

Towards Next-Generation iPEPS Algorithms



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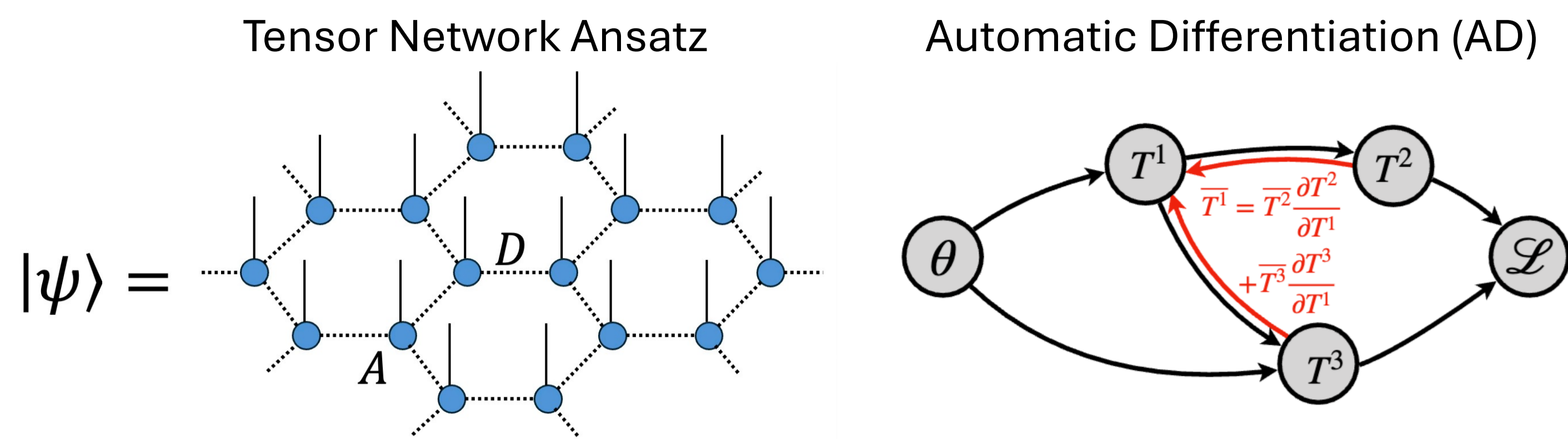
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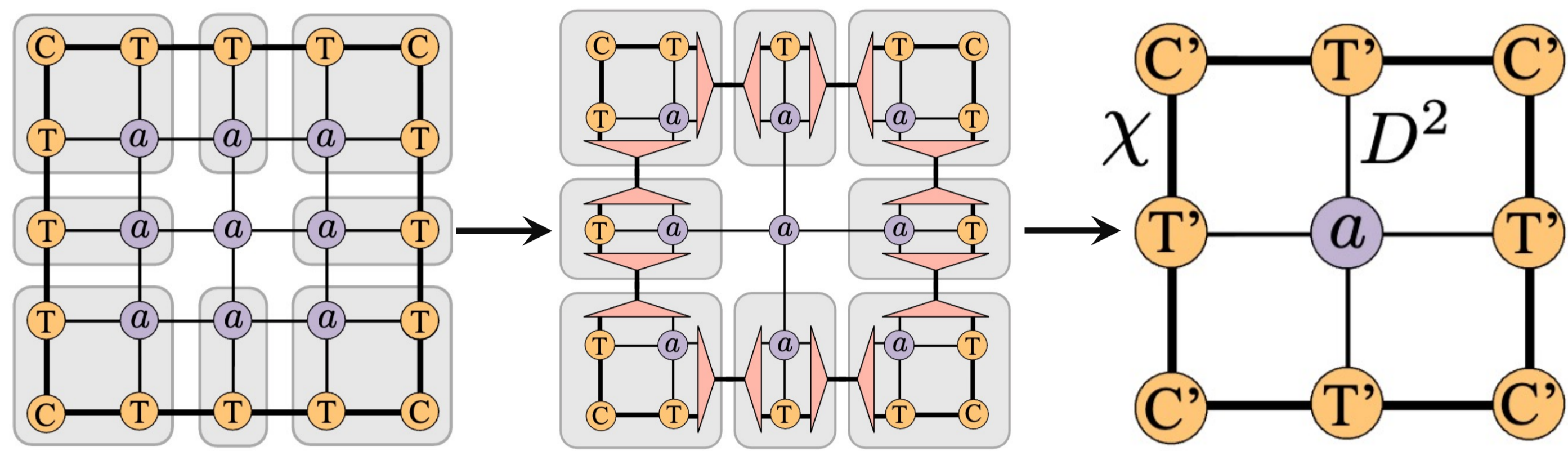
Next-Generation iPEPS Toolbox



