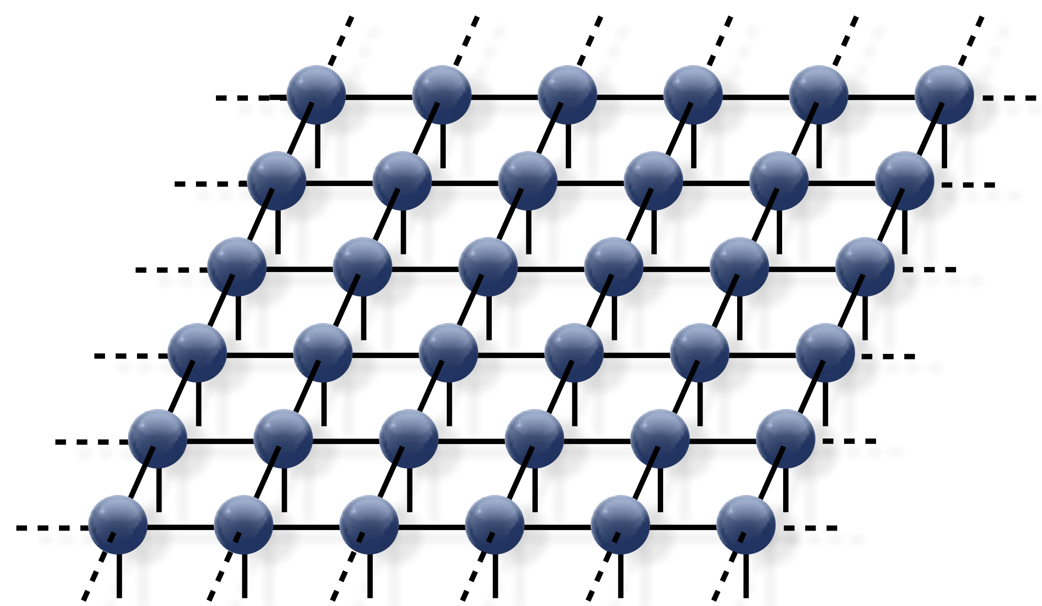
Lectures on
1: Introduction to iPEPS
2: Advanced iPEPS techniques

Philippe Corboz, Institute for Theoretical Physics, University of Amsterdam



Outline of today's lecture

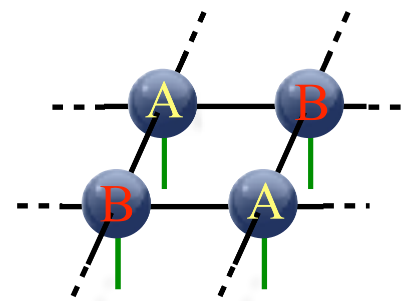
- iPEPS at finite temperature
  - *Imaginary time evolution of density operator (or purification)*
- Finite correlation length scaling
  - *Study of critical phenomena and order parameter extrapolations in gapless systems*
- Spiral iPEPS
  - *efficient simulation of incommensurate spin spiral phases*
- Excitations & spectral functions
  - *Excitation ansatz & real-time evolution*
- Extensions to 3D
  - *iPEPS for 3D quantum systems*
  - *iPEPS for layered systems in 3D*

iPEPS at finite temperature

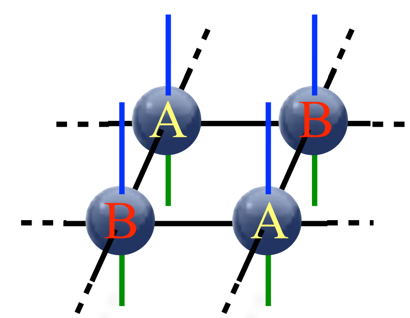
Finite temperature simulations with iPEPS

- 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), …

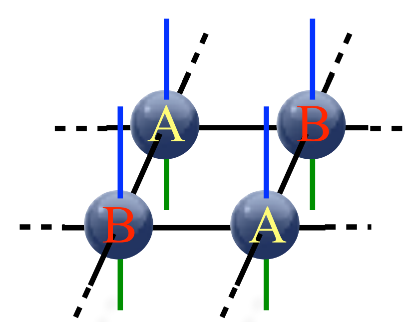
- Wave-function: $|\Psi\rangle \approx$



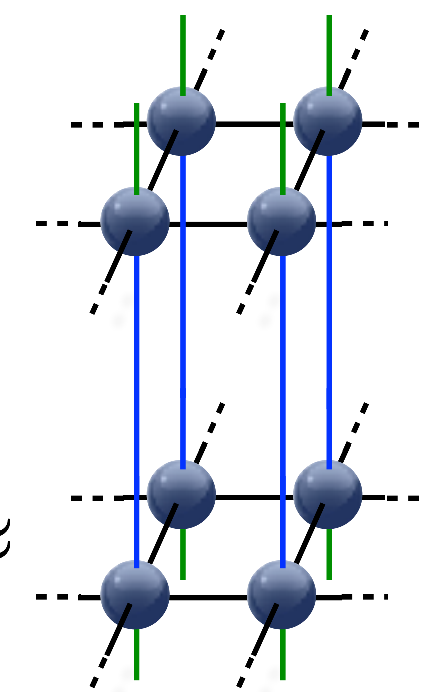
- Density-operator: $\hat{\rho} = e^{-\beta \hat{H}} \approx$



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



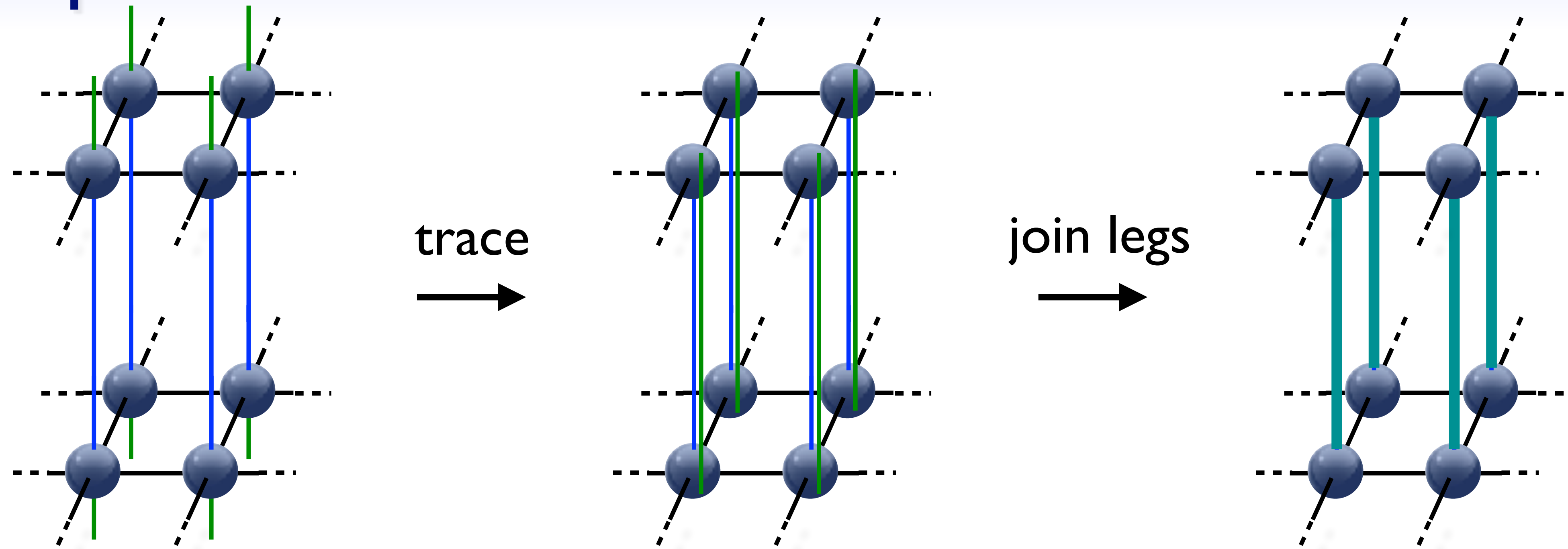
$\hat{\rho}(\beta) \approx$



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

Finite temperature simulations with iPEPS

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



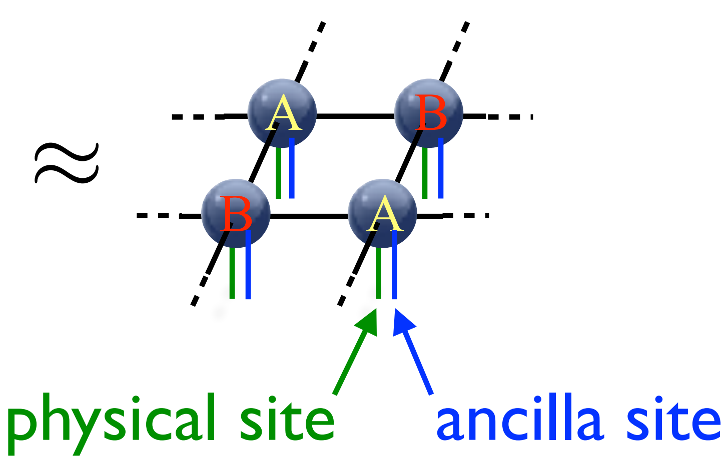
$\langle \tilde{\Psi} | \tilde{\Psi} \rangle$

same structure as
for wave functions

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

Other (equivalent) formulation using purification:

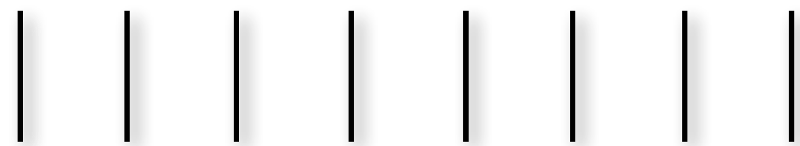
$|\tilde{\Psi}\rangle \approx$



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

Imaginary time evolution

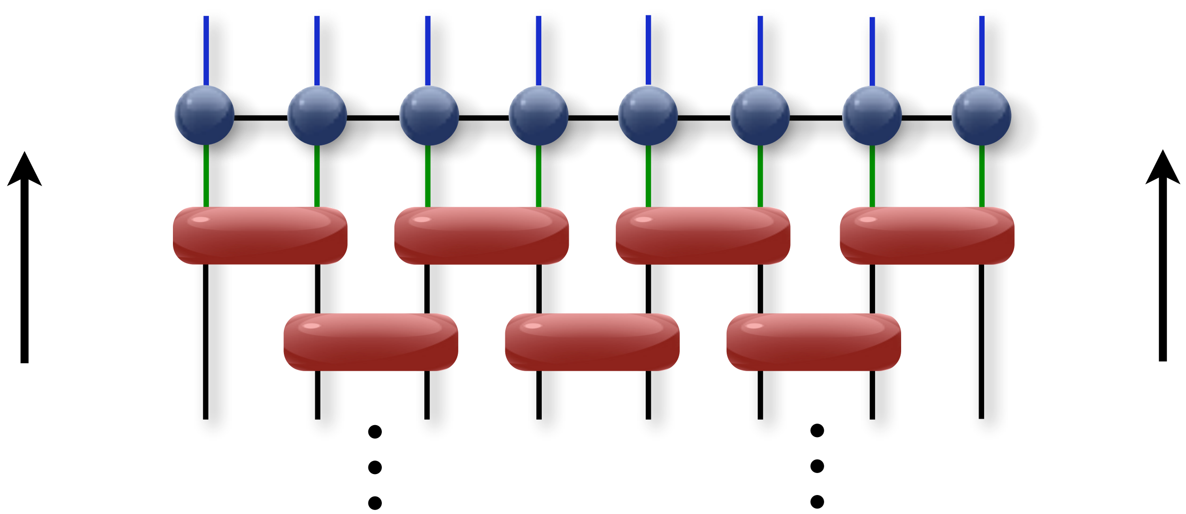
Czarnik, Dziarmaga & PC, PRB 99 (2019)

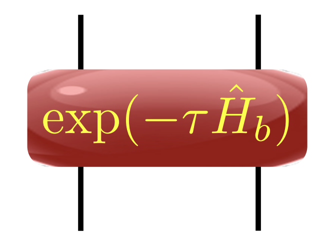
- Start at infinite temperature: $\hat{\rho}(\beta = 0) = \mathbb{I}$
- Initial state:  exact!
- Evolve in imaginary time: $\hat{\rho}(\beta) = e^{-\beta \hat{H}/2} \hat{\rho}(0) e^{-\beta \hat{H}/2}$

$\tau = \beta/n$

Trotter-Suzuki decomposition:

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

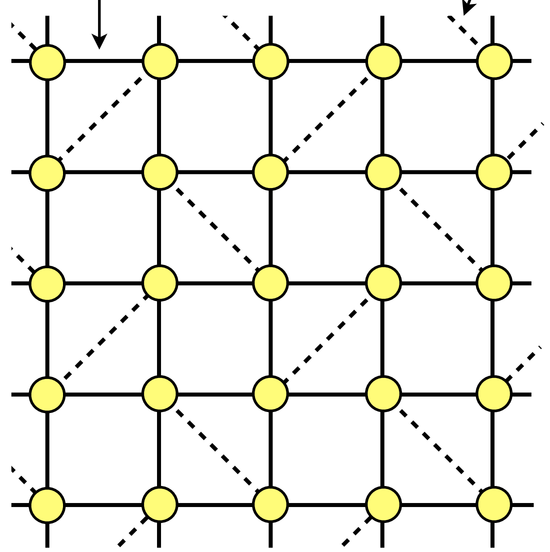




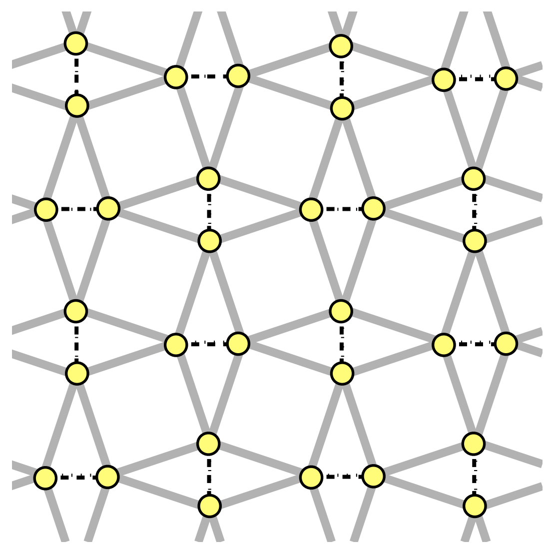
- Truncate after each step using e.g. simple / full update
- Evolve up to target $\beta/2$

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

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

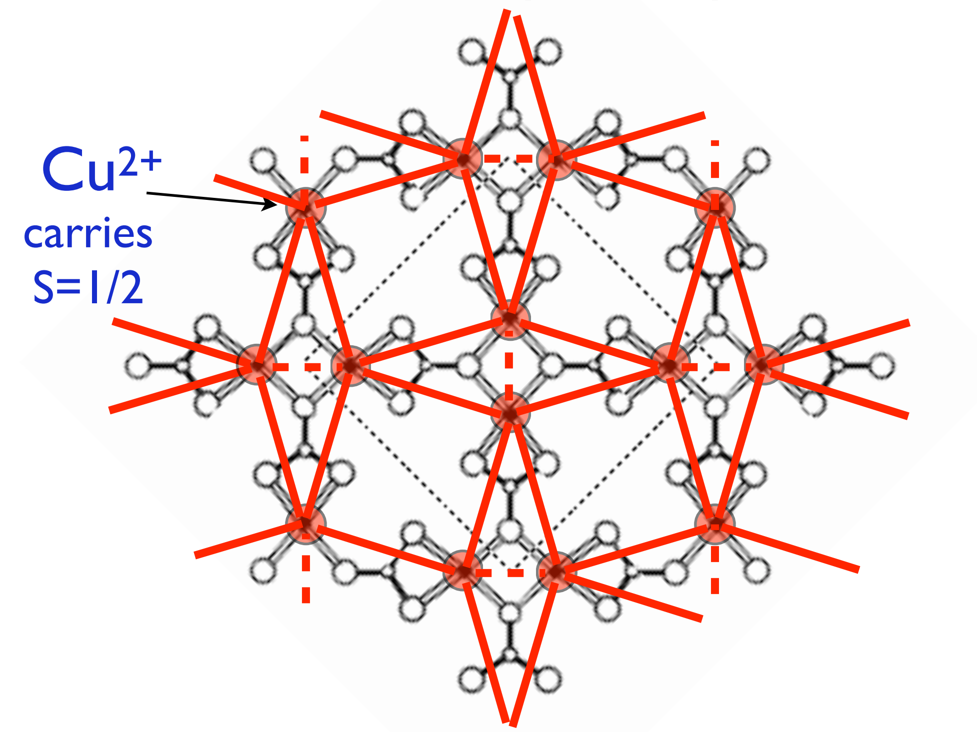


↔



↔

$SrCu_2(BO_3)_2$



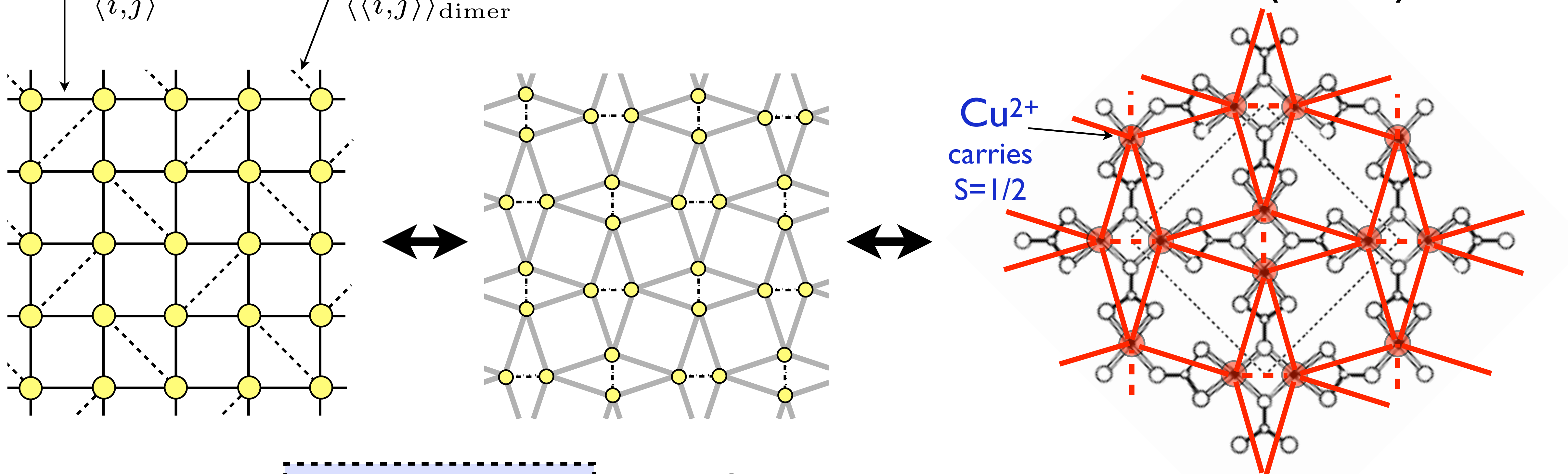
Shastry & Sutherland, Physica B+C **108** (1981)

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

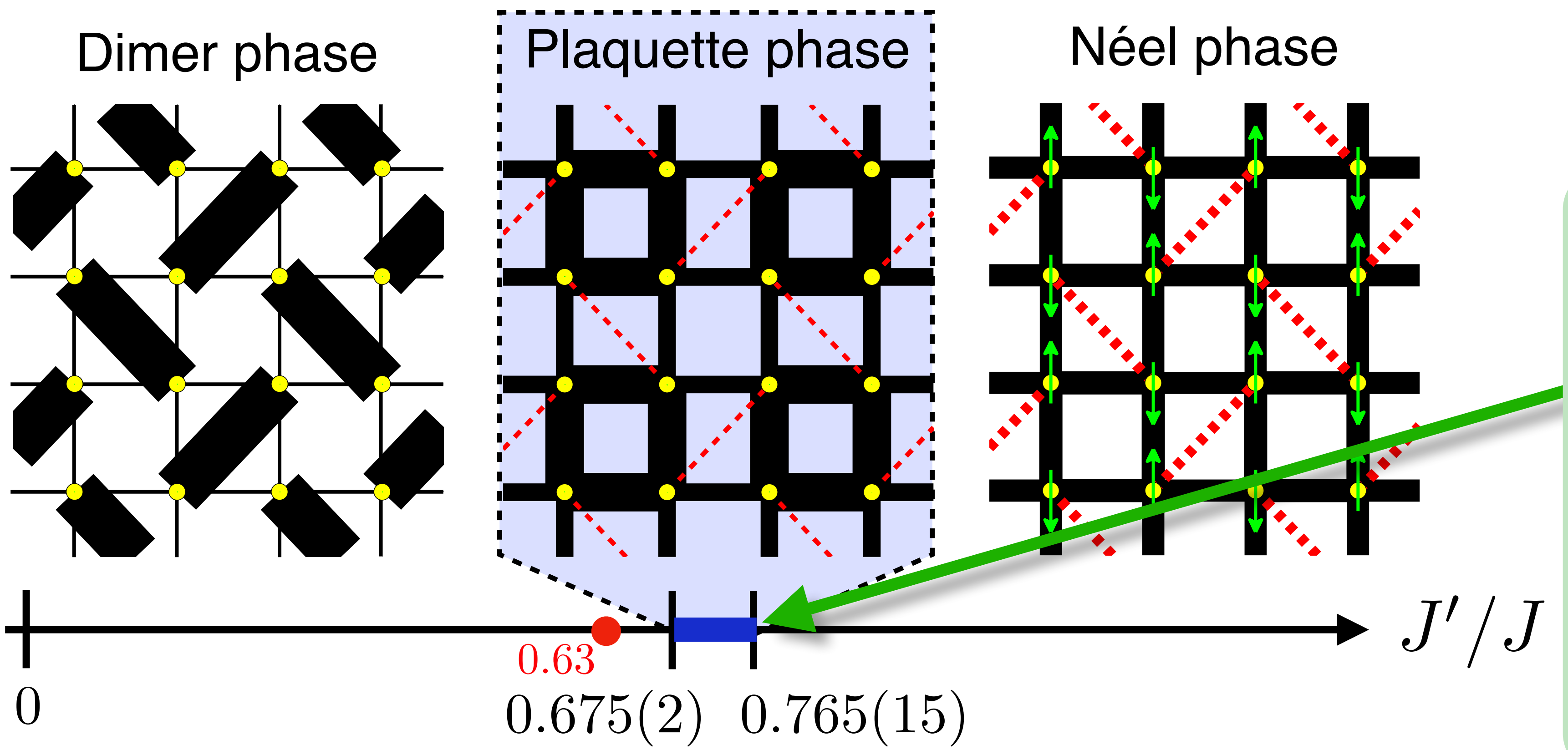
The Shastry-Sutherland model and $SrCu_2(BO_3)_2$

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

$SrCu_2(BO_3)_2$



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



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

Deconfined QCP

Lee, You, Sachdev & Vishwanath, PRX 9 (2019)
Liu et al, PRL 133 (2024)

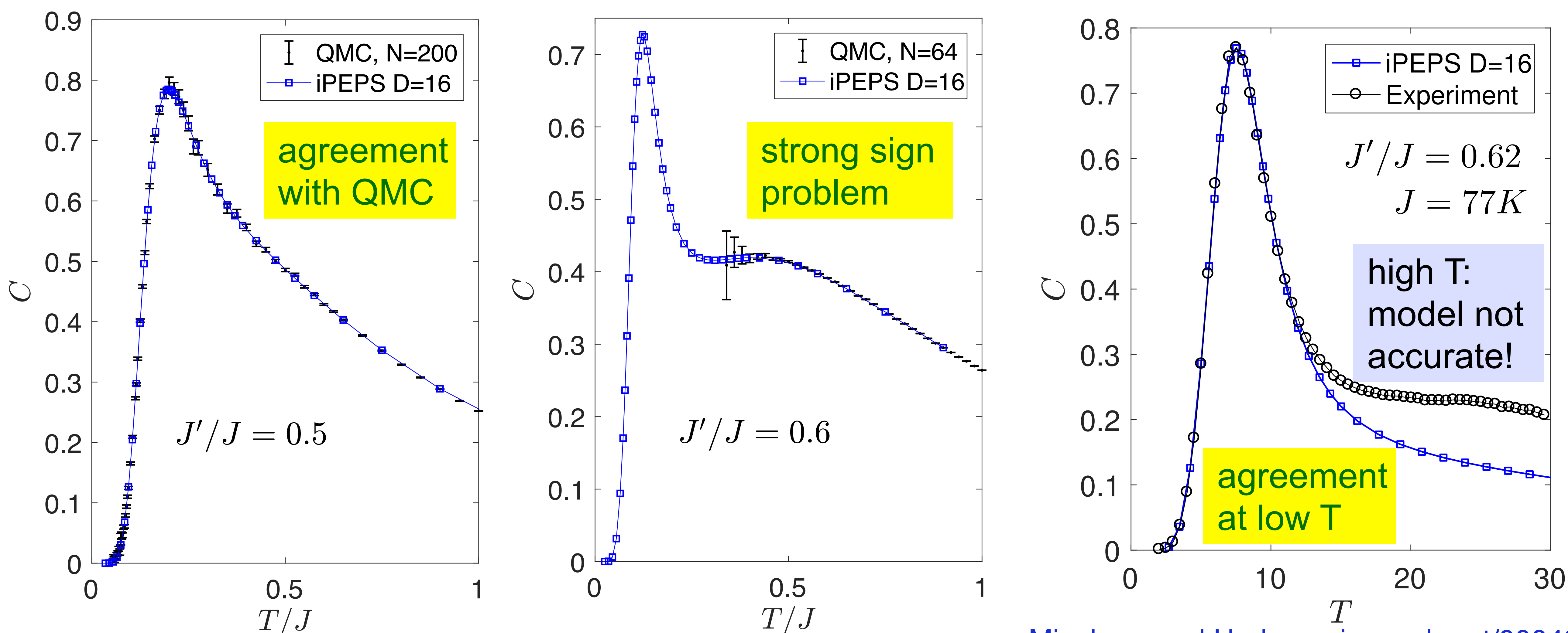
Intermediate QSL phase?

