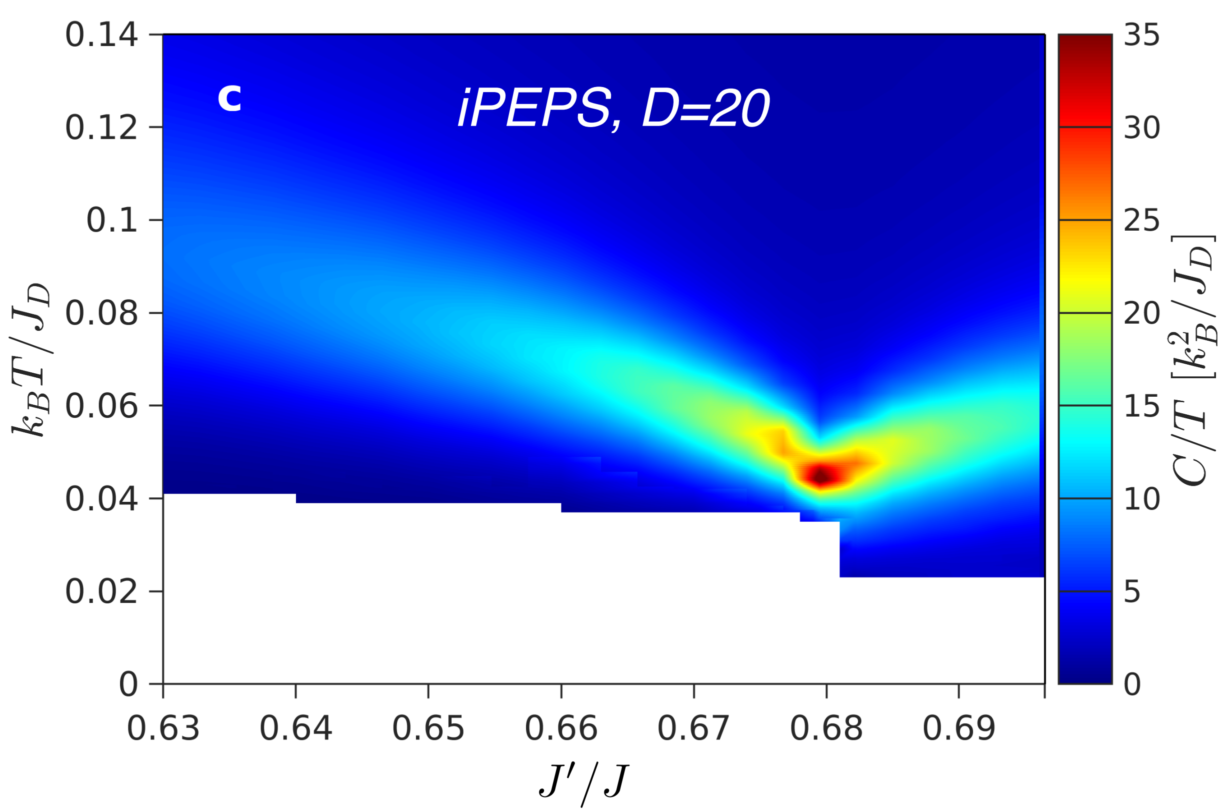
Can we reproduce this with iPEPS?

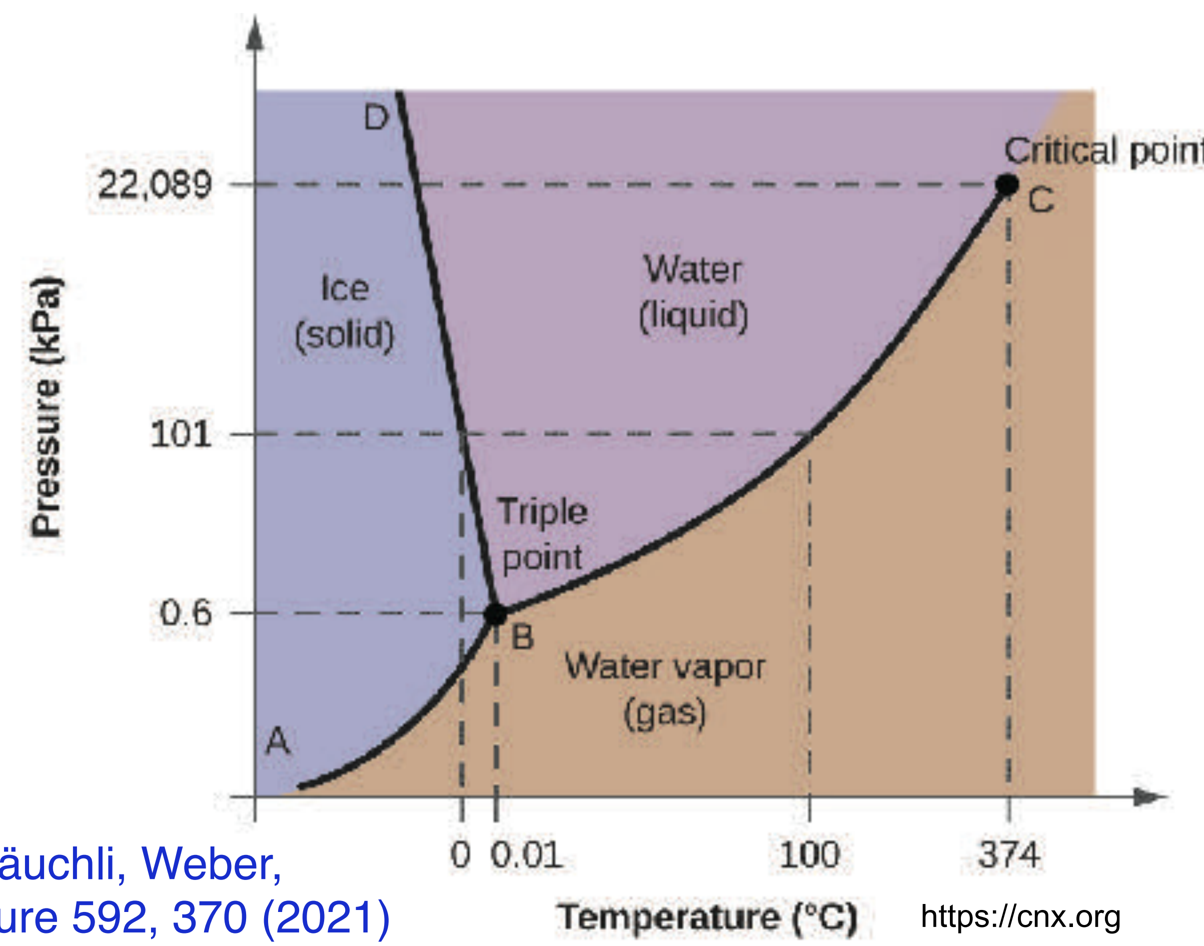


Specific heat data (group of H. M. Rønnow)





