QRCTM: scalable iPEPS simulation for frustrated quantum magnets

Qi Yang (仰旗)

CTMRG ~ ~~SVD~~ → QR

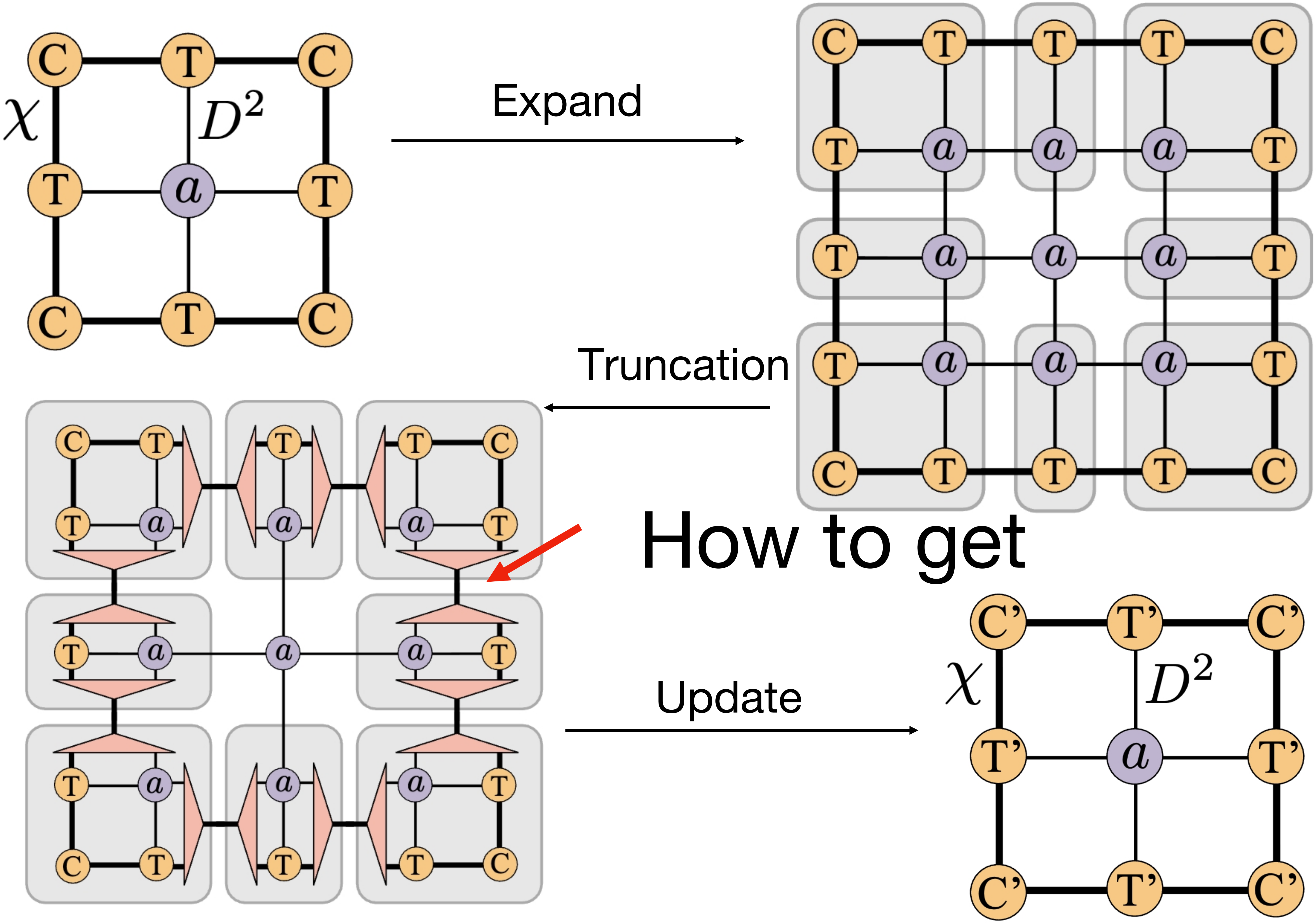
1996 → 2025

EuroHPC Joint Undertaking

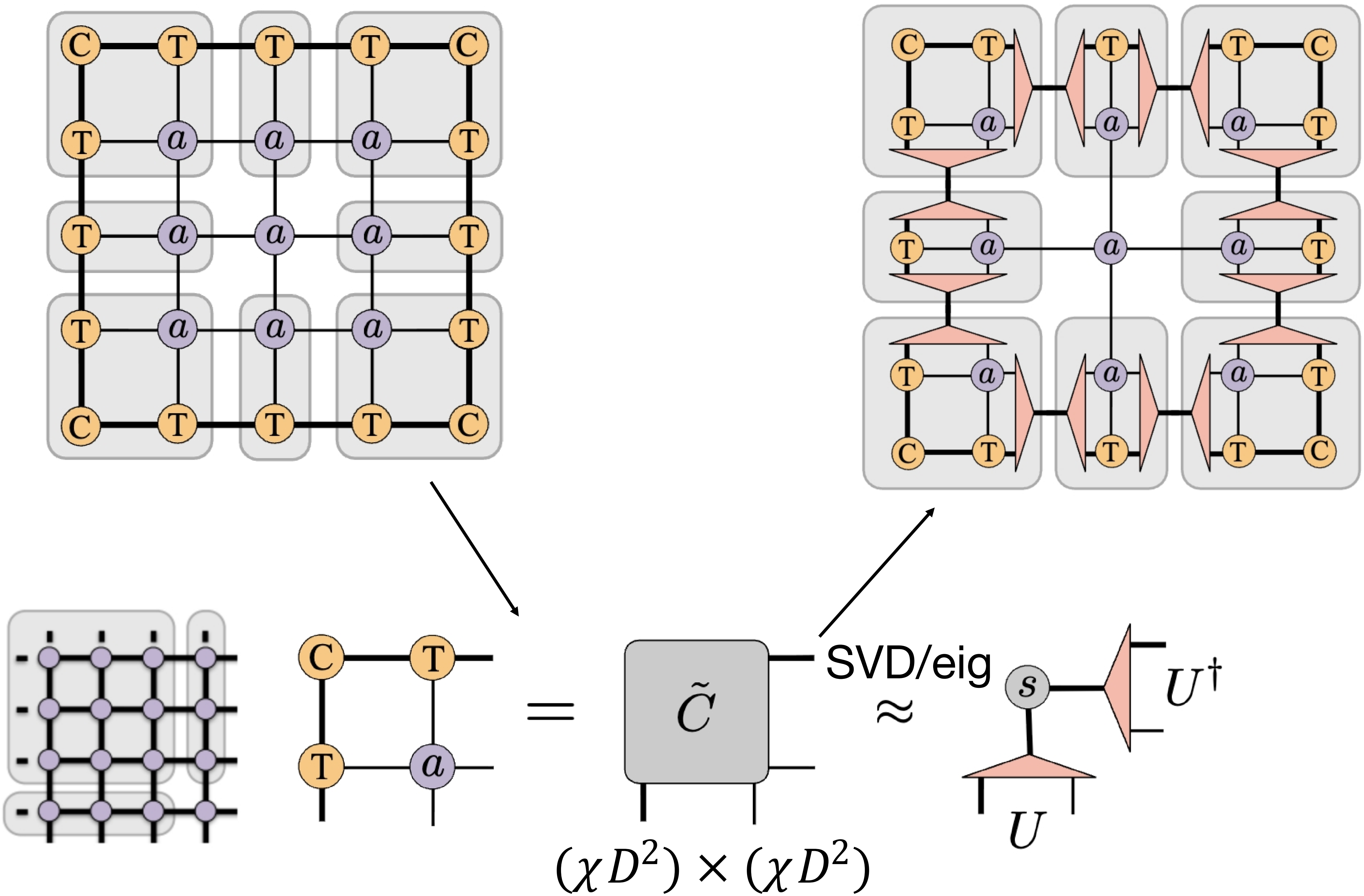
erc

UNIVERSITY OF AMSTERDAM

Textbook (C4v) CTMRG iterations