Yang et al, PRB 105 (2022)
Wang et al, CPL 39 (2022)
Viteritti et al, arxiv: 2311.16889
Maity et al., arXiv:2501.00096

Finite temperature simulation examples

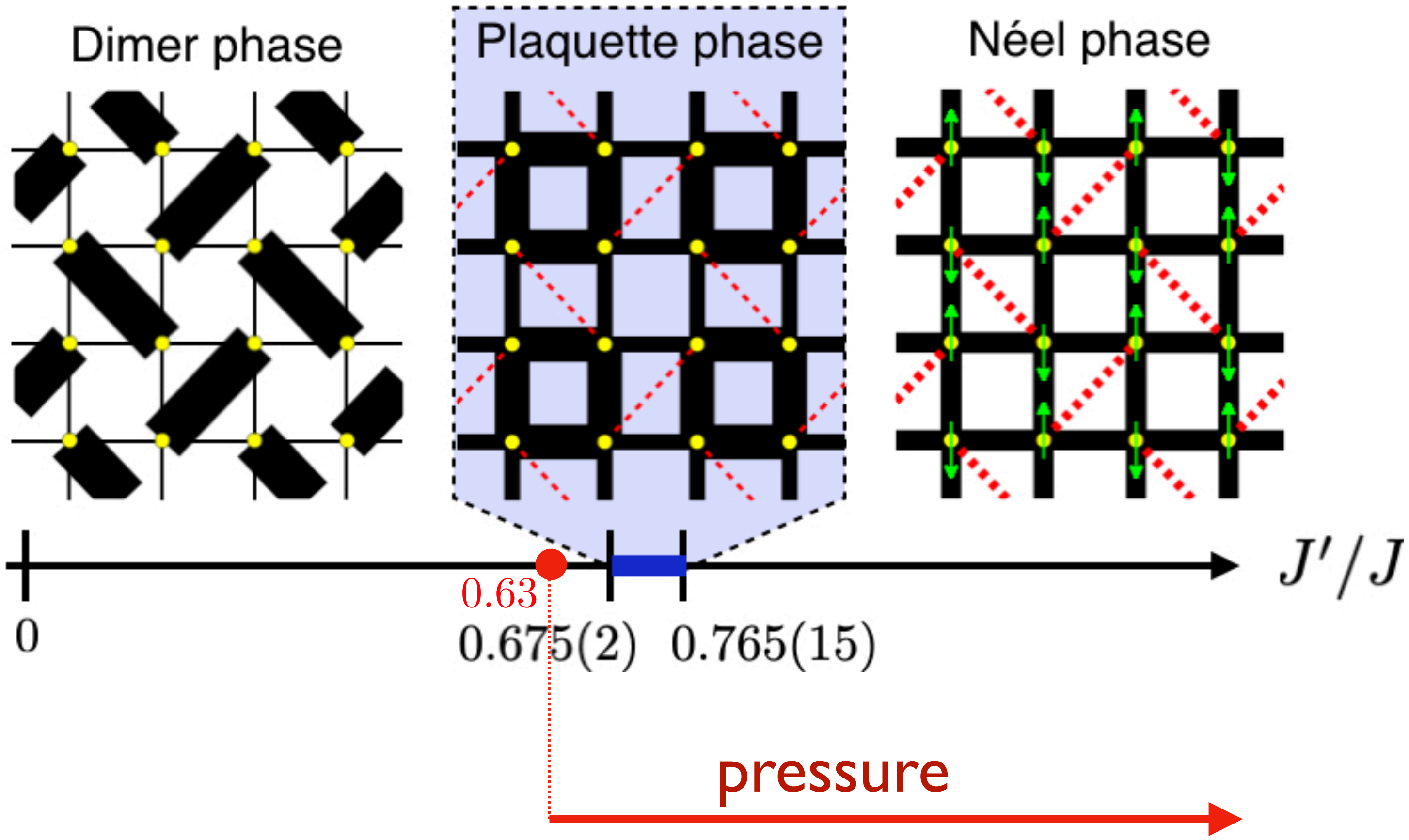
Wietek, PC, Wessel, Normand, Mila, and Honecker, PRR 1 (2019)

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



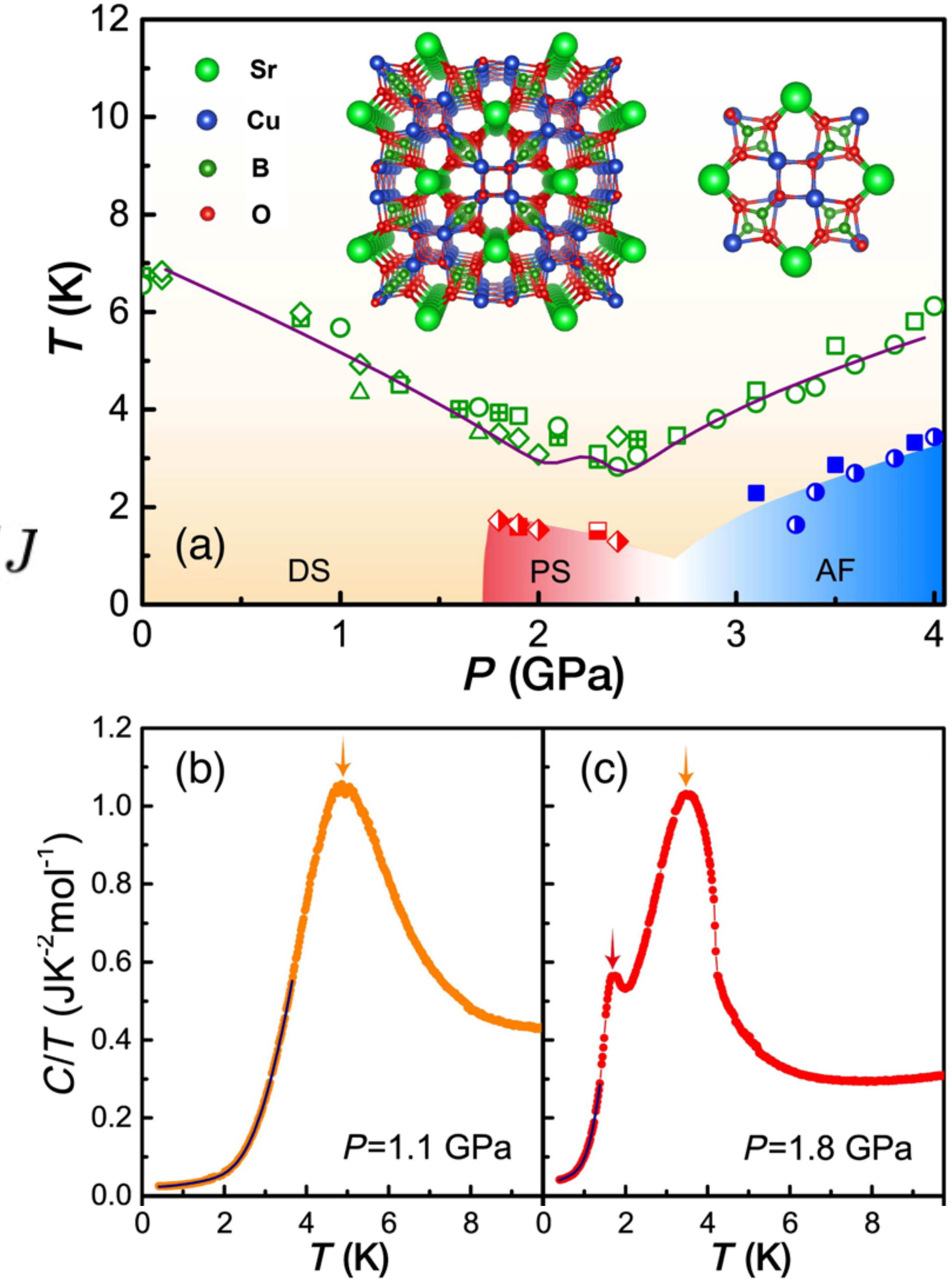
Miyahara and Ueda, arxiv:cond-mat/0004260

$SrCu_2(BO_3)_2$ under pressure



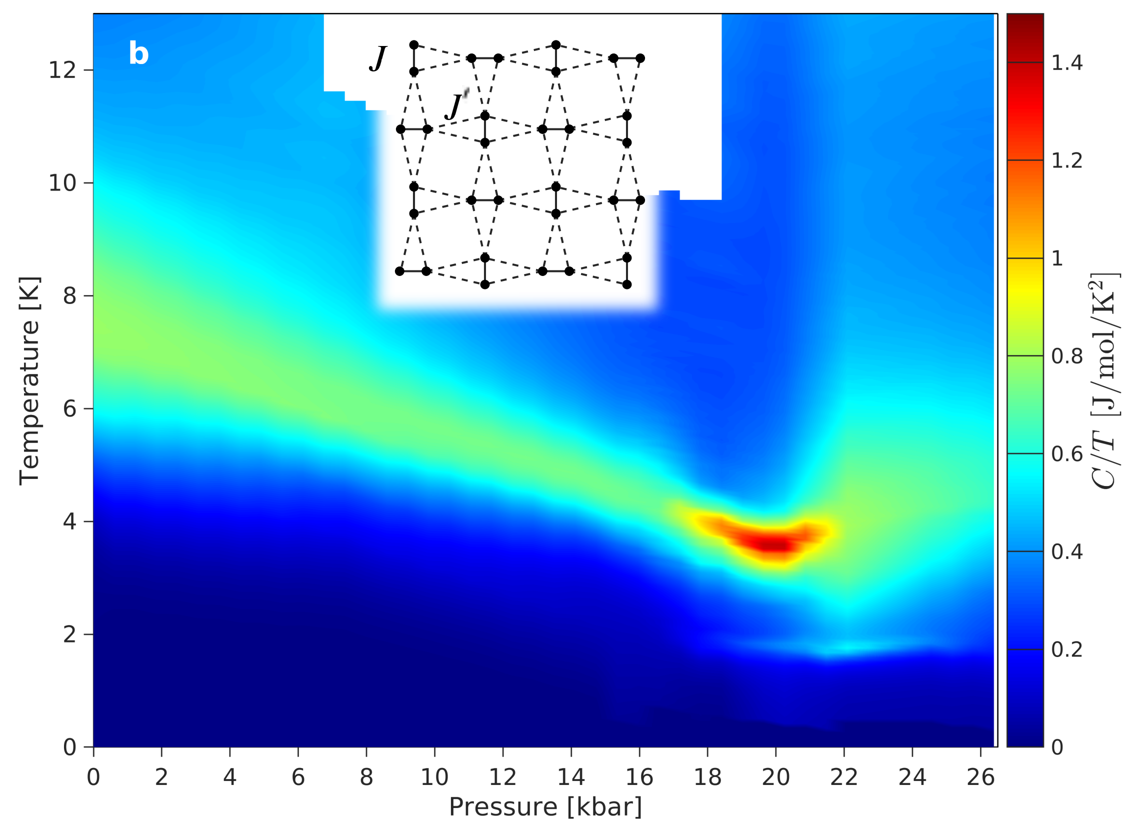
Drive system across the phase transitions!

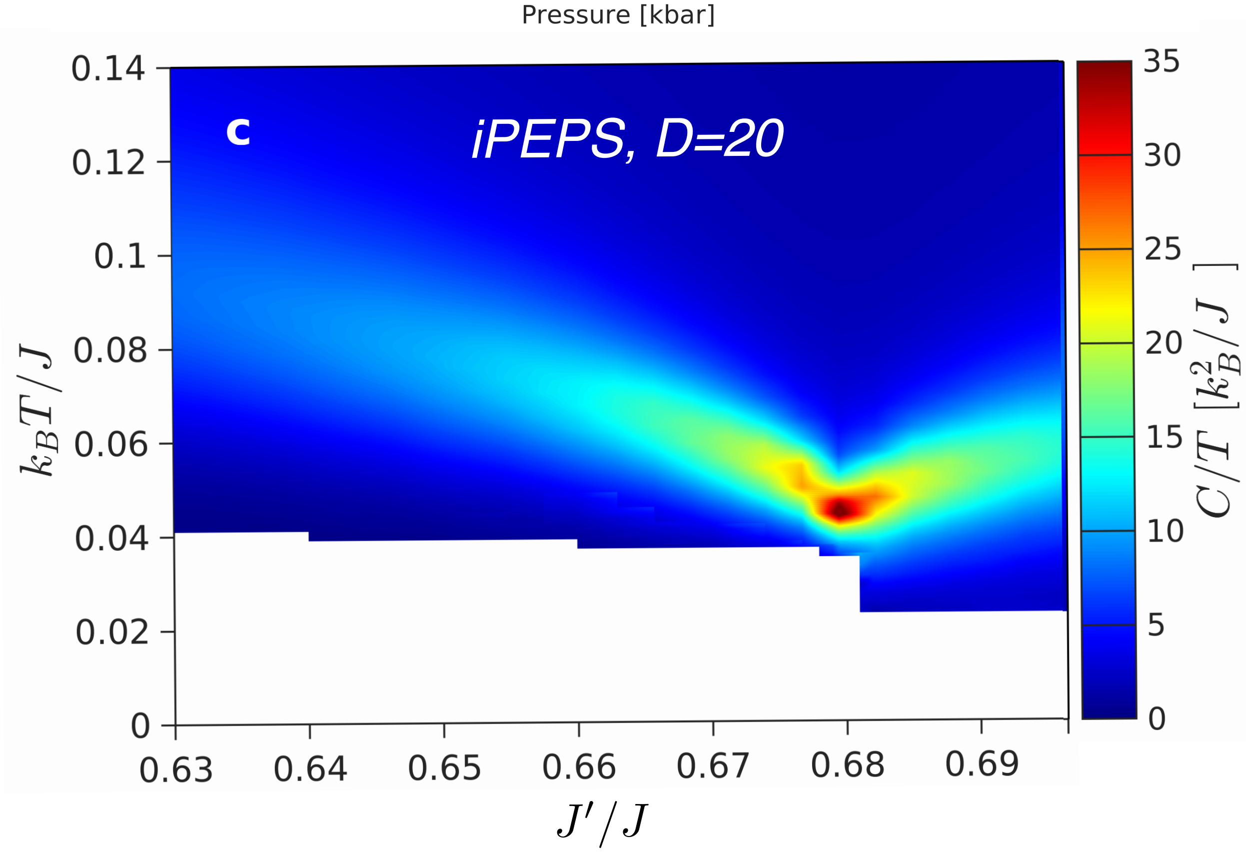
Waki, et al. J. Phys. Soc. Jpn. 76, 073710 (2007)
Haravifard, et al. Nat. Commun. 7, 11956 (2016)
Zayed, et al., Nat. Phys. 13, 962 (2017)
Sakurai, et al., J. Phys. Soc. Jpn. 87, 033701 (2018)
Guo, et al., PRL 124, 206602 (2020)
Bettler, et al,. Phys. Rev. Research 2, 012010 (2020)



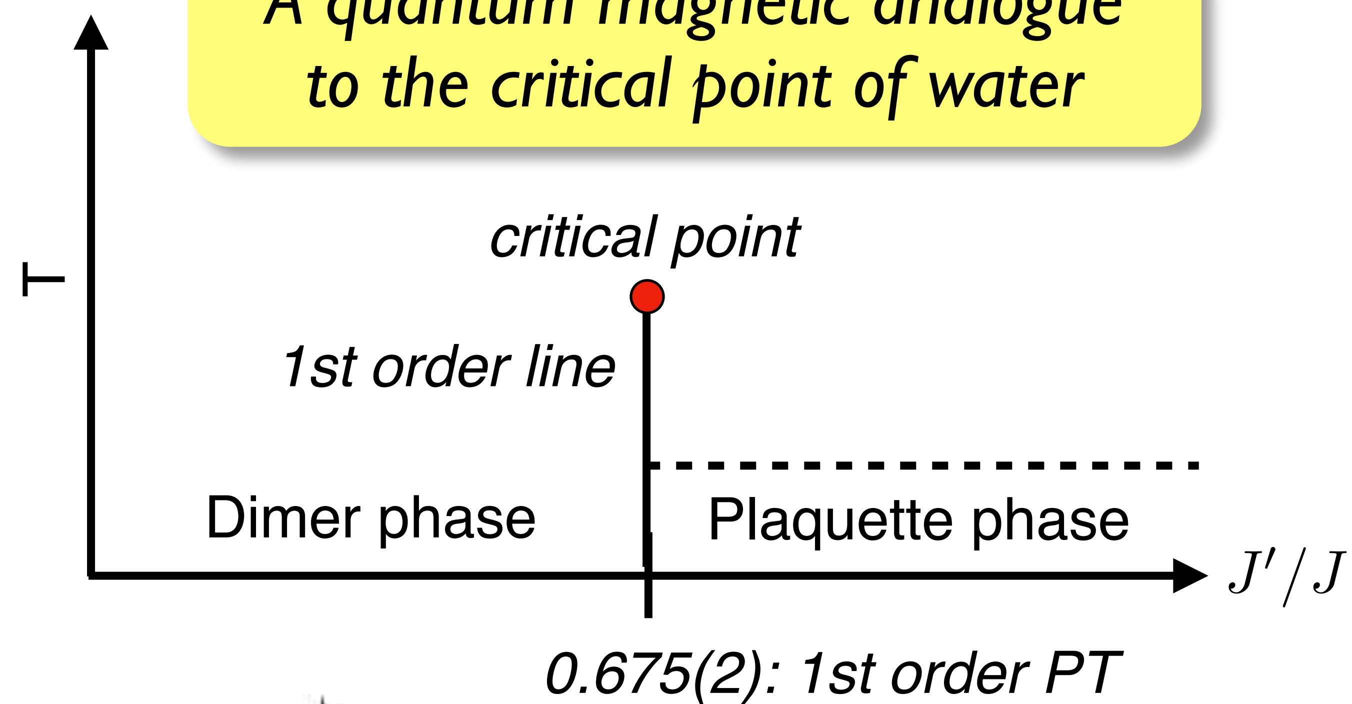
Guo, et al., PRL 124, 206602 (2020)

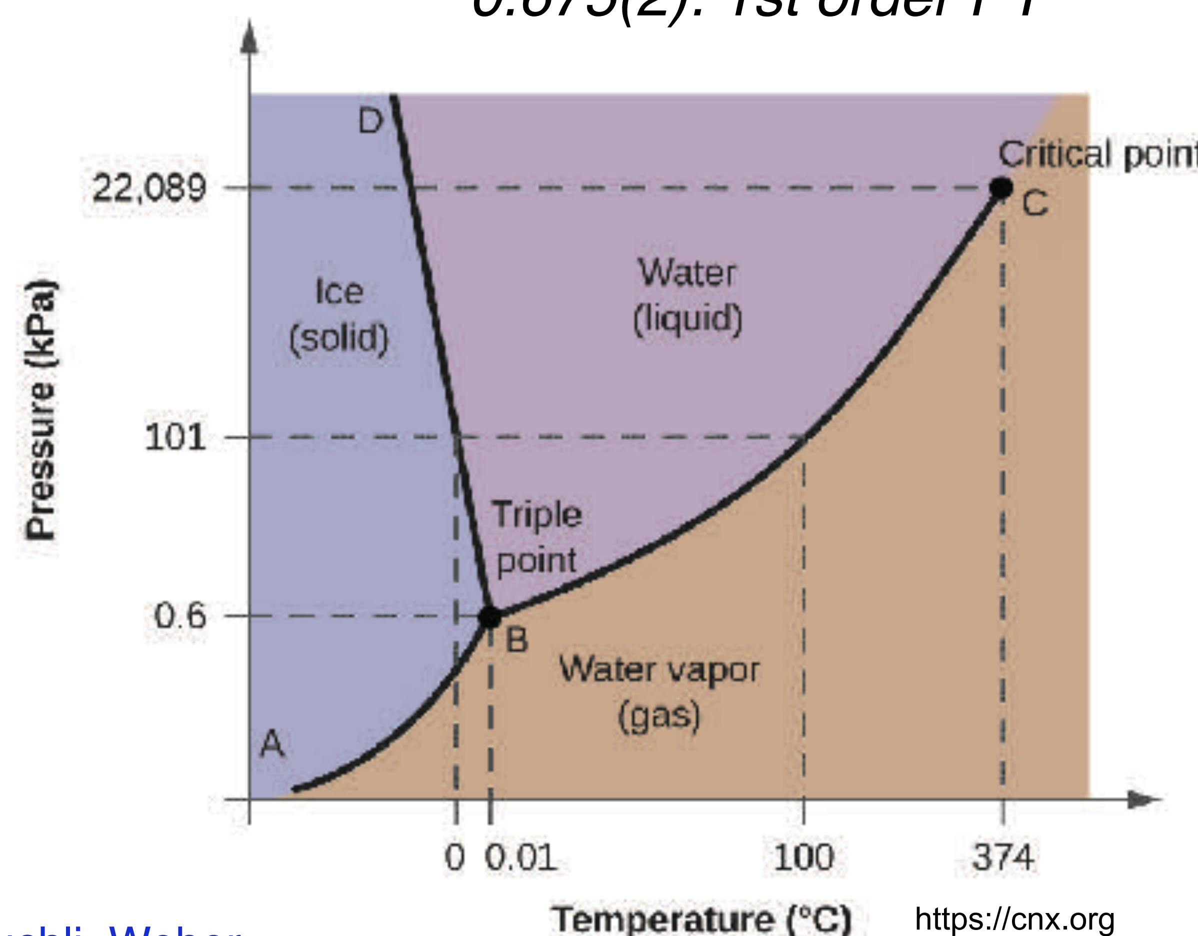
Specific heat data (group of H. M. Rønnow)





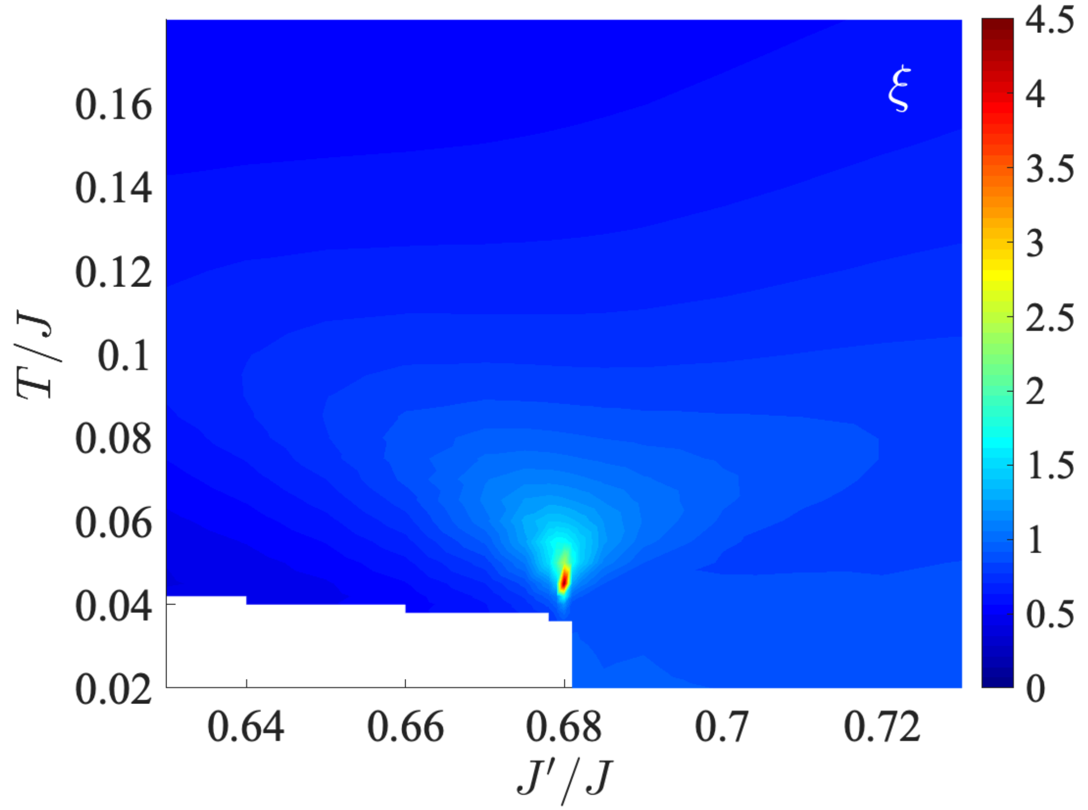
A quantum magnetic analogue to the critical point of water

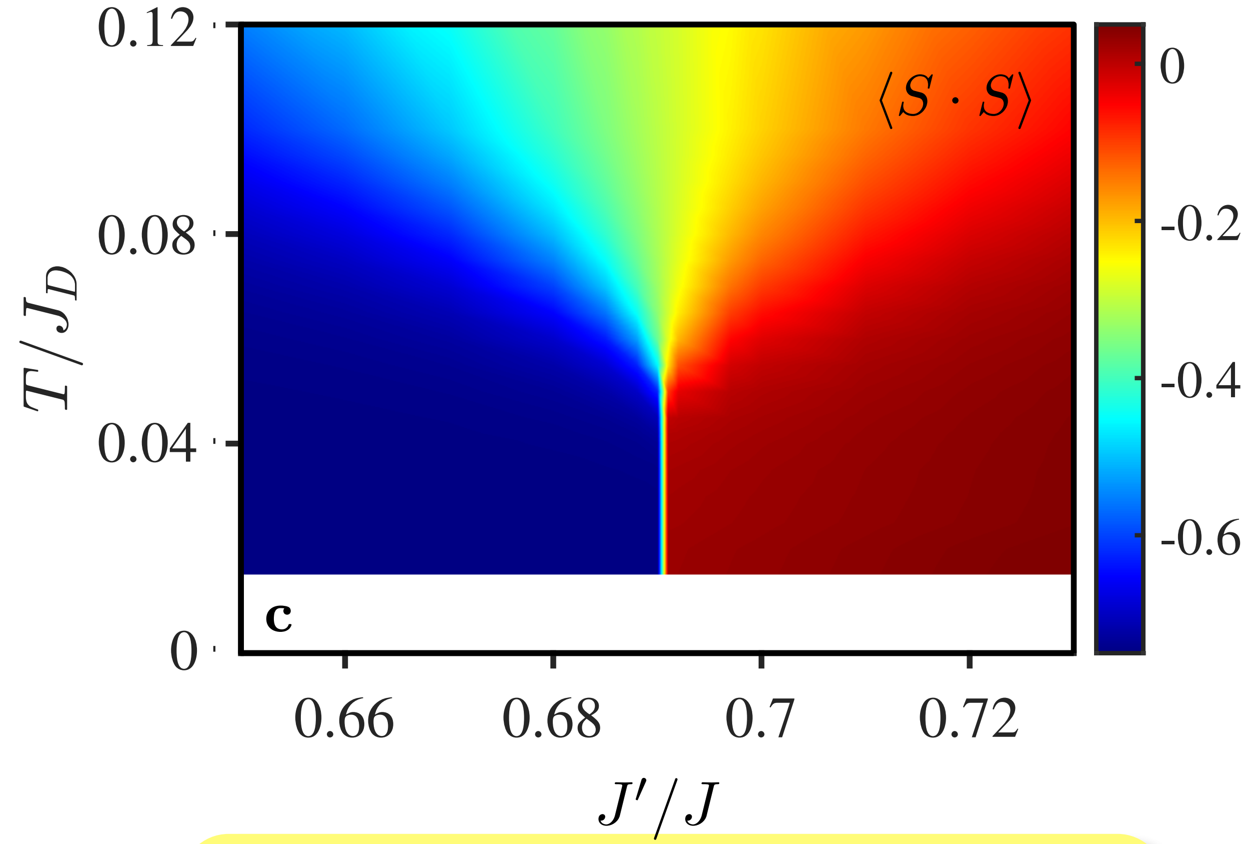




Jiménez, Crone, Fogh, Zayed, Lortz, Pomjakushina, Conder, Läuchli, Weber,
Wessel, Honecker, Normand, Rüegg, PC, Rønnow & Mila, Nature 592, 370 (2021); see also Wang et al, PRL 131 (2023)

Correlation length & jump in <S · S> on dimer

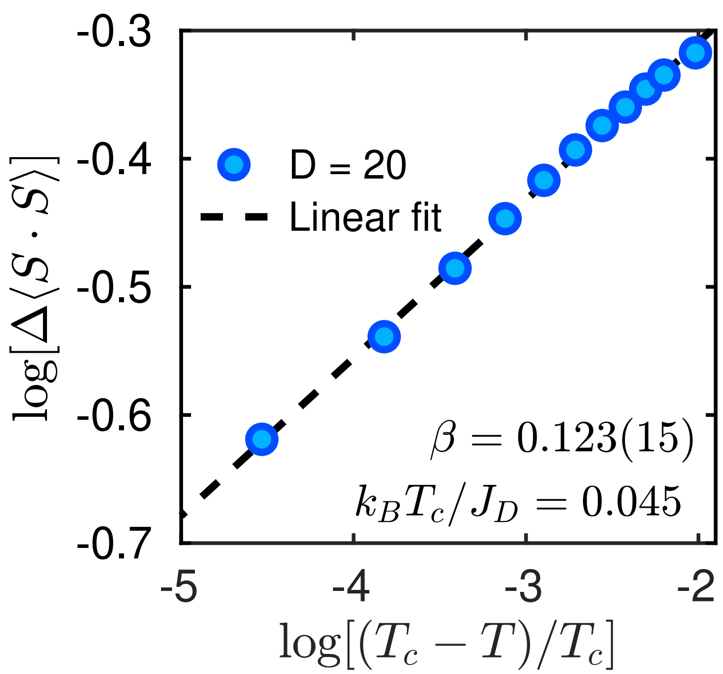




Diverging correlation length

Jump in <S · S> on dimer below Tc

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



also confirmed with MPS:

Wang, Li, Xi, Gao, Yan, Li, Su, PRL 131, 116702 (2023)

Other examples

PHYSICAL REVIEW B 100, 165147 (2019)

Tensor network simulation of the Kitaev-Heisenberg model at finite temperature

Piotr Czarnik,[1] Anna Francuz,[2] and Jacek Dziarmaga[2]
[1]*Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, PL-31342 Kraków, Poland*
[2]*Marian Smoluchowski Institute of Physics, Jagiellonian University, ulitsa Prof. S. Lojasiewicza 11, PL-30-348 Kraków, Poland*

PHYSICAL REVIEW B 103, 075113 (2021)

Tensor network study of the $m = \frac{1}{2}$ magnetization plateau in the Shastry-Sutherland model at finite temperature

Piotr Czarnik,[1] Marek M. Rams,[2] Philippe Corboz,[3] and Jacek Dziarmaga[2]
[1]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*
[2]*Institute of Theoretical Physics, Jagiellonian University, Łojasiewicza 11, PL-30348 Kraków, Poland*
[3]*Institute for Theoretical Physics, Delta Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands*

SciPost Phys. 10, 019 (2021)

Finite-temperature symmetric tensor network for spin-1/2 Heisenberg antiferromagnets on the square lattice

Didier Poilblanc[1*], Matthieu Mambrini[1] and Fabien Alet[1]

PHYSICAL REVIEW LETTERS 128, 227202 (2022)

Thermal Ising Transition in the Spin-1/2 J_1-J_2 Heisenberg Model

Olivier Gauthé[*] and Frédéric Mila
Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

PHYSICAL REVIEW B 106, 195105 (2022)

Finite-temperature tensor network study of the Hubbard model on an infinite square lattice

Aritra Sinha,[1] Marek M. Rams,[1] Piotr Czarnik,[1,2] and Jacek Dziarmaga[1]
[1]*Jagiellonian University, Institute of Theoretical Physics, ulica Łojasiewicza 11, 30-348 Kraków, Poland*
[2]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

PHYSICAL REVIEW B 111, 014428 (2025)

Weakly first-order melting of the 1/3 plateau in the Shastry-Sutherland model

Samuel Nyckees,[1] Philippe Corboz,[2] and Frédéric Mila[1]
[1]*Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland*
[2]*Institute for Theoretical Physics and Delta Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands*

Forestalled Phase Separation as the Precursor to Stripe Order

Aritra Sinha[1] and Alexander Wietek[1]
[1]*Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, Dresden 01187, Germany*

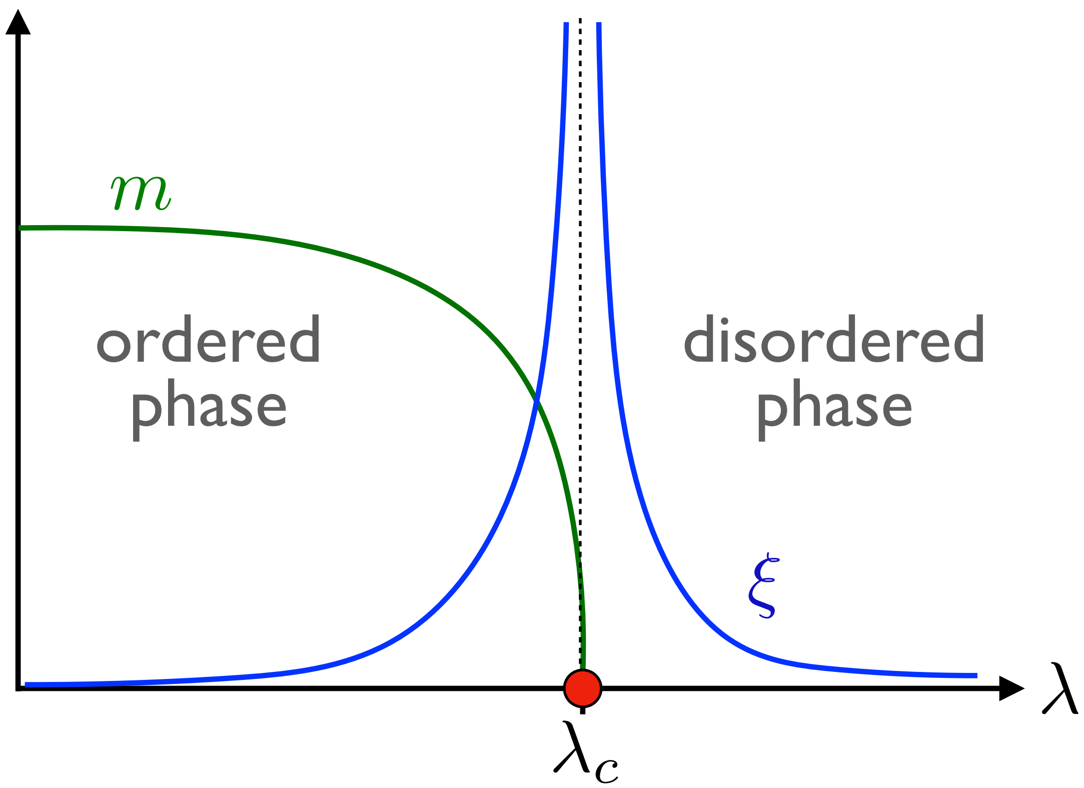
(Dated: November 26, 2024)

Obtaining accurate results at low-T challenging! Room for improvement!

