Towards Next-Generation iPEPS Algorithms

UNIVERSITY OF AMSTERDAM
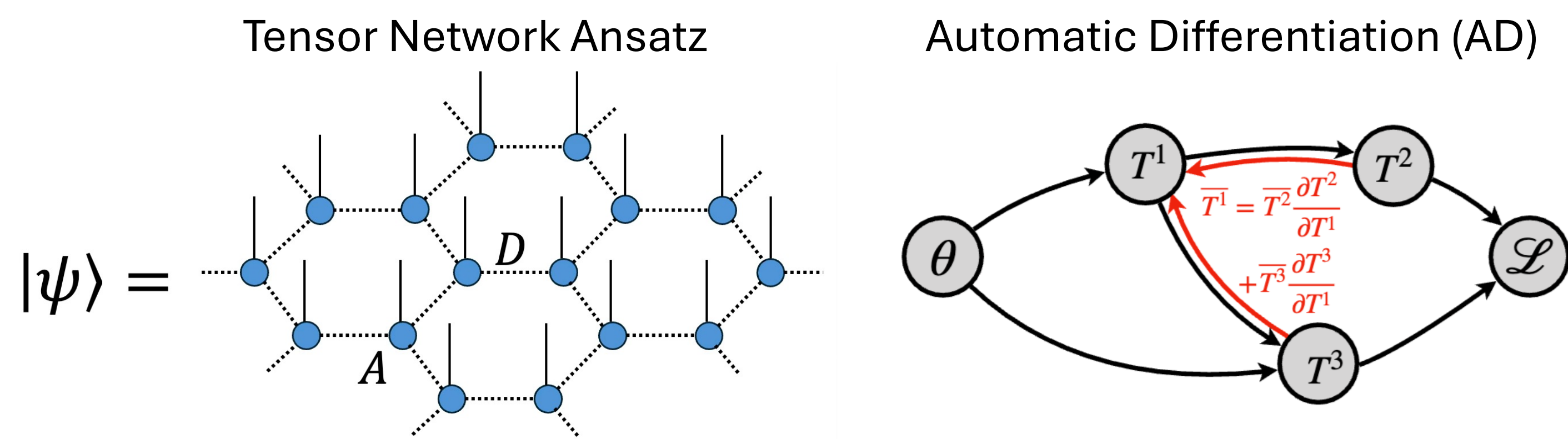**Qi Yang** (Presenter), Philippe Corboz
GHENT UNIVERSITY
Xingyu Zhang, Yuchi He, Wei Tang, Jutho Haegeman
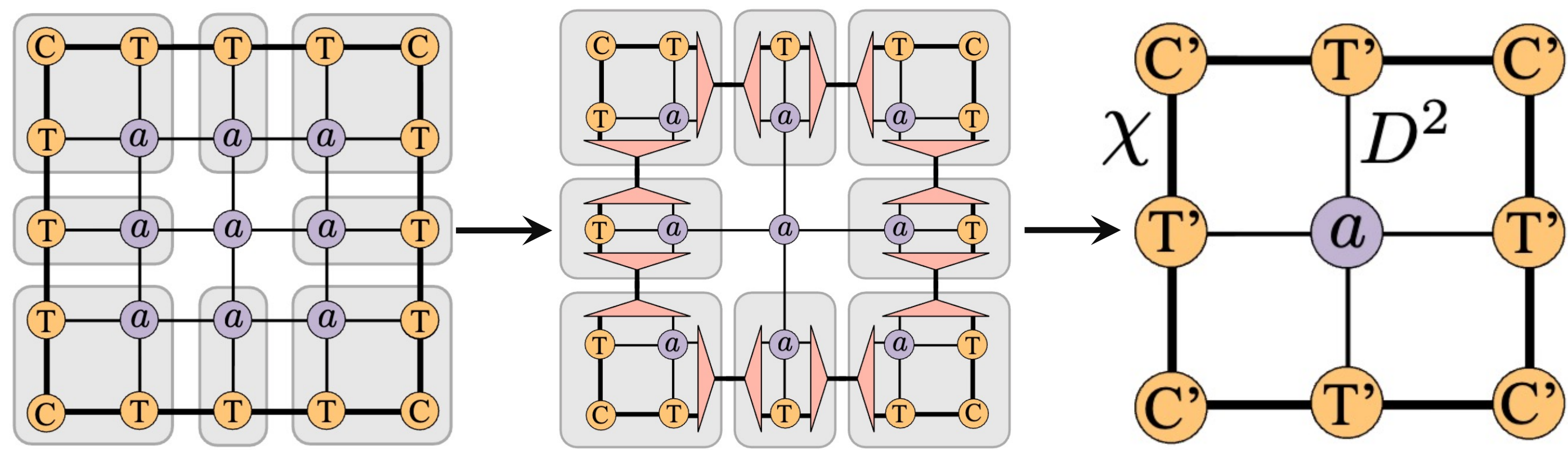erc
EuroHPC Joint Undertaking