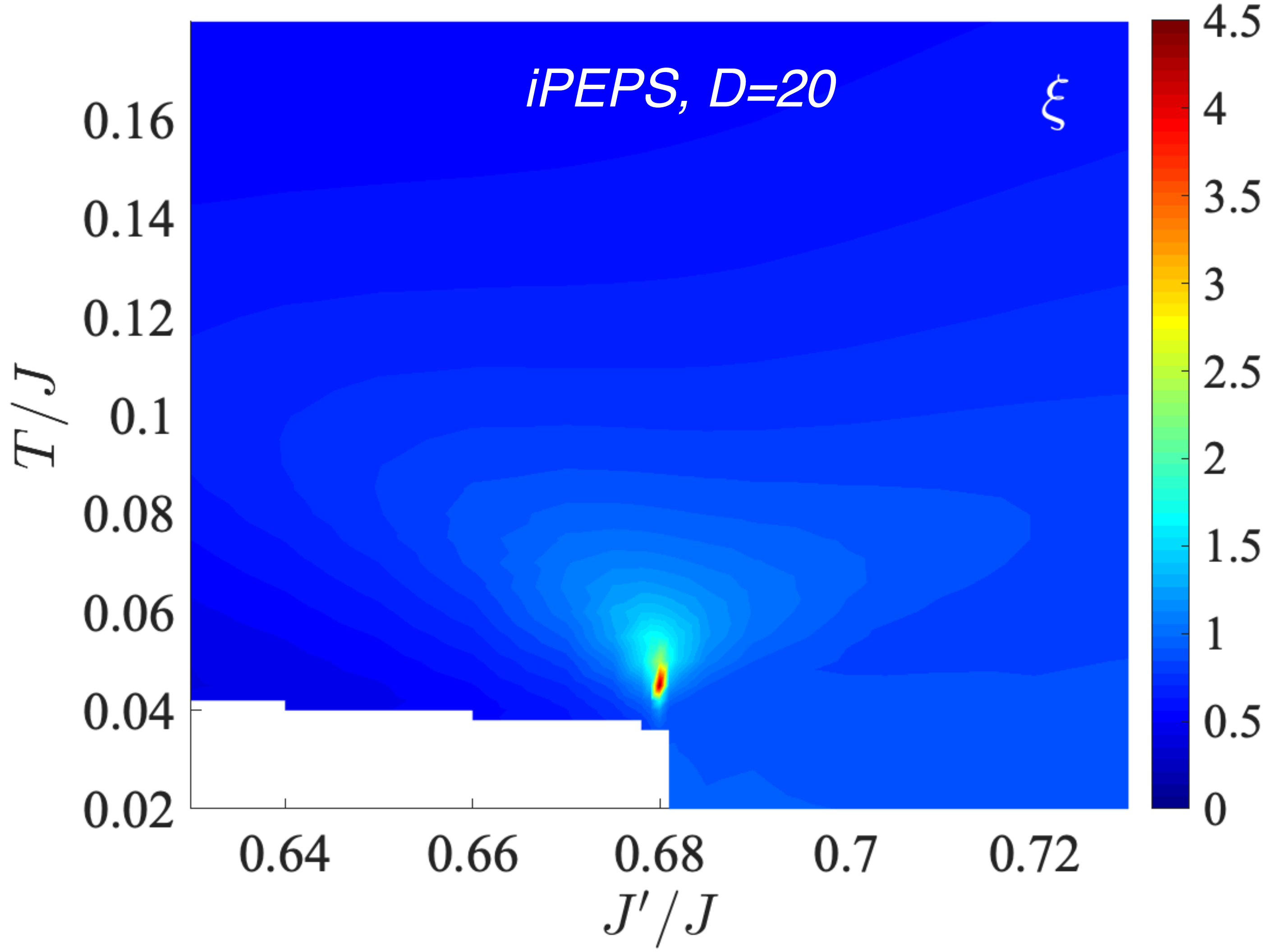




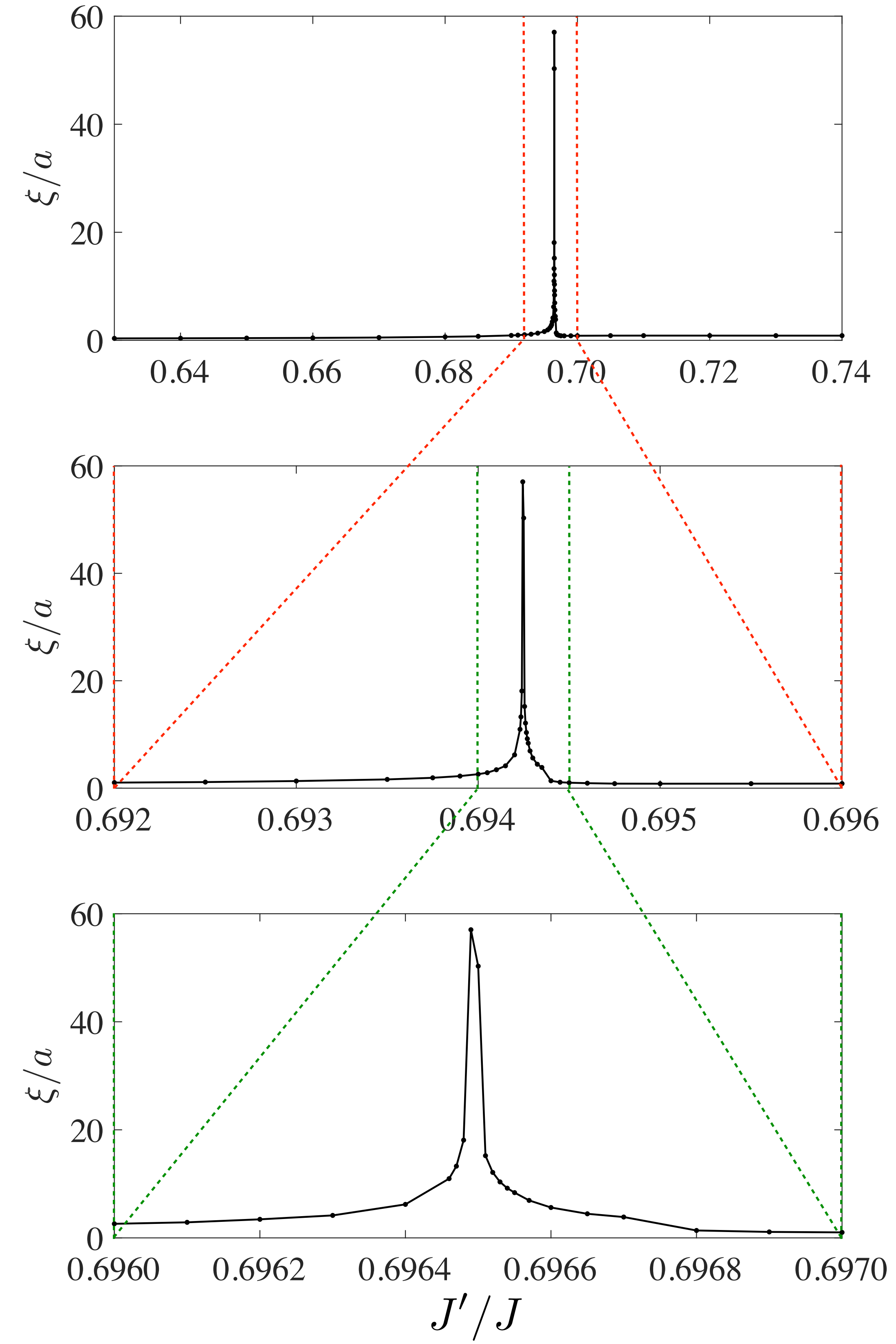
https://cnx.org

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

Correlation length



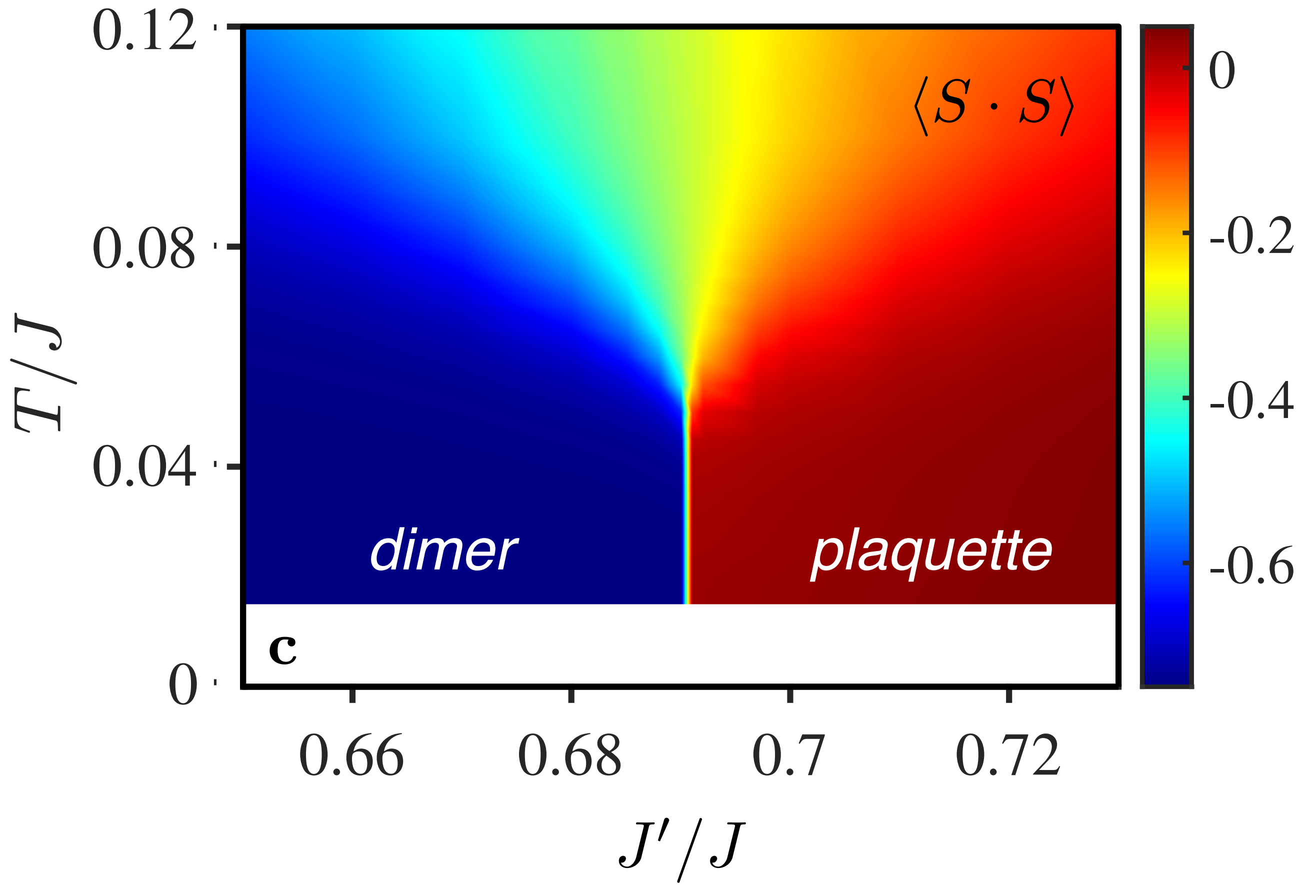
Zooming-in (D=8)



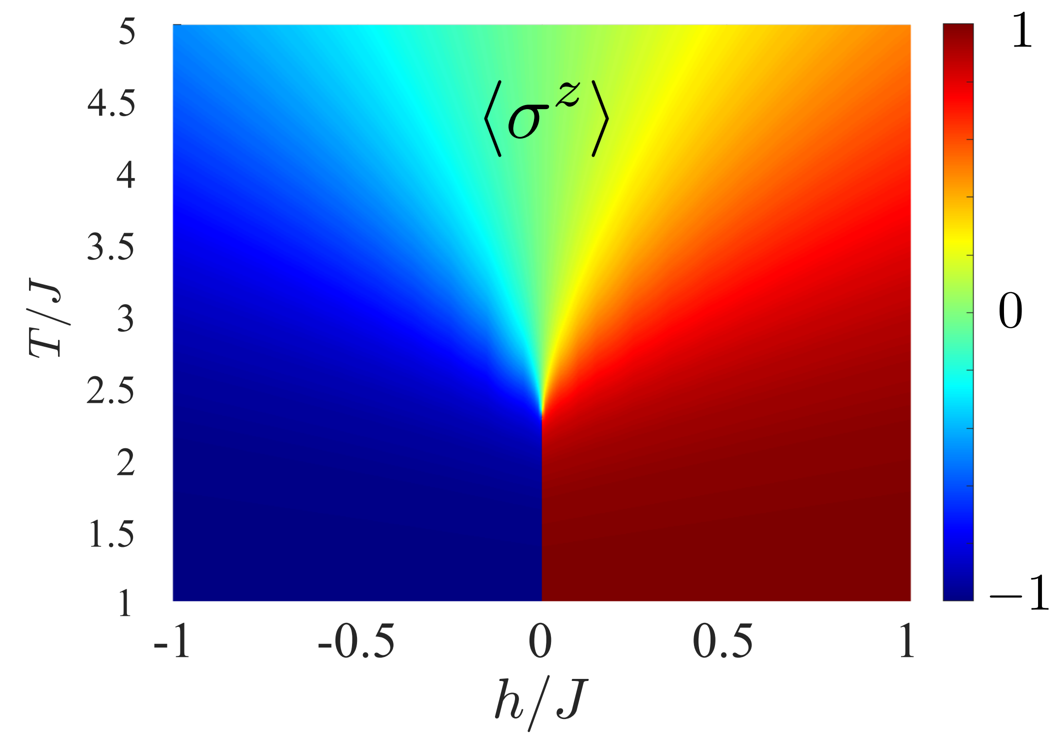
Diverging correlation length compatible with a critical point

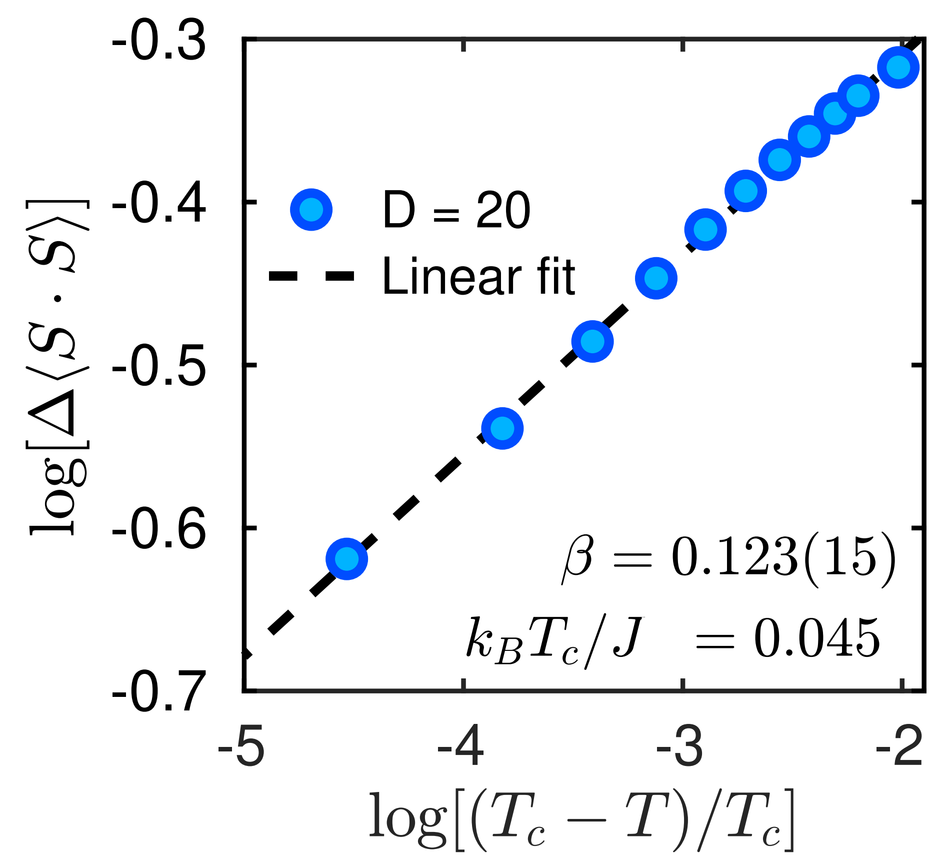
Jump in <S · S> on dimer

iPEPS D=10 (with DM)