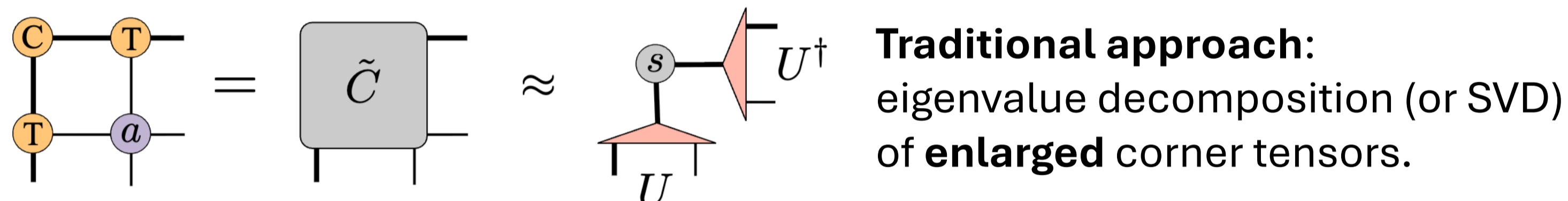
Background: Automatic differentiation enables high-precision iPEPS studies of 2D quantum many-body systems.

QRCTM

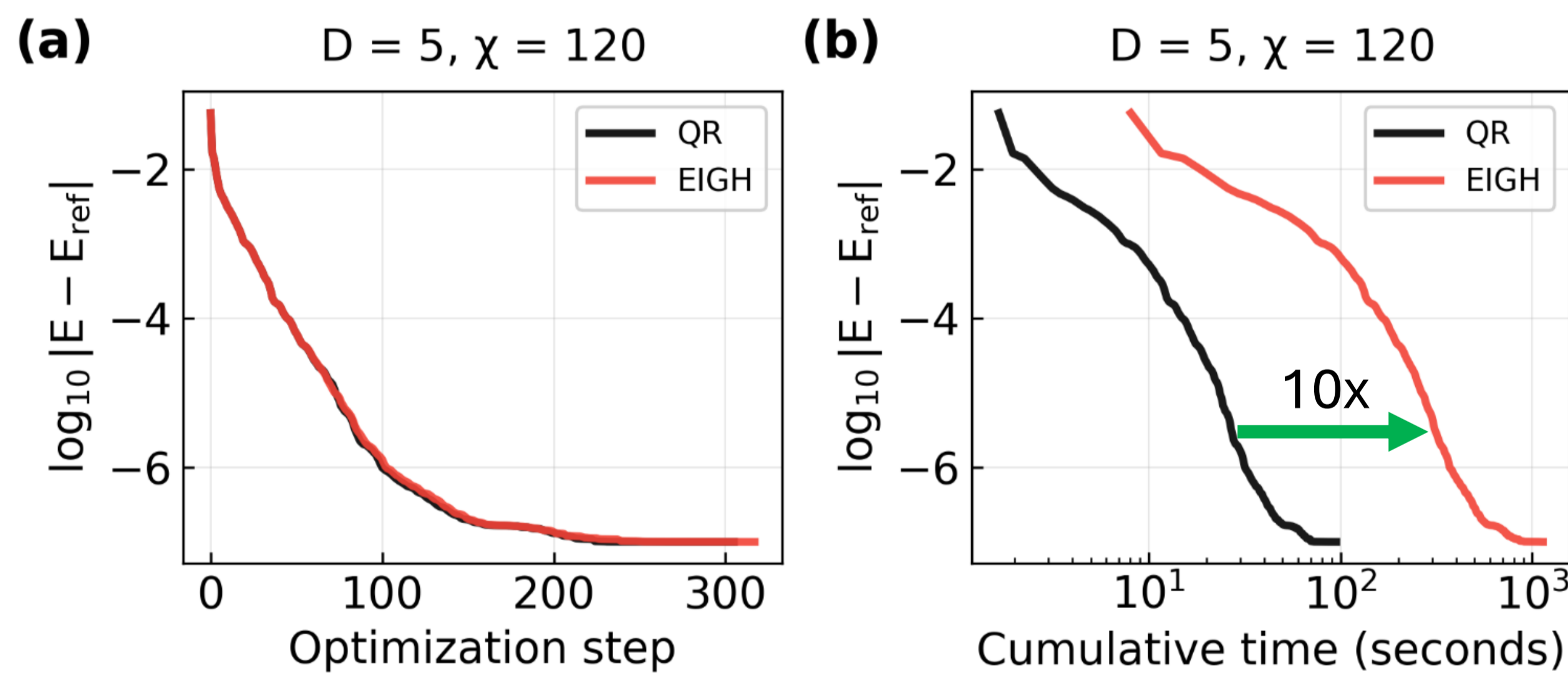
Pedagogical,
Newcomer-friendly (user-tested)
ready-to-run demo:



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



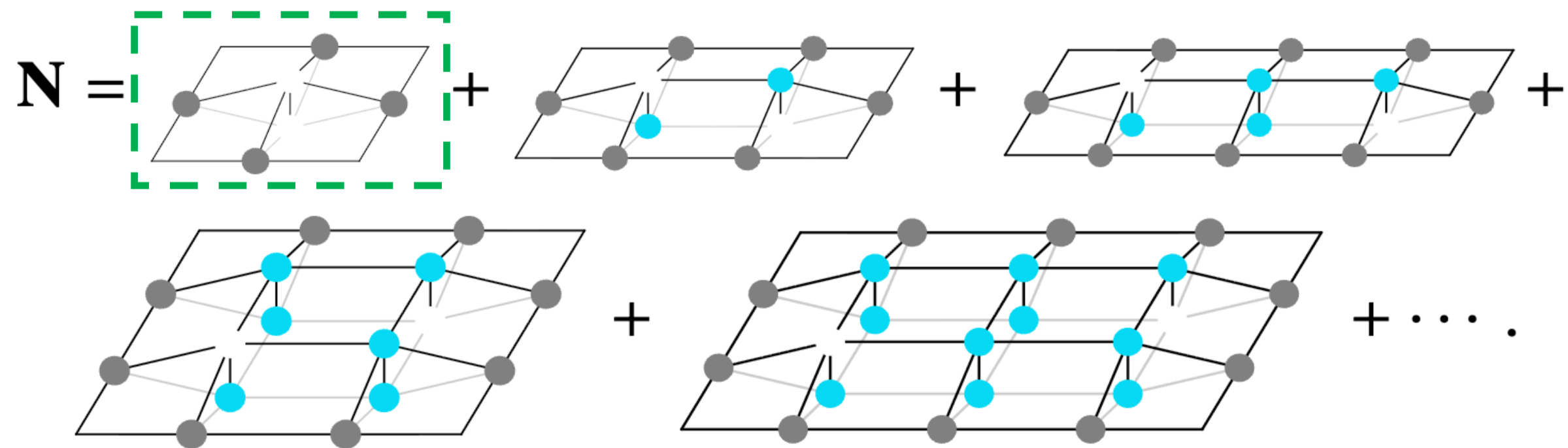
Benchmark: 2D AFM Heisenberg model on the honeycomb lattices