Next-Generation iPEPS Toolbox

Tensor Network Ansatz
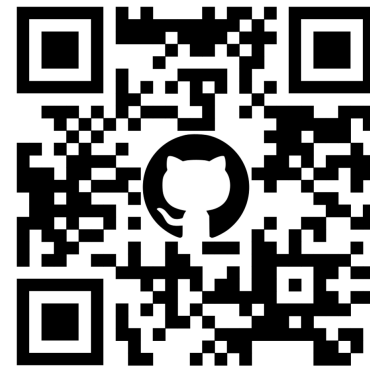

$|\psi\rangle =$ ... D ... A

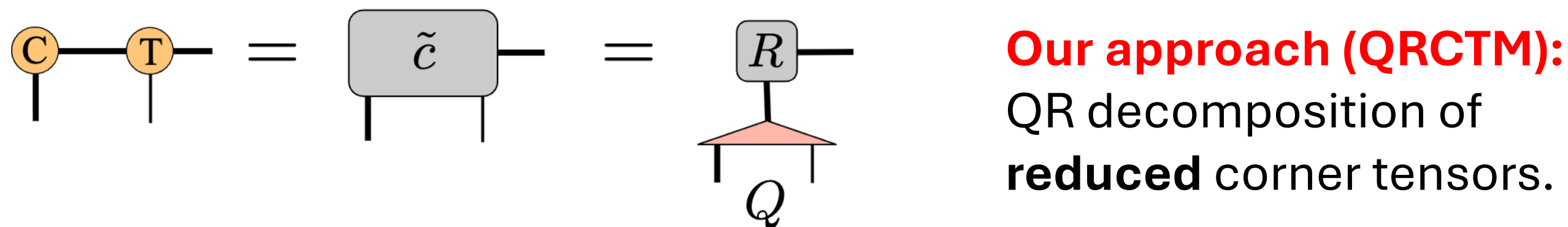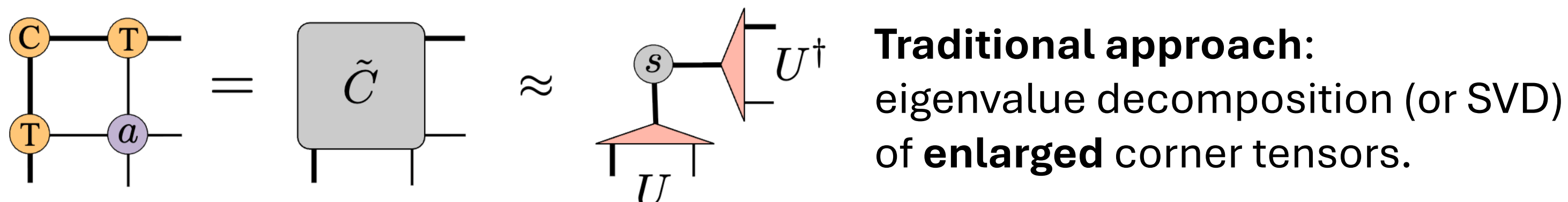Automatic Differentiation (AD)