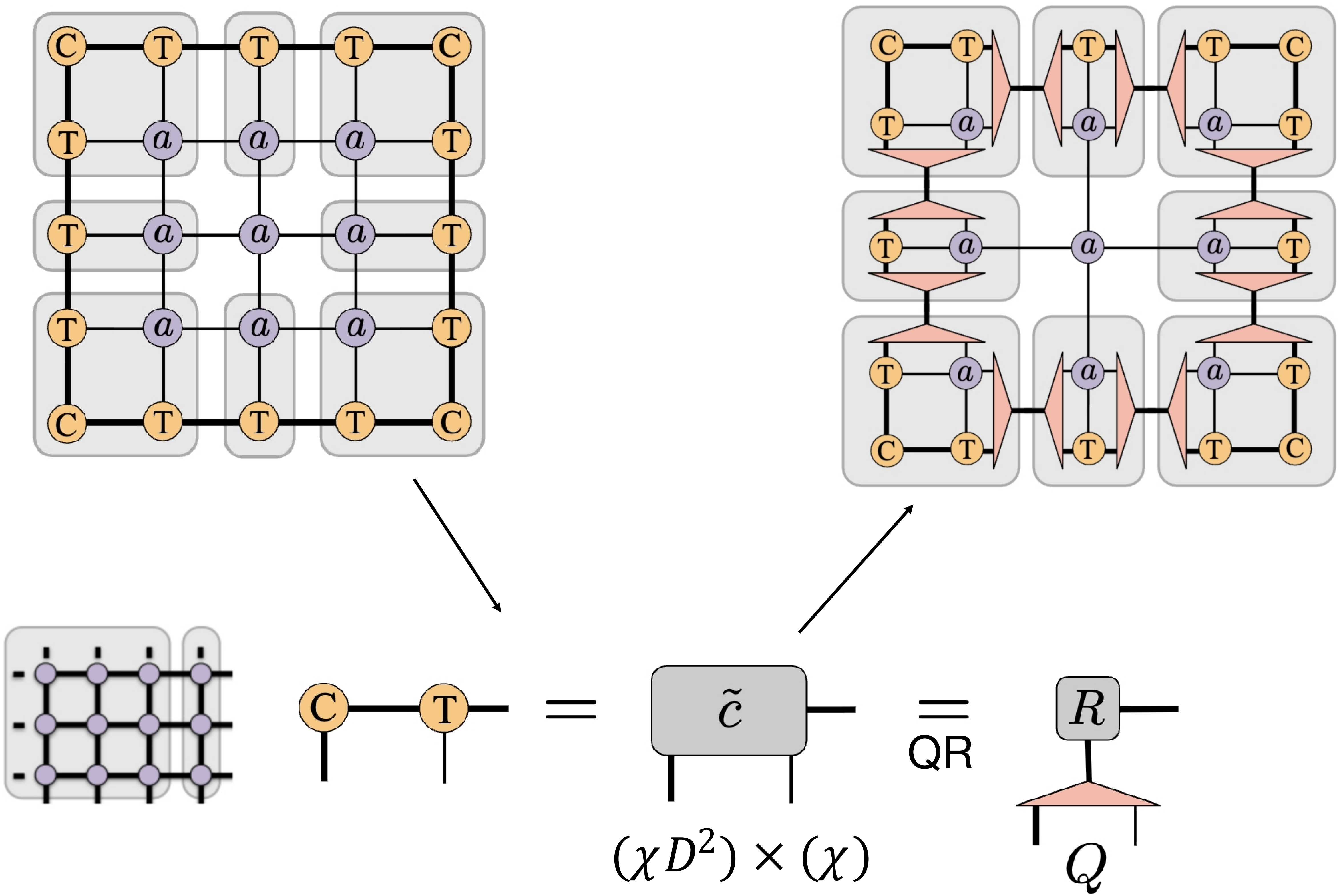


By diagonalizing enlarged corner



Nishino & Okunishi, **1996** , JPSJ 65, 891

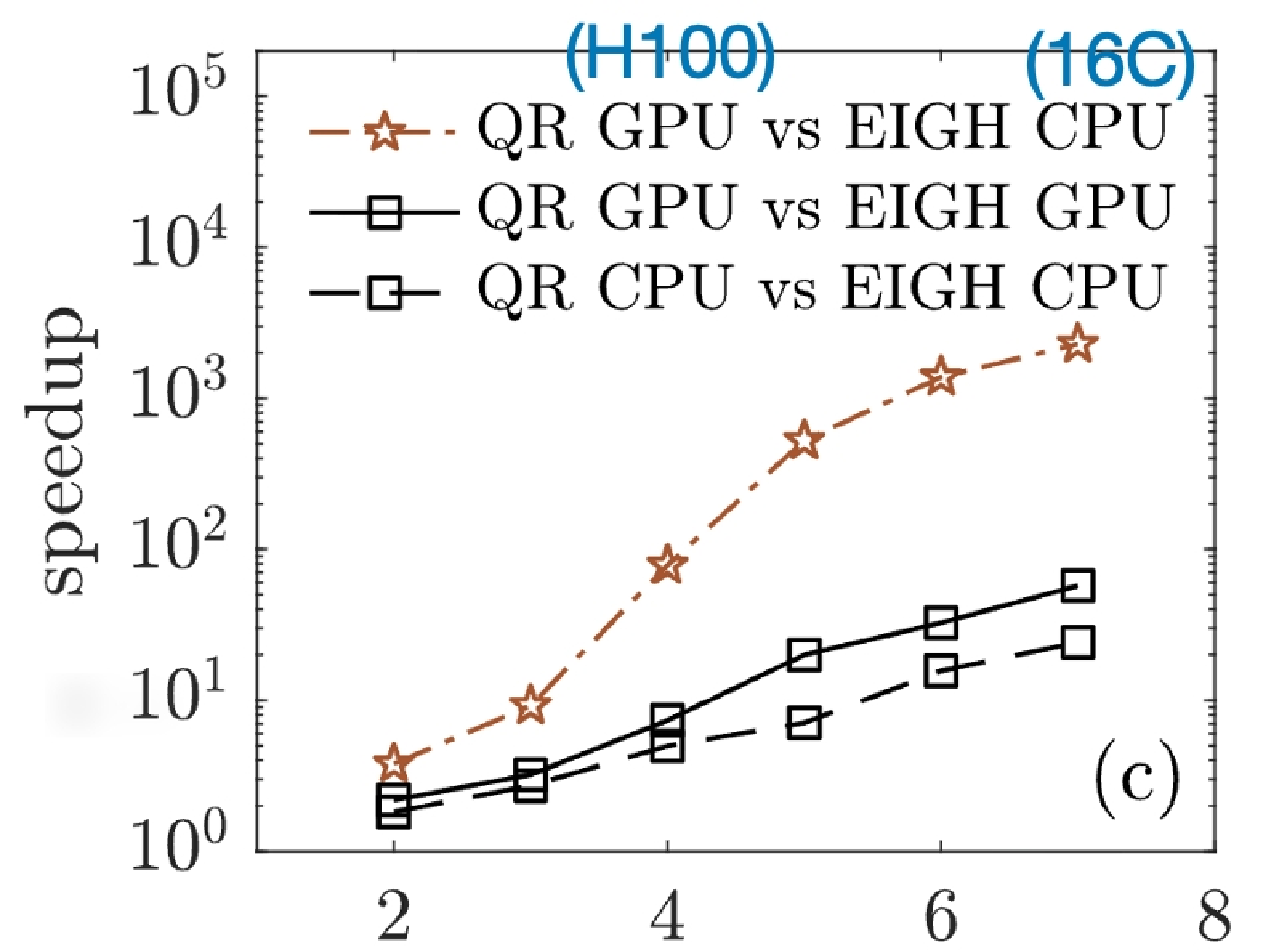
A simpler approach missing for ~30 years?



Y. Zhang* & Q. Yang* & P. R. Corboz (**2025**) arXiv:2505.00494

Advantages?