Finite correlation length scaling: “finite size scaling” with iPEPS

$$L \to \xi_D$$

Motivation: study of quantum phase transitions



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

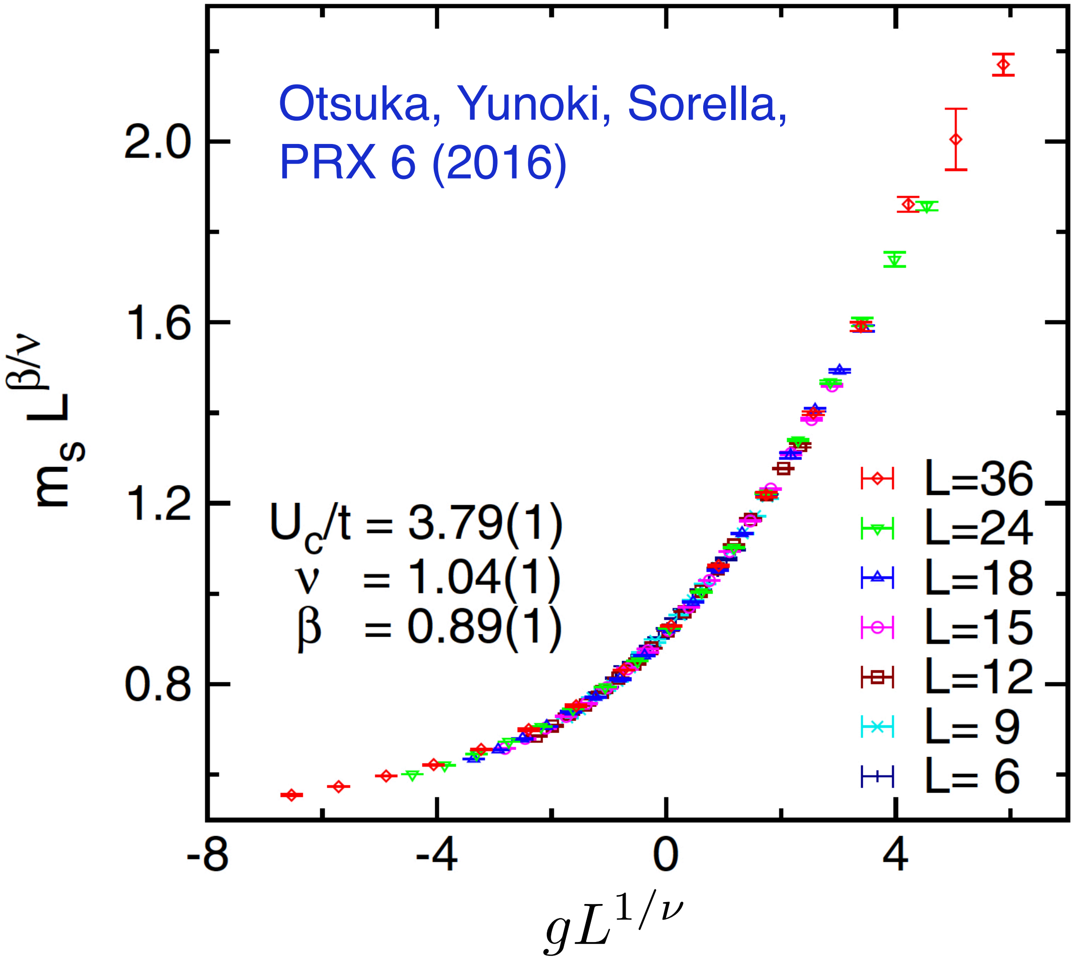
$$\xi \sim |g|^{-\nu}$$

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

Critical coupling?
Universal critical exponents?
Challenging!

- Strong finite size effects in the vicinity of the critical point
- Powerful approach: *finite size scaling:* $m(g,L) = L^{-\beta/\nu}\mathcal{F}(gL^{1/\nu})$

Motivation: study of quantum phase transitions



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

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

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

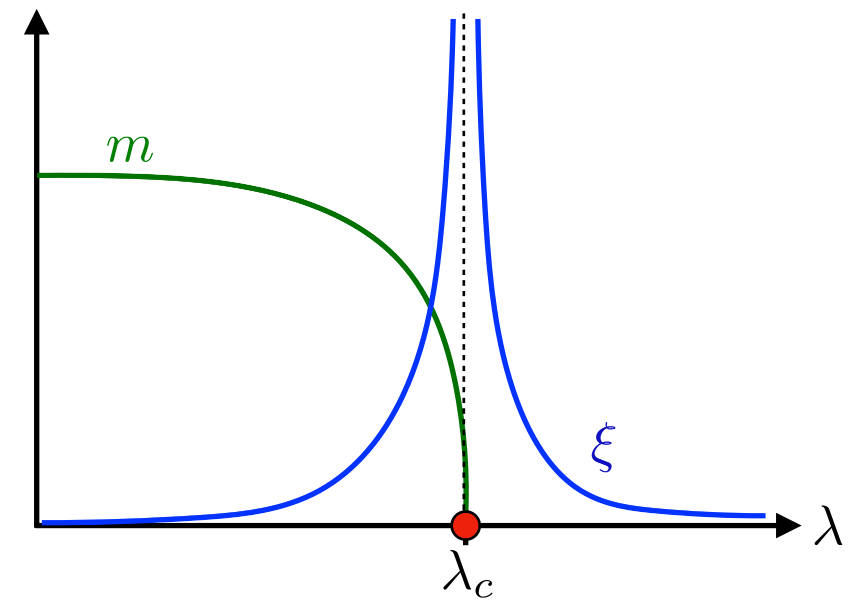
- Strong finite size effects in the vicinity of the critical point

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

- Can we do something similar with iPEPS?

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?

PC, P. Czarnik, G. Kapteijns, L. Tagliacozzo, PRX 8 (2018); M. Rader and A. M. Läuchli, PRX 8 (2018)

- 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: $z = 1$ $\xi_{time} \sim \xi_{space}^z \sim \xi_{space}$

- 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!

Finite correlation length scaling with iPEPS

PC, P. Czarnik, G. Kapteijns, L. Tagliacozzo, PRX 8 (2018); M. Rader and A. M. Läuchli, PRX 8 (2018)

- Complication: there are two bond dimensions:

Bond dimension of the TN ansatz: $D \to \xi_D$

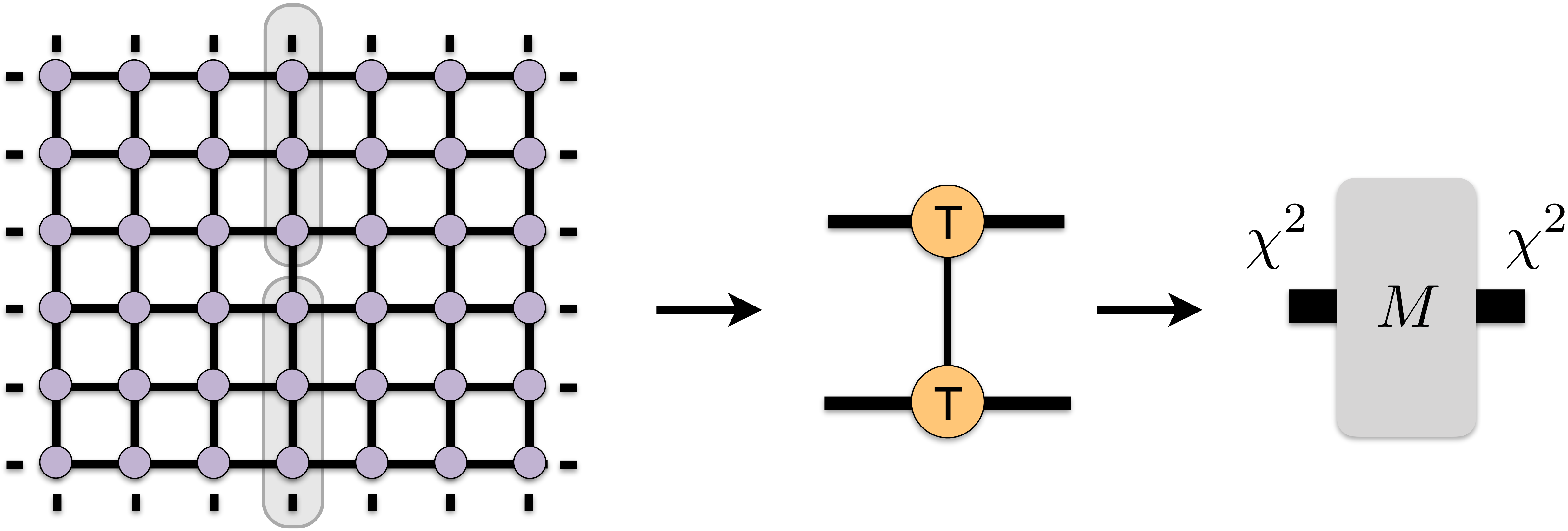
Boundary dimension in contraction: $\chi \to \xi_\chi$

- 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 MPS (1D) case:

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

Computing the correlation length with CTM

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



Transfer matrix made of
an infinite column of tensors

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

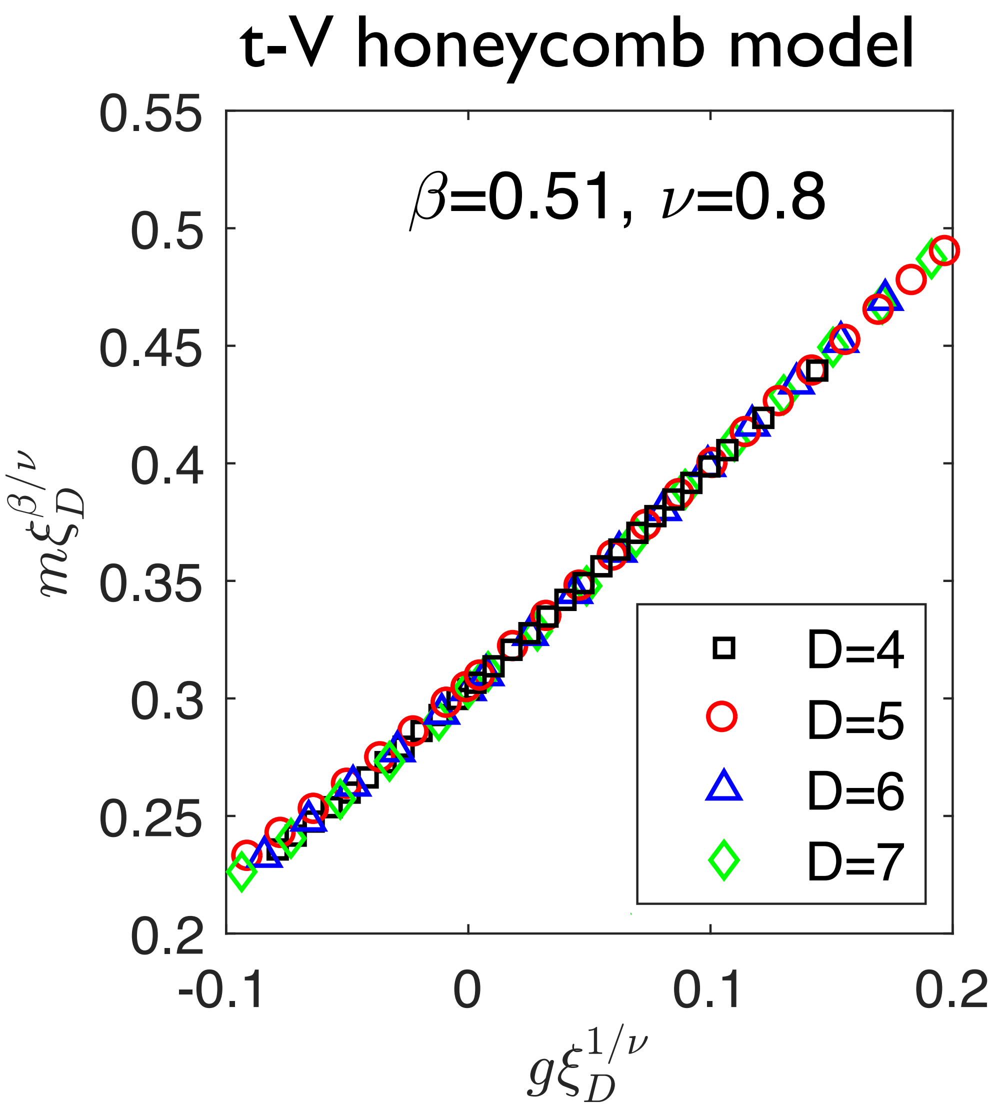
1st and 2nd lowest
eigenvalue of M

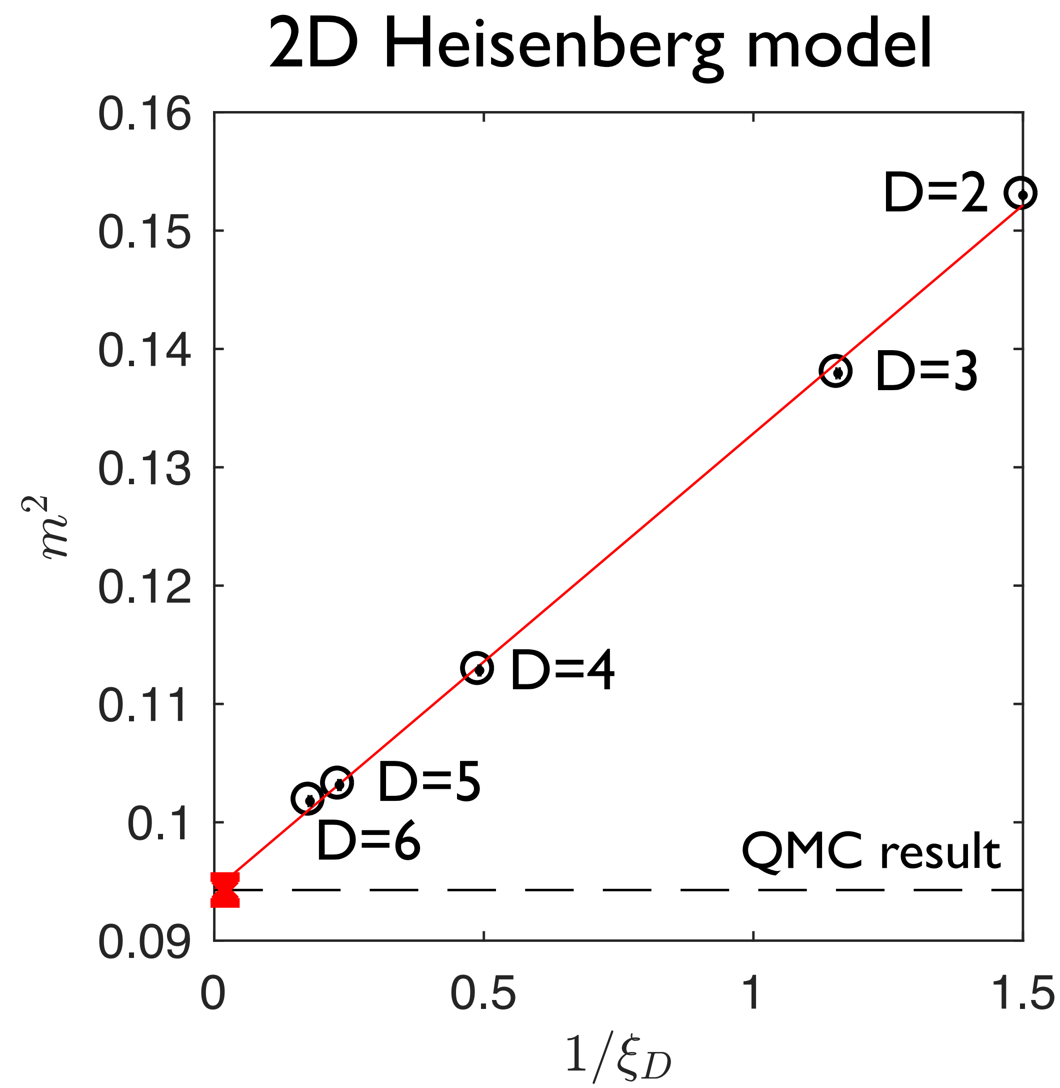
★ Accurate $\chi \to \infty$ extrapolation technique:

Rams, Czarnik & Cincio, PRX 8, 041033 (2018)

Application examples

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





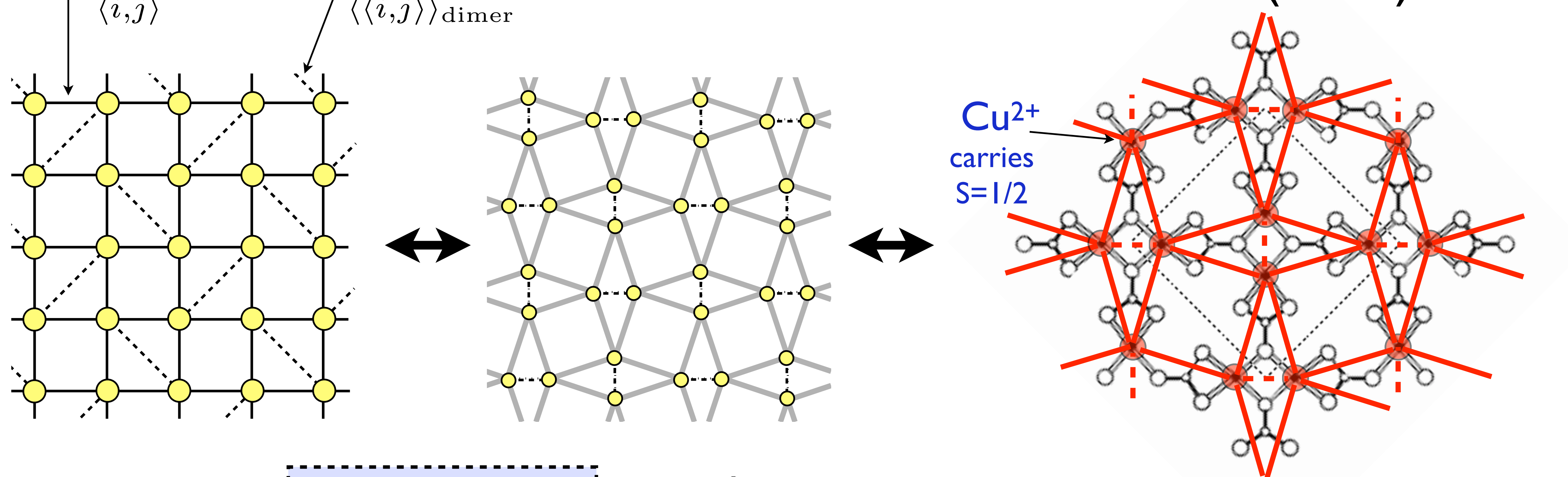
- TF Ising & XY model — M. Rader and A. M. Läuchli, PRX 8 (2018)
- J_1-J_2 Heisenberg model — Hasik, Poilblanc, Becca, SciPost Physics 10 (2021)
- *t-V* model at finite T — Czarnik, PC, PRB 99 (2019)
- Kagome HM — Ferrari, et. al, SciPost Phys. 14, 139 (2023)
- Anisotropic triangular HM — Hasik, PC, PRL 133, 176502 (2024)

⋮ ⋮

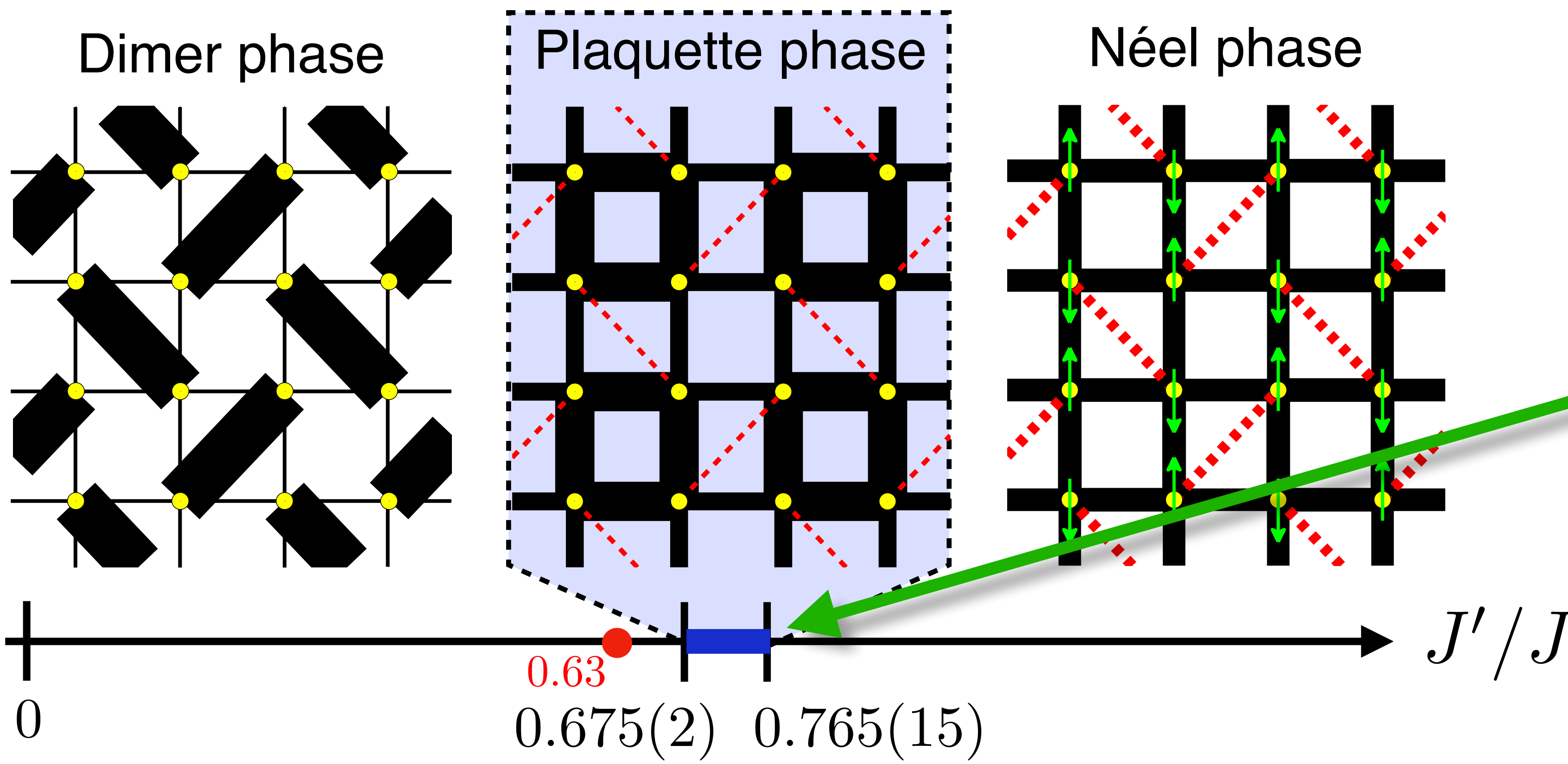
The Shastry-Sutherland model revisited

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

SrCu₂(BO₃)₂



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



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

Deconfined QCP

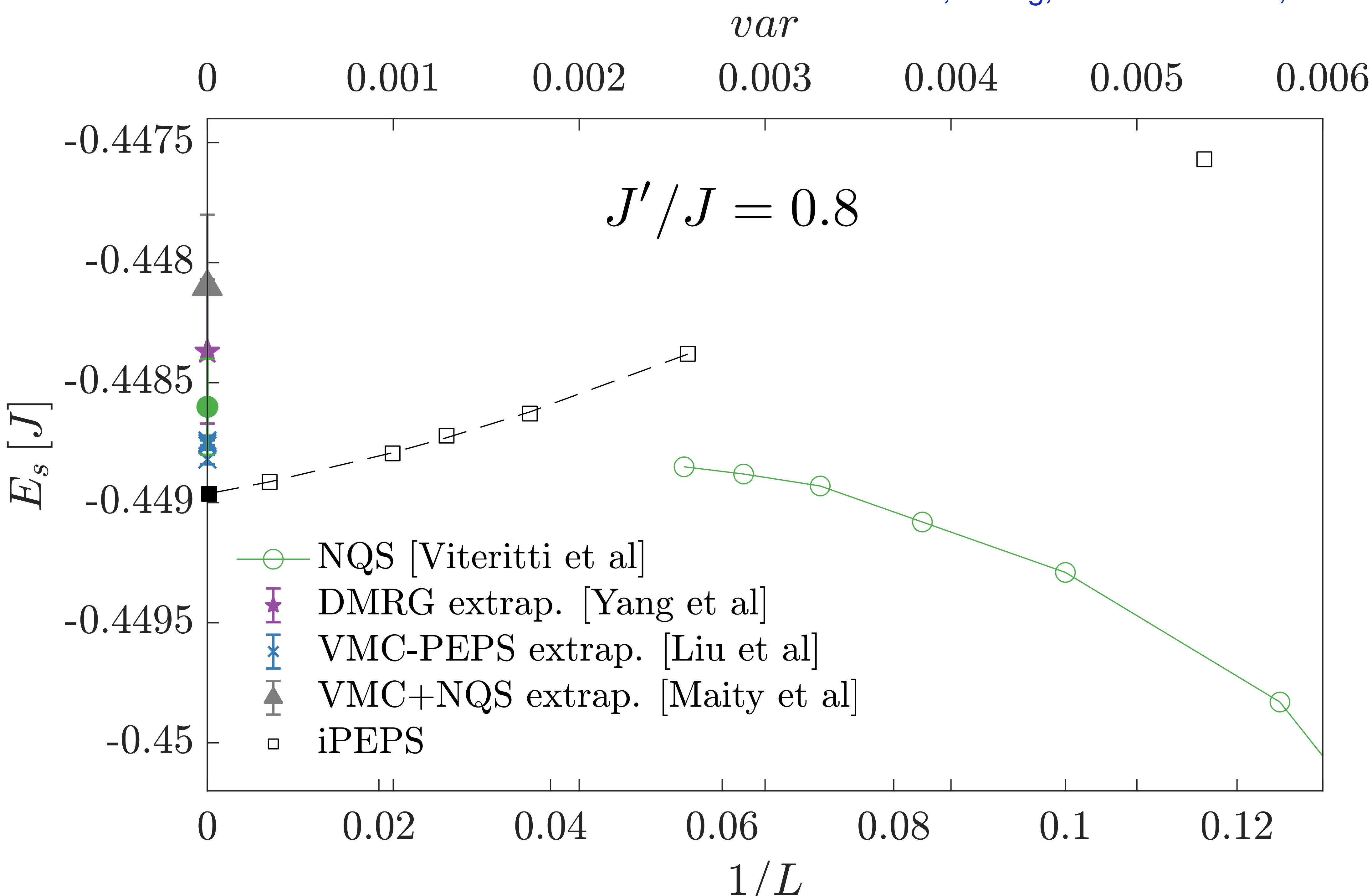
Lee, You, Sachdev & Vishwanath, PRX 9 (2019)
Liu et al, PRL 133 (2024)