2D classical Ising model in a field





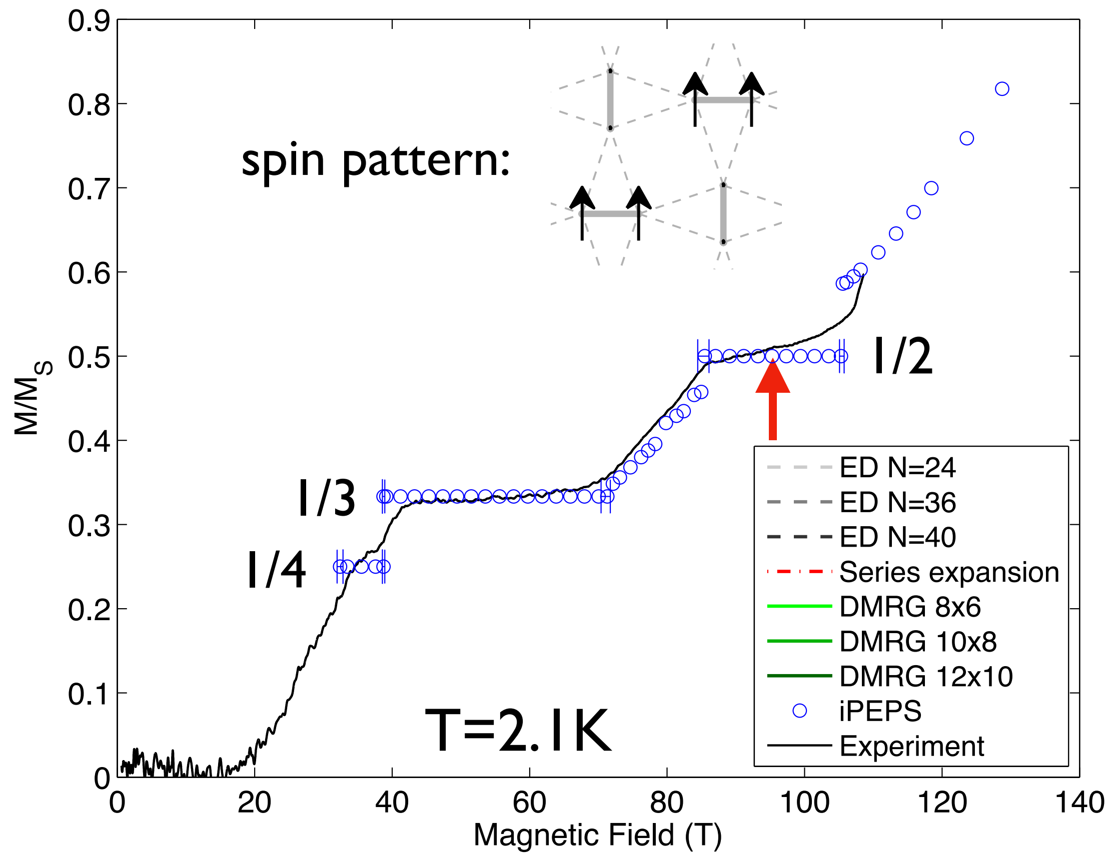
Clear evidence of a first order line with a critical point compatible with the 2D Ising universality class

exact value:
$\beta = 0.125$

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

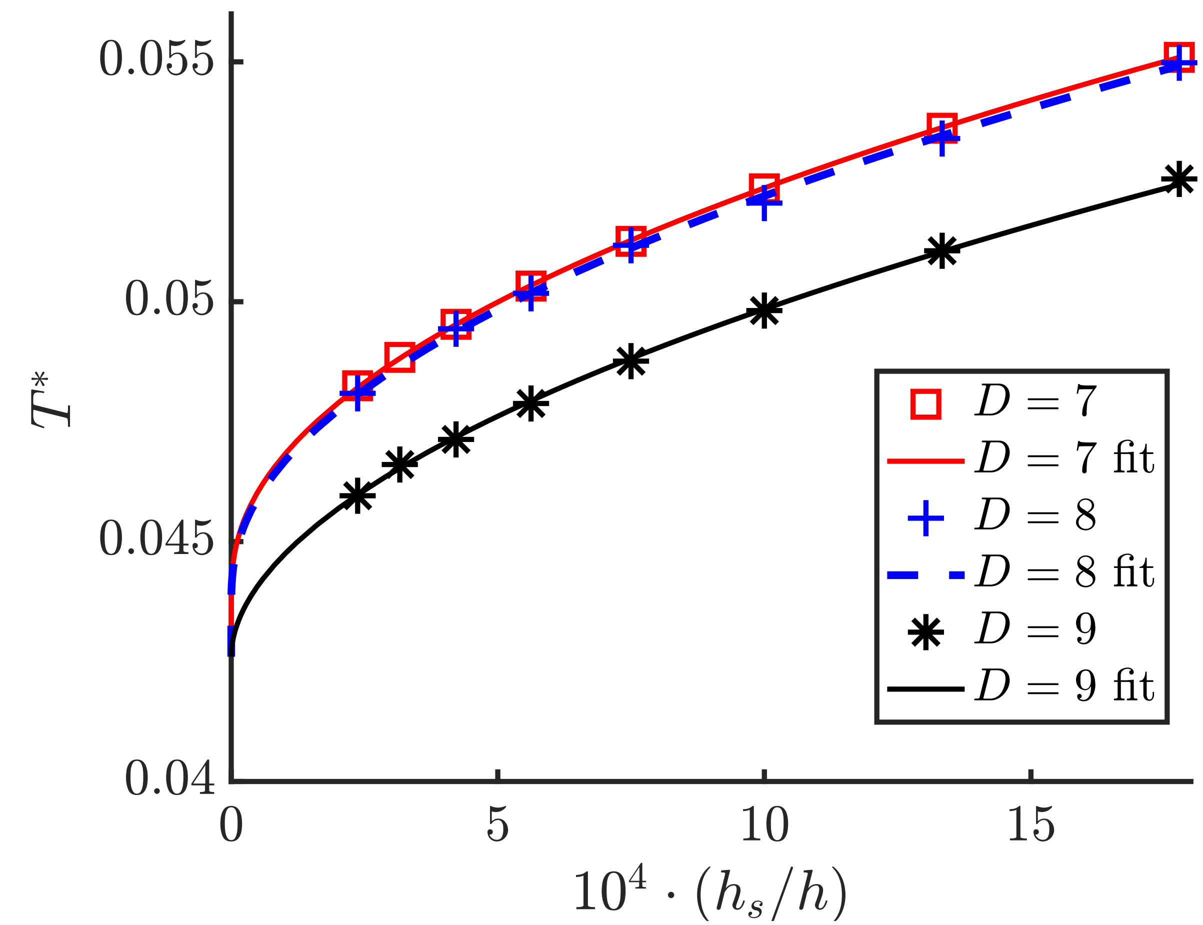
P. Czarnik, M. M. Rams, PC, and J. Dziarmaga, PRB 103, 075113 (2021)

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

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

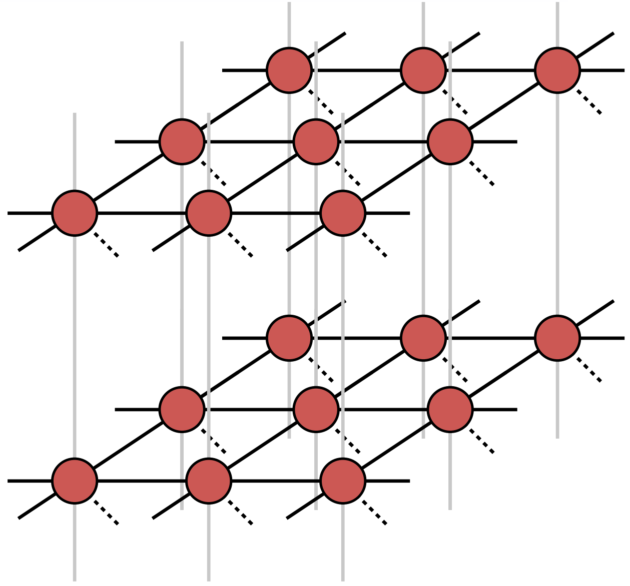
iPEPS for 3D quantum systems

Motivation: success of TN in 1D & 2D

- iPEPS: 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)
S. Yang, T. B. Wahl, H.-H. Tu, N. Schuch, and J. I. Cirac, PRL 114, 106803 (2015)
T. Liu, W. Li, A. Weichselbaum, J. von Delft, and G. Su, PRB 91, 060403 (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.-W. Li, B. Bruognolo, A. Weichselbaum, and J. von Delft, PRB 103, 075127 (2021)
J. Hasik, D. Poilblanc, and F. Becca, SciPost Physics 10, 012 (2021)
… and many more …

Tensor networks for 3D quantum systems?

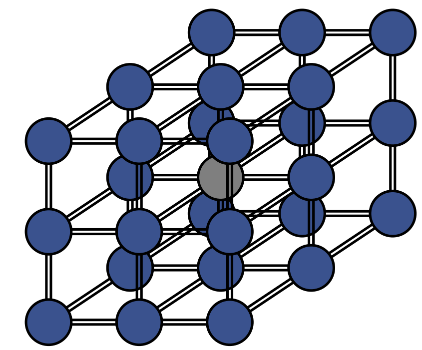


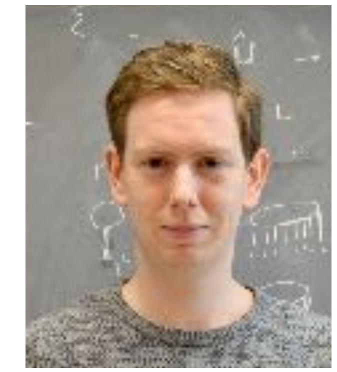
- **Main challenge: how to contract it??**
- Several works in the context of 3D classical or 2+1D:
  - **3D HOTRG:**
    Xie, Chen, Qin, Zhu, Yang, Xiang, PRB 86, 045139 (2012)
  - **Corner-transfer matrix (CTM) in 3D:**
    Nishino and Okunishi, J. Phys. Soc. Jpn. 67, 3066 (1998)
    Orús, Phys. Rev. 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); Vlaar & PC, arxiv:2208.06423