1. Reduced
2. Prefactor
3. GPU



2D Heisenberg model, $\chi = 5D^2$

GEMM
Permute, QR
SVD, Eigh

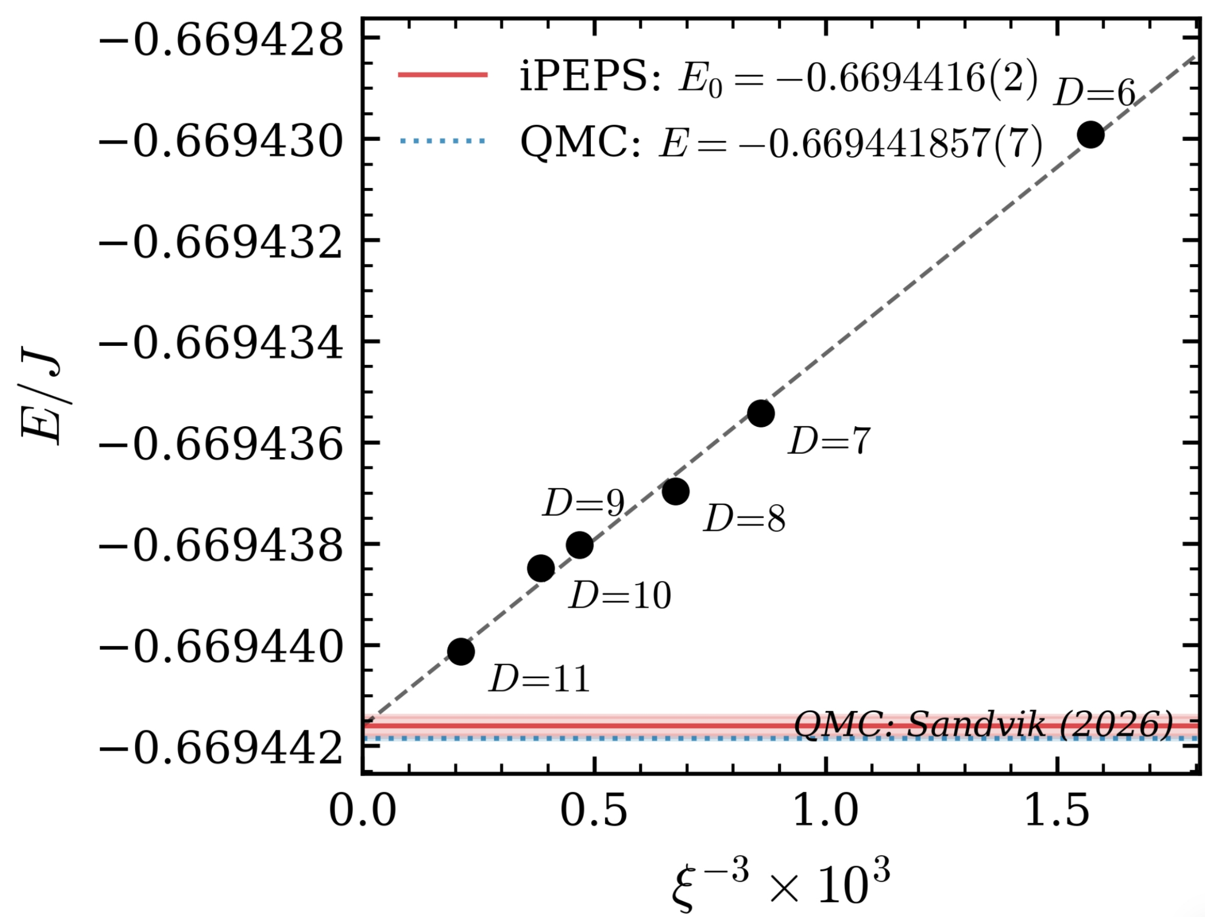
Fixed-point agrees at machine precision

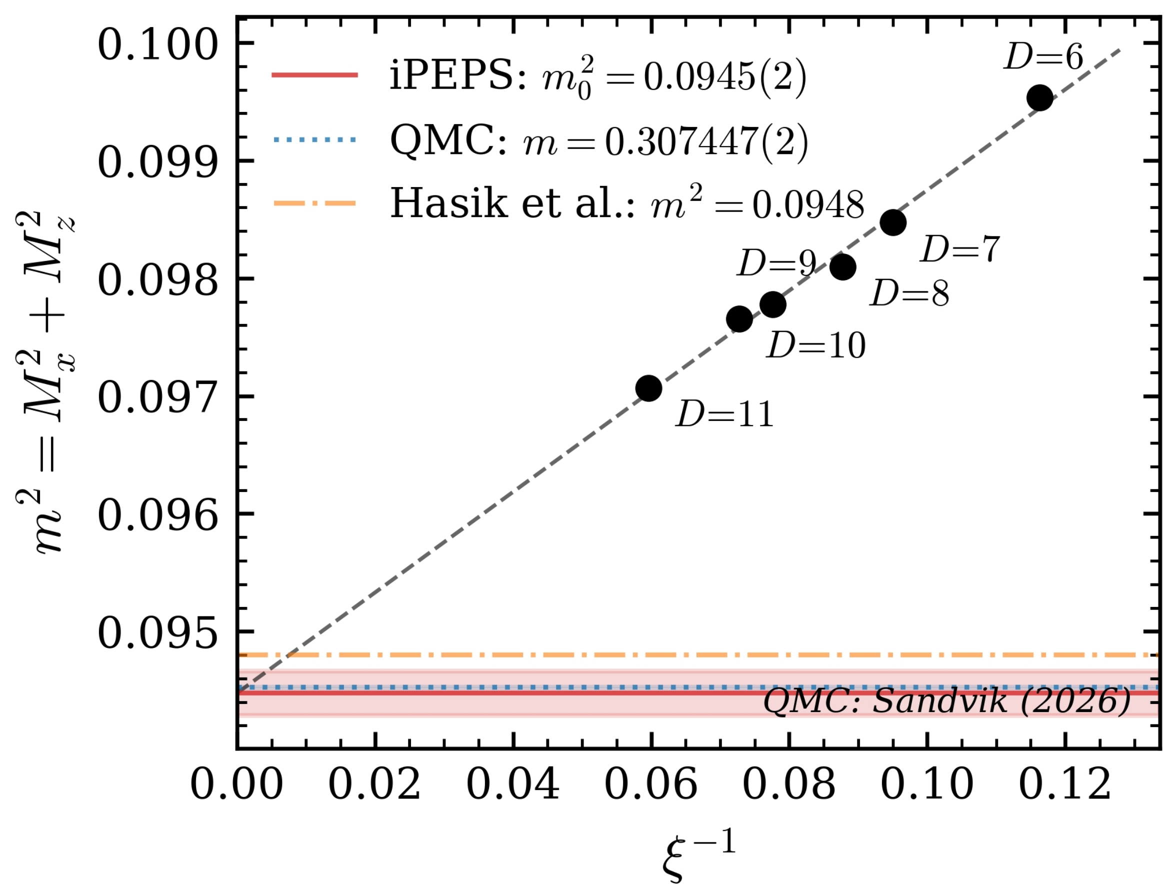
Even better with AD! $\frac{1}{s_j^2 - s_i^2}$

Liao et al. PRX 9, 031041 (2019)