Intermediate QSL phase

Yang et al, PRB 105 (2022)
Wang et al, CPL 39 (2022)
Viteritti et al, arxiv: 2311.16889
Maity et al., arXiv: 2501.00096

Benchmark comparison of variational energies

PC, Zhang, Ponsioen & Mila, arXiv:2502.14091



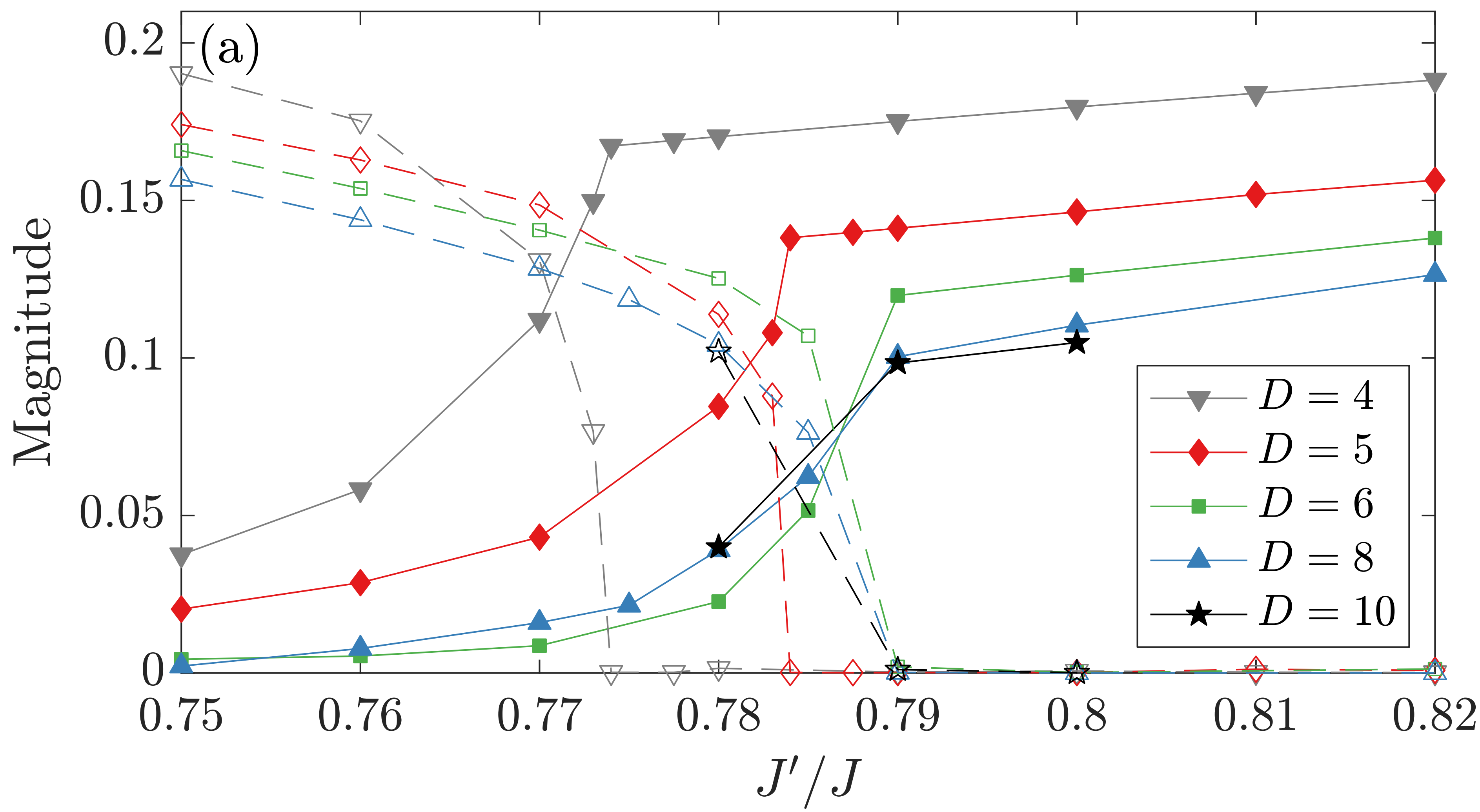
★ iPEPS yields lowest variational energy in the thermodynamic limit

Plaquette - “AF” phase transition at finite D

PC, Zhang, Ponsioen & Mila, arXiv:2502.14091

Plaquette order

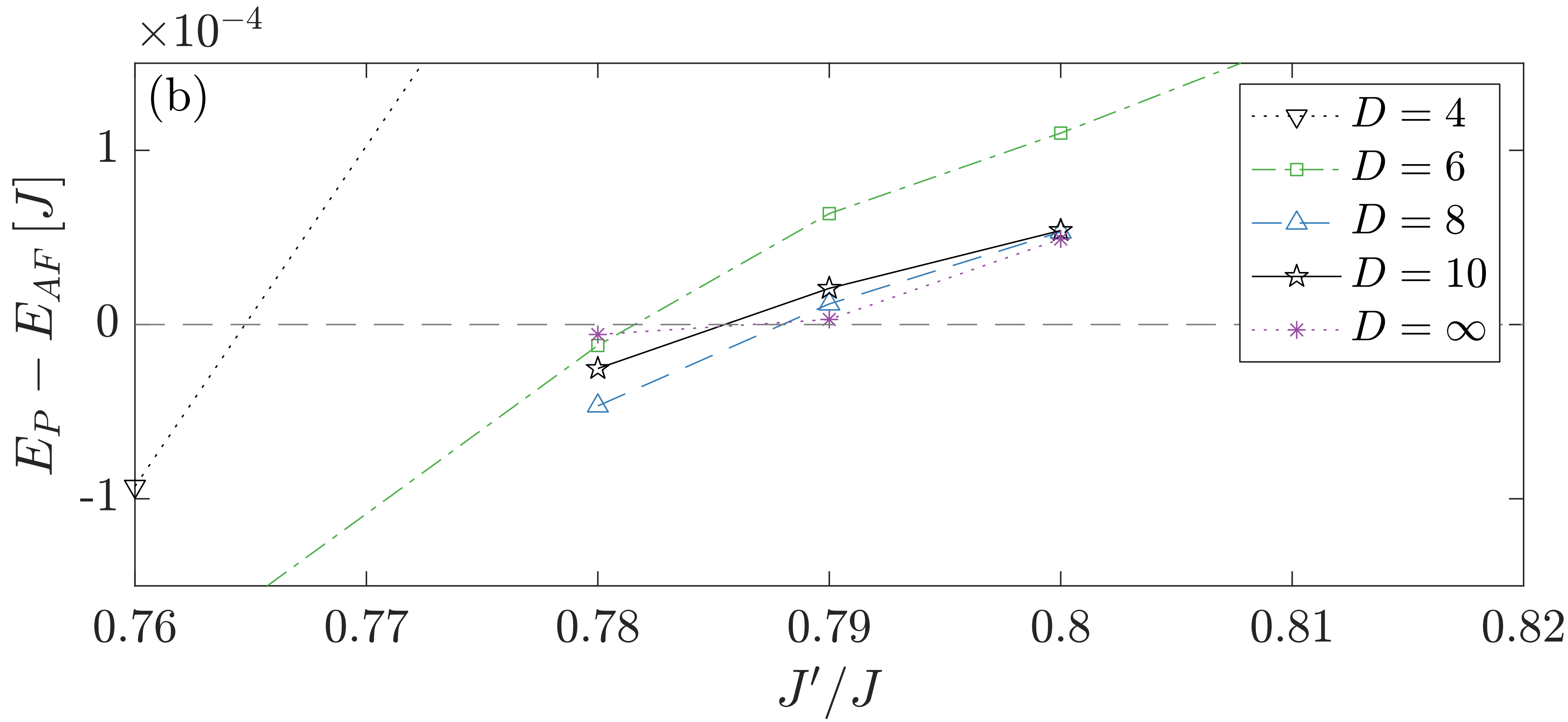
AF order (at finite D)



★ Phase transition between 0.78 and 0.79 for large D

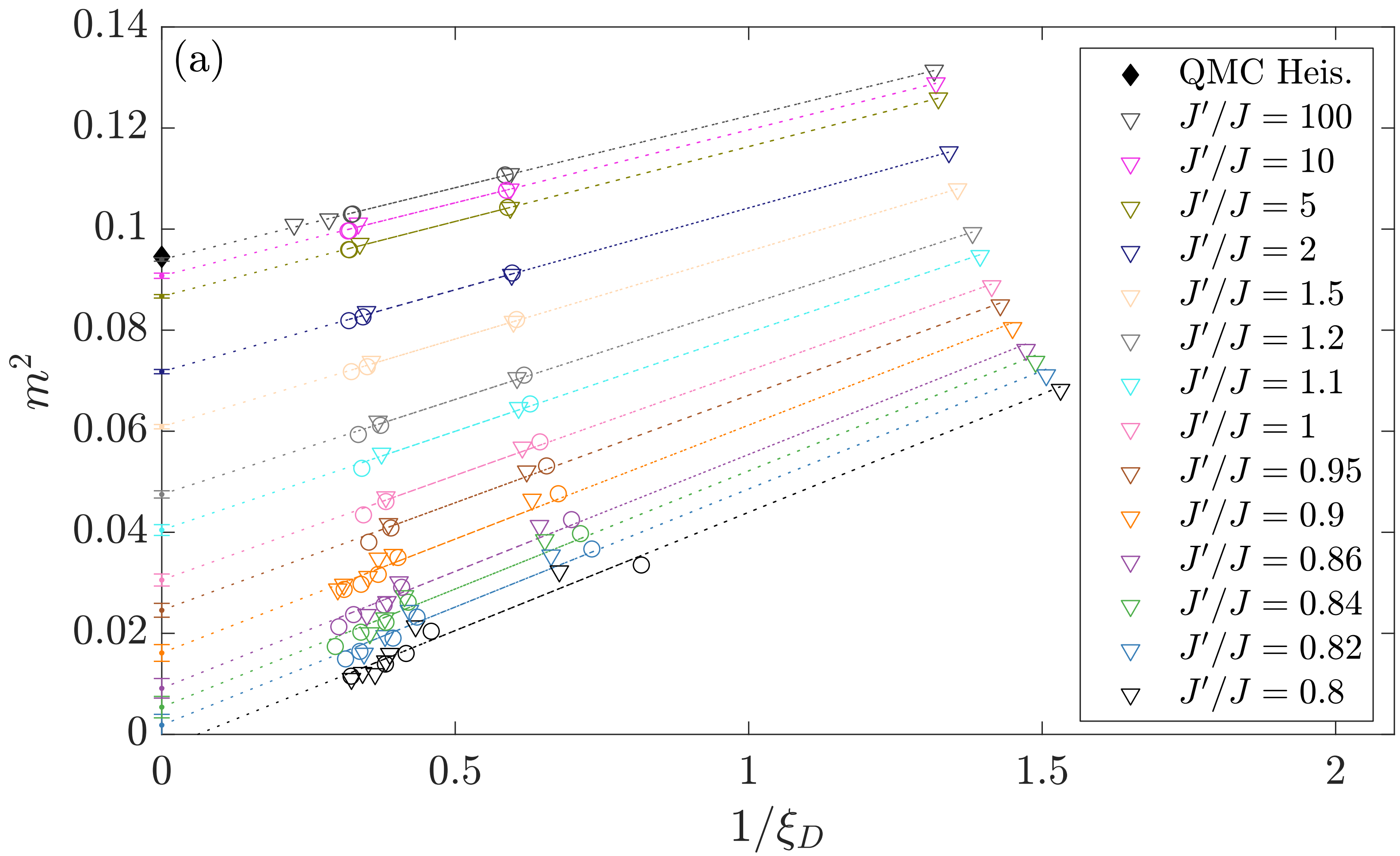
P - "AF" transition using constrained iPEPS

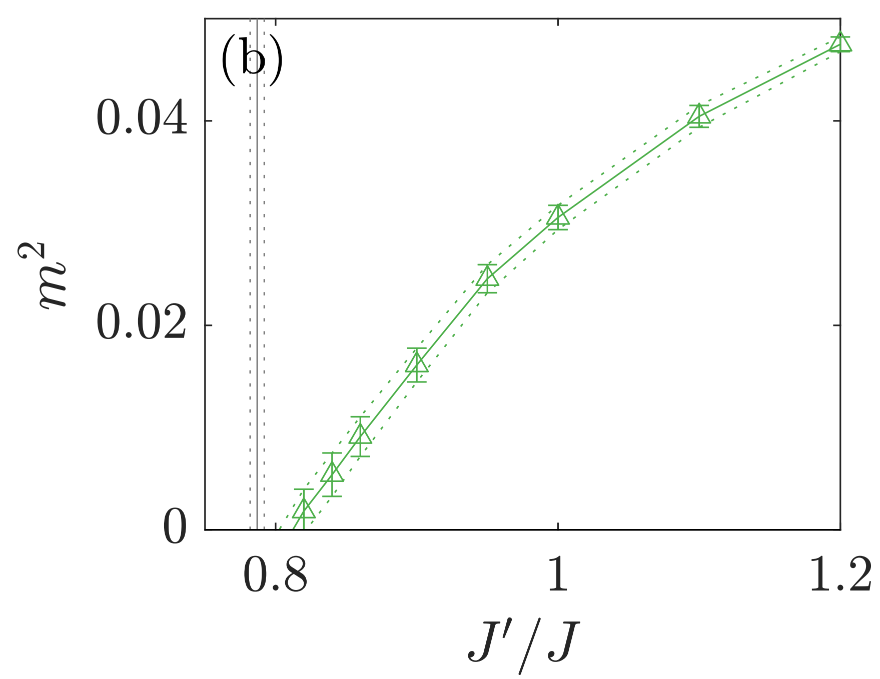
PC, Zhang, Ponsioen & Mila, arXiv:2502.14091

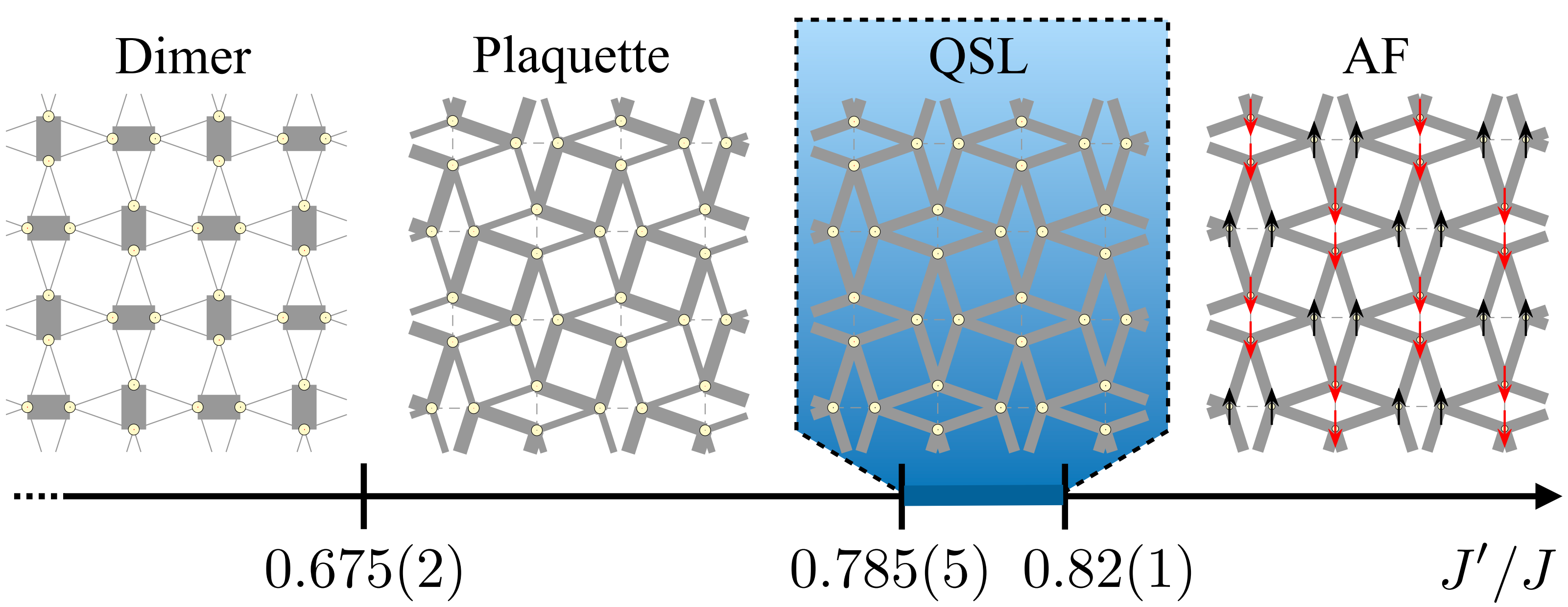


★ Phase transition between 0.78 and 0.79 for large and infinite D

Finite correlation length scaling

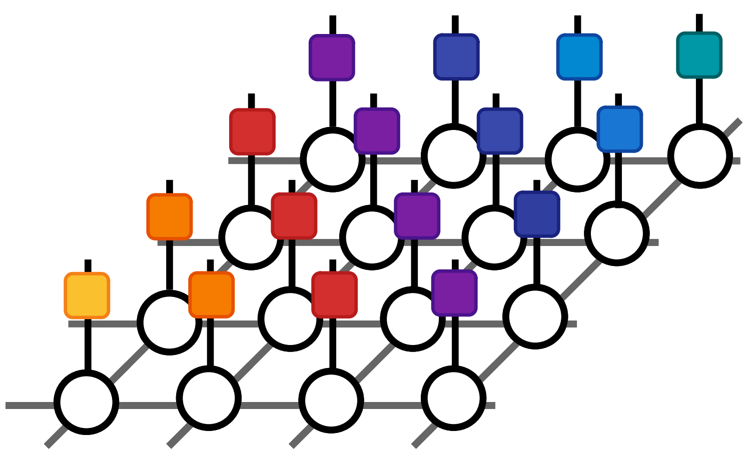




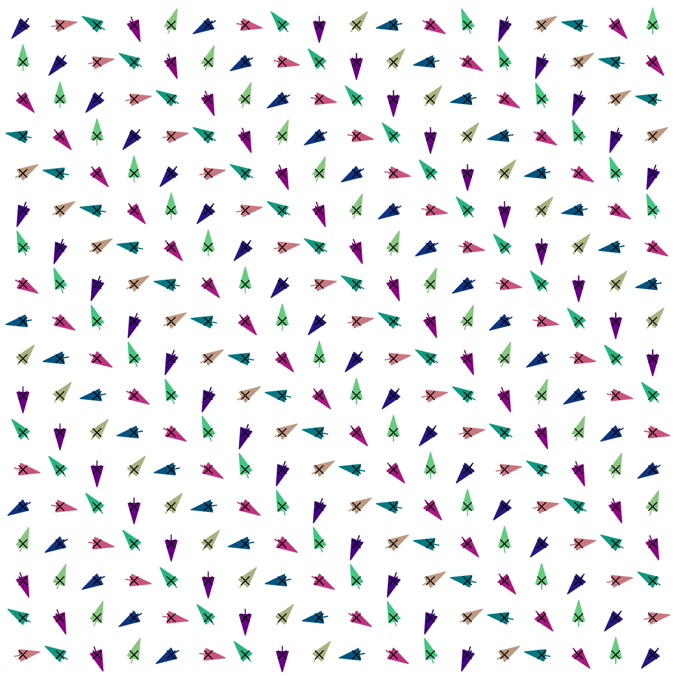


★ In agreement with DMRG and NQS

Study of incommensurate spin spiral phases: **spiral iPEPS**



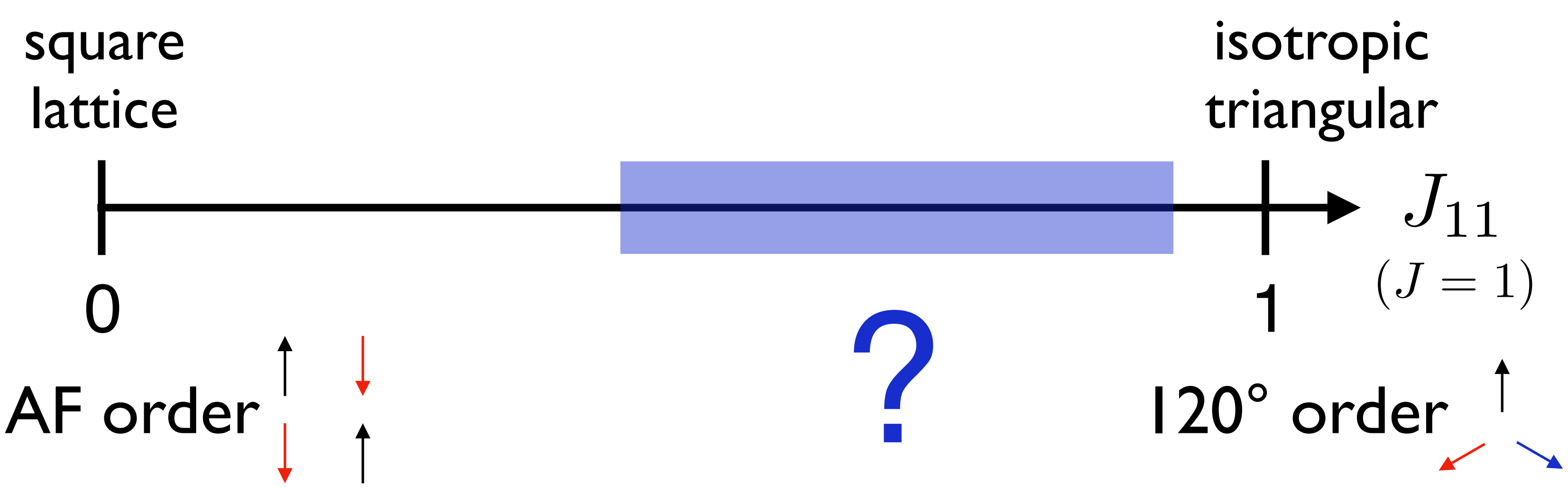
Juraj Hasik

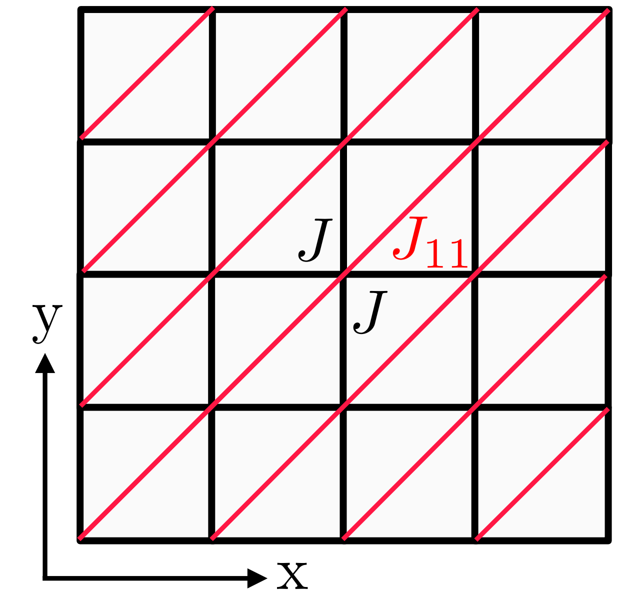


J. Hasik, PC, PRL 133, 176502 (2024)

Anisotropic triangular lattice Heisenberg model

$$H = \sum_{\mathbf{r}} J(\mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{x}} + \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{y}}) + J_{11} \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}+\hat{x}+\hat{y}}$$





- Mean-field theory: Spin spiral order between [0.5, 1] with $\mathbf{q} = (\pi, \pi) \ldots (2\pi/3, 2\pi/3)$
- Spin-wave theory: 0-flux quantum spin liquid (QSL) for [0.77, 0.88] Hauke et al, NJP 13 (2011)
- Schwinger boson theory: nematic QSL between [0.6, 0.9] Gonzales et al, PRB 102 (2020)
- Series expansion: dimerized state between [0.7, 0.9] Weihong et al, PRB 59 (1999)
- DMRG: weak spatial symmetry breaking? Weichselbaum & White, PRB 84 (2011)
- VMC: competing QSL and spiral phase between [0.7, 0.8] Ghorbani et al, PRB 93 (2016)

Numerical study of spin spiral phases

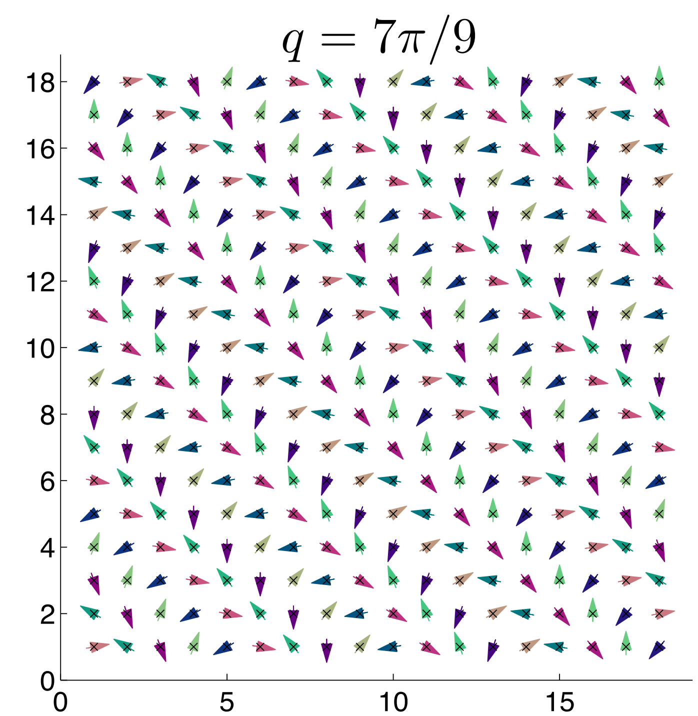
- **Challenge:** system size needs to be commensurate with the wavelength of the spin spiral

- VMC: only specific wave vectors can be realized → **bias**

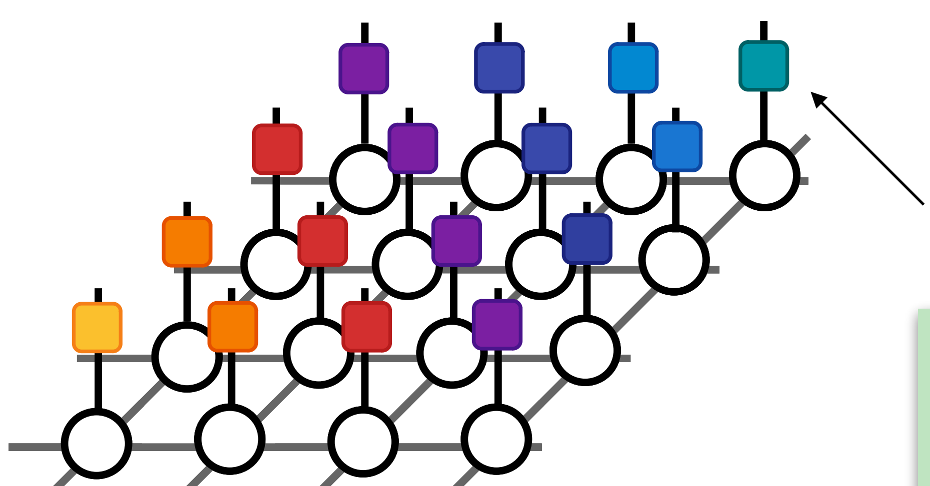
- iPEPS: large unit cells are in principle possible…