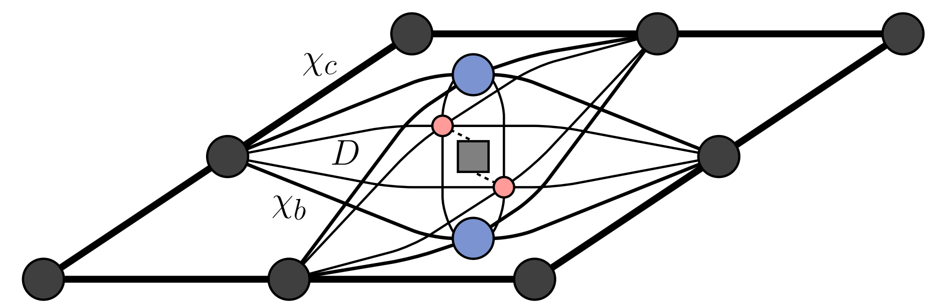
- **Cluster contractions:**
  - ✦ Contract finite clusters instead of full network
  - ✦ cheap & simple
  - ✦ Not very accurate, but useful for quick results



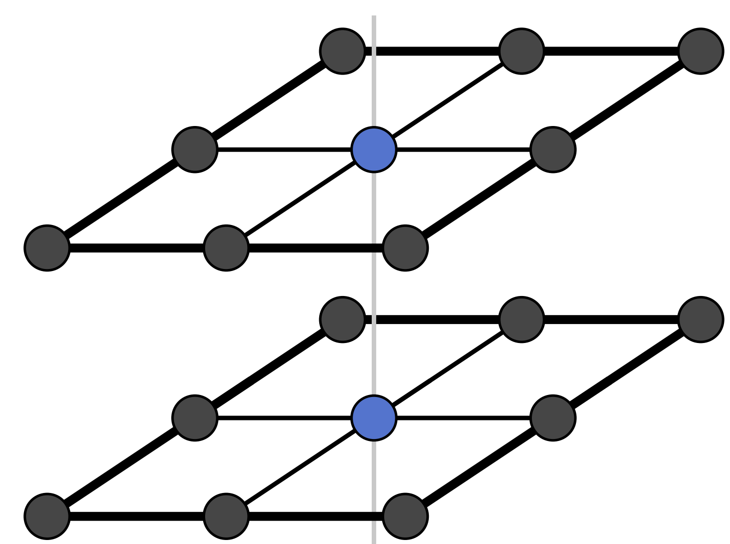


Patrick Vlaar

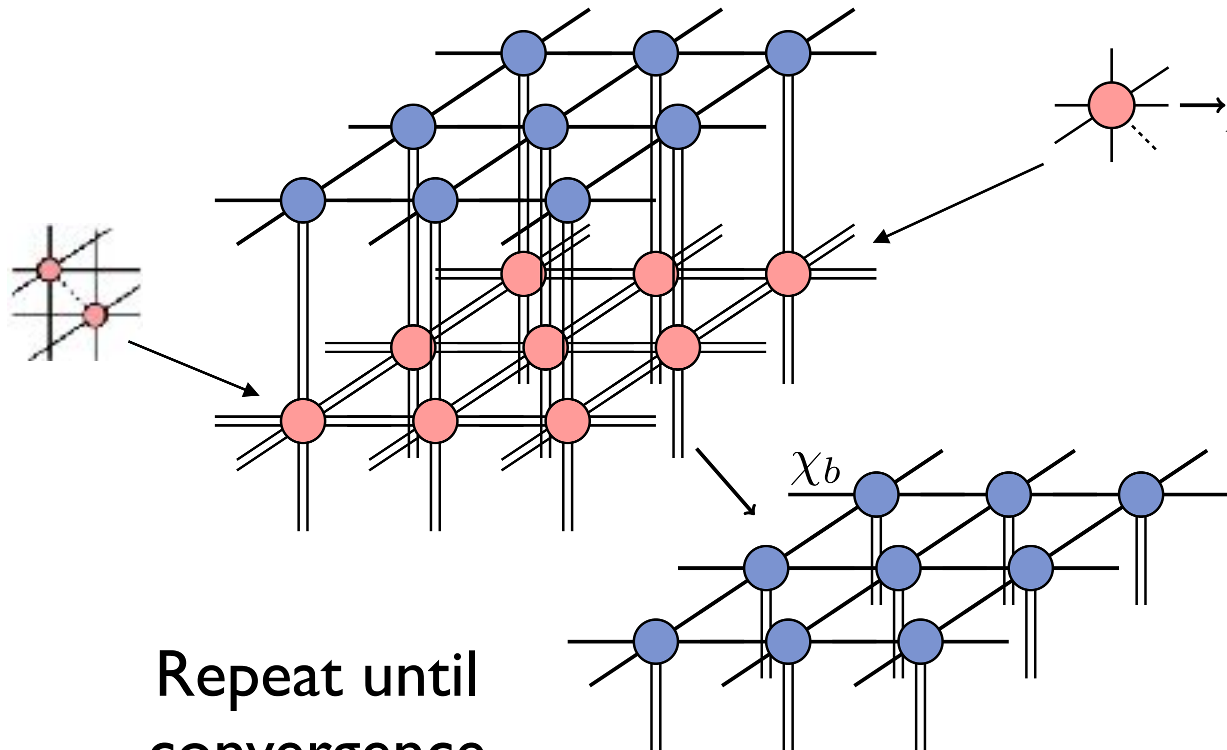
- **Full 3D contraction: the SU + CTM approach**
  - ✦ Boundary iPEPS approach
  - ✦ Combination of simple update (SU) truncation + CTM method
  - ✦ Good accuracy & convergence & tractable cost

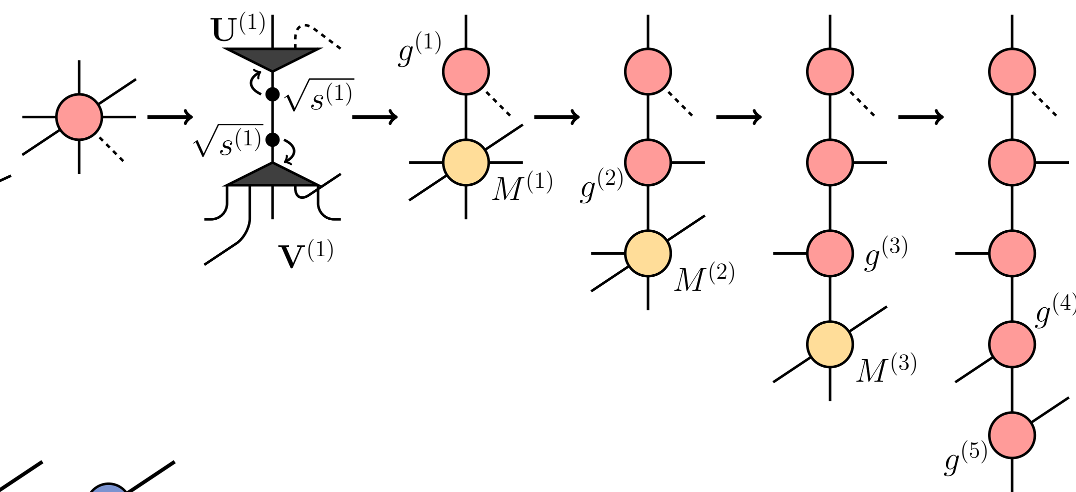


- **Contraction of layered systems: LCTM**
  - ✦ Decouple layers away from the center → use CTM to contract 2D layers
  - ✦ Good accuracy for anisotropic systems
  - ✦ Lower cost than full 3D algorithm