AFM Heisenberg on square lattice

Scale: $D \to 11$, $\chi_{\text{opt}} \to 968$, $\chi_{\text{measure}} \to 1864$, without U(1) symmetry





$$E_{QMC} = -0.669437(5)$$

$$E_{QMC} = -0.669441857(9)$$

$$E_0 = -0.6694416(2)$$

$$m_{QMC} = 0.3070(3)$$

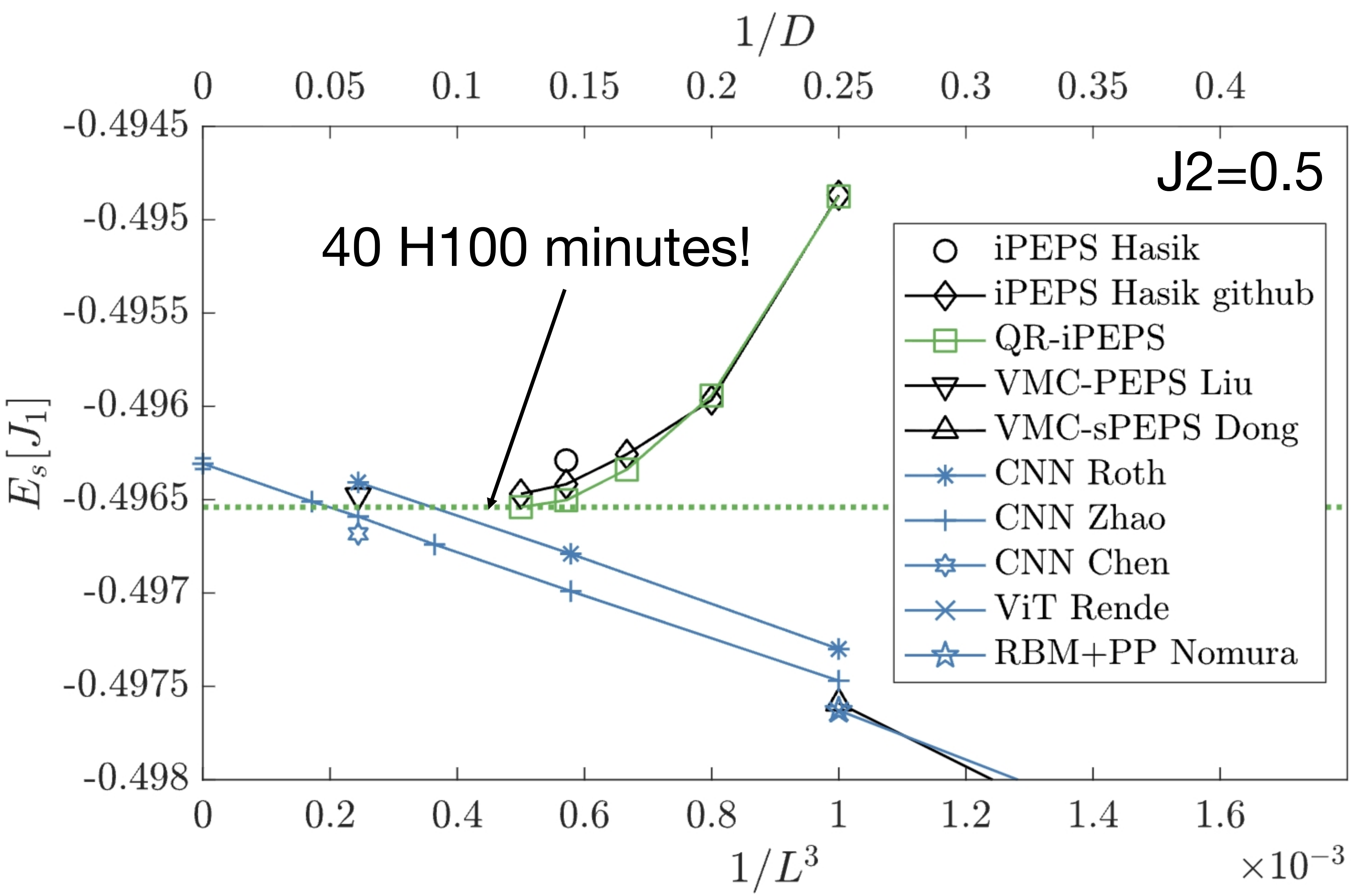
Sandvik PhysRevB.56.11678 (1997)

$$m_{QMC} = 0.307447(2)$$

Sandvik arxiv:2601.20189 (2026)