  … but rather cumbersome/expensive

- **Spiral iPEPS:** single-tensor ansatz with position dependent local unitaries



iPEPS with 18 tensors

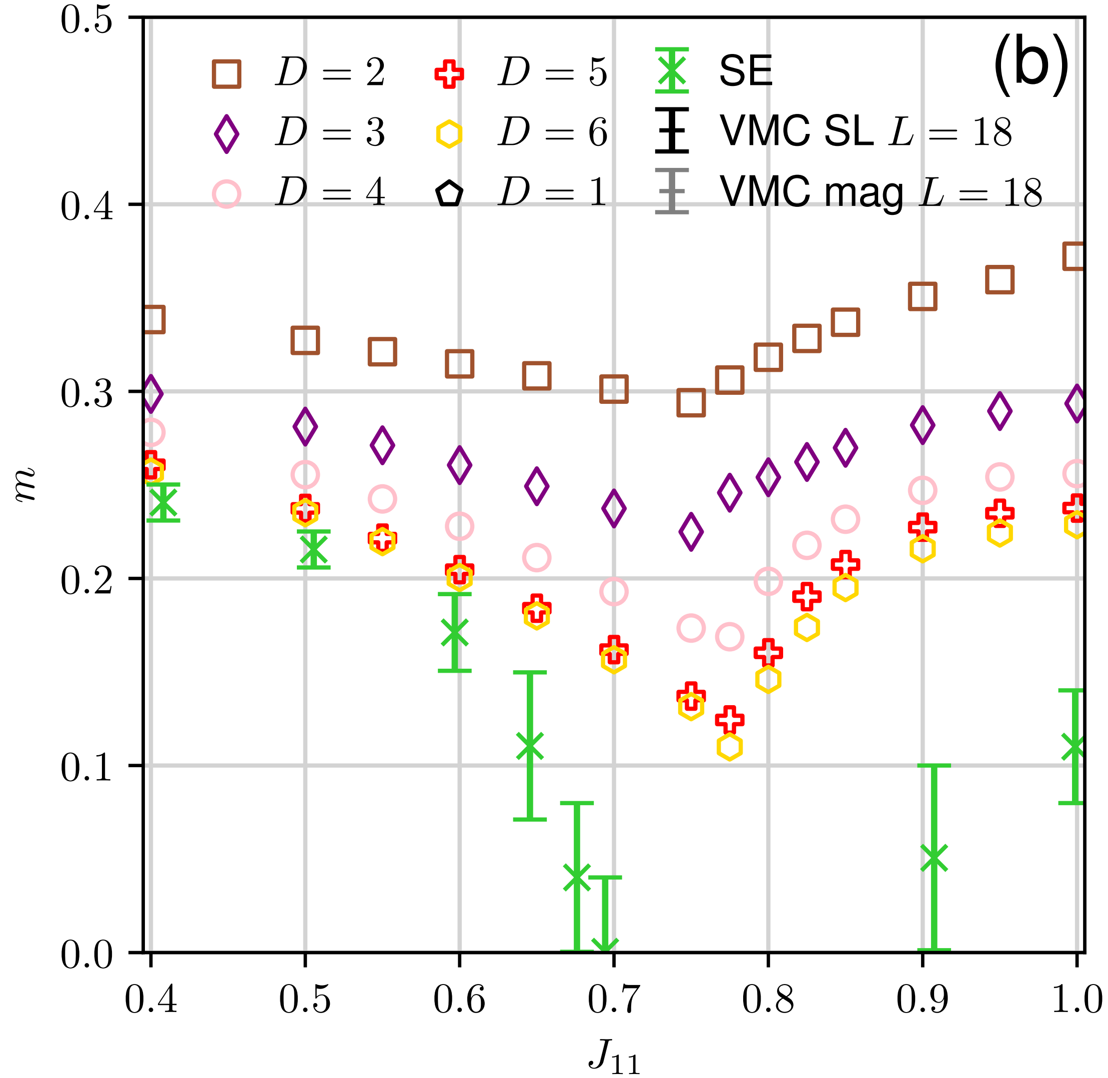


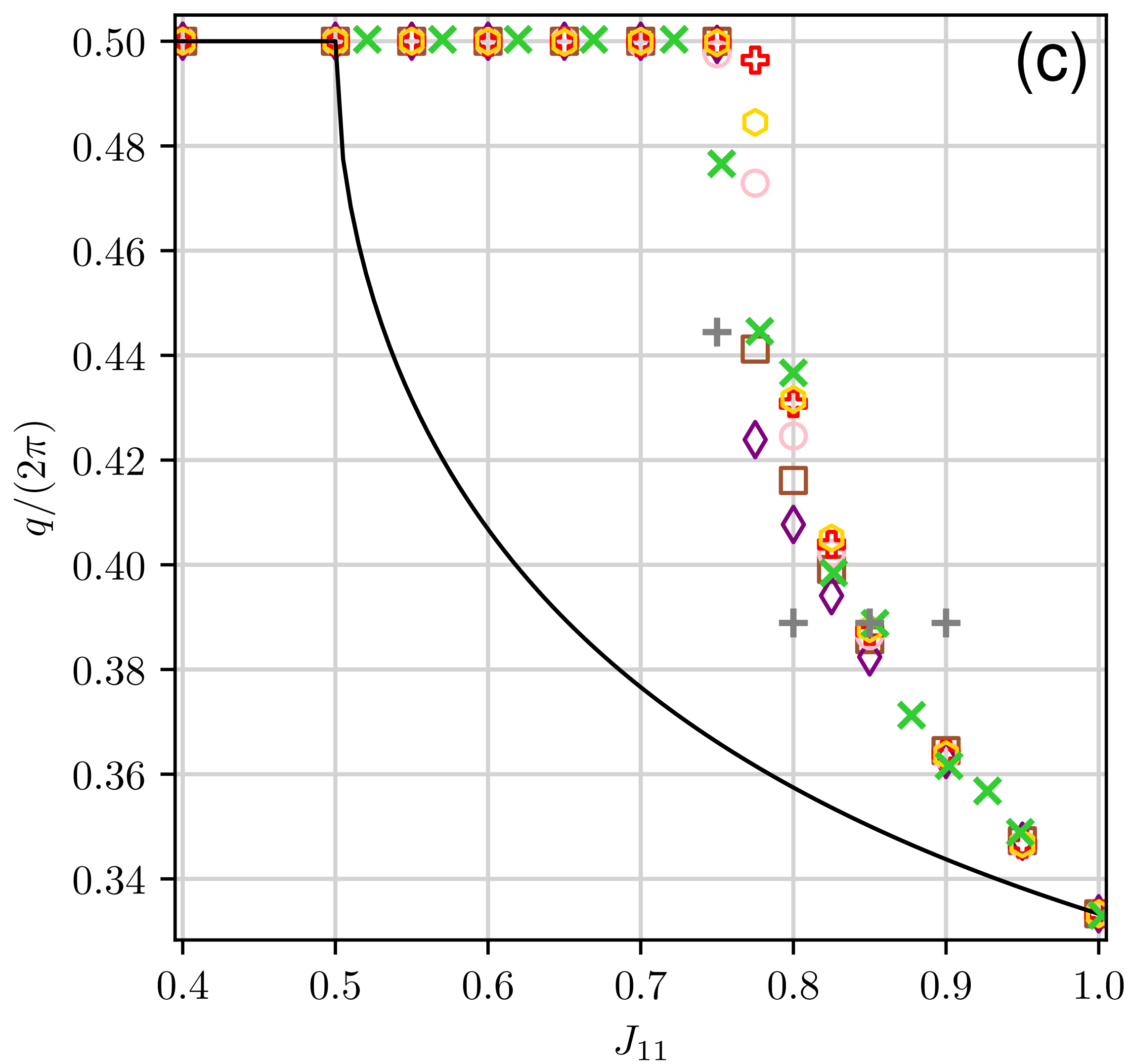
$$u_{\mathbf{r}}(\mathbf{q}, \mathbf{r}') = \exp[i\pi(\mathbf{q}\cdot\mathbf{r}')S^y_{\mathbf{r}}]$$

rotates the spin in the x-z plane, turning the spiral into a (correlated) ferromagnet, with wavevector ***q*** *as variational parameter*

Similar approach used for MPS in 1D: Ueda & Maruyama, PRB 86 (2012)

Optimal *q* as a function of J_{11}

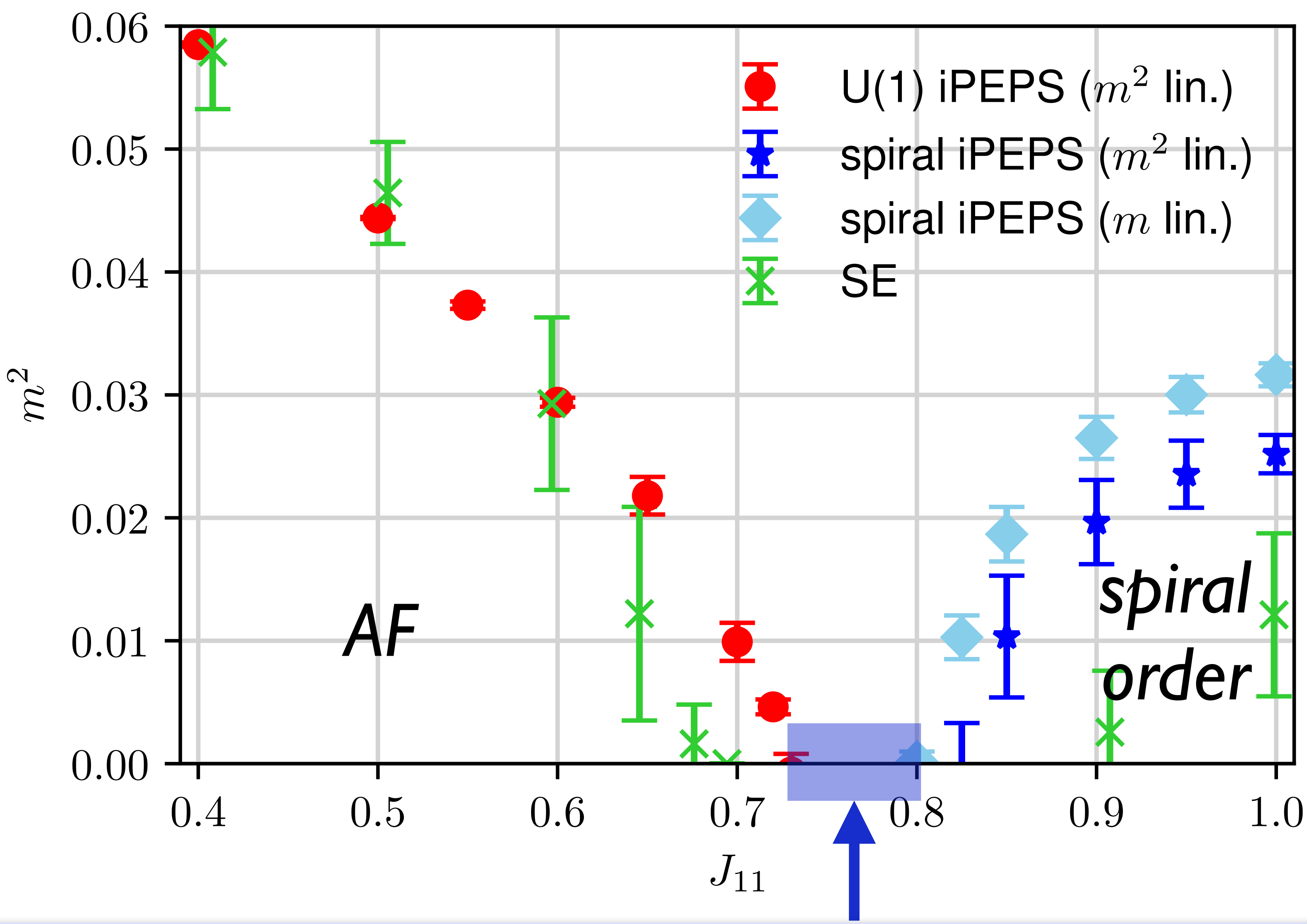




- m suppressed around [0.7, 0.8]

- Optimal $q=(\pi,\pi)$ up to $J_{11}\sim 0.75$

Extrapolated order parameter



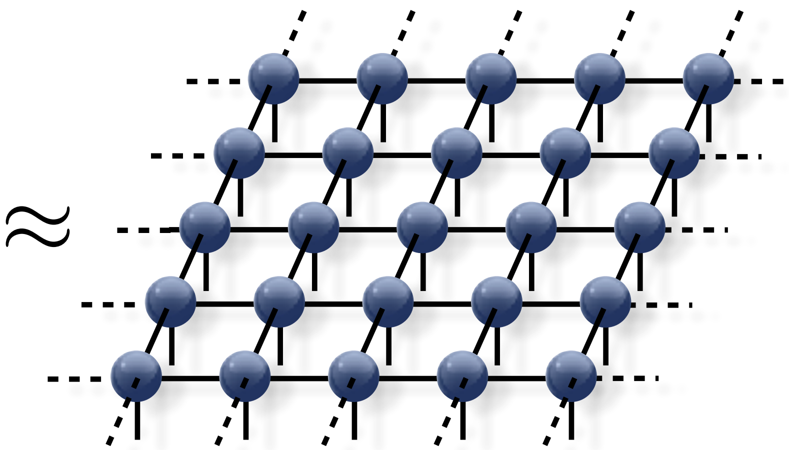
- ***Quantum spin liquid*** *for* $J_{11} \in [0.73(1), 0.80(2)]$

Unbiased simulation of spiral order is crucial for resolving the competition with QSL !

Excitations with iPEPS

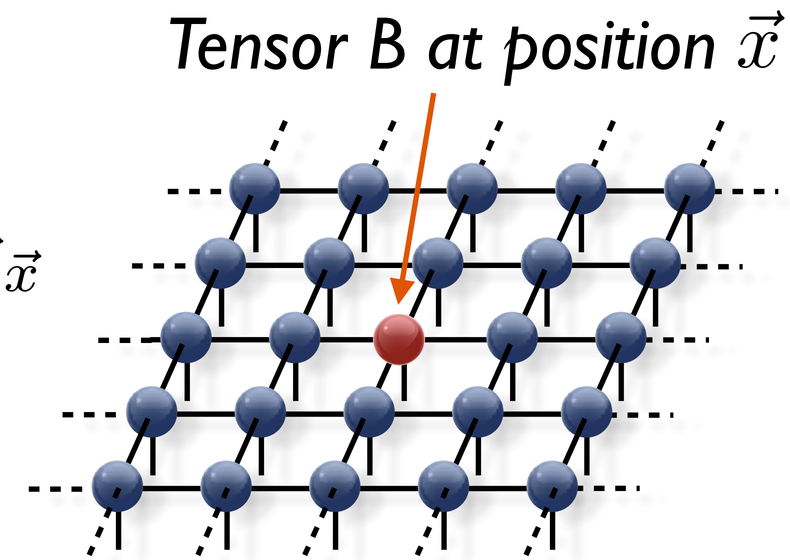
iPEPS excitation ansatz

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



- Excitation on top of ground state with momentum k

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

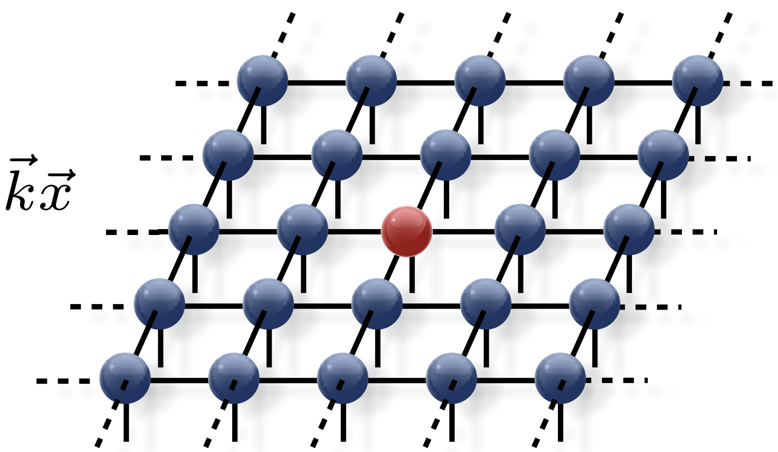


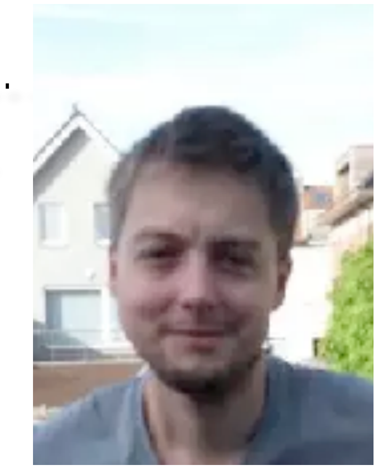
Haegeman, Pirvu, Weir, Cirac, Osborne, Verschelde, and Verstraete, PRB 85, 100408(R) (2012).
Haegeman, Michalakis, Nachtergaele, Osborne, Schuch, and Verstraete, PRL 111, 080401 (2013).
Haegeman, Osborne, and Verstraete, PRB 88, 075133 (2013).
Zauner, Draxler, Vanderstraeten, Degroote, Haegeman, Rams,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

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





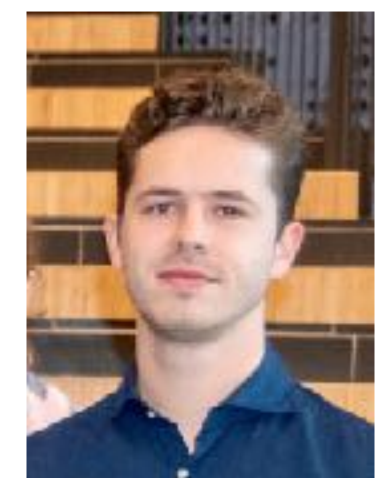
Laurens Vanderstraeten

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)

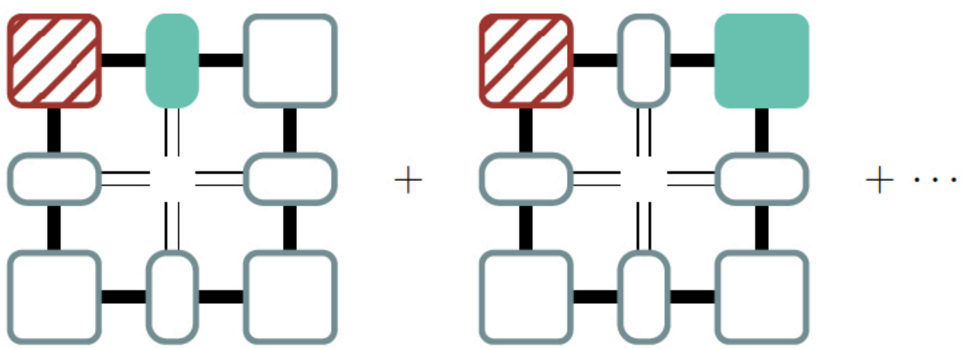
CTM approach Ponsioen and PC, PRB 101, 195109 (2020)

CTM + AD approach Ponsioen, Assaad, PC, SciPost Physics, 12, 006 (2022)
Ponsioen, Hasik, PC, PRB 108 (2023)

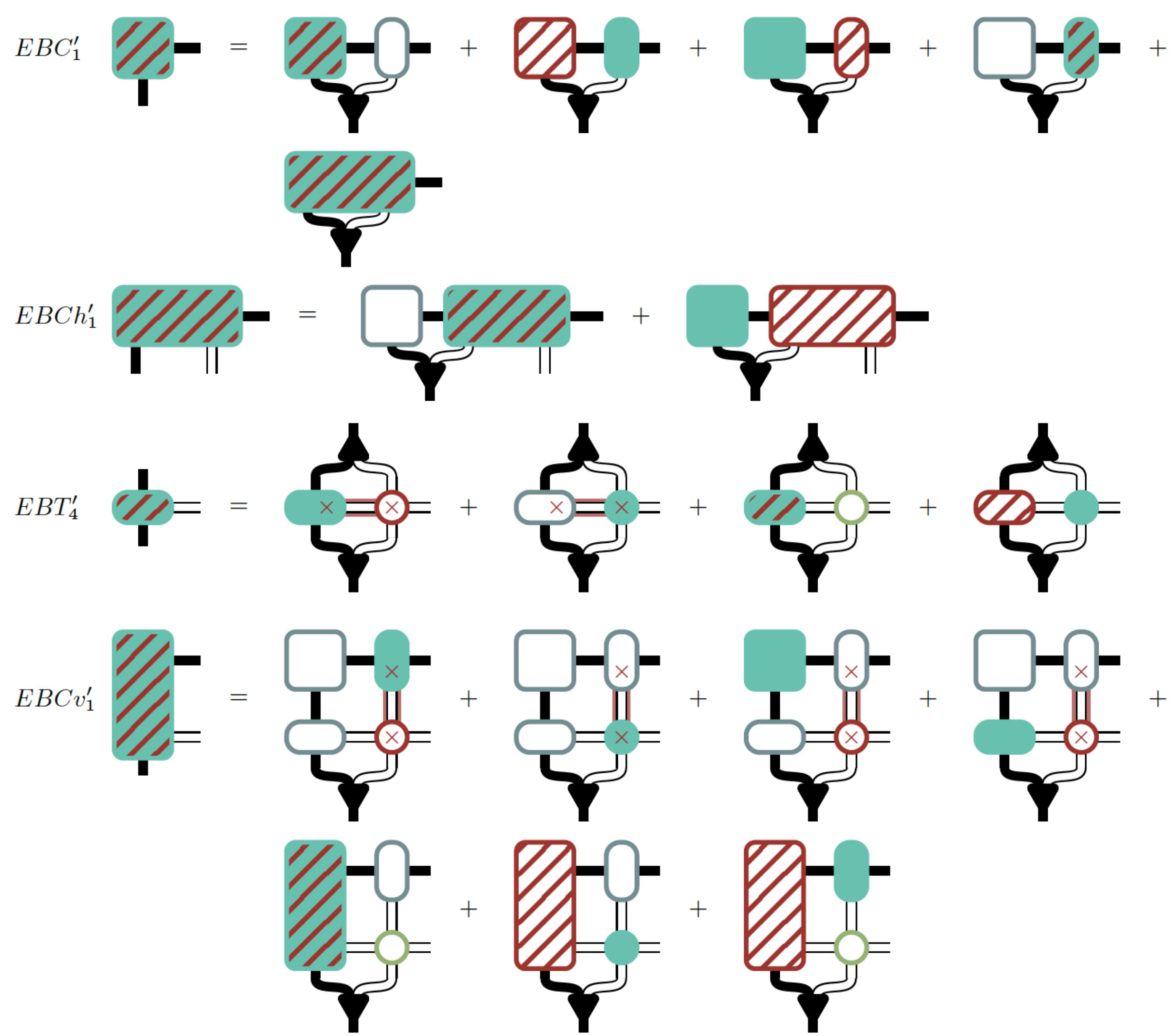
Generating function Tu, Vanderstraeten, Schuch, Lee, Kawashima, Chen, PRX Quantum ’24

Systematic summation using CTM

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



Left move examples:



Norm

Energy

Excitation

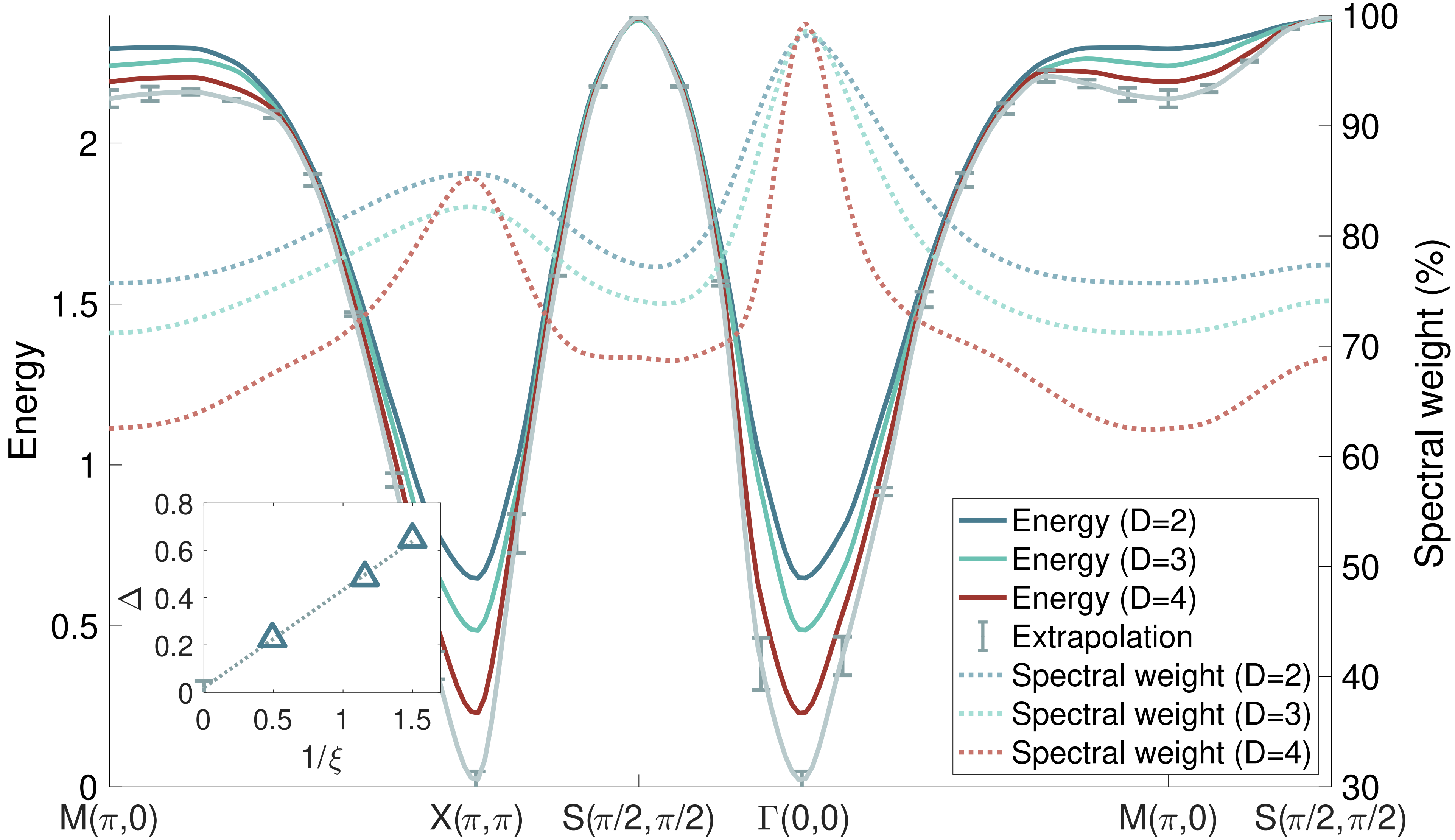
Energy + excitation

Ponsioen & PC, PRB 101 (2020)

Simpler: *use AD to avoid the summation of energy terms*

Ponsioen, Assaad, PC, SciPost Physics, 12, 006 (2022)
Ponsioen, Hasik, PC, PRB 108 (2023)
Tu, Vanderstraeten, Schuch, Lee, Kawashima, Chen, PRX Quantum ’24

Benchmark: 2D Heisenberg model

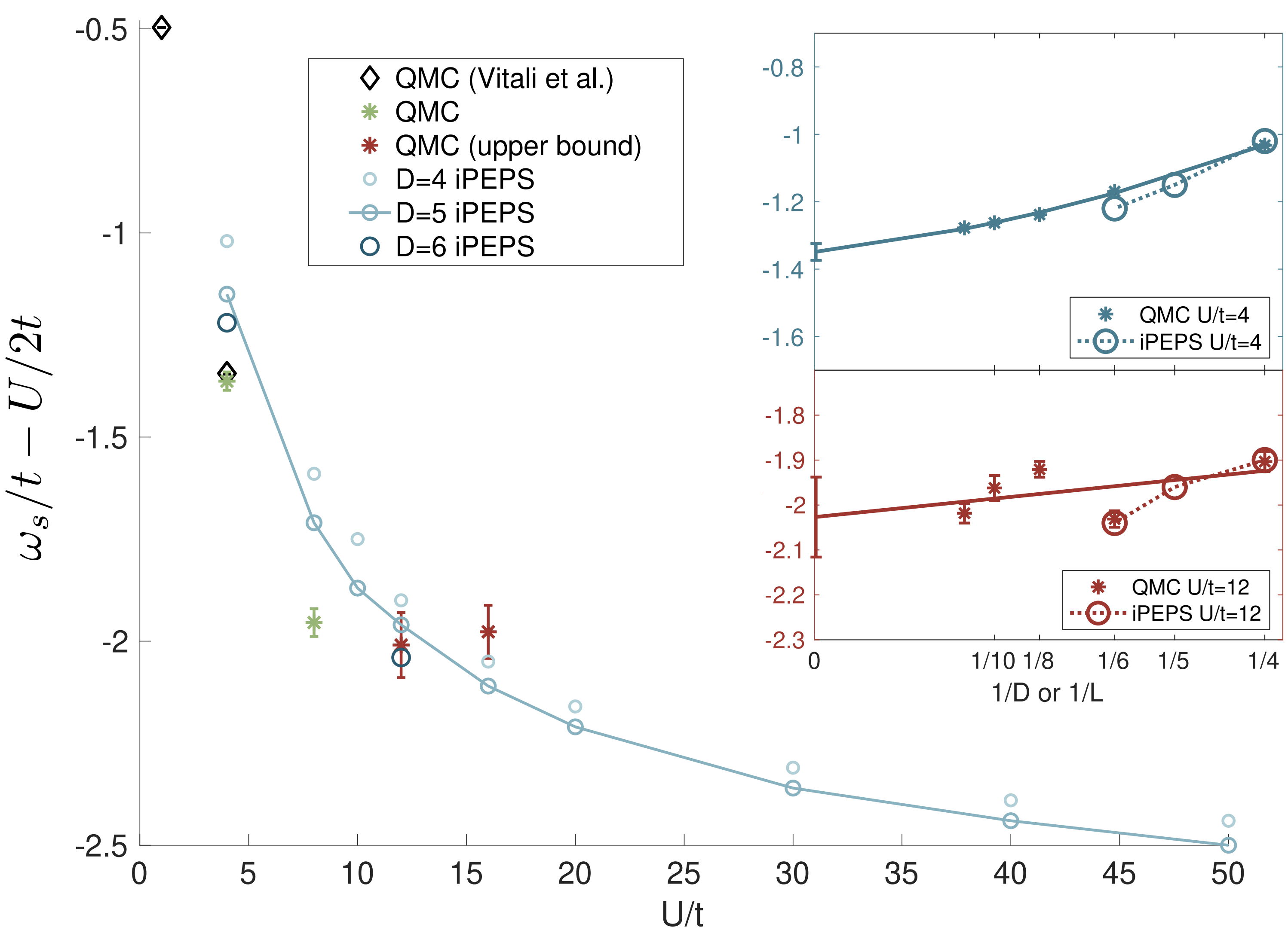


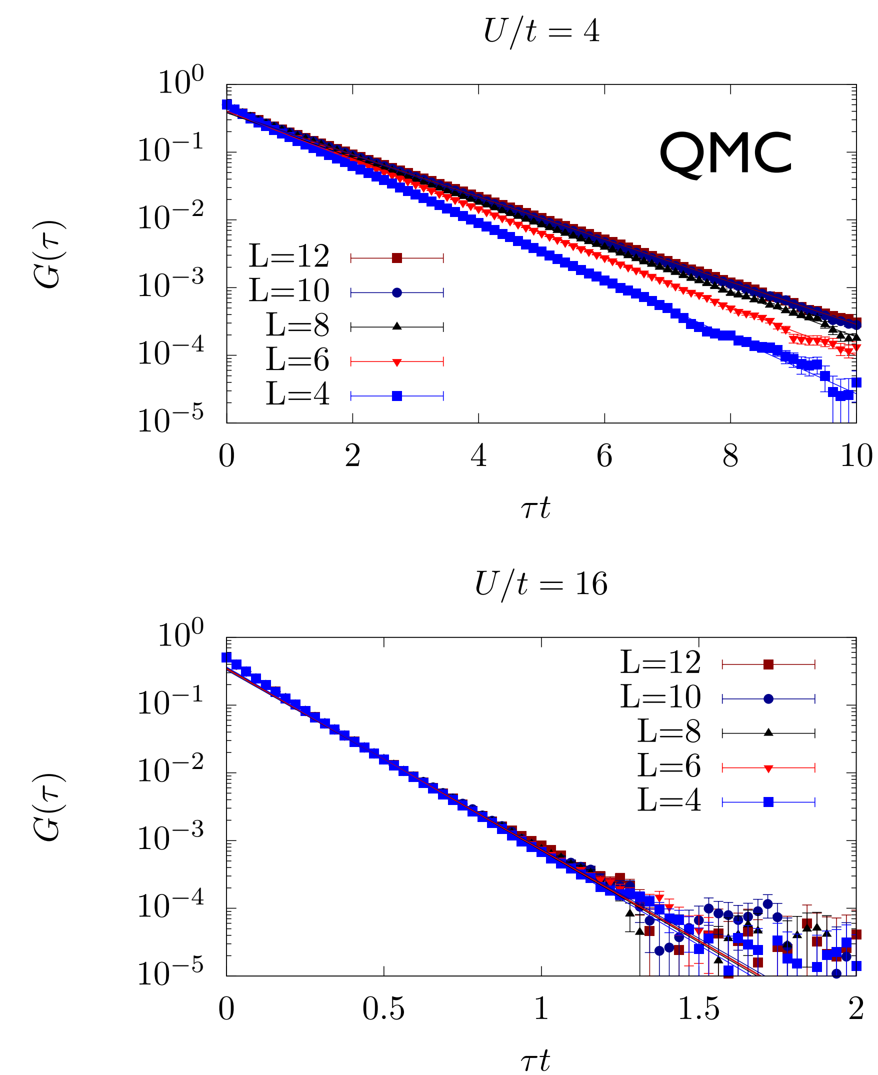
Ponsioen and PC, PRB 101, 195109 (2020)

similar results in:
Vanderstraeten, Haegeman, Verstraete, PRB 99, 165121 (2019)