Background: Automatic differentiation enables high-precision iPEPS studies of 2D quantum many-body systems.
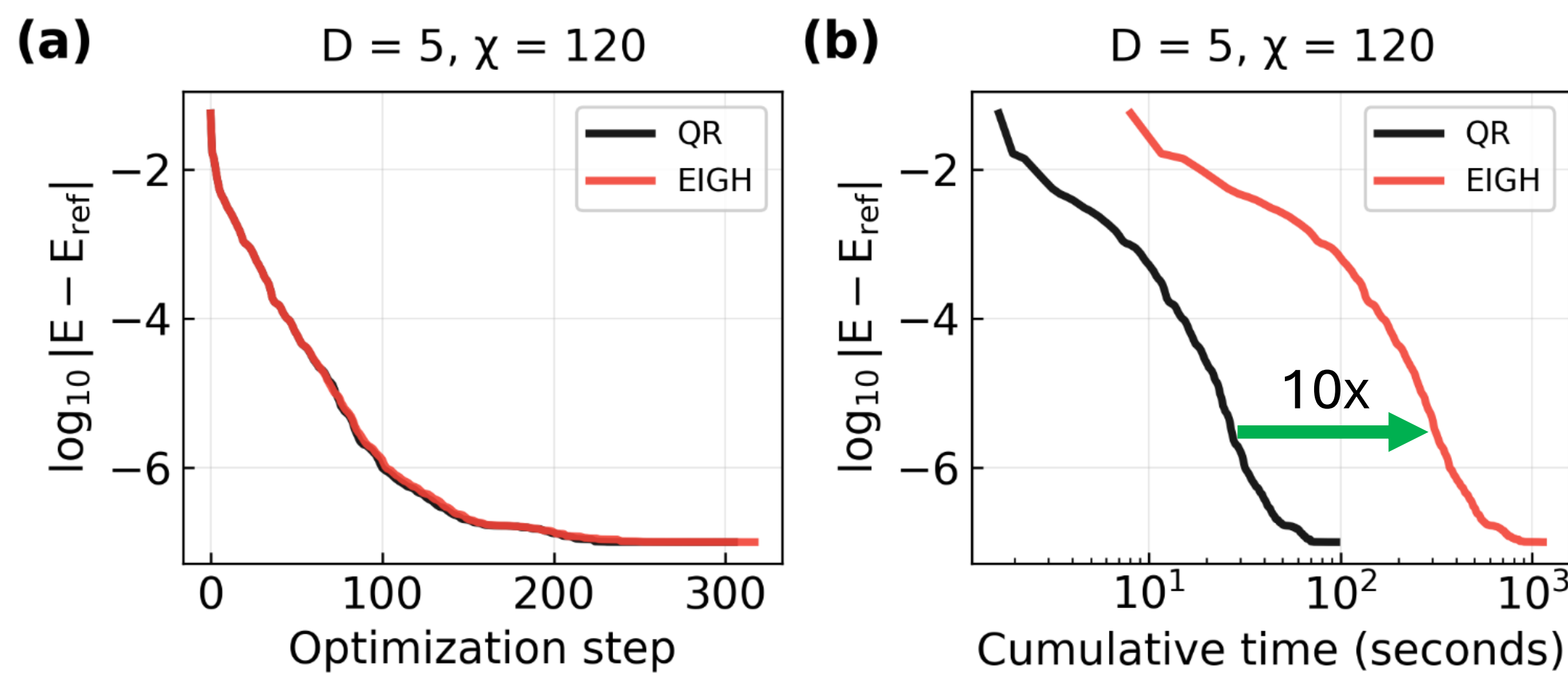
QRCTM

Pedagogical, Newcomer-friendly (user-tested) ready-to-run demo:

Corner Transfer Matrix Renormalization Group (CTMRG): use a **projector** to coarse-grain the 2D many-body system.
To compute the **projector**:

Traditional approach: eigenvalue decomposition (or SVD) of **enlarged** corner tensors.

Our approach (QRCTM): QR decomposition of **reduced** corner tensors.

Benchmark: 2D AFM Heisenberg model on the honeycomb lattices

(a) $D = 5, \chi = 120$

(b) $D = 5, \chi = 120$

10x

Results: [1,2] QRCTM yields an _order-of-magnitude_ speed-up for iPEPS contractions _without loss of accuracy_.