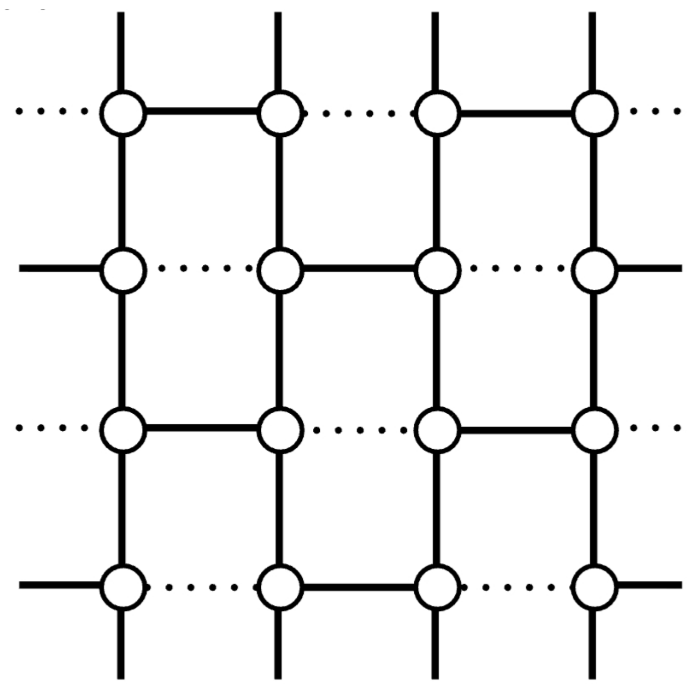
$$m_0 = 0.3073(3)$$

J1-J2 on Square lattice: SOTA energy



iPEPS on the Honeycomb Lattice: Brick-Wall Approach

Brick Wall



PhysRevX.2.041013

Large Unit Cell VUMPS

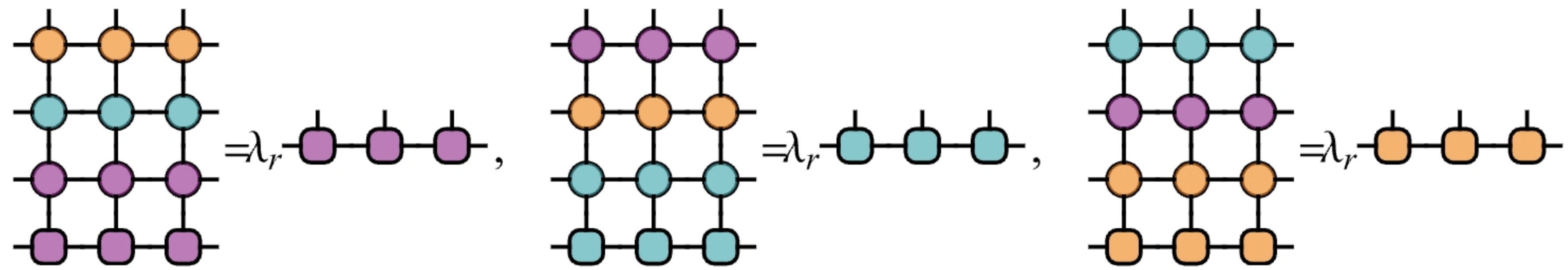


Fig: PhysRevB.108.085103

Large Unit Cell CTMRG

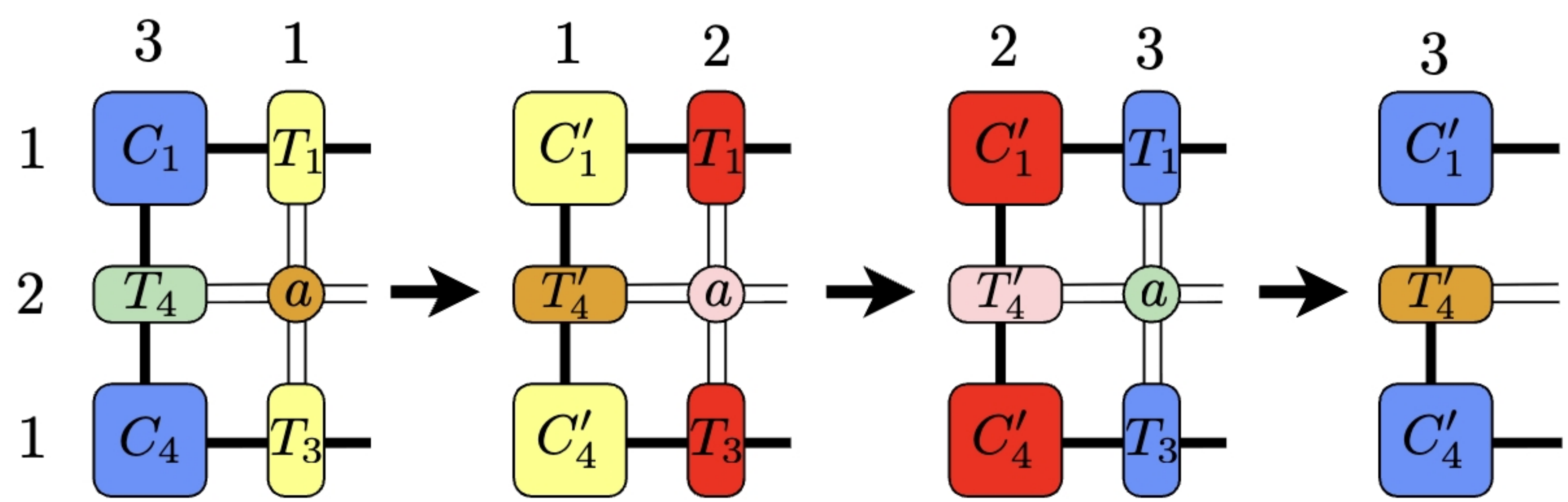


Fig: Philippe Corboz's slides@tnqmp2016

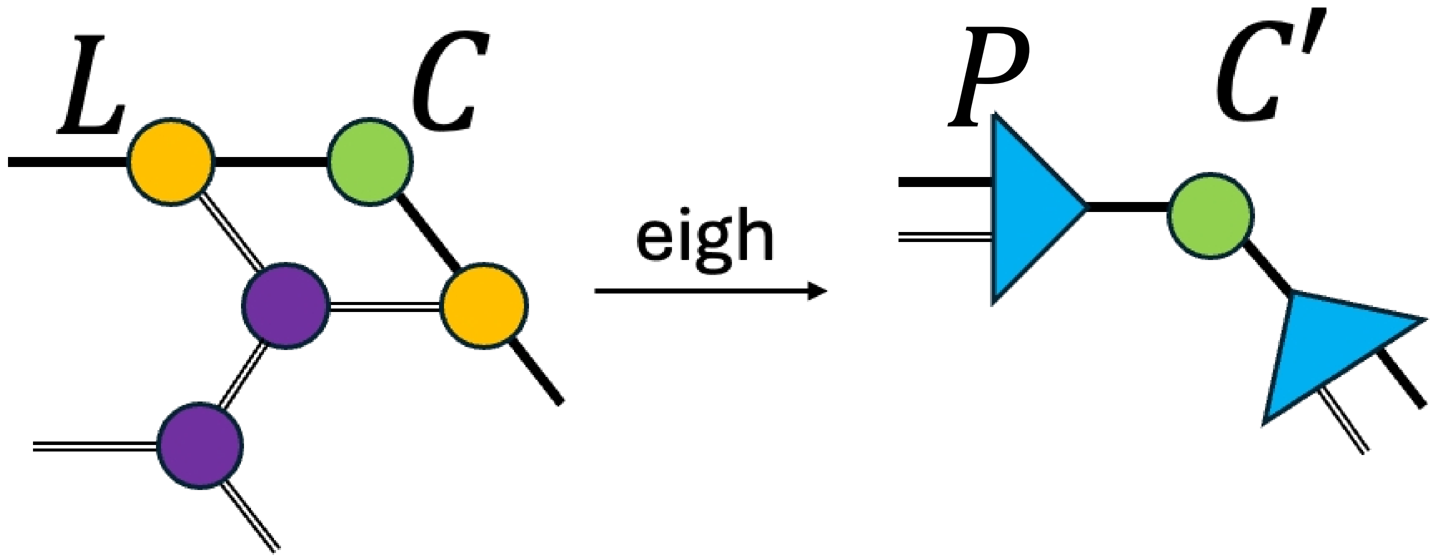
Complex Coding, Unstable convergence

Figures shown for illustration only; credit for large–unit–cell algorithms goes to the original authors.

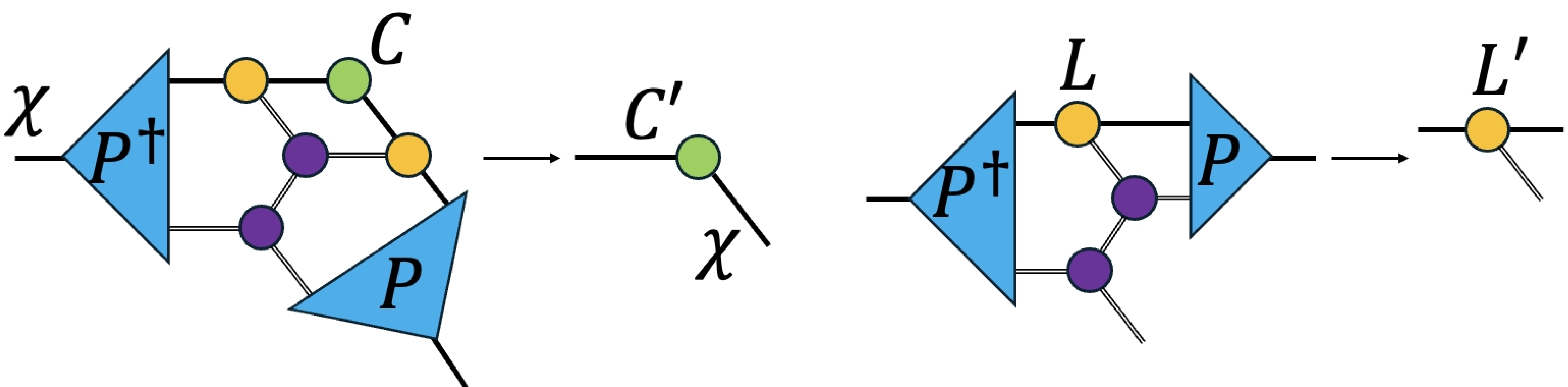
CTMRG for uniform C_{3v} iPEPS

Lukin et al., PhysRevB.107.054424(2023)