Charge gap in the half-filled Hubbard model

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



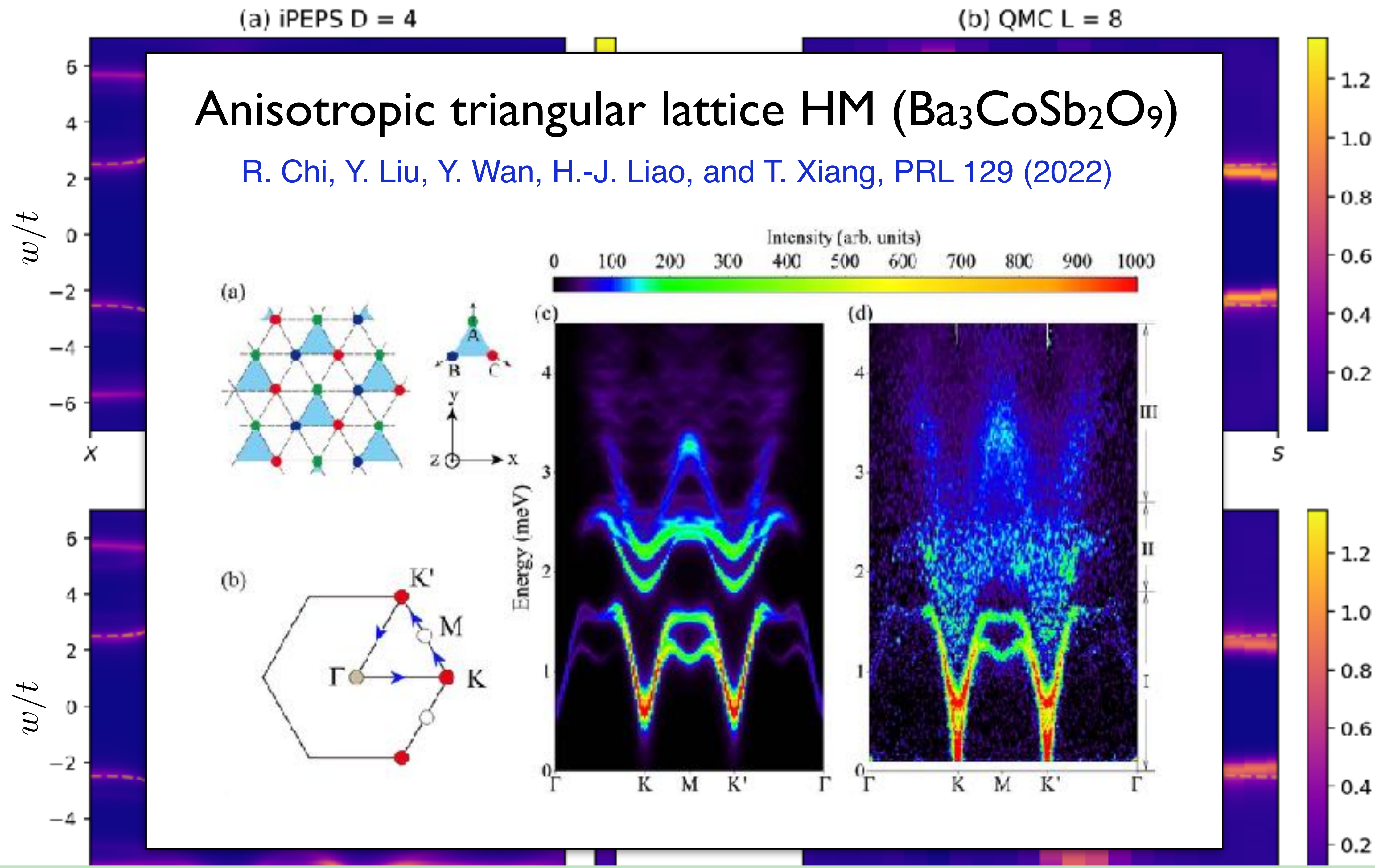


★ Systematic improvement with D, approaching QMC for U/t=4 and U/t=8

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

Spectral function A(ω, k) for U/t=8 (half filling)

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



Anisotropic triangular lattice HM ($Ba_3CoSb_2O_9$)

R. Chi, Y. Liu, Y. Wan, H.-J. Liao, and T. Xiang, PRL 129 (2022)

Already a powerful tool, but computationally rather expensive.
Further improvements desirable!

Spectral function via real-time evolution

Juan Diego
Arias Espinoza

$$S(\mathbf{k},\omega) = \int dt e^{i\omega t} \sum_{\mathbf{r}} e^{-i\mathbf{k}\mathbf{r}} \underbrace{\langle O_{\mathbf{r}}(t) O_0 \rangle}$$

$$\downarrow$$

$$e^{iE_0 t} \langle \Psi_0 | O_{\mathbf{r}} e^{-i\hat{H}t} O_0 | \Psi_0 \rangle$$

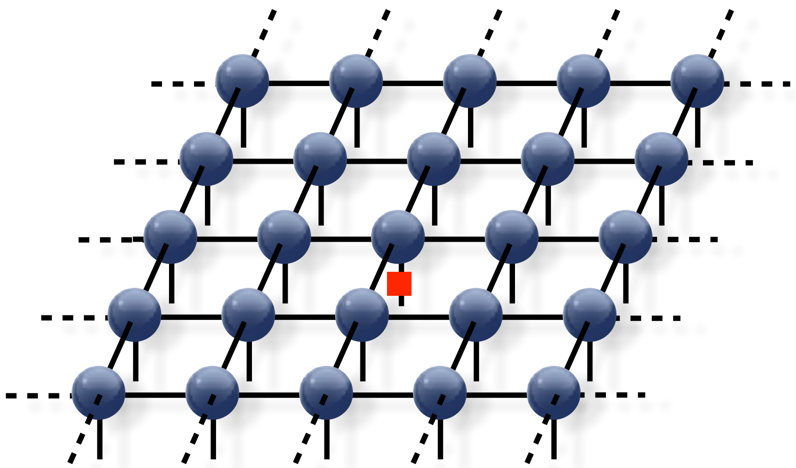
➡ Real time evolution of iPEPS with O applied

Approach:

Arias Espinoza, PC, PRB 110 (2024)

- Start from uniform GS (1-site unit cell)
- Extend unit cell size to L x L
- Apply operator O in the center of unit cell
- Time evolve $O_0|\Psi_0\rangle$ up to t_f with FU

  Czarnik, Dziarmaga, Corboz, PRB 99 (2019)

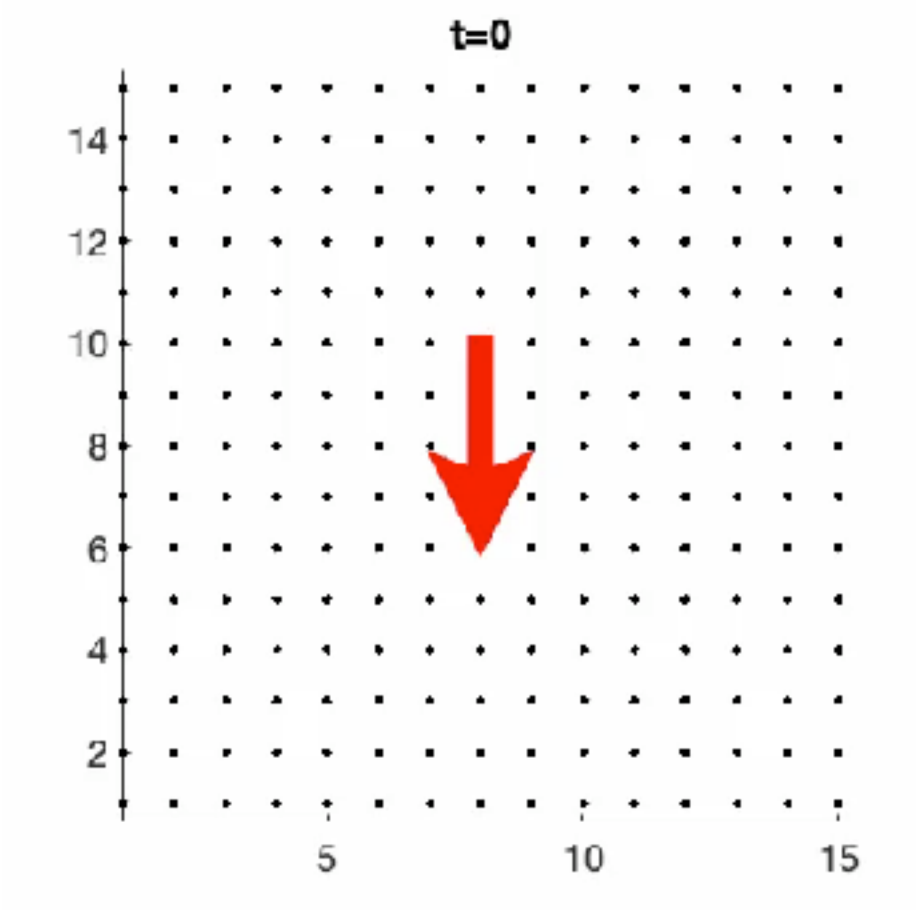


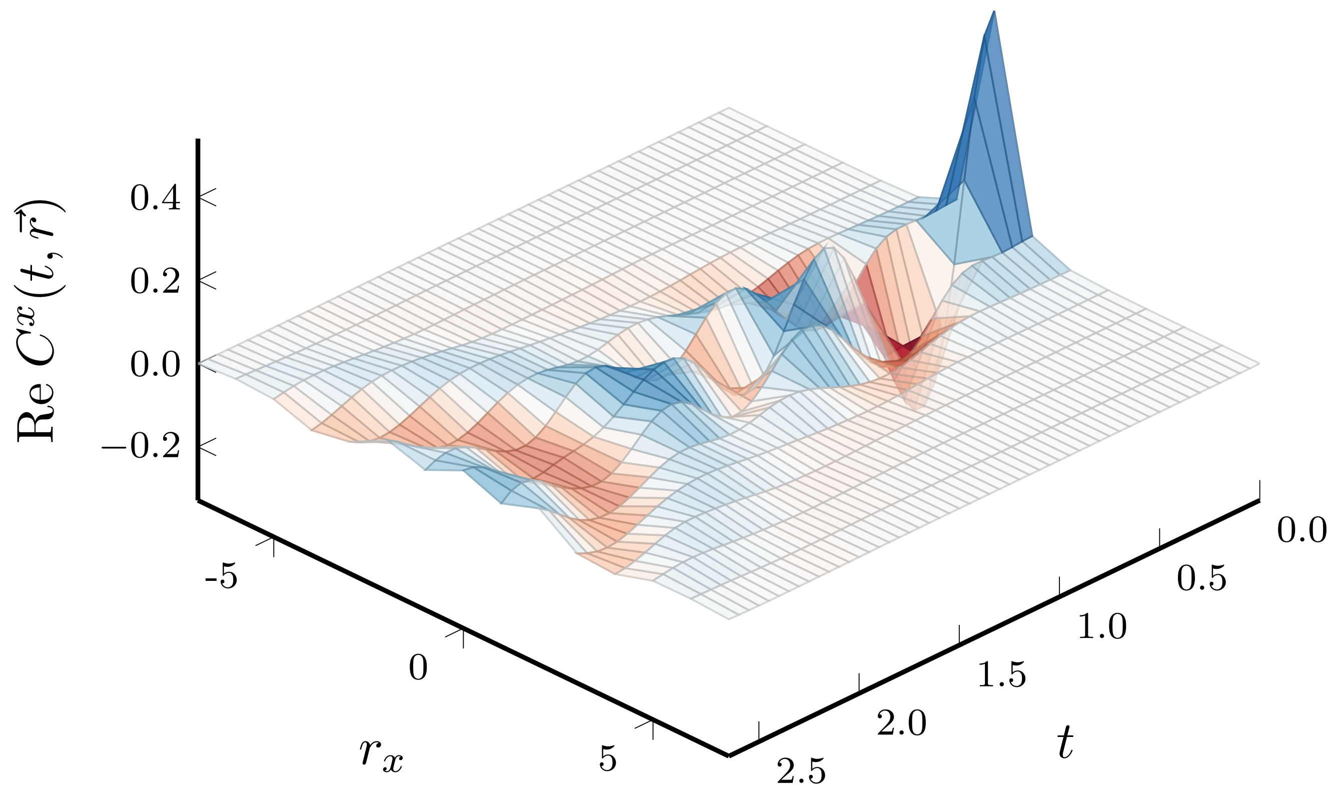
- Compute overlaps with $\langle\Psi_0|O_{\mathbf{r}}$ for all r and t
- Compute spatial FT and then temporal FT (convoluted with Gaussian)

Dynamical structure factor via real-time evolution

Test-case: transverse field Ising model $\hat{H} = -\sum_{\langle i,j \rangle} \hat{\sigma}_i^z \hat{\sigma}_j^z - \lambda \sum_i \hat{\sigma}_i^x$

$\lambda = 2.5, L = 15$



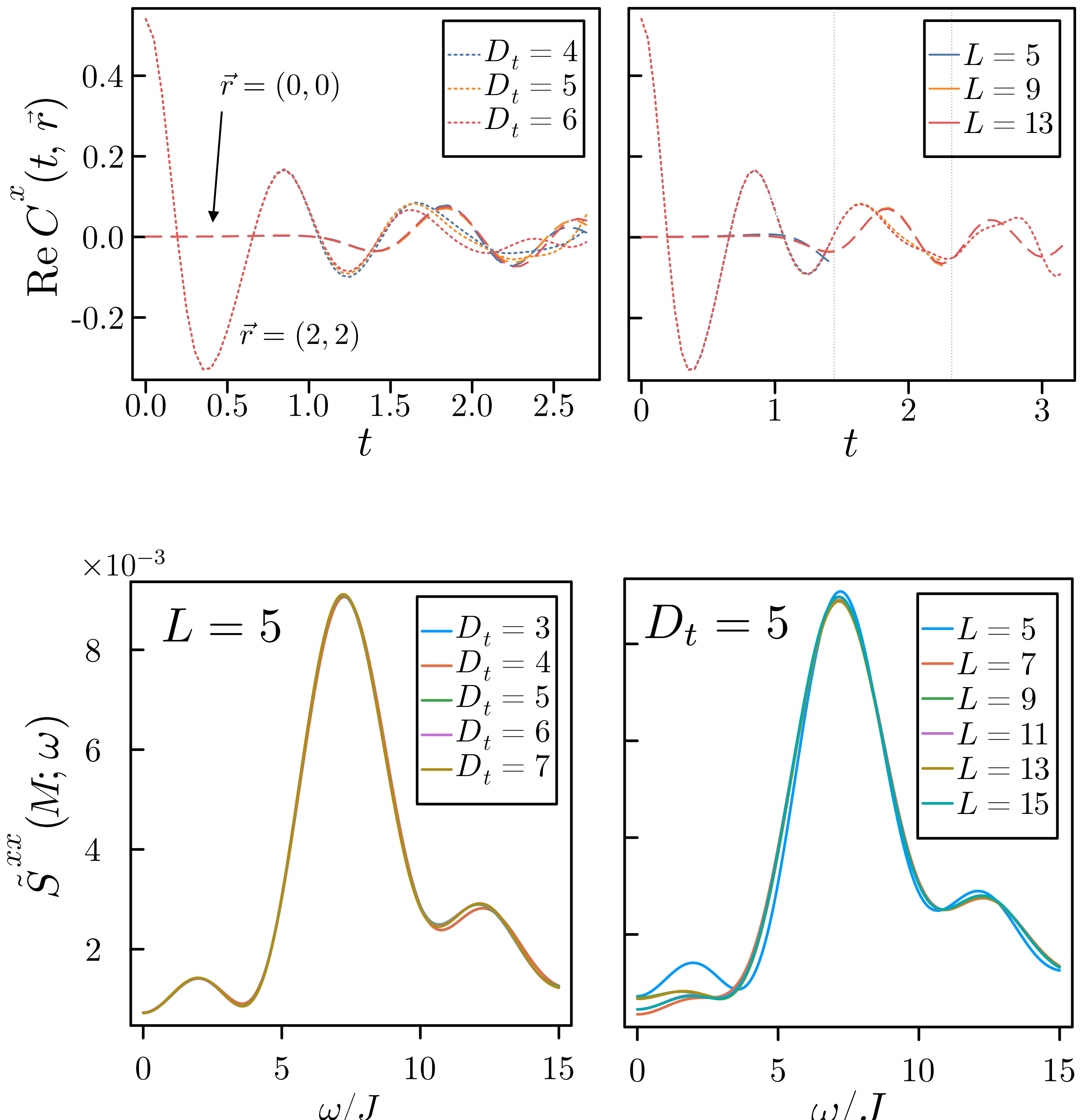


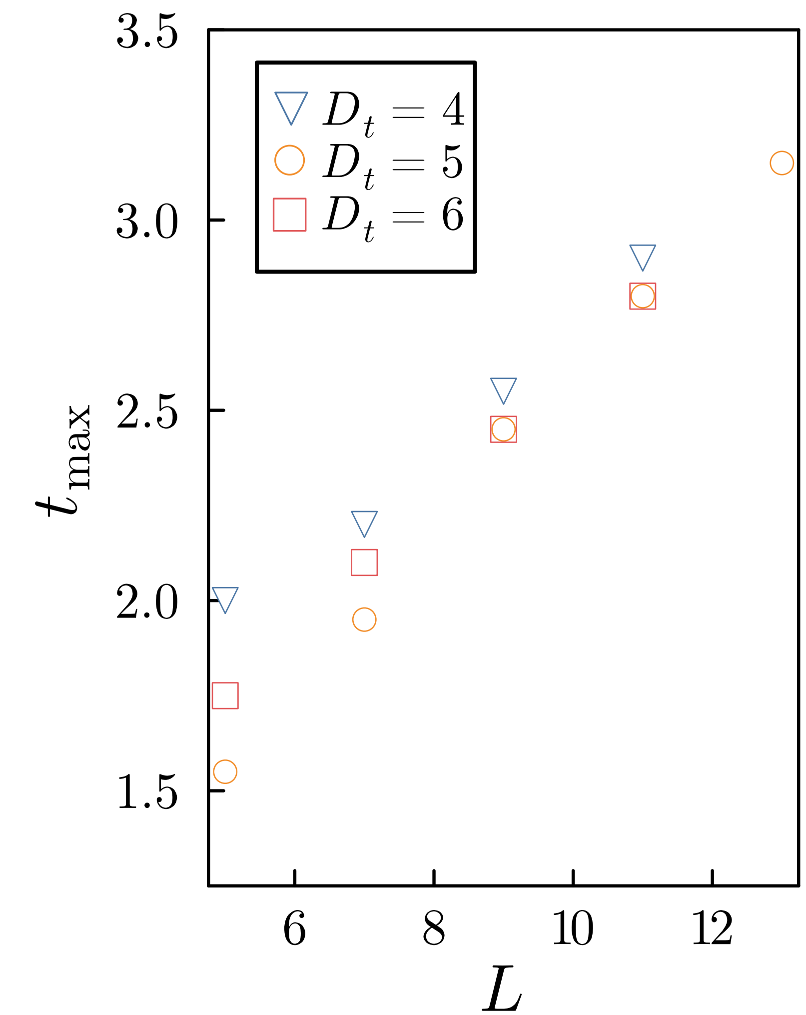
$\langle \tilde{\Psi}(t) | \hat{\sigma}_r^z | \tilde{\Psi}(t) \rangle - \langle \Psi_0 | \hat{\sigma}_r^z | \Psi_0 \rangle$

$C^x(t, \vec{r}) = \langle \hat{\sigma}_{\vec{r}}^x(t) \hat{\sigma}_0^x(0) \rangle_c$

$|\tilde{\Psi}(t)\rangle = e^{-i\hat{H}t} \hat{\sigma}_0^x |\Psi_0\rangle$

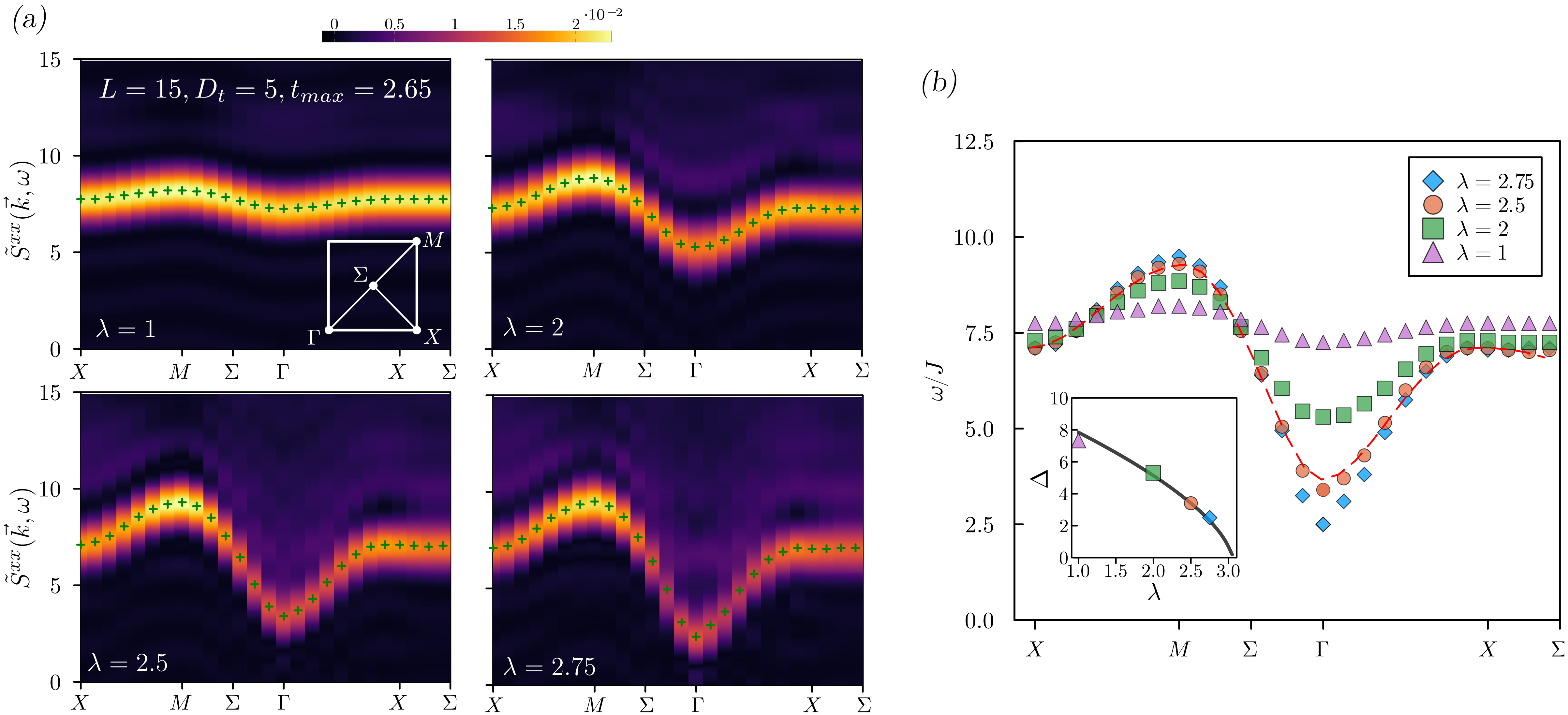
Finite D, L effects and maximal time (λ=2.5)





★ Finite *D* and finite cell size *L* effects relatively small, but t_{max} limited by *L*!