Preconditioning for iPEPS energy minimization

Consider the metric for iPEPS tensors,

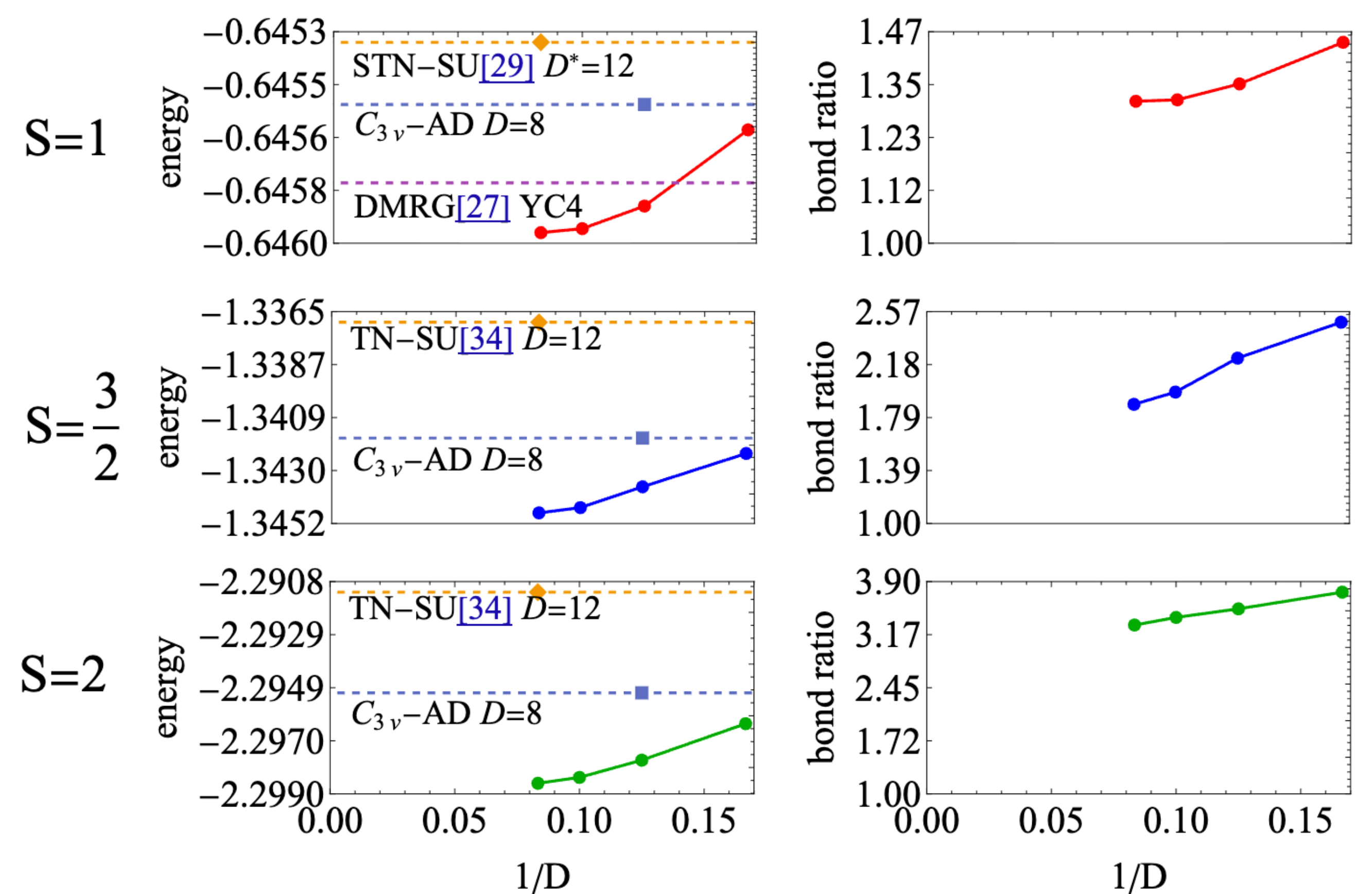