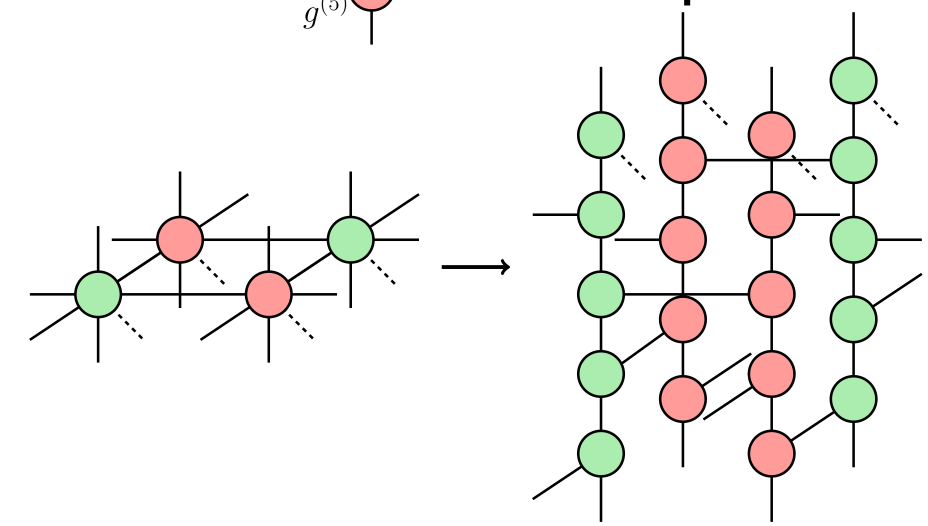
Full 3D contraction: SU + CTM approach





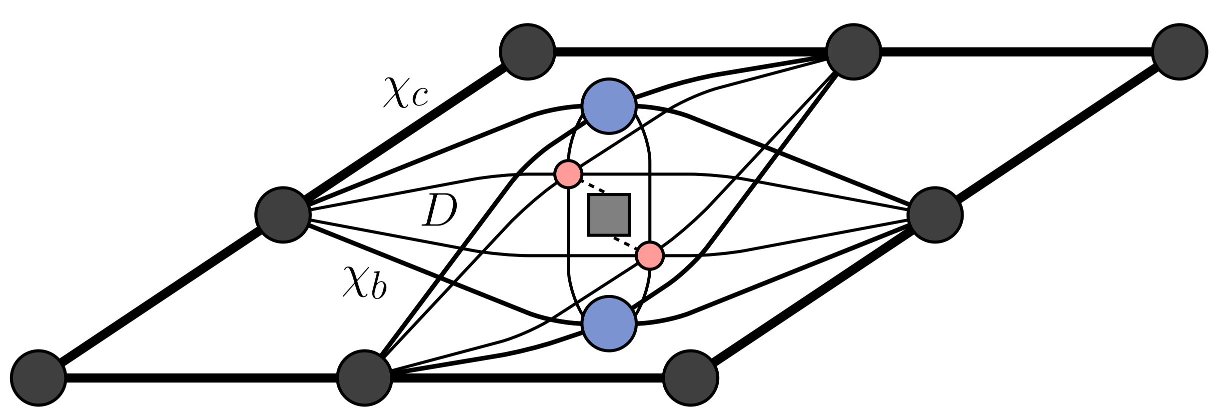
Split with SVDs

Sequence of 2-site operators



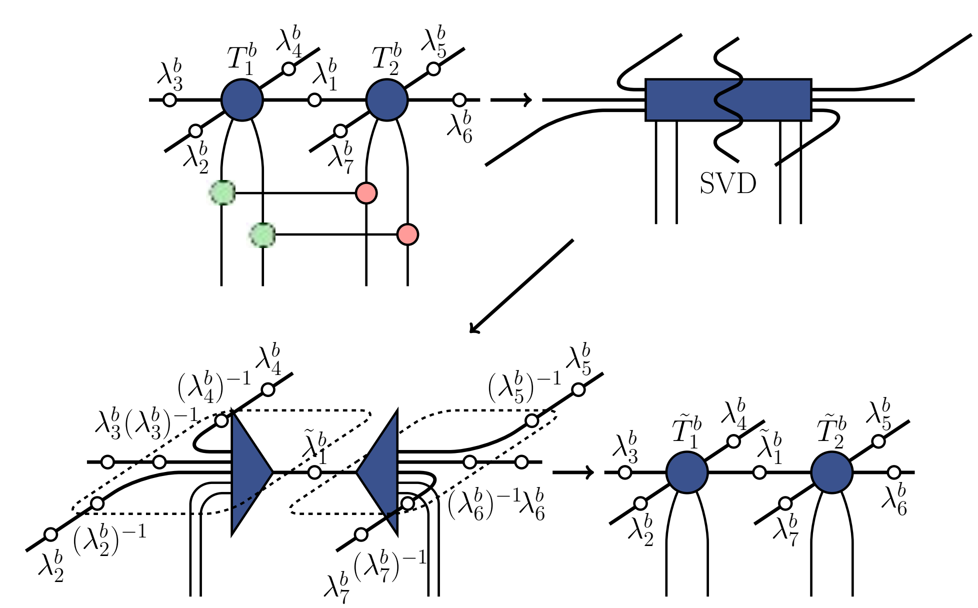
Repeat until convergence

use CTM to contract resulting 3-layer network



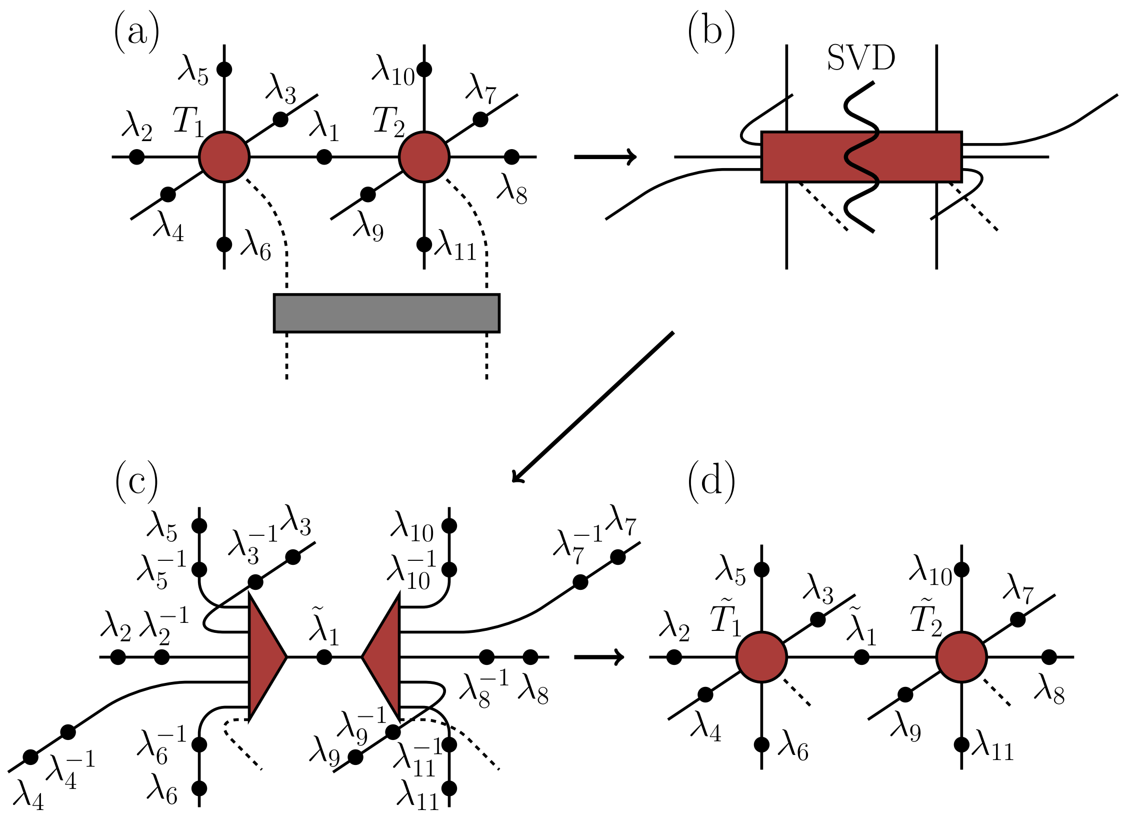
$\mathcal{O}(\chi_c^3\chi_b^4D^4 + \chi_c^2\chi_b^6D^6 + \chi_c^2\chi_b^4D^9)$

Apply and use SU to truncate

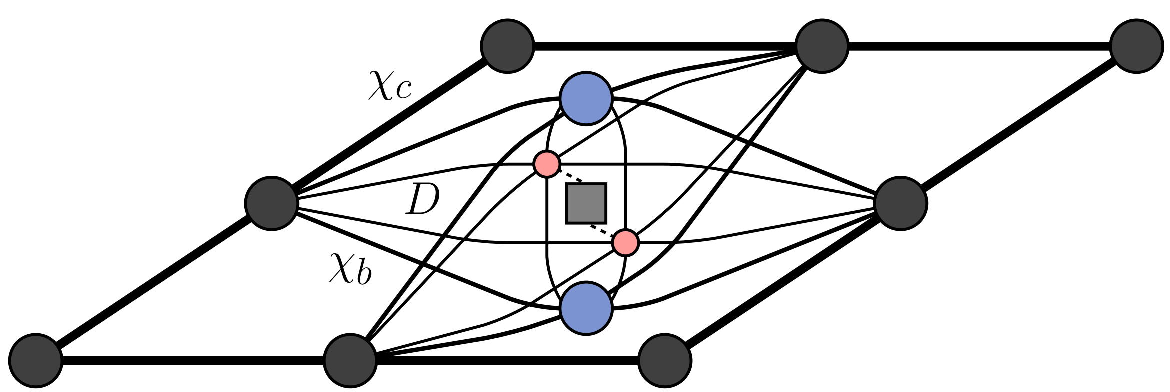


Benchmark results: 3D Heisenberg model

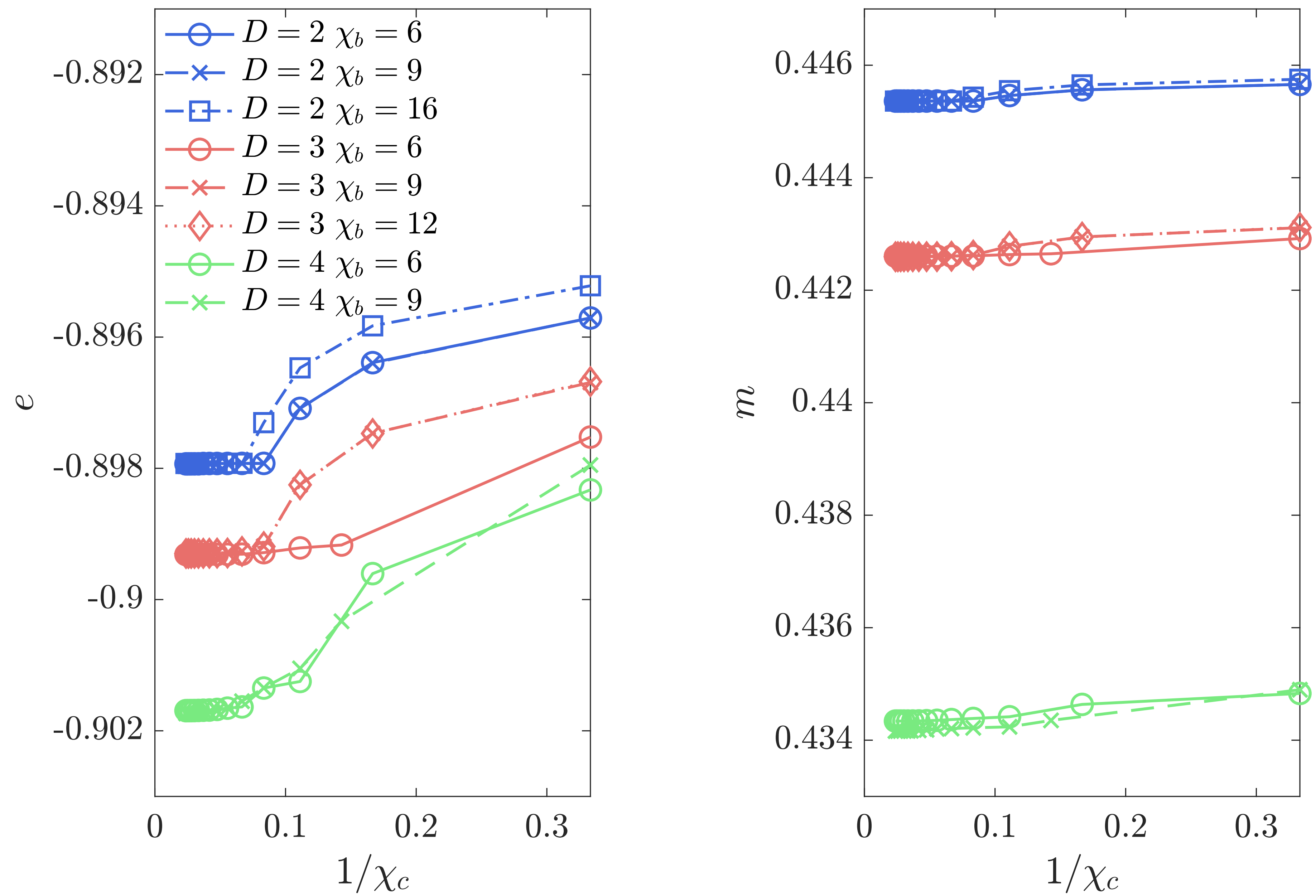
- Optimization: imaginary time evolution based on SU in 3D