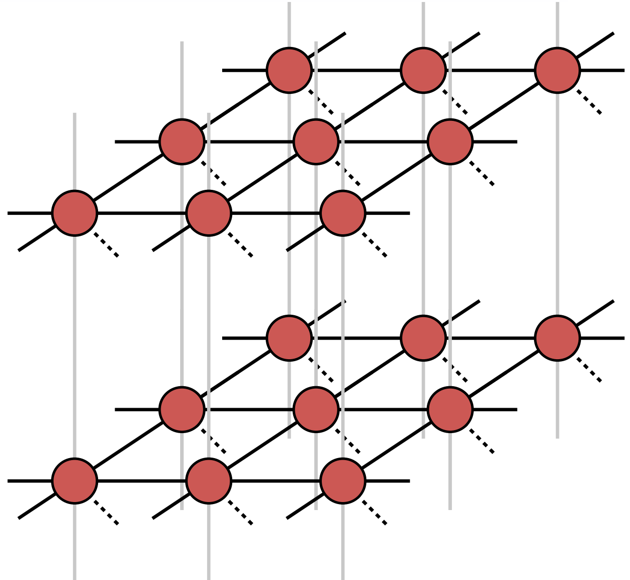
Dynamical structure factor via real-time evolution



- Overall good agreement with results from excitation ansatz
- Reaching long times is challenging: increasing cell size required to avoid interaction effects between nearby cells

Extensions to 3D

Tensor network methods for 3D quantum systems



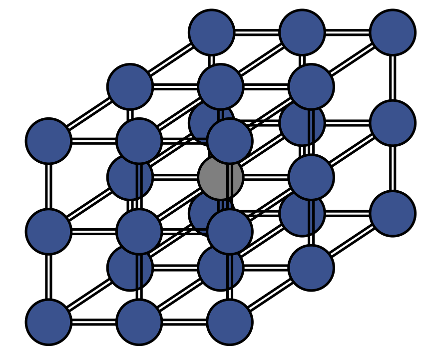
- **Main challenge: how to contract it??**

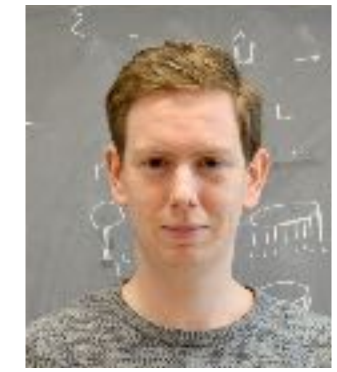
- Several works in the context of 3D classical or 2+1D:
  - **3D HOTRG:**
    Xie, Chen, Qin, Zhu, Yang, Xiang, PRB 86 (2012)
  - **Corner-transfer matrix (CTM) in 3D:**
    Nishino and Okunishi, J. Phys. Soc. Jpn. 67, 3066 (1998)
    Orús, PRB 85, 205117 (2012)
  - **Approaches based on a boundary iPEPS:**
    Nishino, et al, Nucl. Phys. B 575 (2000); Nishino, et al, Prog. Theor. Phys. 105 (2001)
    Gendiar, Nishino, PRE 65, 046702 (2002); Gendiar and Nishino, PRB 71 (2005)
    Gendiar, Maeshima, and Nishino, Prog. Theor. Phys. 110 (2003)
    Vanderstraeten, Vanhecke, and Verstraete, PRE 98, 042145 (2018)
  - **Other approaches:**
    Ran, Piga, Peng, Su, and Lewenstein, PRB 96, (2017)
    Jahromi and Orús, PRB 99 (2019); Sci. Rep. 10 (2020)
    Tepaske and Luitz, PRR 3 (2021); Magnifico, et al, Nat. Comm. 12 (2021)
    Gray, Chan, PRX 14 (2014)

Overview

Vlaar & PC, PRB 103 (2021); PRL 130 (2023)

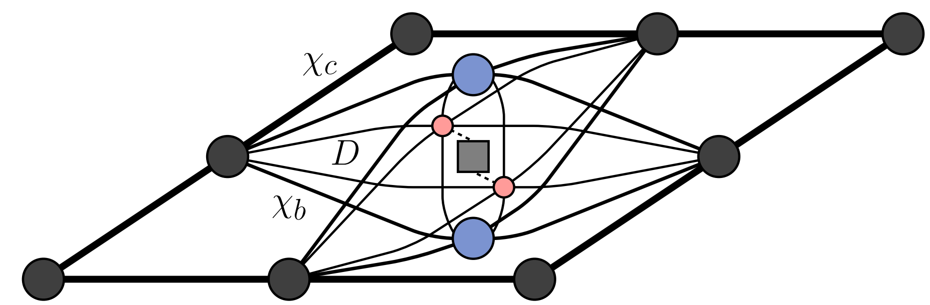
- **Cluster contractions:**
  - ✦ Contract finite clusters instead of full network
  - ✦ cheap & simple
  - ✦ Not very accurate, but useful for quick results



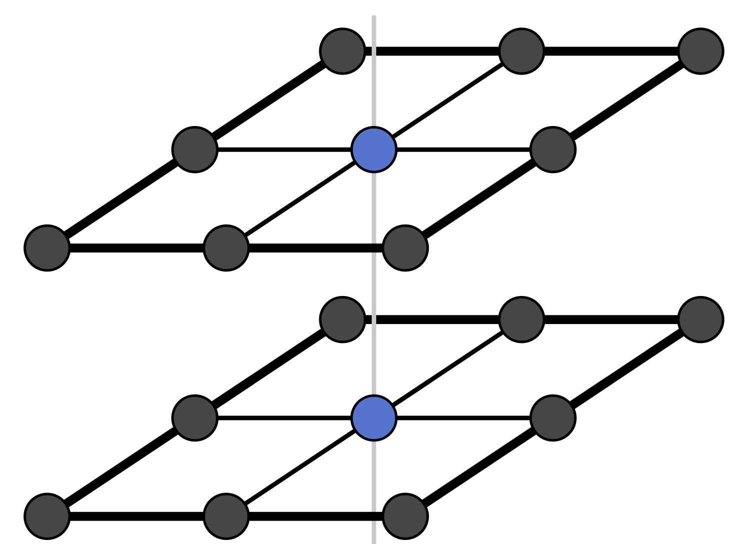


Patrick Vlaar

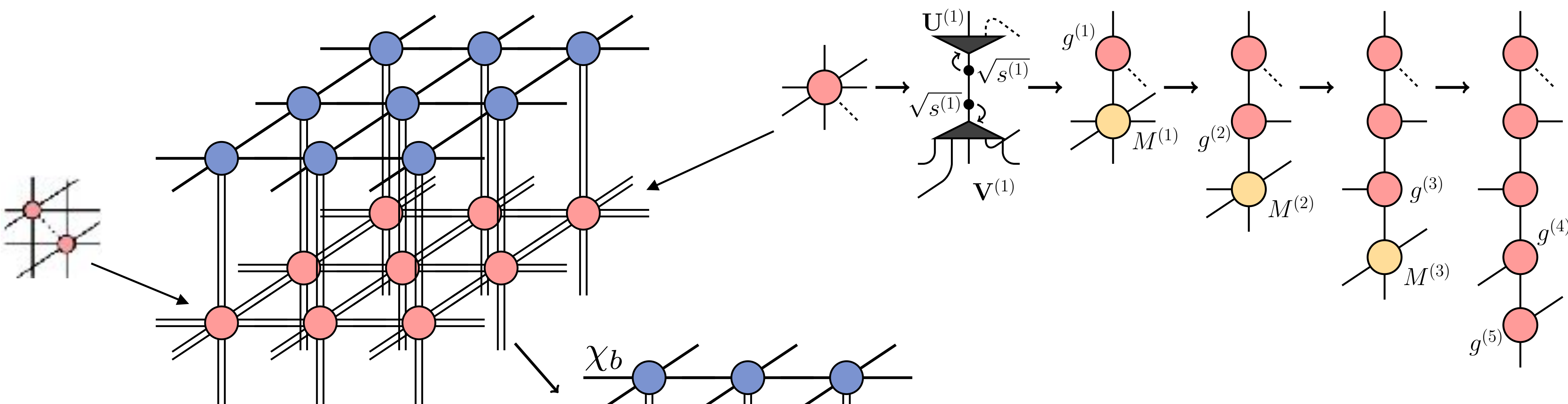
- **Full 3D contraction: the SU + CTM approach**
  - ✦ Boundary iPEPS approach
  - ✦ Combination of simple update (SU) truncation + CTM method
  - ✦ Good accuracy & convergence & tractable cost



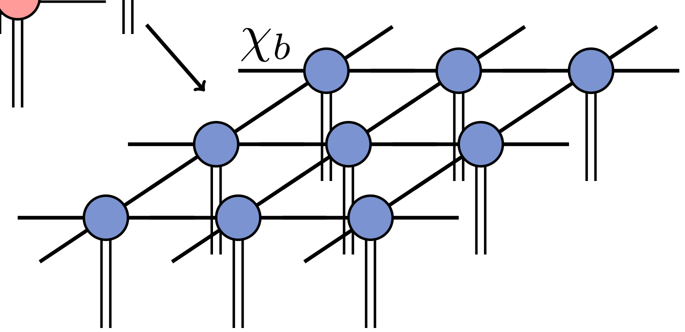
- **Contraction of layered systems: LCTM**
  - ✦ Decouple layers away from the center → use CTM to contract 2D layers
  - ✦ Good accuracy for anisotropic systems
  - ✦ Substantially lower cost than full 3D algorithm



Full 3D contraction: SU + CTM approach



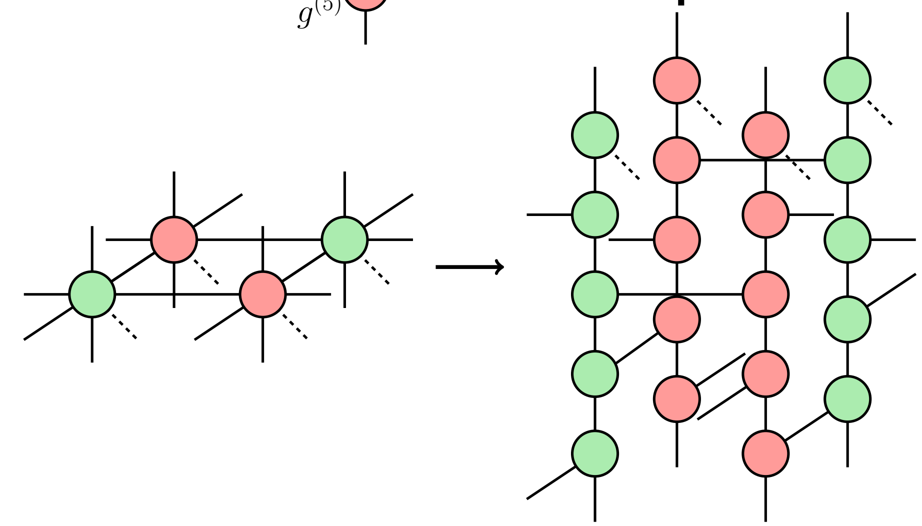
Split with SVDs



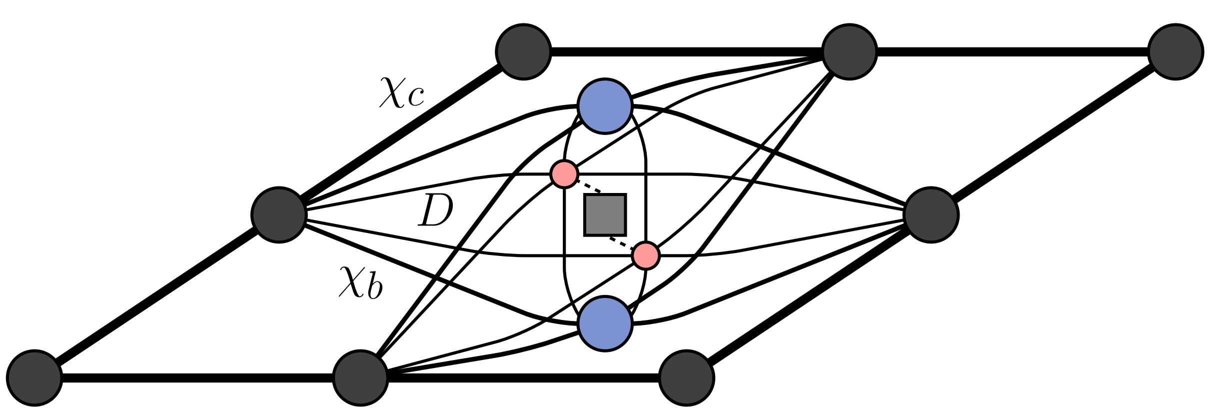
Repeat until convergence

↓

Sequence of 2-site operators

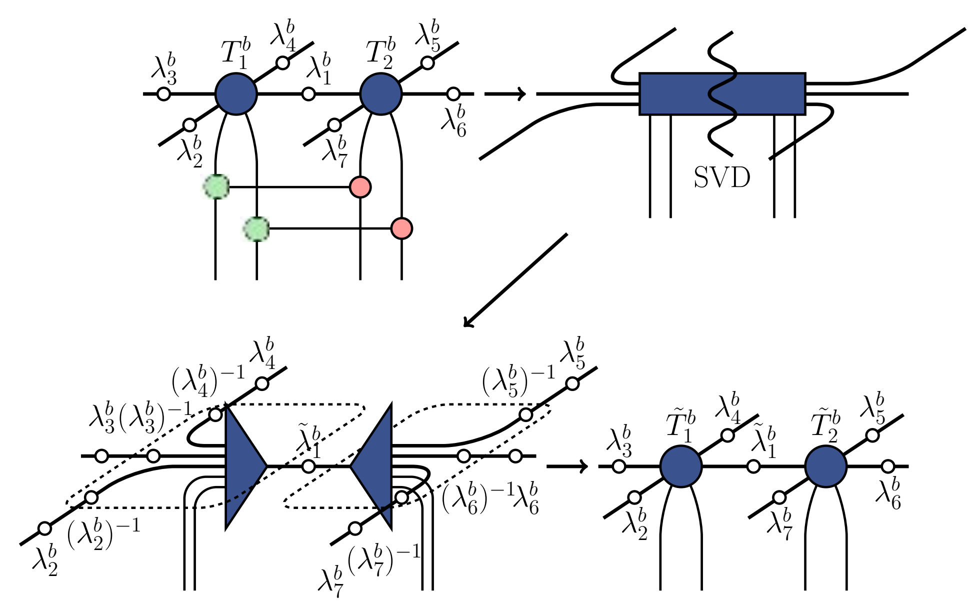


use CTM to contract resulting 3-layer network

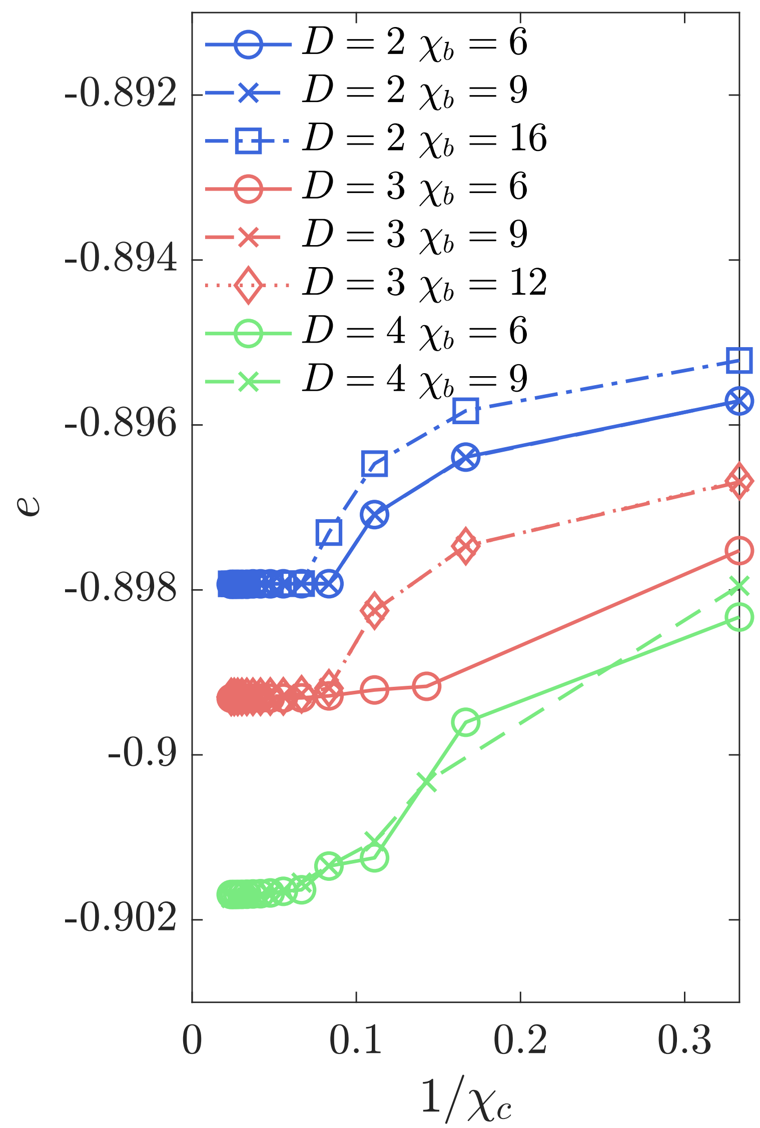


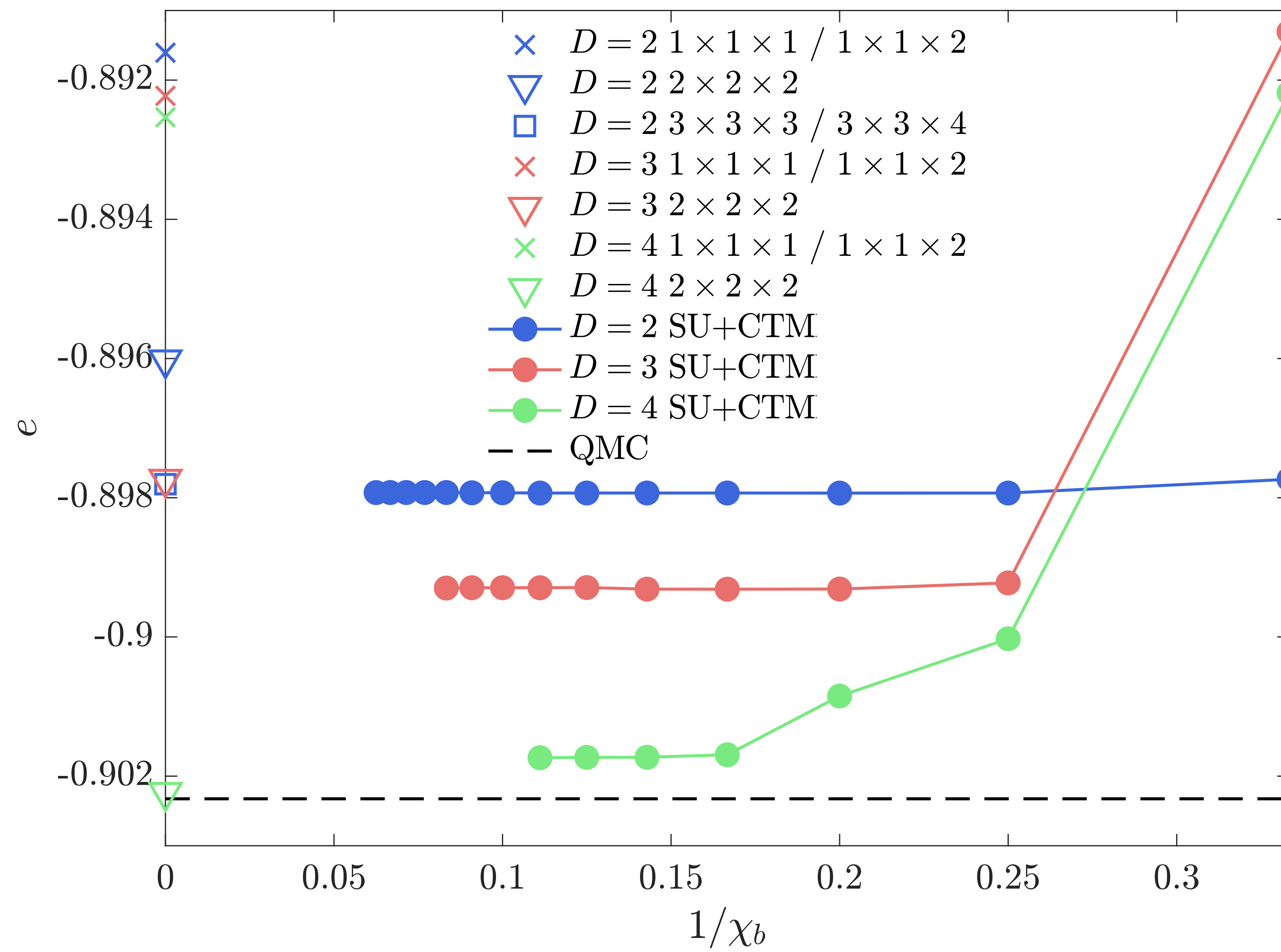
$$\mathcal{O}(\chi_c^3\chi_b^4D^4 + \chi_c^2\chi_b^6D^6 + \chi_c^2\chi_b^4D^9)$$

Apply and use SU to truncate



Convergence in χ_c and χ_b (3D Heisenberg model)

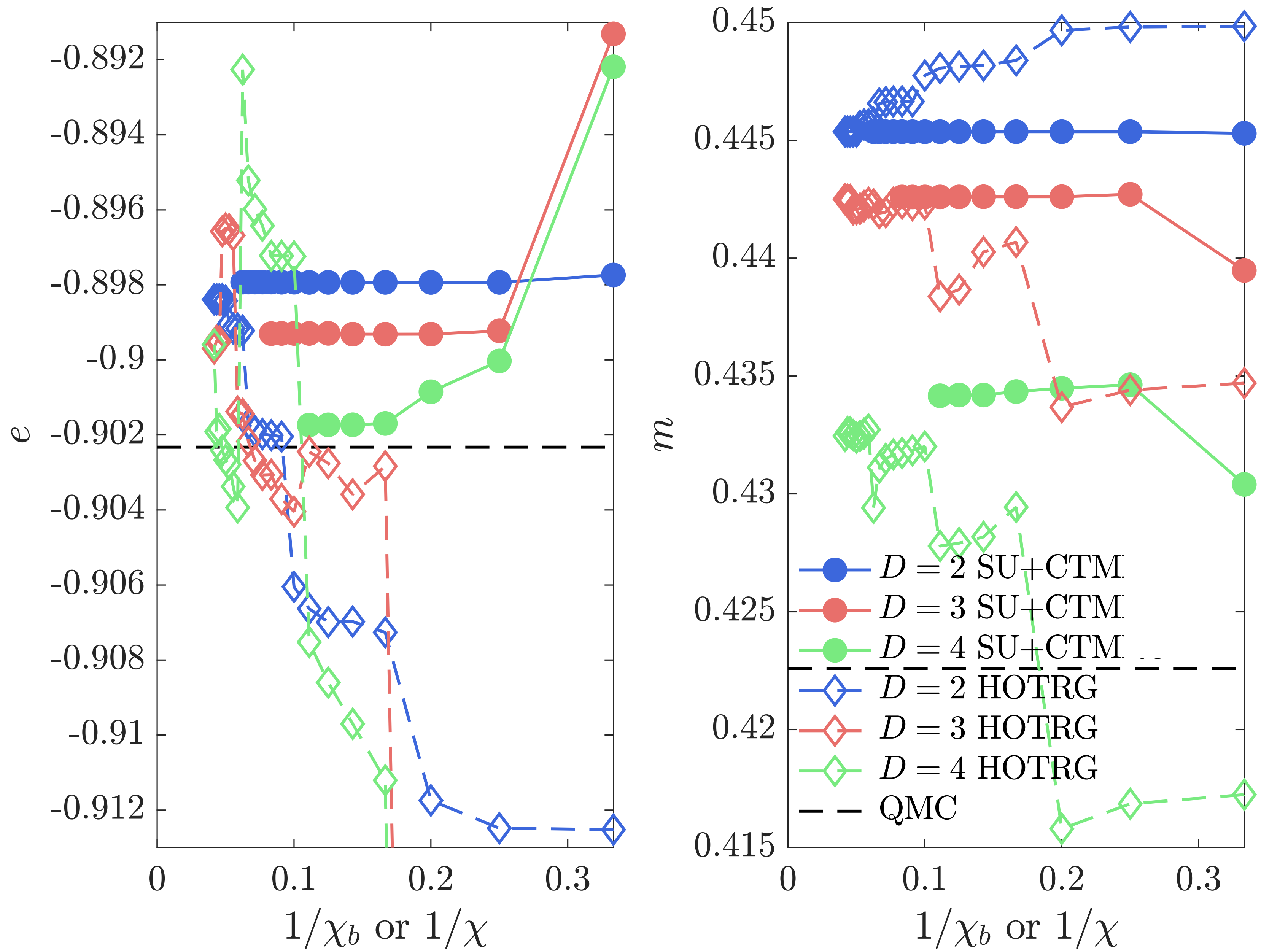




★ Systematic convergence in χ_c and χ_b

Comparison with 3D HOTRG

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

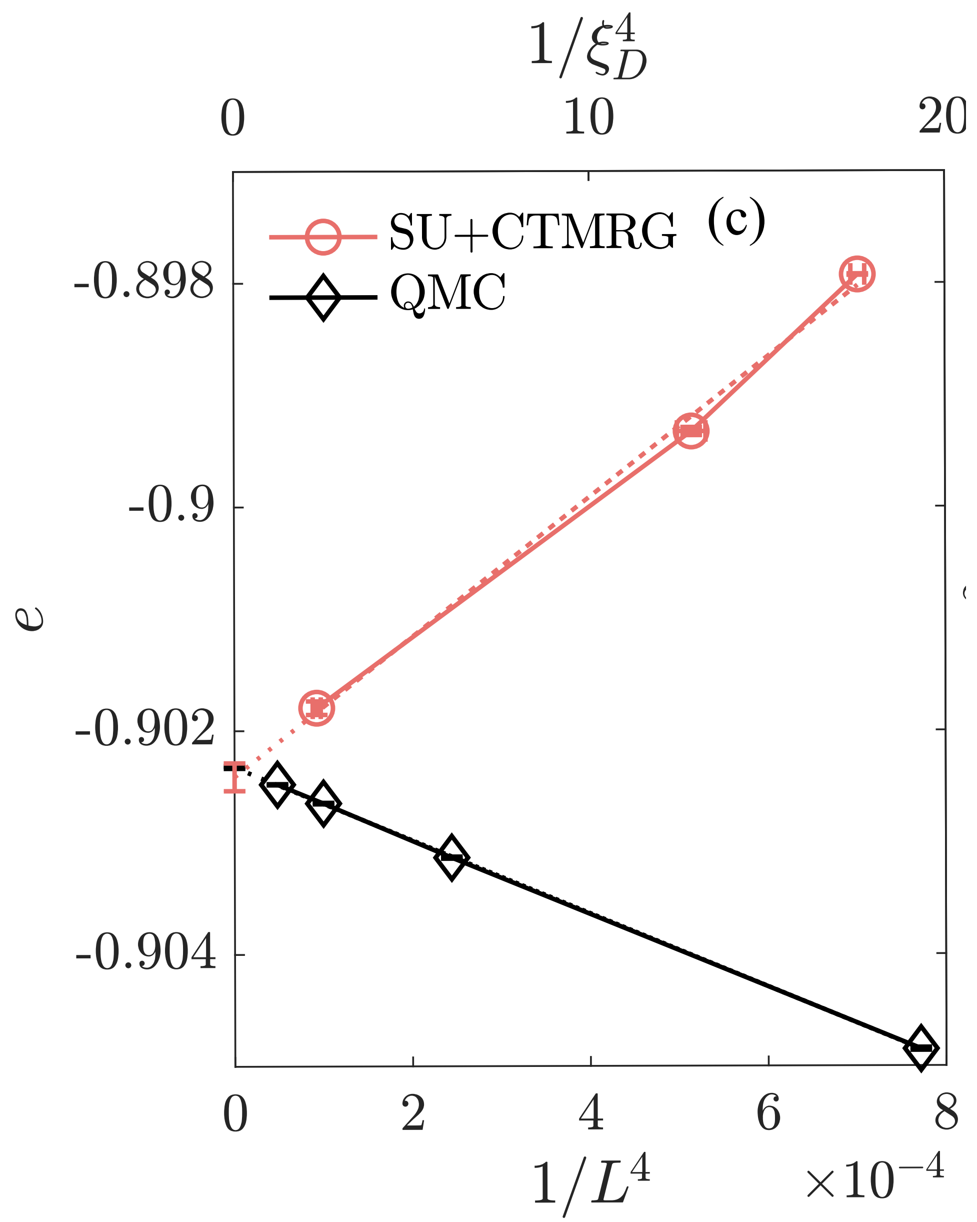


★ Very irregular convergence with HOTRG, in contrast to SU+CTM

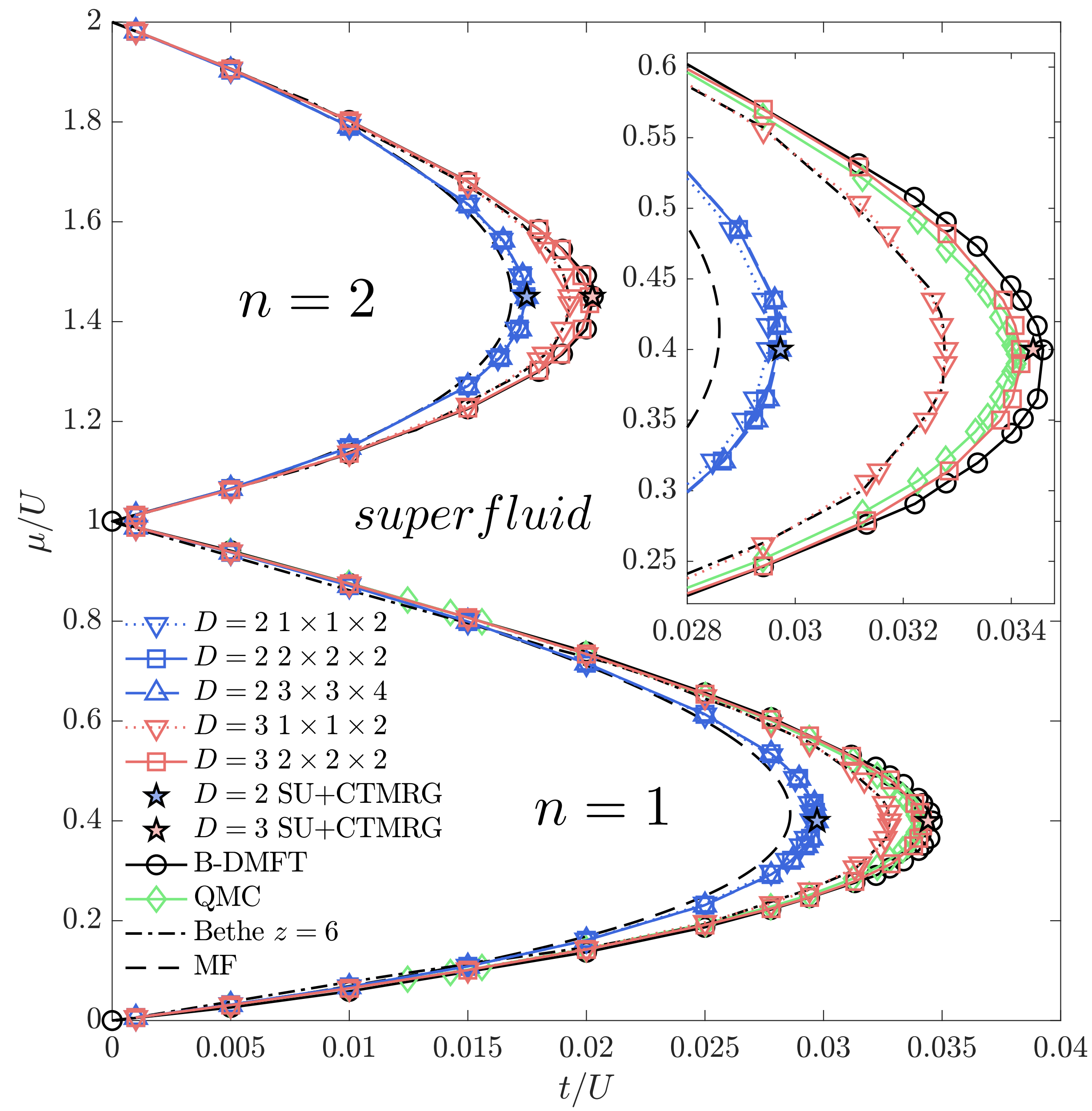
Benchmark results in 3D

Vlaar & PC, PRB 103 (2021)