Step 1: Build projector. (expensive EVD) ~95% time



Step 2: Update edge and corner tensors. ~ 5% time

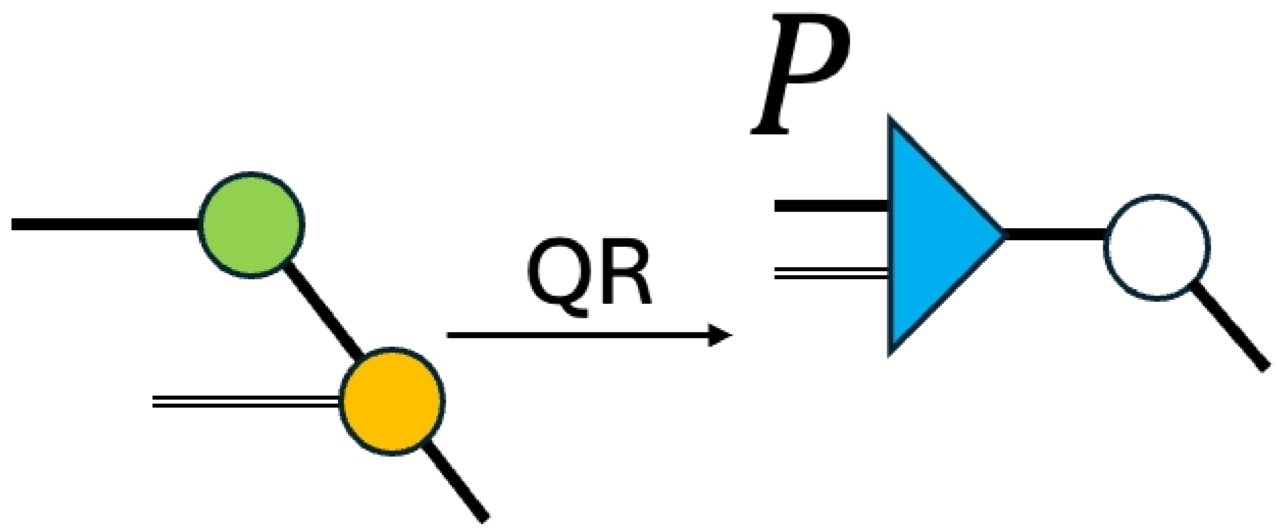


H100, double, very large D>6 and chi>600

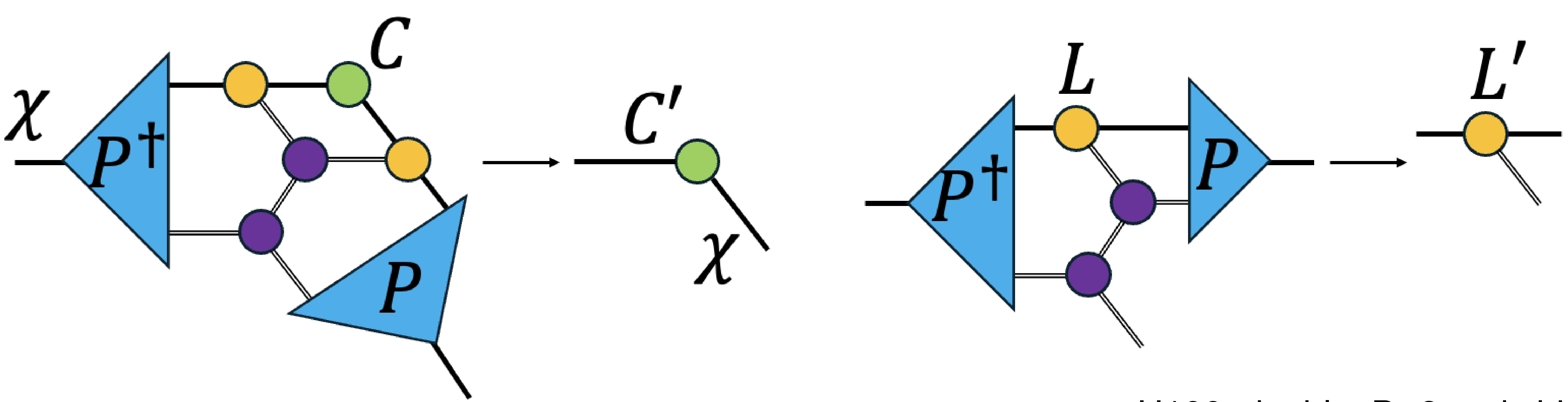
QRCTM for uniform C_{3v} iPEPS

Yang et al.PhysRevB.113(8),085109(2026)

Step 1: Build projector via QR (cheap) ~10% time



Step 2: Update edge and corner Tensors. ~90% time

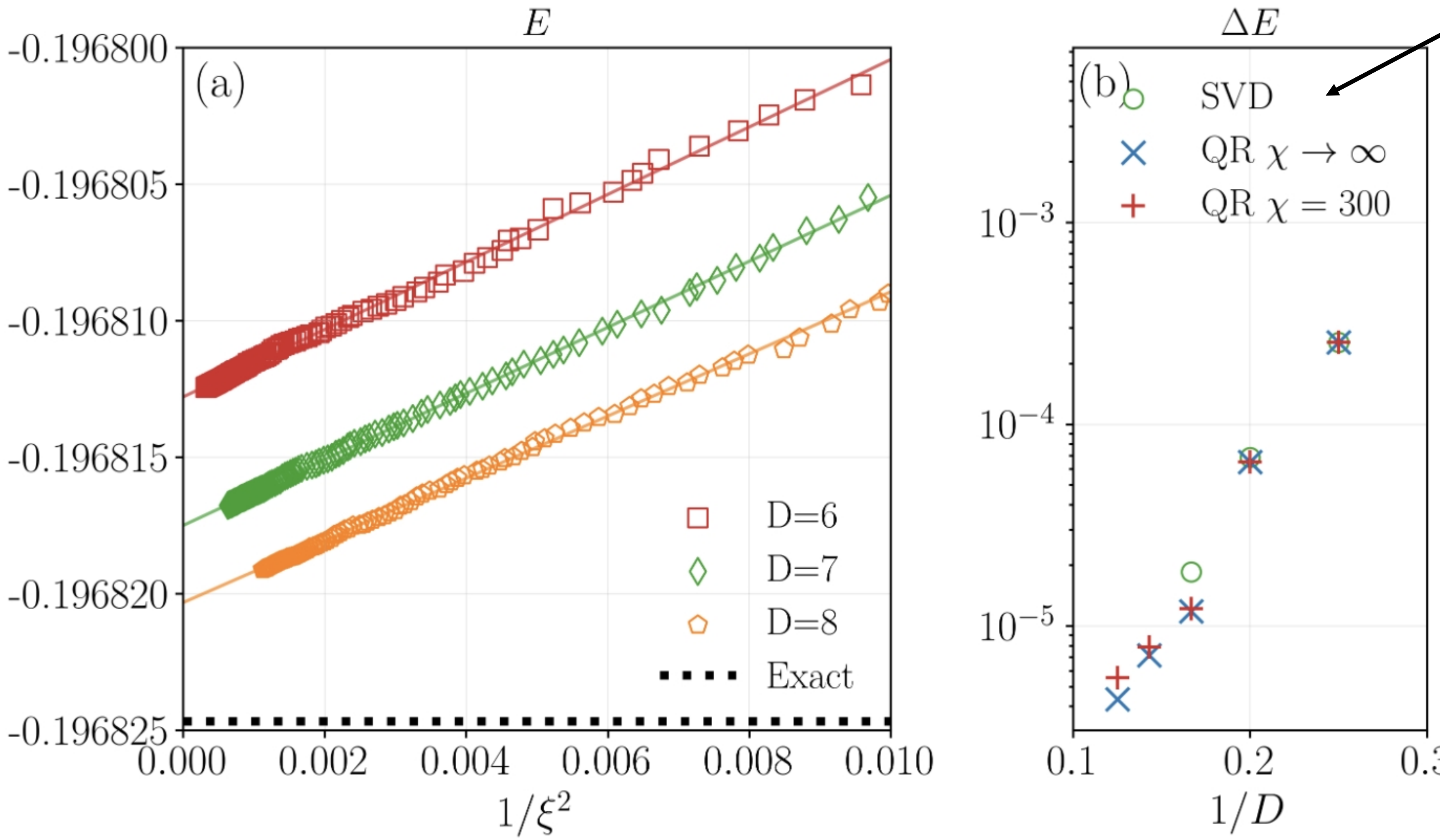


H100, double, D=6 and chi=600

Isotropic Kitaev model (S=1/2) energy

j.aop.2005.10.005

Lukin et al., PhysRevB.107.054424(2023)



Critical SG $D = 8, \| \Delta E/E \| = 7 \times 10^{-5}$ PhysRevLett.123.087203(2019)