- Study of convergence in χ_c, χ_b, D with comparisons to QMC

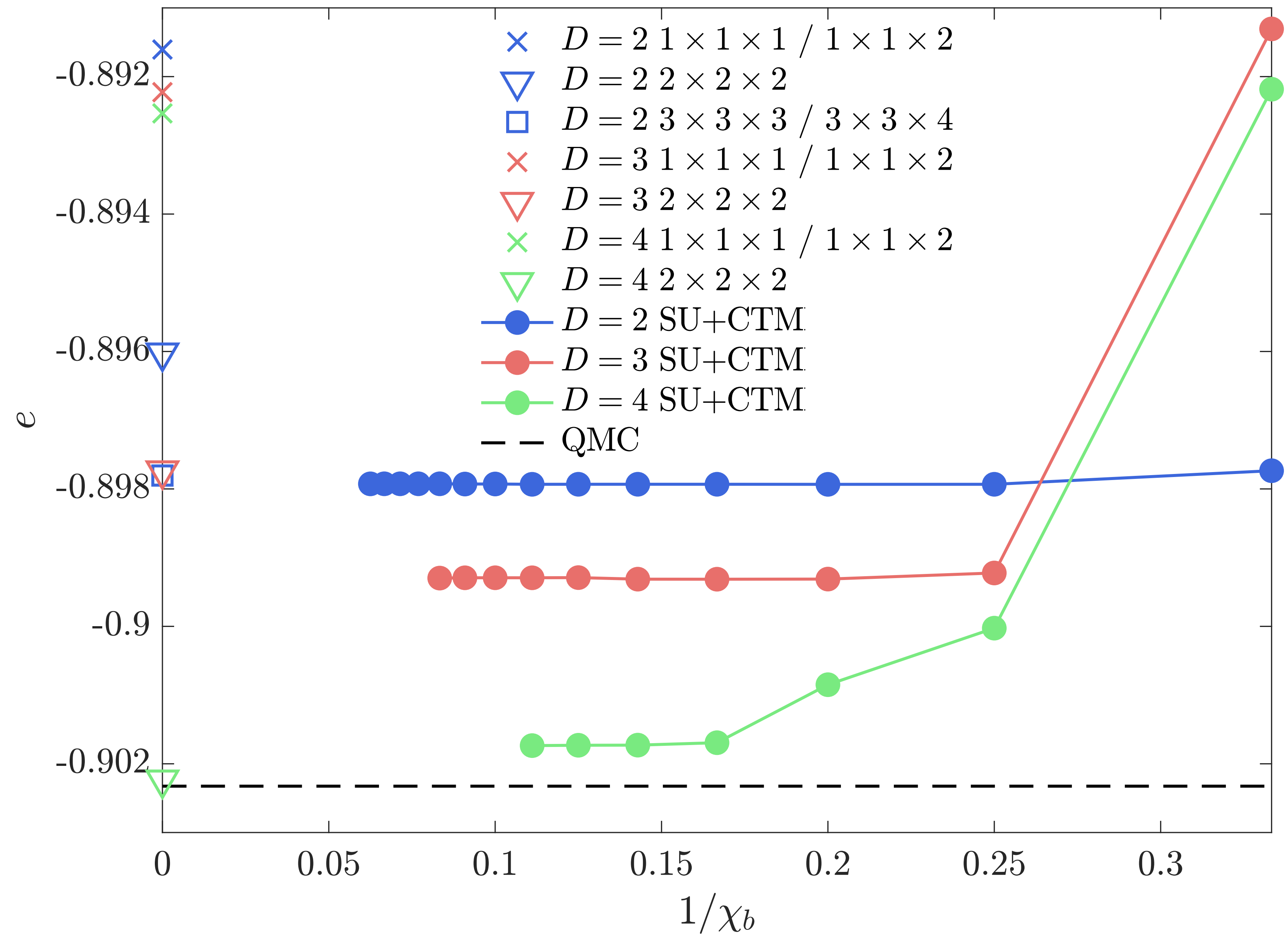


Convergence in χ_c



★ Systematic convergence in χ_c

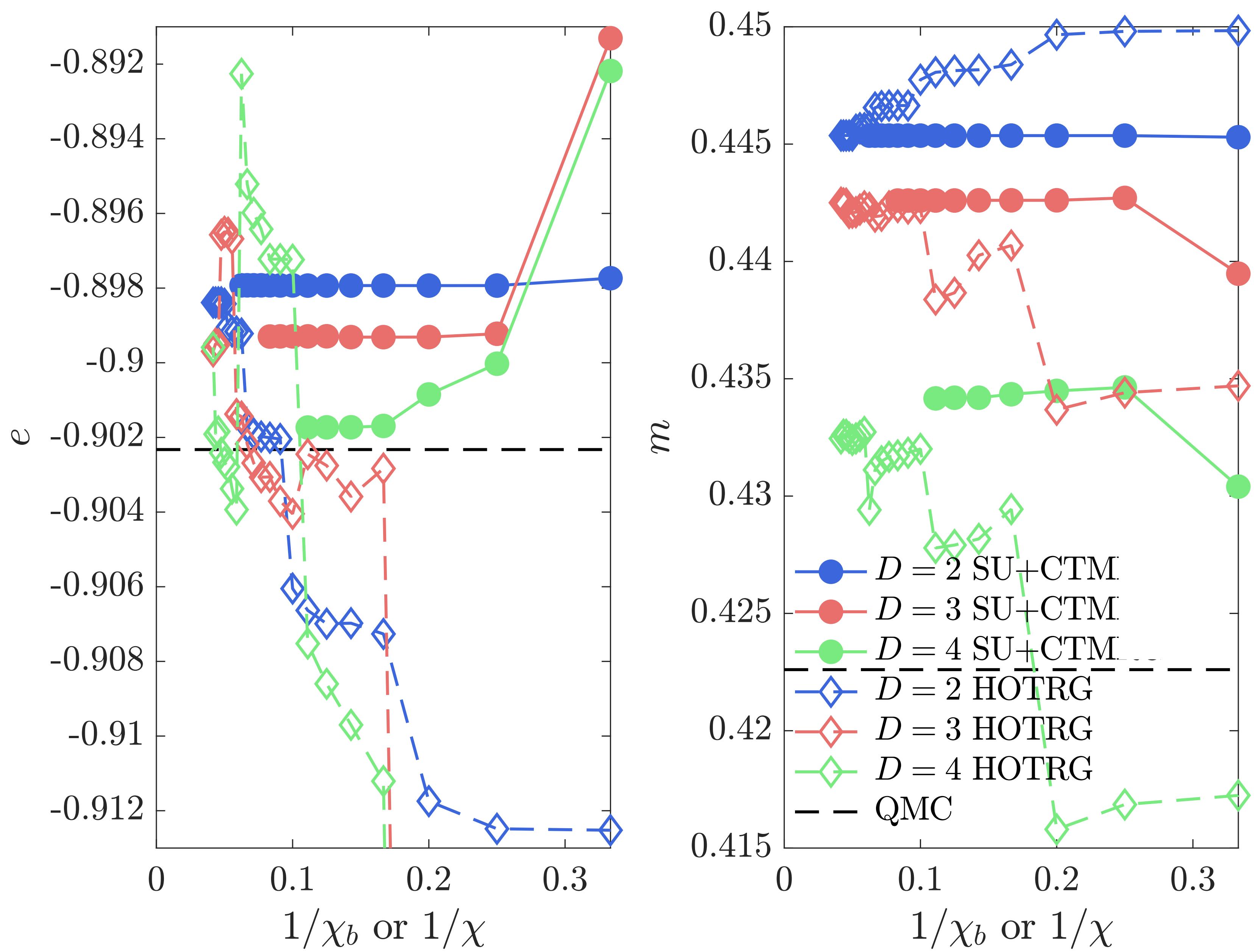
Convergence in χ_b & cluster results: *energy*