3D Heisenberg model



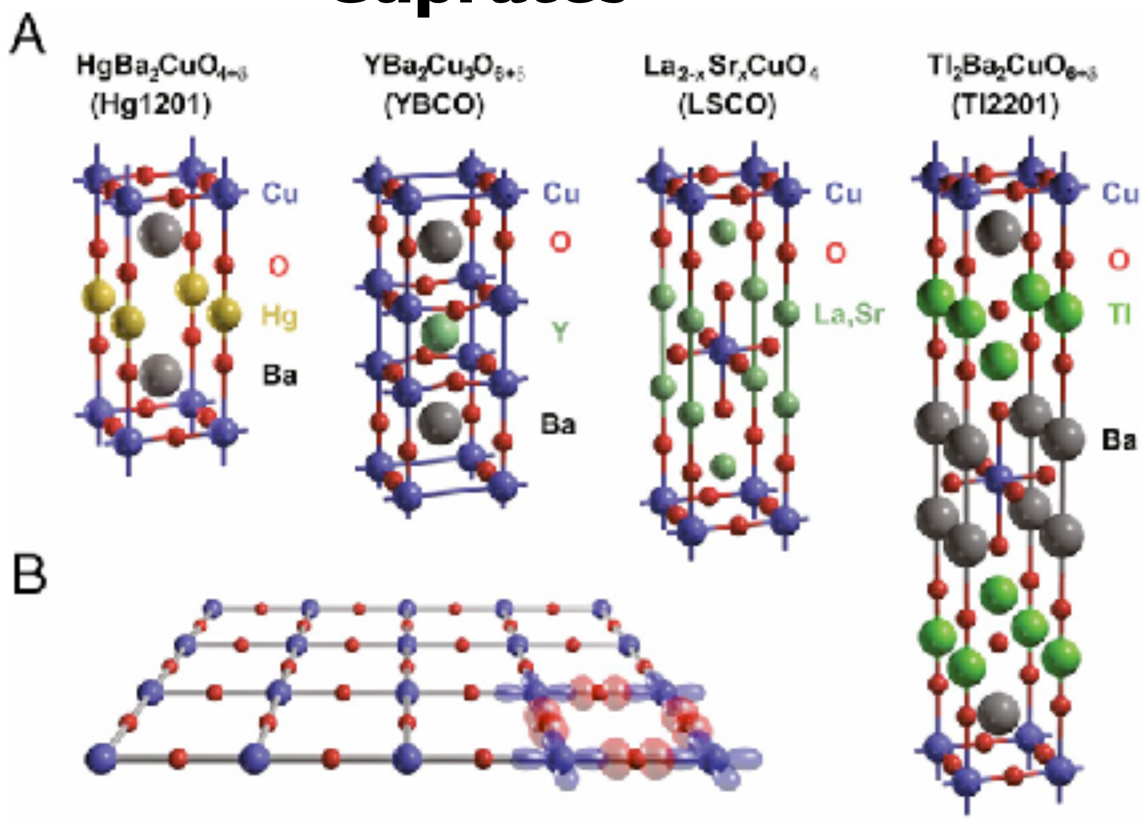
3D Bose-Hubbard model

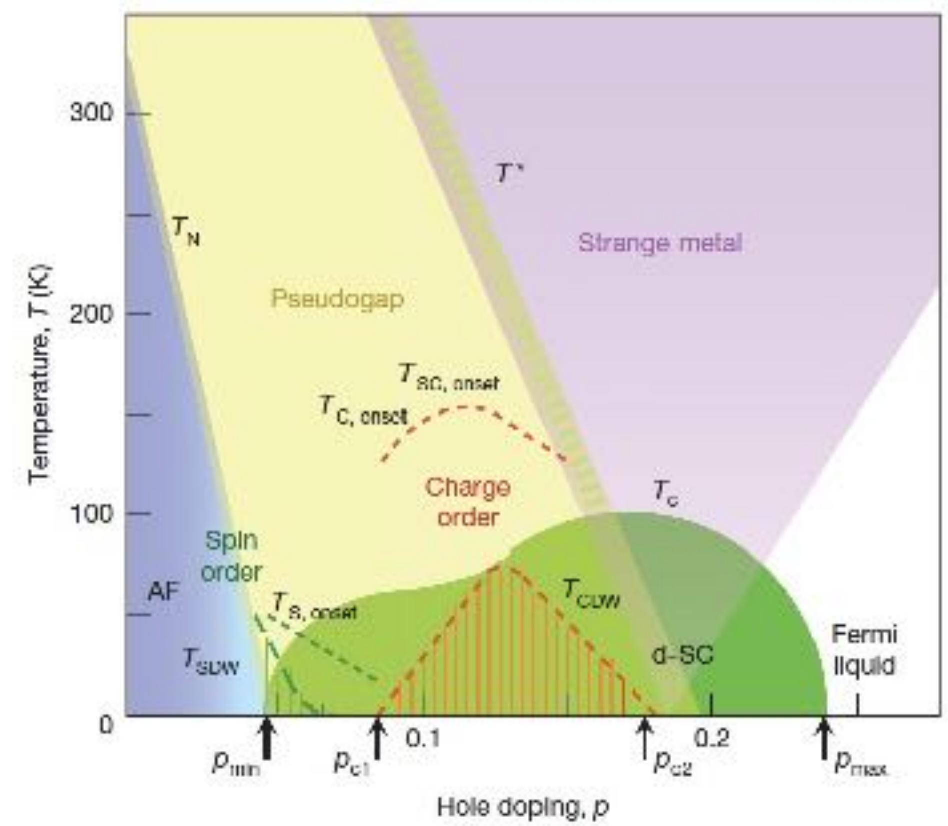


★ SU+CTM: promising approach for 3D problems

Layered systems (anisotropic 3D)

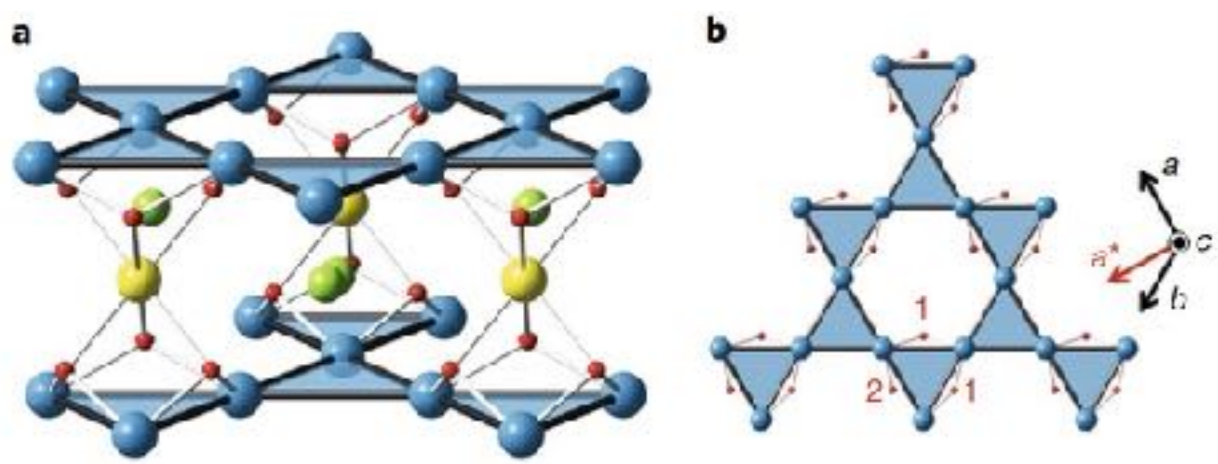
Cuprates



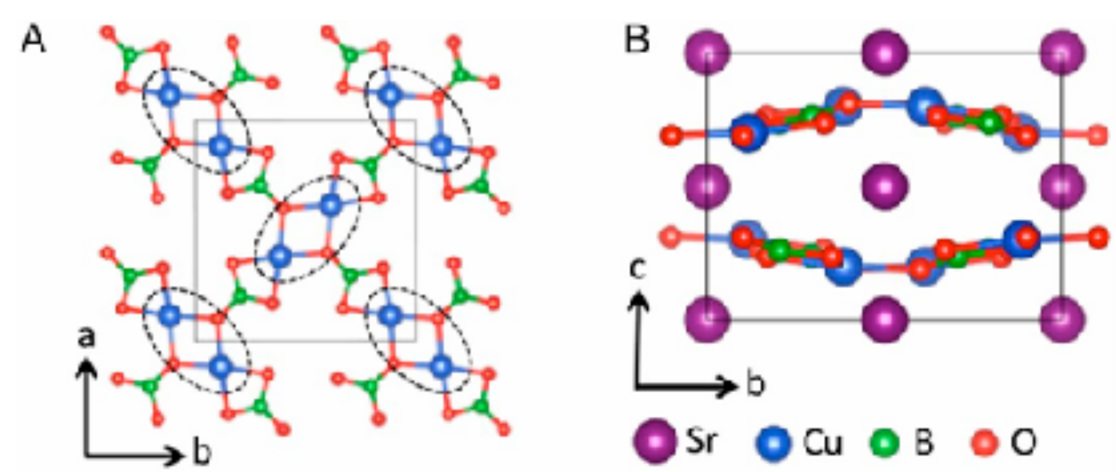


Barišić, et al., PNAS 110, 12235 (2013)

Herbertsmithite



$SrCu_2(BO_3)_2$

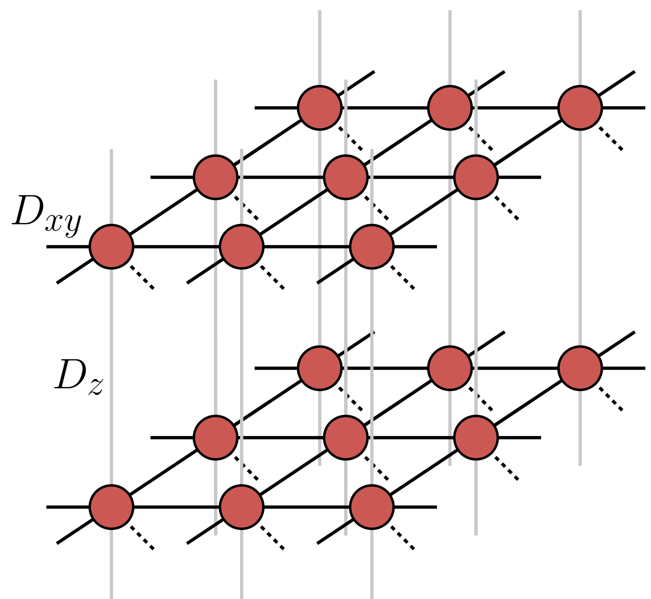


Khuntia et al., Nature Physics 16, 469 (2020)

Radtke et al., PNAS 112 (2015)

iPEPS for layered systems

Vlaar, PC, arxiv:2208.06423

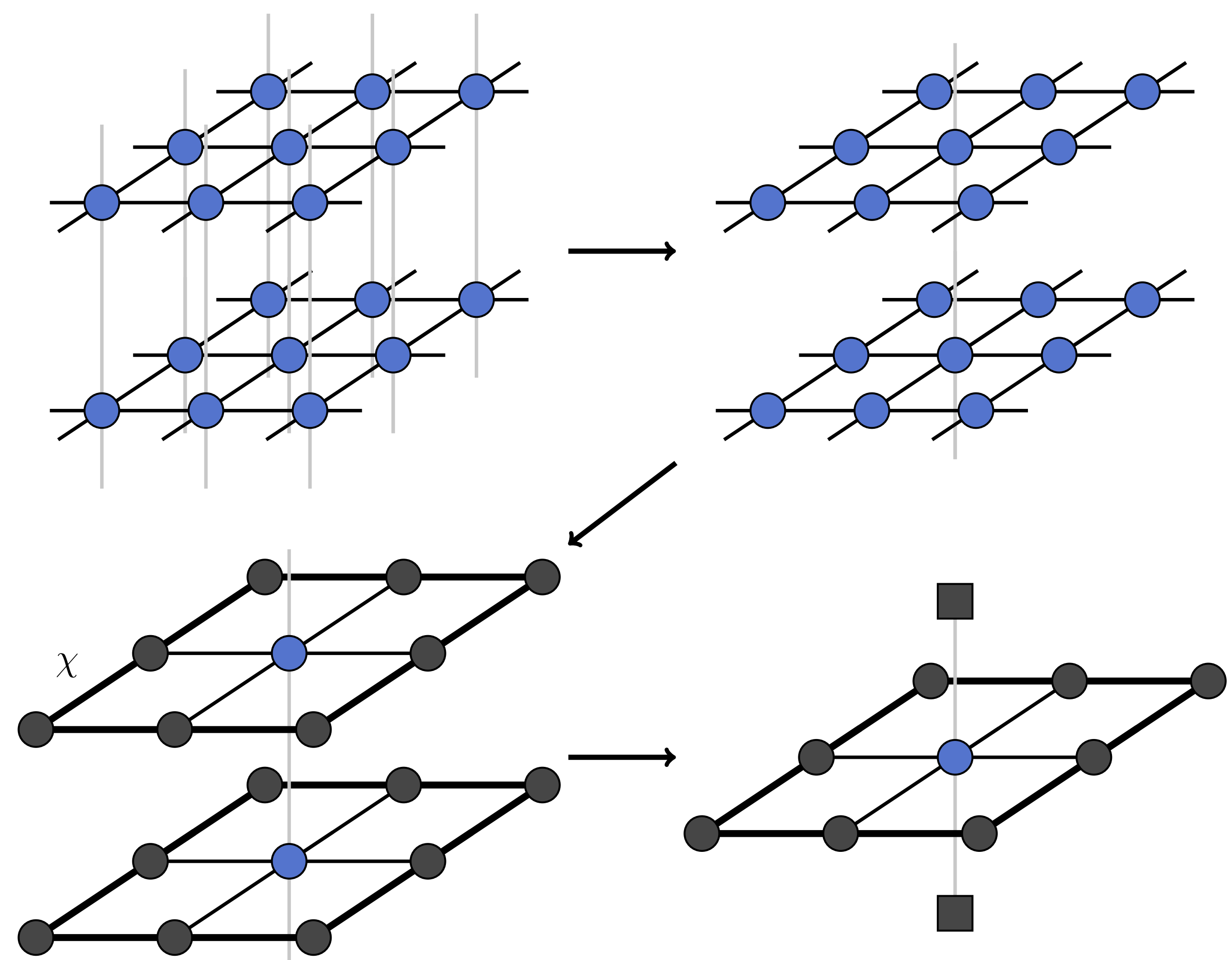


Ansatz:

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

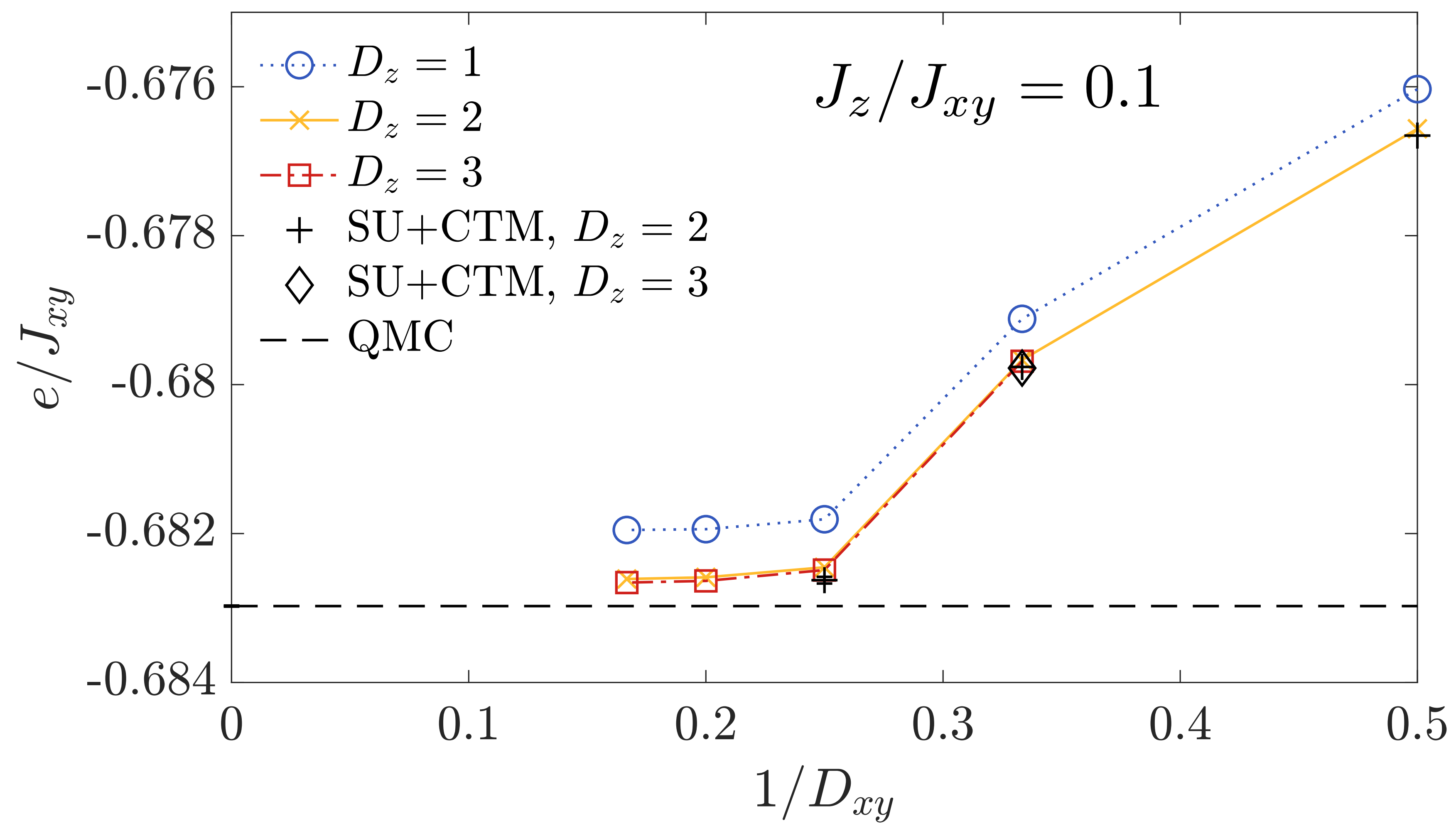
Contraction:

- $D_z = 1$: contract individual layers (2D)
- $D_z > 1$: perform effective decoupling away from center using full update $\rightarrow$ 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)

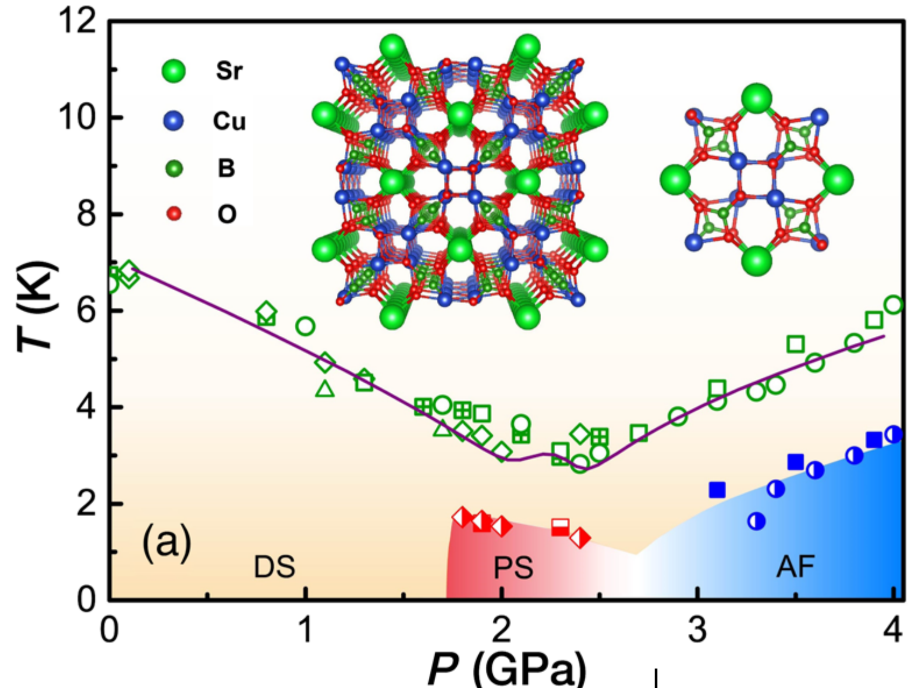


- Substantial improvement from $D_z = 1$ to $D_z = 2$
- Values close to the extrapolated QMC result
- In agreement with more expensive full 3D contraction

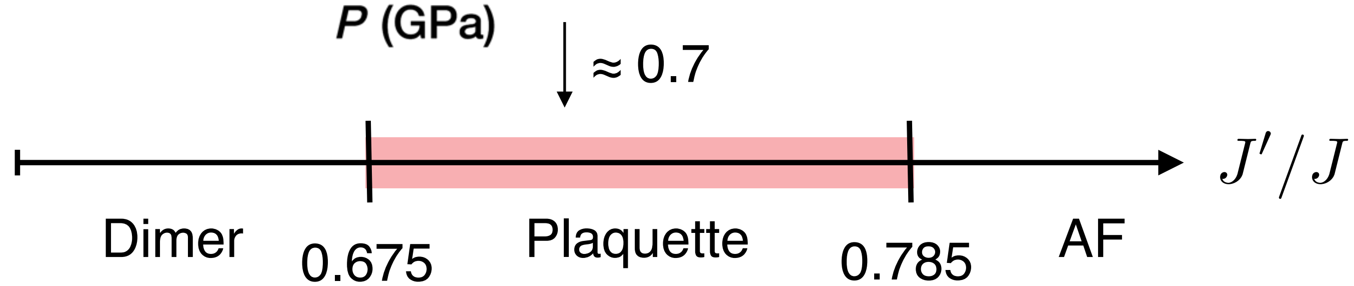
Vlaar & PC, PRB 103, 205137 (2021)

Limitations of the Shastry-Sutherland model

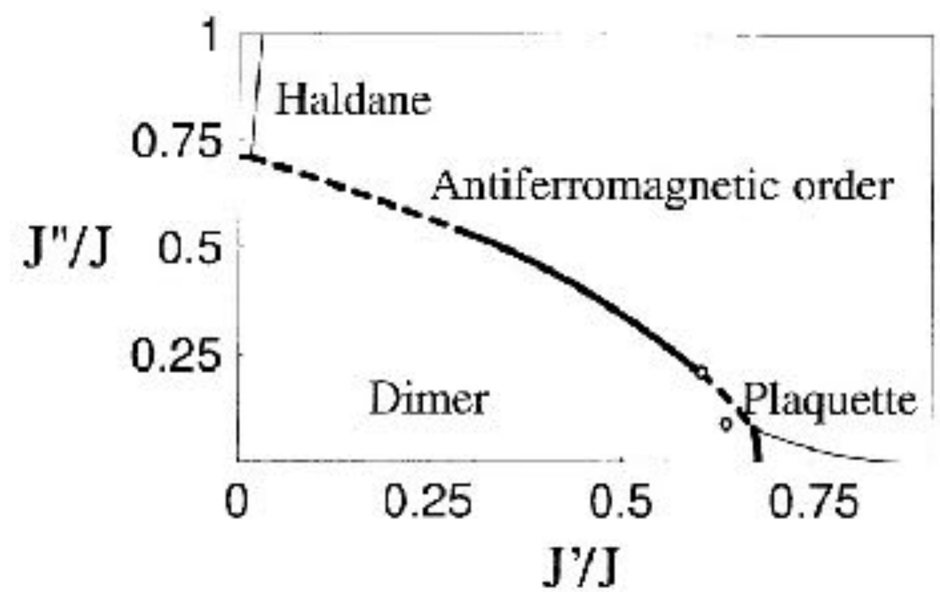
- Extent of the plaquette phase is smaller in experiments than in theory



Guo, et al (2020)

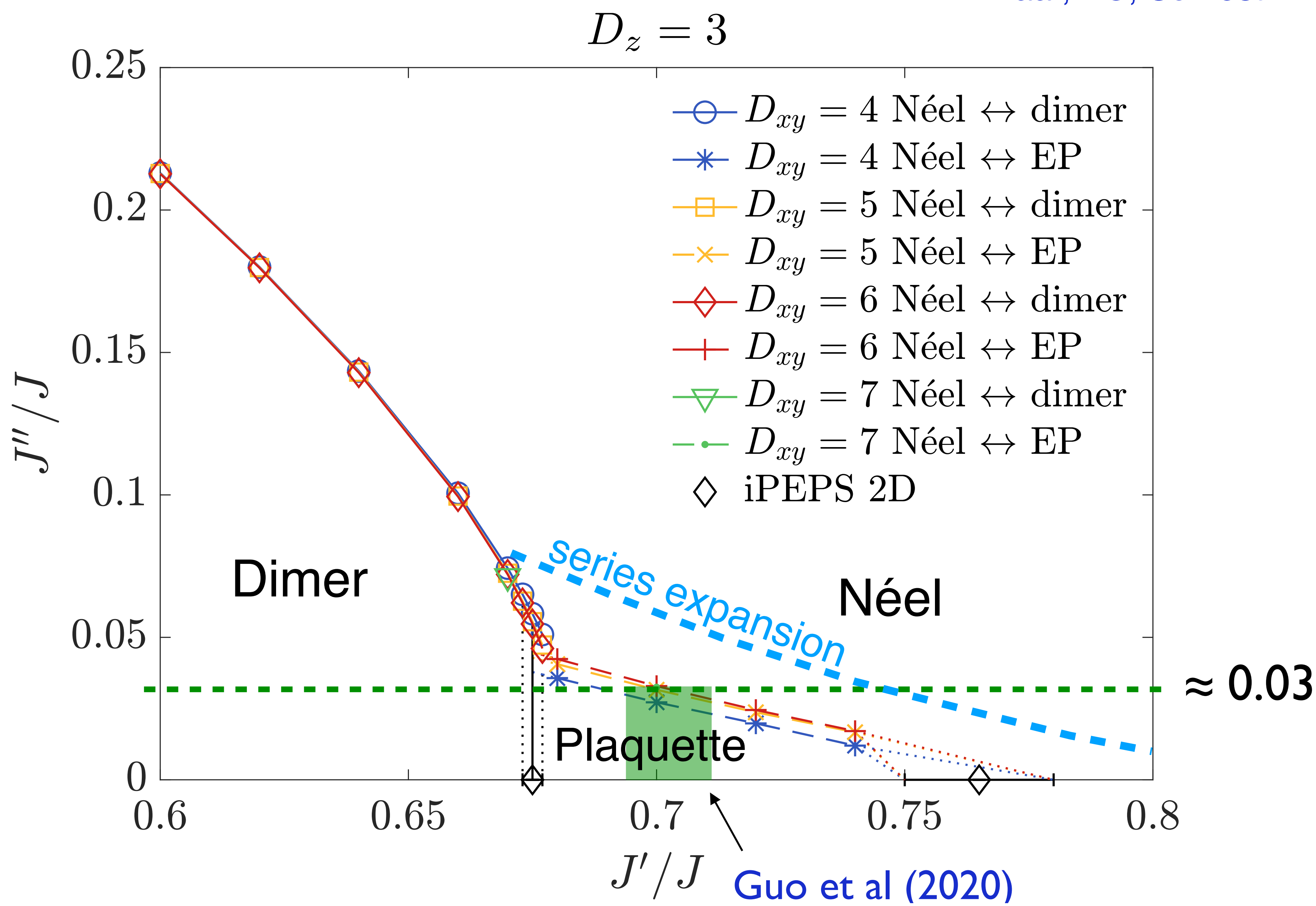


- Series expansion results Koga, JPSJ 69 (2000)
    - ✦ A interlayer coupling reduces the extent of the plaquette phase



iPEPS phase diagram of 3D Shastry-Sutherland model

Vlaar, PC, SciPost Physics 15, 126 (2023)



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

LCTM: useful tool to study layered systems in 3D

Conclusion

✓ **iPEPS: powerful & versatile tool**

- ★ Finite temperature simulations
- ★ Study of gapless systems using *finite correlation length scaling*
- ★ *Spiral iPEPS: simple and efficient ansatz to represent spin spiral states*
- ★ Excitations & spectral functions
- ★ Extensions to 3D and layered systems

✓ Still room for improvement & extensions & new applications!

Thank you for your attention!

Acknowledgements:
P. Vlaar, J. Hasik, B. Ponsioen, S. Crone, J.D. Arias Espinoza, S. Kleijweg, E. Cortes Estay, Y. Zhang, Q. Yang, N. Kamar, P. Czarnik, J. Dziarmaga, L. Tagliacozzo, F. Mila, F. F. Assaad

erc
European Research Council
established by the European Commission