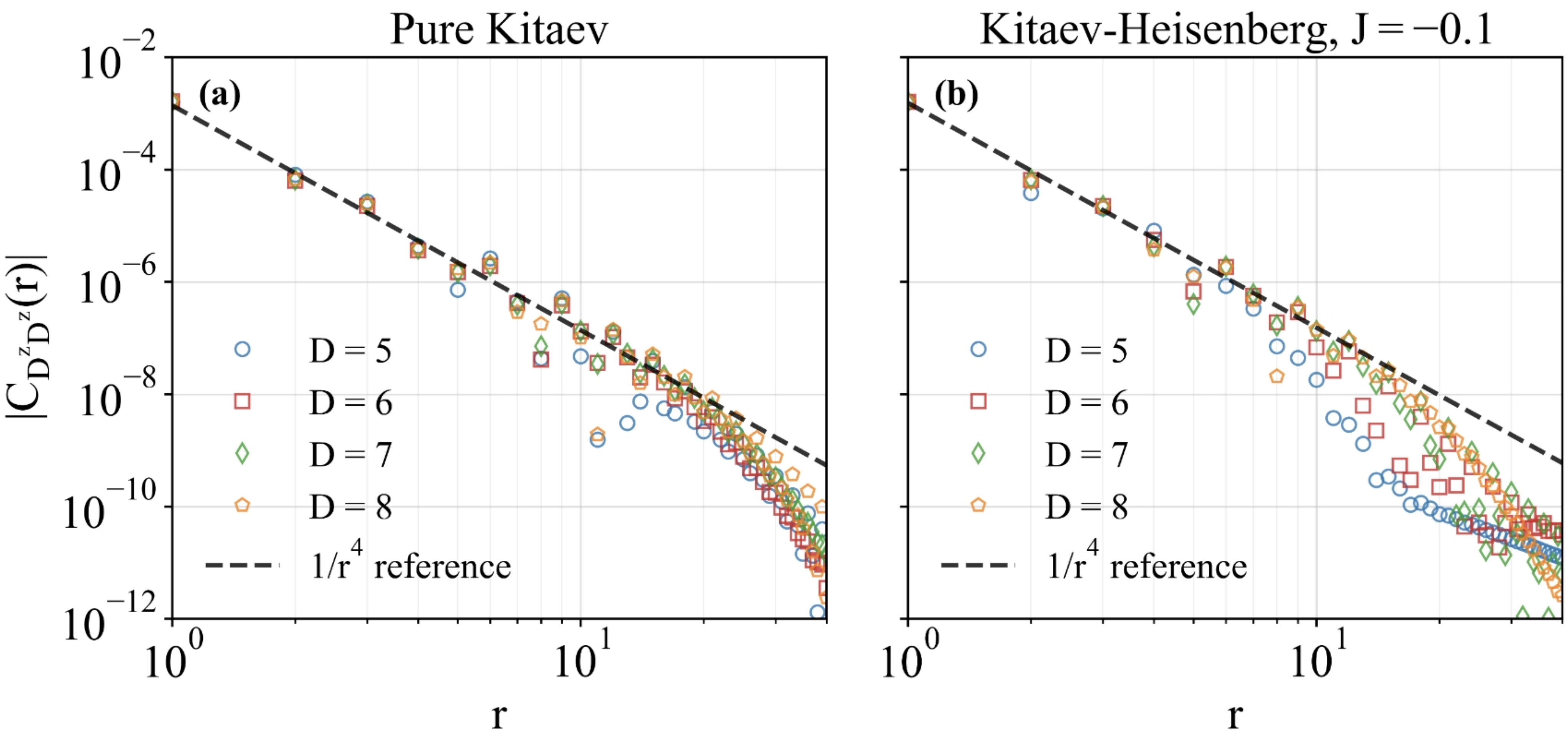
AD+CTMRG $D = 6, \| \Delta E/E \| = 9 \times 10^{-5}$ PhysRevB.107.054424(2023)

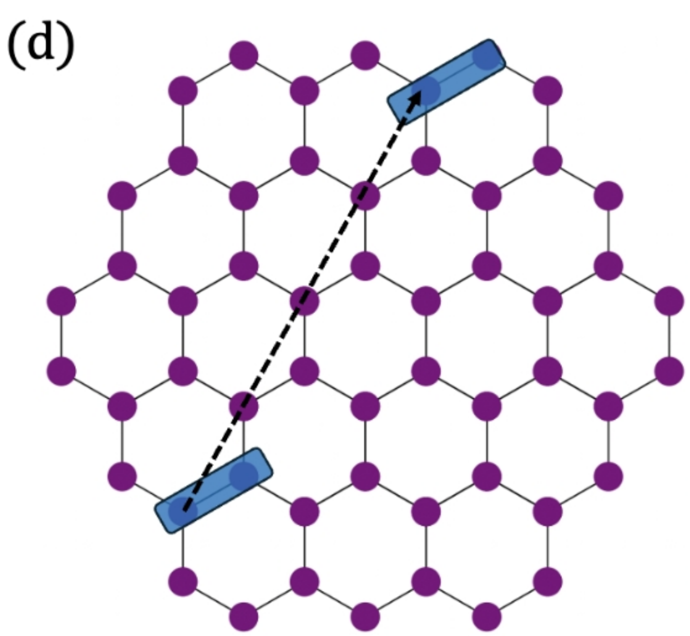
AD+QRCTM $D = 8, \| \Delta E/E \| = 2 \times 10^{-5}$

SOTA reported energy with AD+iPEPS

Not extrapolated, energy per site.

Dimer-Dimer correlation decay





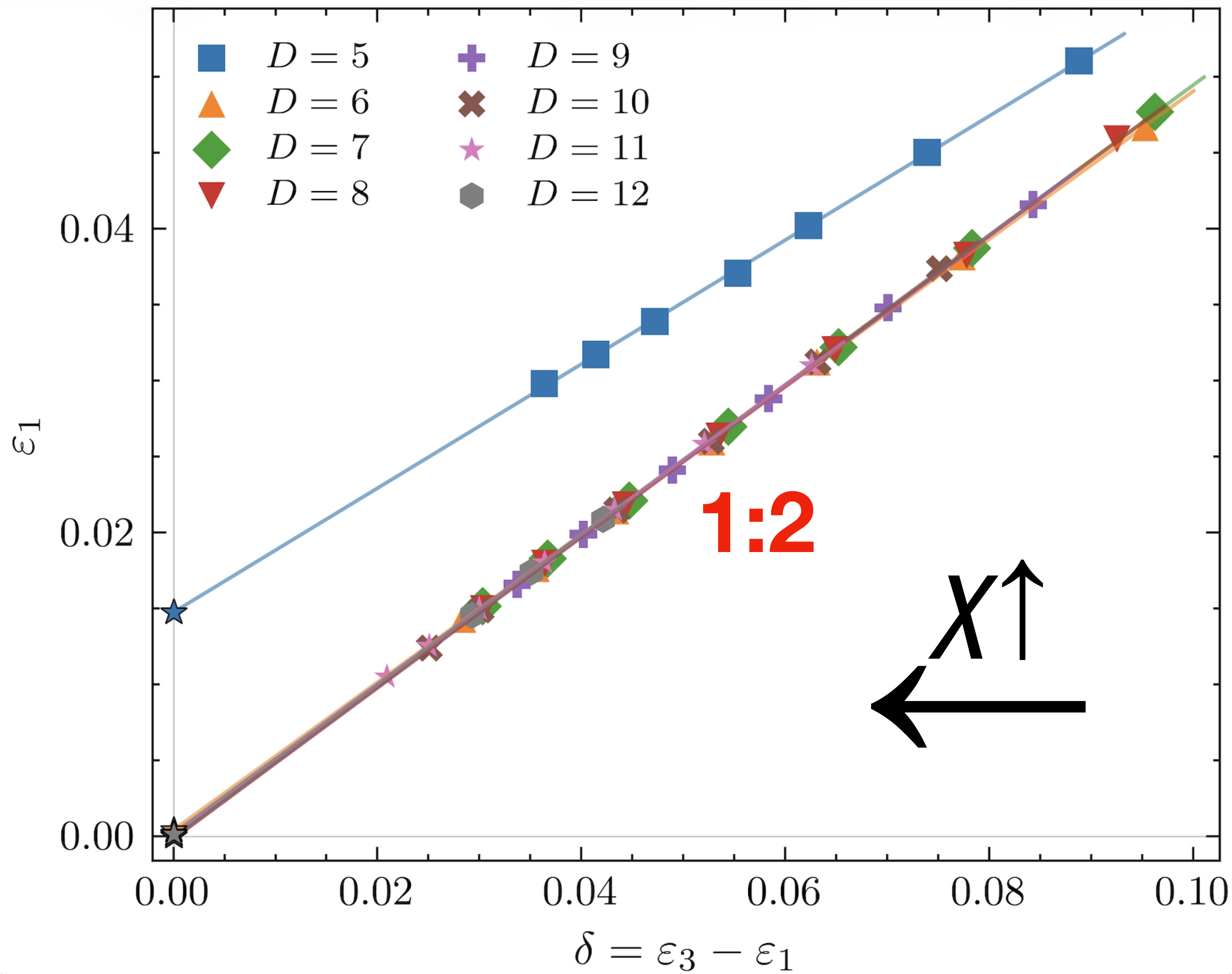
J=0, exactly solvable. J≠0?