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

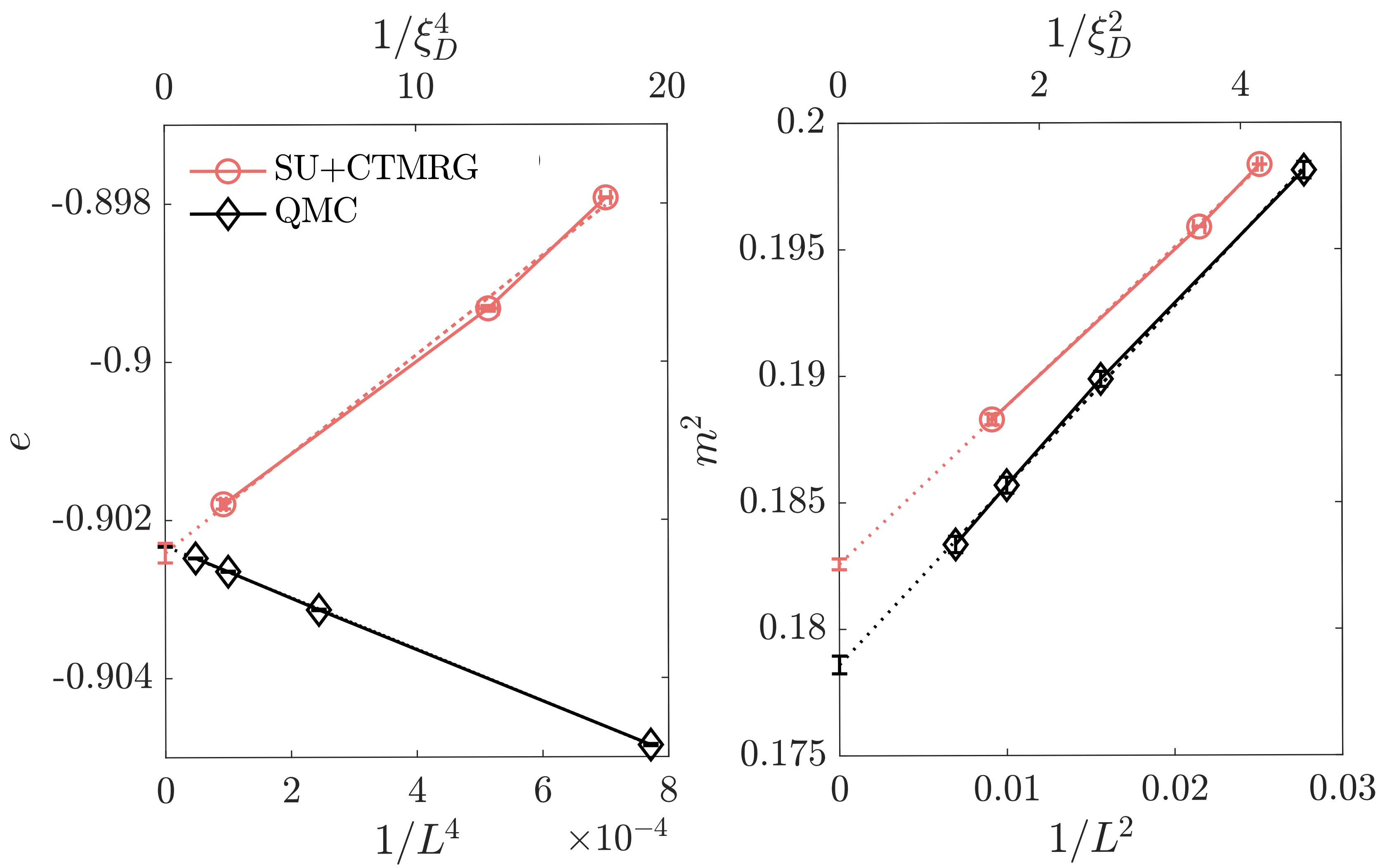
Comparison with HOTRG

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



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

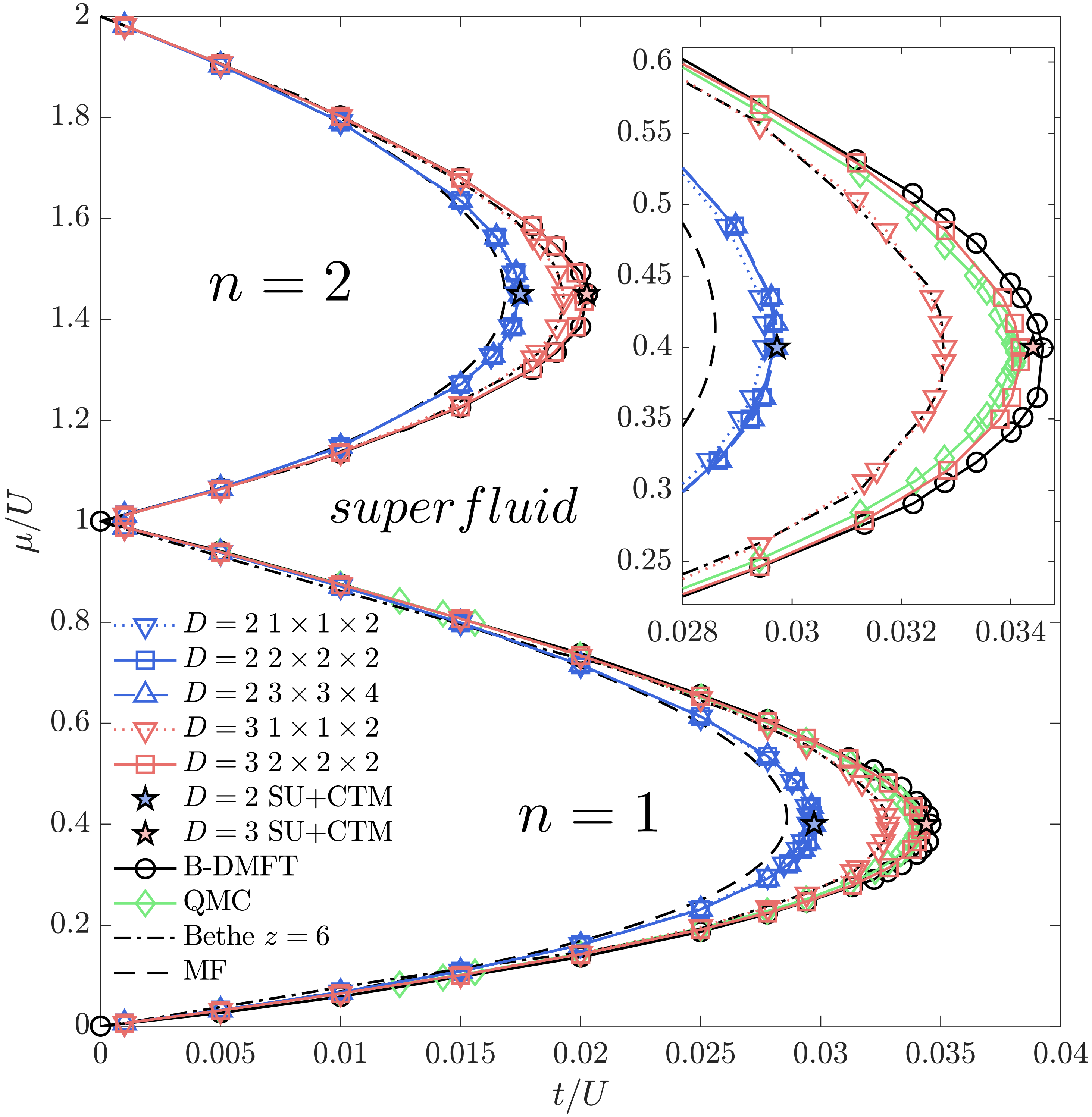
Finite correlation length scaling



- ★ 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

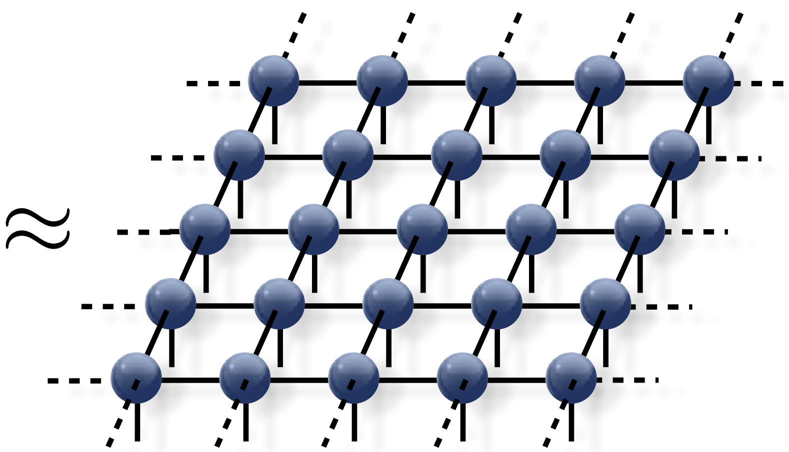
★ D=3: close to QMC result, better than B-DMFT

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

Excitations with iPEPS

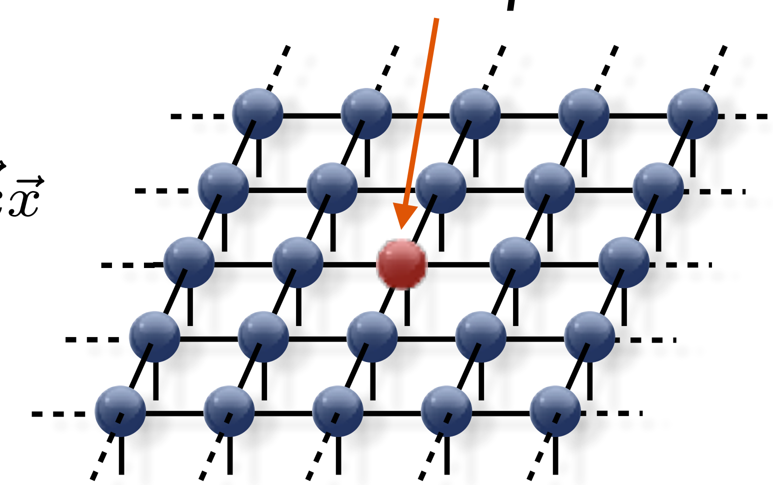
iPEPS excitation ansatz

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



- Excitation on top of ground state with momentum k

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

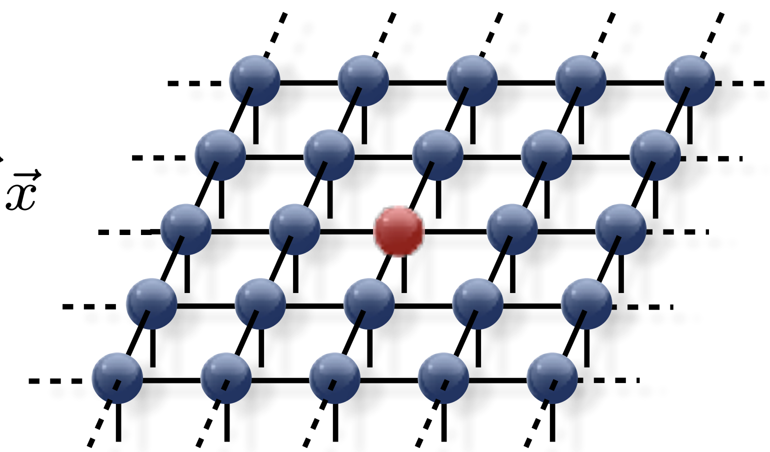


Haegeman, Pirvu, Weir, Cirac, Osborne, Verschelde, and Verstraete, PRB 85, 100408(R) (2012).
Haegeman, Michalakis, Nachtergaele, Osborne, Schuch, and Verstraete, PRL 111, 080401 (2013).
Haegeman, Osborne, and Verstraete, PRB 88, 075133 (2013).
Zauner, Draxler, Vanderstraeten, Degroote, Haegeman, Rams, 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

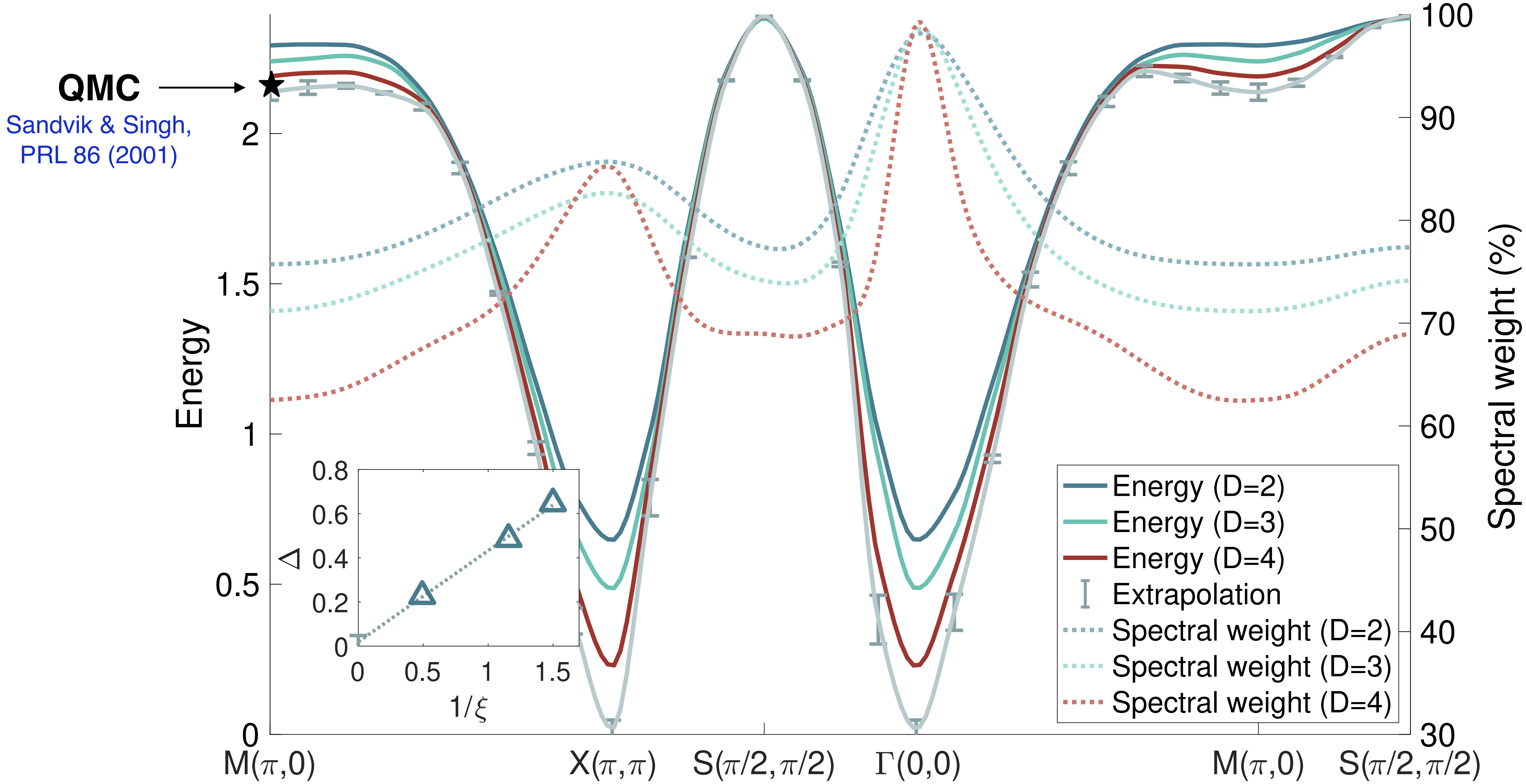
- Use systematic summation:

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



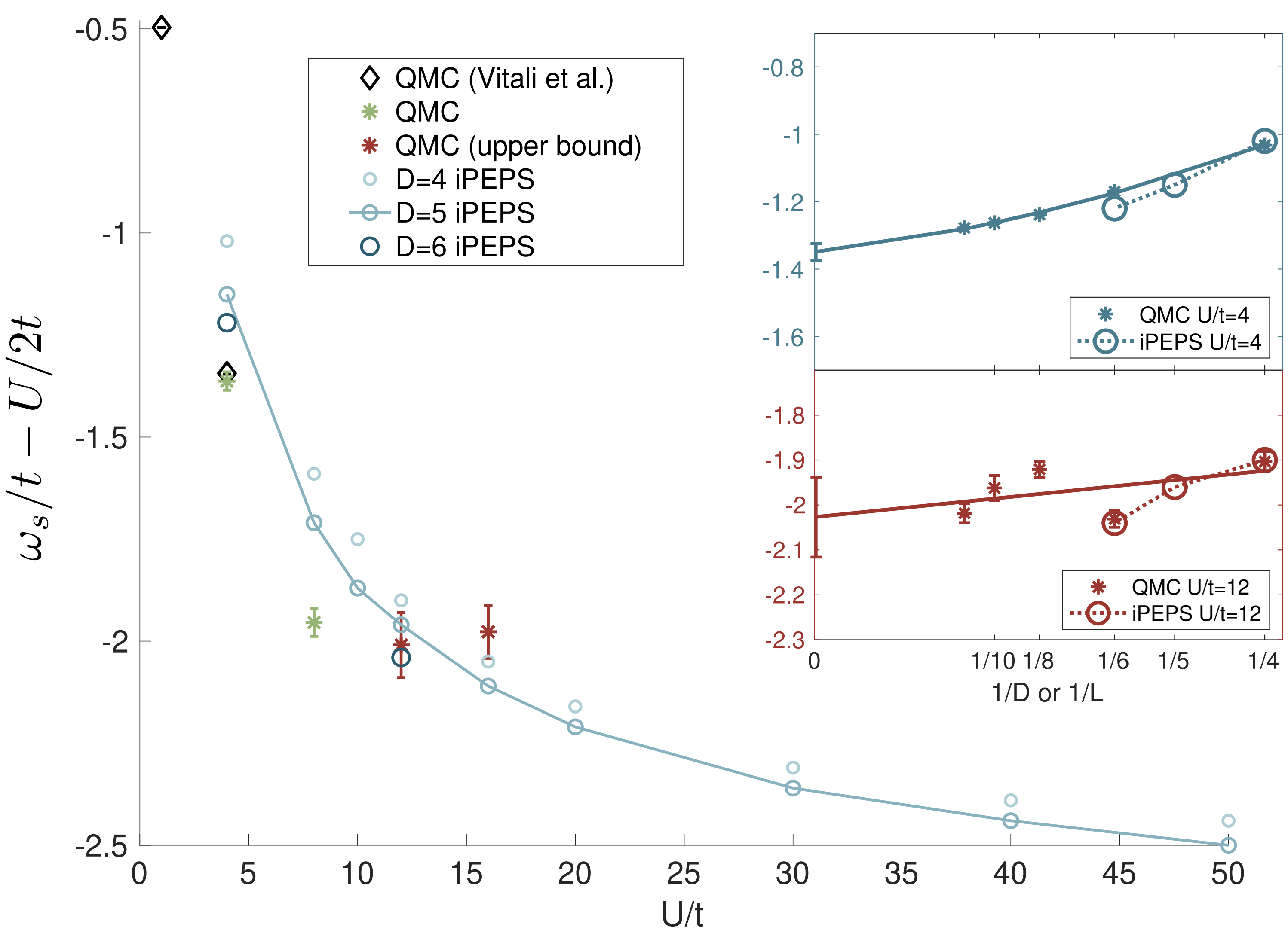
Ponsioen and PC, PRB 101, 195109 (2020)

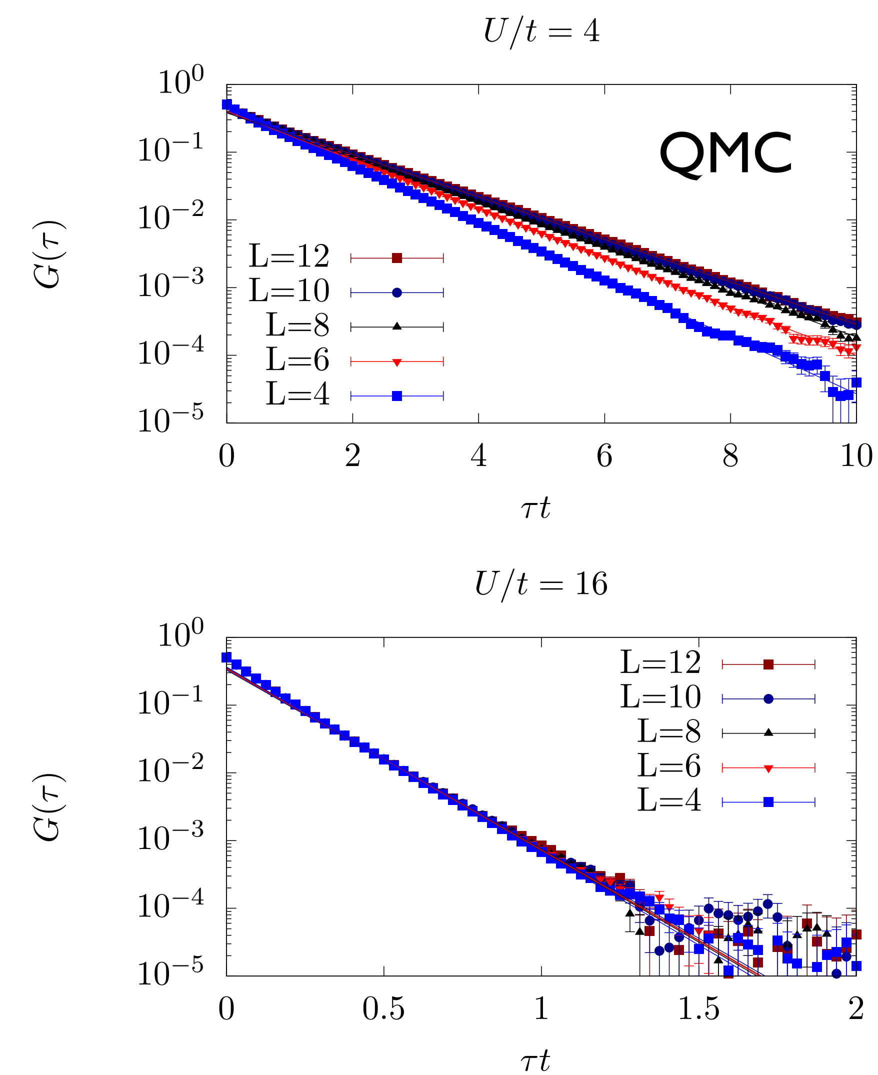
similar results in: Vanderstraeten, Haegeman, Verstraete, PRB 99 (2019)

★ Vanishing gap with extrapolation based on FCL scaling

Charge gap in the half-filled Hubbard model

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

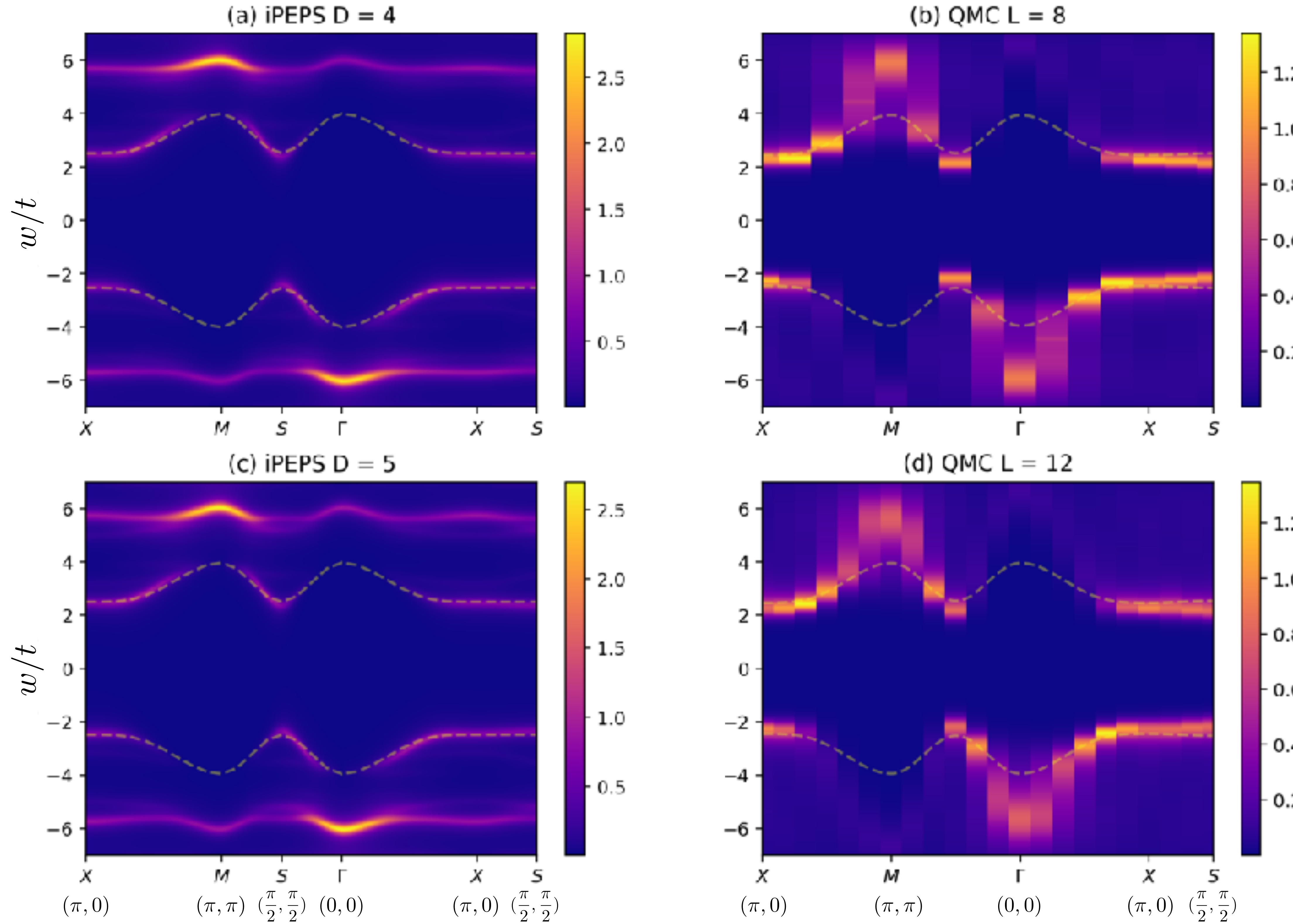




★ Systematic improvement with D, approaching QMC for U/t=4 and U/t=8

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

Spectral function A(ω, k) for U/t=8



Summary

- ✓ Finite correlation length scaling with iPEPS provides a powerful tool for the study of continuous phase transitions & extrapolations of OPs
- ✓ Various applications of FCL & new developments with iPEPS:
  - ★ 2D ground state calculations
  - ★ Extension to finite temperature
  - ★ iPEPS in 3D
  - ★ iPEPS excitation ansatz
- ✓ Still room for improvement

Thank you for your attention!

Acknowledgements:
P. Vlaar, B. Ponsioen, S. Crone, J.D. Arias Espinoza, M. Peschke, J. Hasik, Y. Zhang, L. Tagliacozzo, G. Kapeijns, P. Czarnik, J. Dziarmaga, F. F. Assaad, M. Rams, H. Rønnow, C. Rüegg, J. Jiménez, L. Weber, A. Wietek, S. Wessel, B. Normand, A. Honecker, A. Läuchli, F. Mila

erc