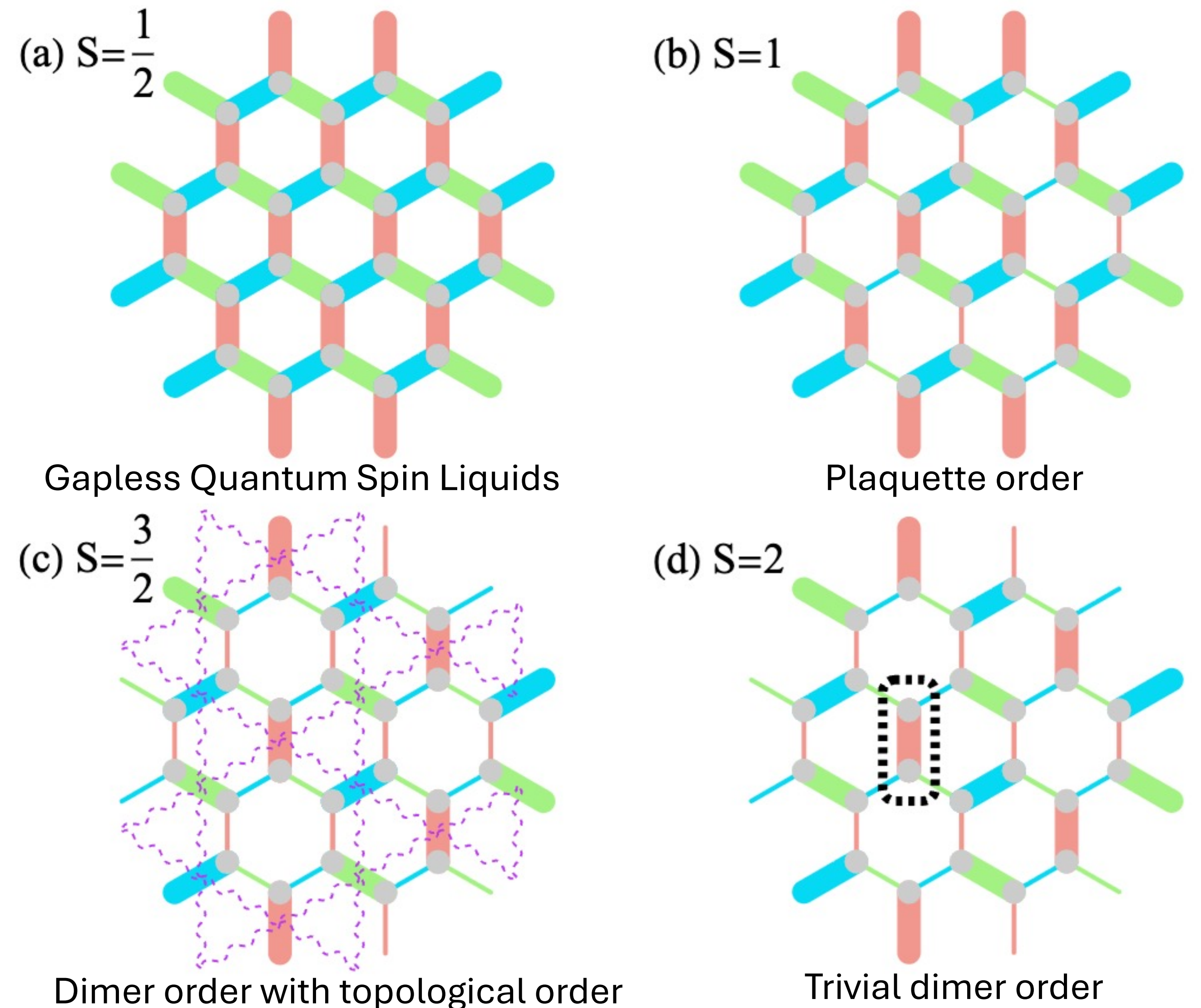$\mathbf{N} = $ ... $+$ ... $+$ ... $+$ ... $+$ ... $+ \cdots$.
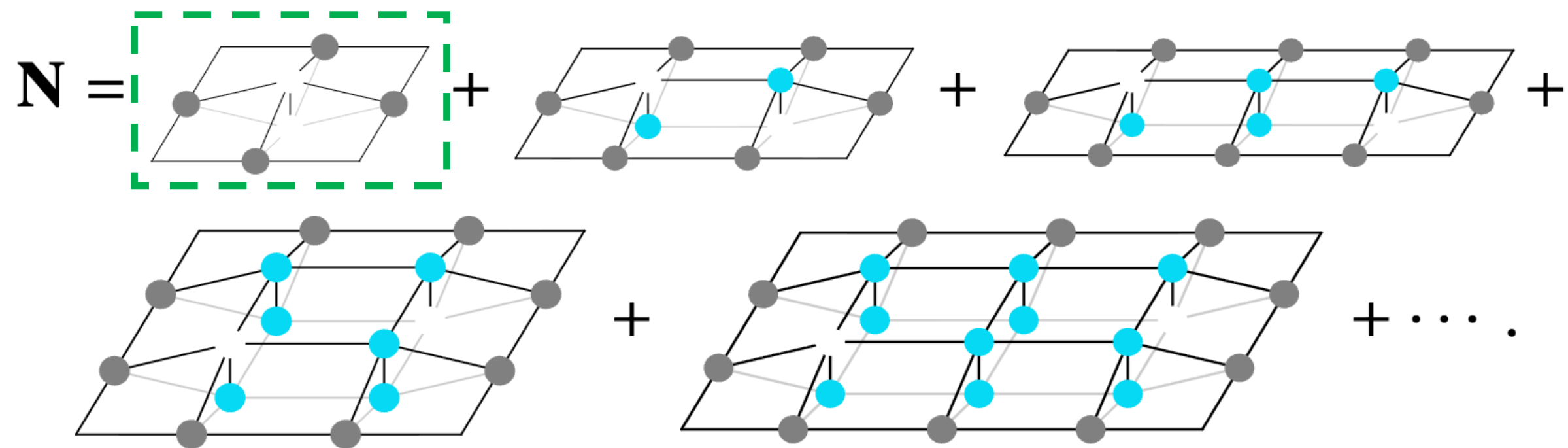
We use the leading term as an approximation to the full metric to **precondition** the problem, **accelerating the convergence** of the L-BFGS optimizer.