Dimer–Dimer r^{-4} tail persists in QSL phase

Phys. Rev. A 78, 012304 (2008)
Phys. Rev. Res. 2, 013005 (2020)

As predicted by field theory; to our knowledge, first confirmed with iPEPS

Transfer matrix spectrum collapse (Kitaev)



Thanks to high accuracy of optimized iPEPS,

Emergent Gapless(CFT) nature is resolved.

Phys. Rev. X 8, 031030 (2018)
Phys. Rev. X 8, 031031 (2018)

Higher Spin Kitaev model

$$H = \sum_{\langle i,j \rangle_\gamma} K_\gamma S_i^\gamma S_j^\gamma$$

$$S > 1/2, K_\gamma = -1$$

Is the ground state a **QSL**?
Any **symmetry breaking**?

Semi-classical analysis

PRB 78, 115116 (2008)
Nat. Commun. 9, 1575 (2018)
....
Results: **Bond order** for Large: S ≧ 2
S=3/2 (unclear), S=1(no SSB)

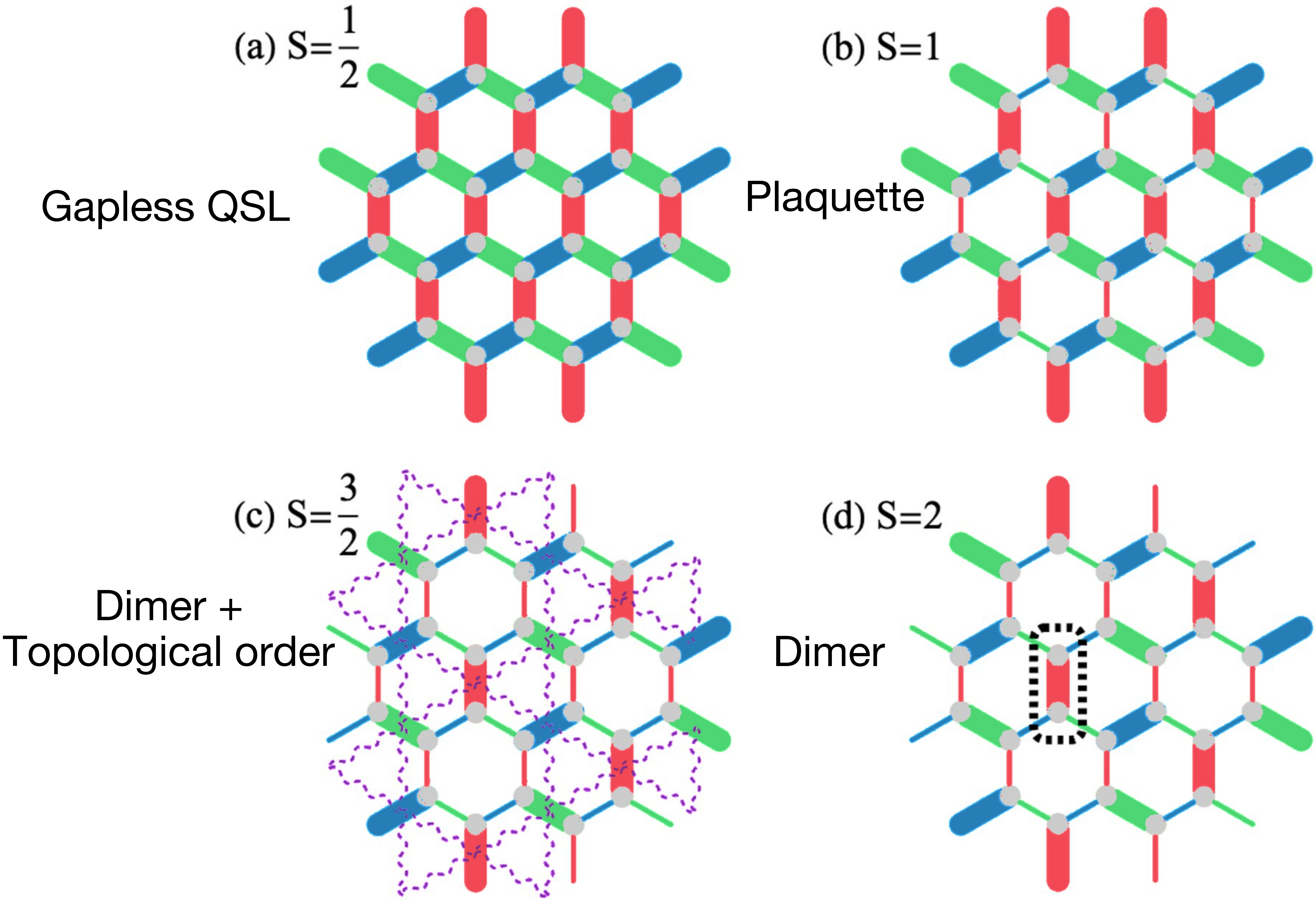
Quantum many-body methods

JPSJ 87, 063703 (2018)
PRR 2, 033318 (2020)
PRR 3, 013160 (2021)
PRB 105, L060403 (2022)
Nat. Commun. 13, 3813 (2022)
PRB 106, 174416 (2022)
SciPost Phys. 16, 100 (2024)
PRR 6, 033077 (2024)
PRB 110, 134402 (2024)
PRR 6, 033168 (2024)
arXiv:2503.24246 (2025)
....
Results: **QSL, no symmetry breaking**

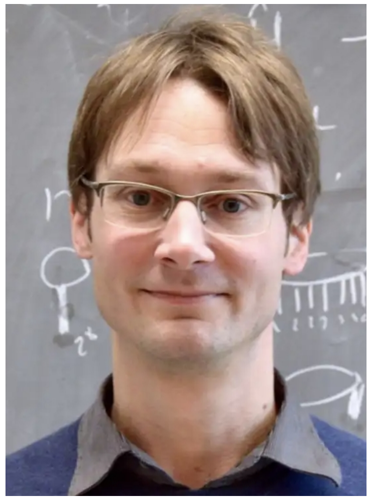
Commun. Phys. 7, 319 (2024)
Result: **(2x2 unit-cell SU), anisotropic**

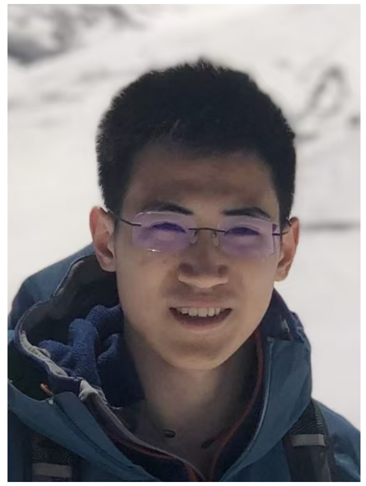
SSB in Higher Spin Kitaev model

arXiv.2511.07415. Collaboration with Xingyu Zhang*, Jutho Heageman, Yuchi He @Ghent

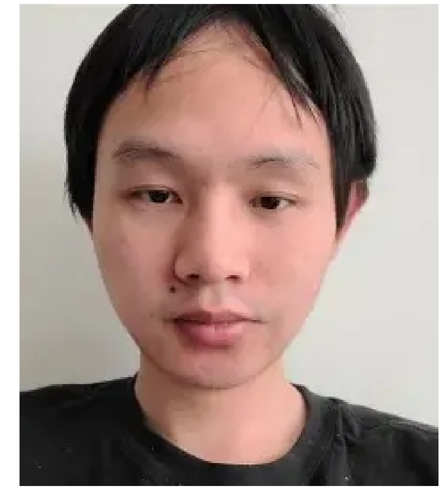


Thanks to my collaborators


Philippe Corboz


Yining Zhang


Jutho Haegeman


Yuchi He


X.Y. Zhang

Philippe Corboz
Qi Yang

Jutho Haegeman
Xingyu Zhang
Yuchi He

Yining Zhang

1. **QRCTM C4v**
2. **QRCTM C3v**
3. **Higher Spin Kitaev**

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Hands on!
Scan me!