Results: Local preconditioning yields faster convergence. See Ref. [3] for more details.

Physical Results for Kitaev-Type Models

Ground states of the spin-S isotropic Kitaev model

Results: [4] Up to S=2, ground states of higher-spin Kitaev models break lattice symmetry.

(a) $S = \frac{1}{2}$ — Gapless Quantum Spin Liquids

(b) $S = 1$ — Plaquette order

(c) $S = \frac{3}{2}$ — Dimer order with topological order

(d) $S = 2$ — Trivial dimer order

S=1 — STN–SU[29] $D^* = 12$; C_{3v}–AD $D = 8$; DMRG[27] YC4

S=$\frac{3}{2}$ — TN–SU[34] $D = 12$; C_{3v}–AD $D = 8$

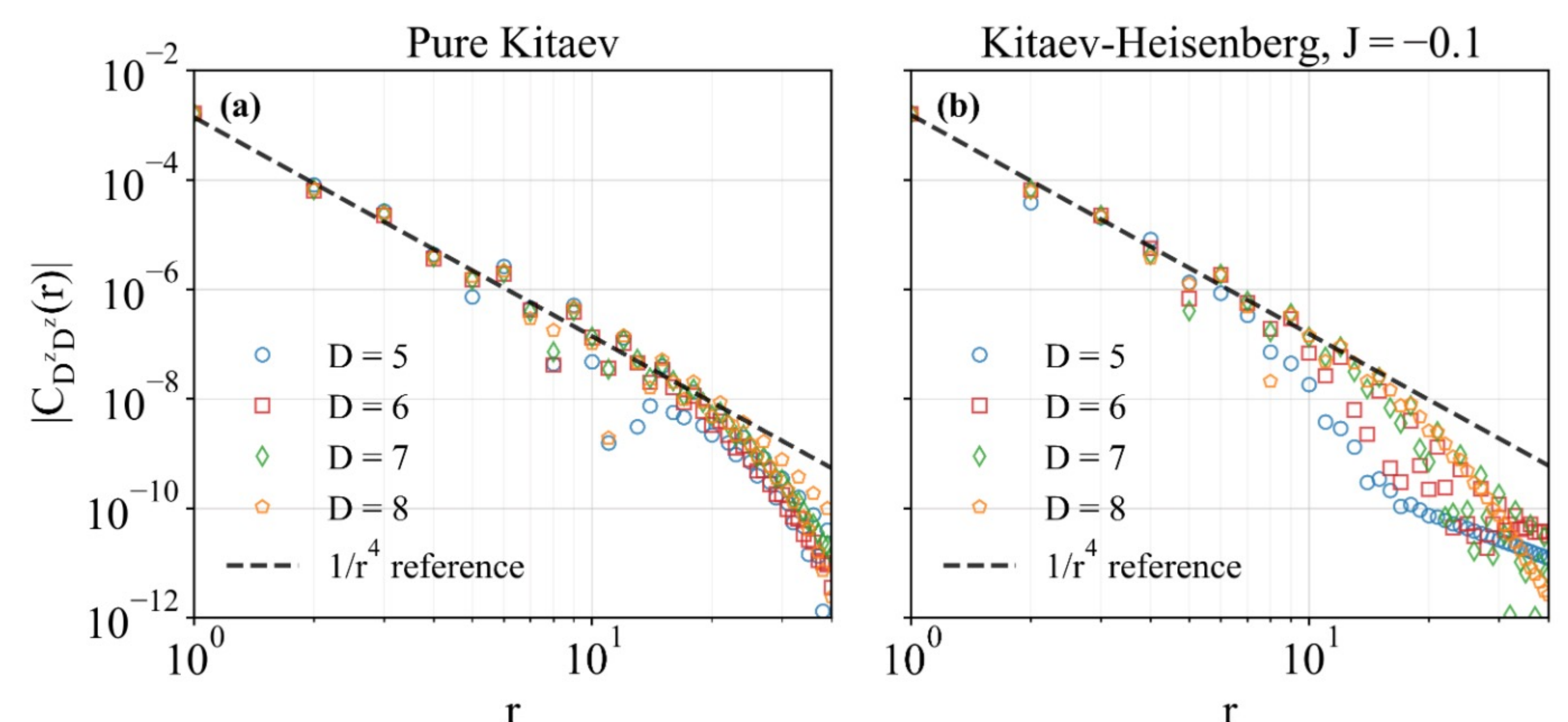S=2 — TN–SU[34] $D = 12$; C_{3v}–AD $D = 8$

Results for spin-1/2 Kitaev-Heisenberg model

Results: [2] iPEPS evidence for the universal 1/r^4 decay of the dimer-dimer correlation function within the QSL regime.

Dimer-dimer correlations:

$$D^z(r) = S_i^z(r) S_j^z(r)$$

$$C_{D^z D^z}(r) = \langle D^z(0) D^z(r) \rangle - \langle D^z(0) \rangle \langle D^z(r) \rangle,$$

(a) Pure Kitaev

(b) Kitaev-Heisenberg, J = −0.1

D = 5, D = 6, D = 7, D = 8, $1/r^4$ reference

* contributed equally.
[1] Y. Zhang∗, **Q. Yang**∗, and P. Corboz. Accelerating two-dimensional tensor network contractions using QR-decompositions.
[2] **Q. Yang** and P. Corboz. Efficient iPEPS Simulation on the Honeycomb Lattice via QR-based CTMRG.
[3] X.-Y. Zhang∗, **Q. Yang**∗, P. Corboz, J. Haegeman, and W. Tang. Accelerating two-dimensional tensor network optimization by preconditioning.
[4] X.-Y. Zhang∗, **Q. Yang**∗, P. Corboz, J. Haegeman, and Y. He. Topological and Trivial Valence-Bond Orders in Higher-Spin Kitaev Models.

Refs:
[1] arXiv: 2505.00494
[2] arXiv: 2509.05090
[3] arXiv: 2511.09546
[4] arXiv: 2511.07415