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 \tilde{N} ,



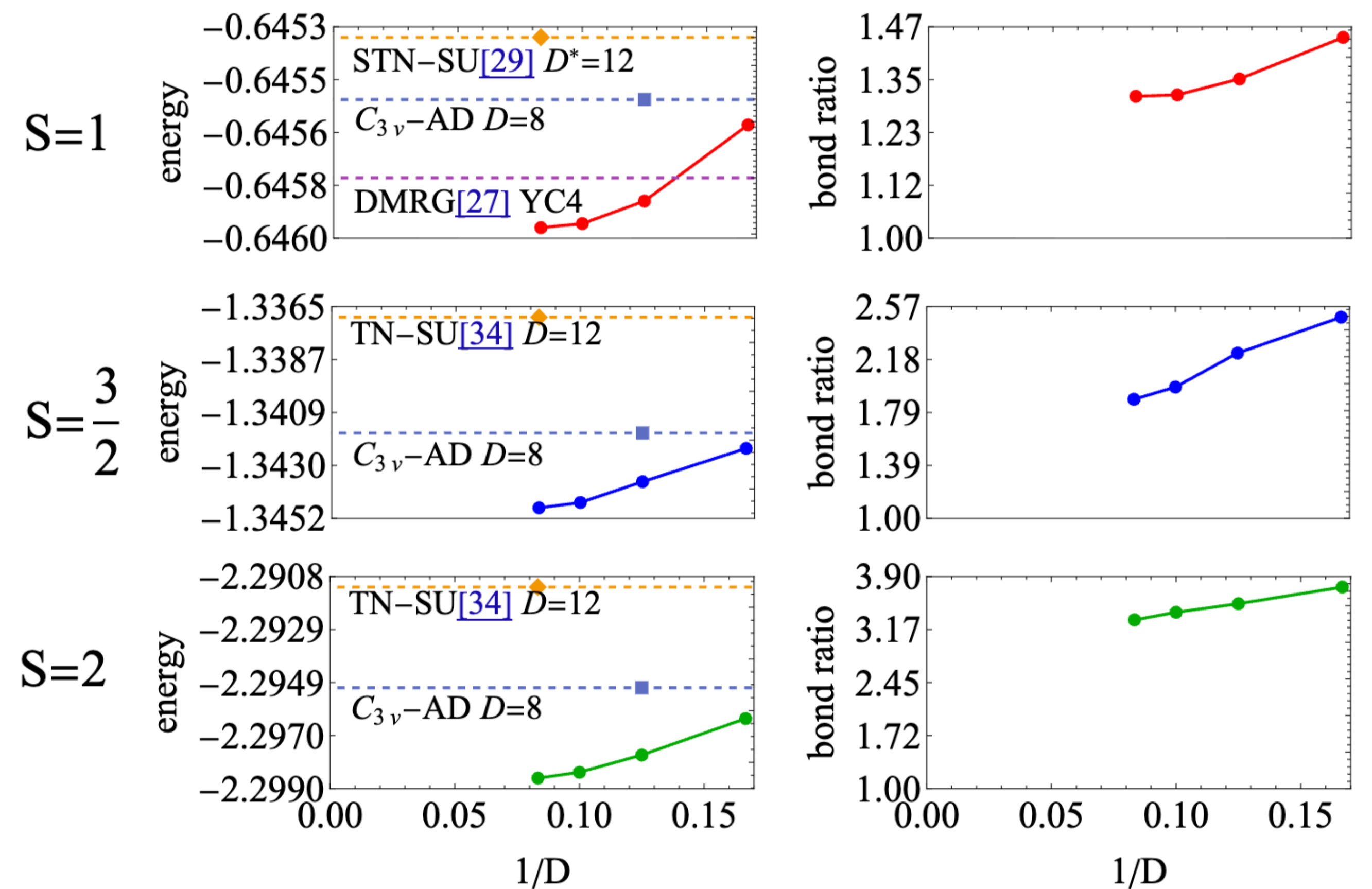
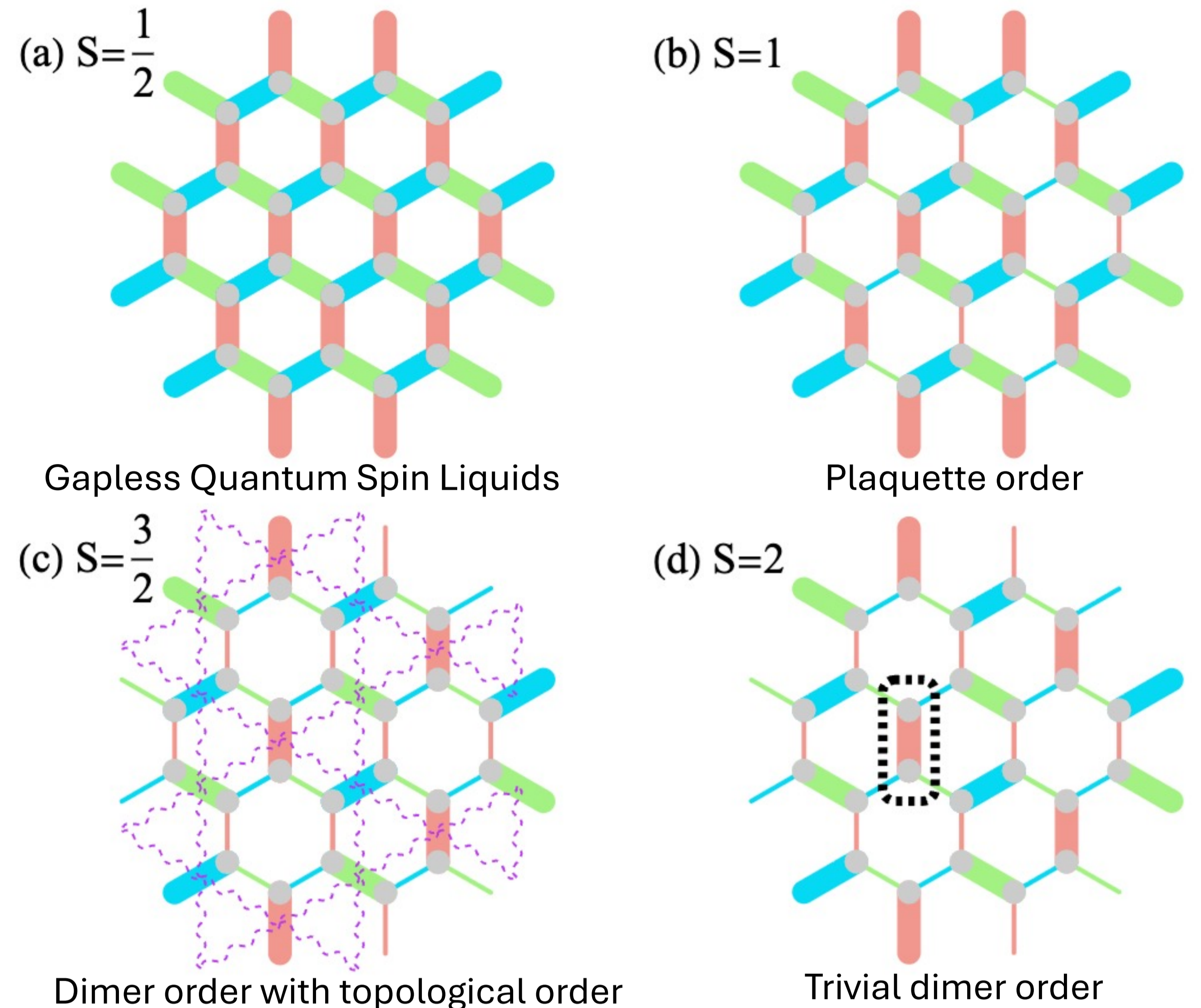
We use the **leading term** as an approximation to the full metric to **precondition** the problem, **accelerating the convergence** of the L-BFGS optimizer.

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.



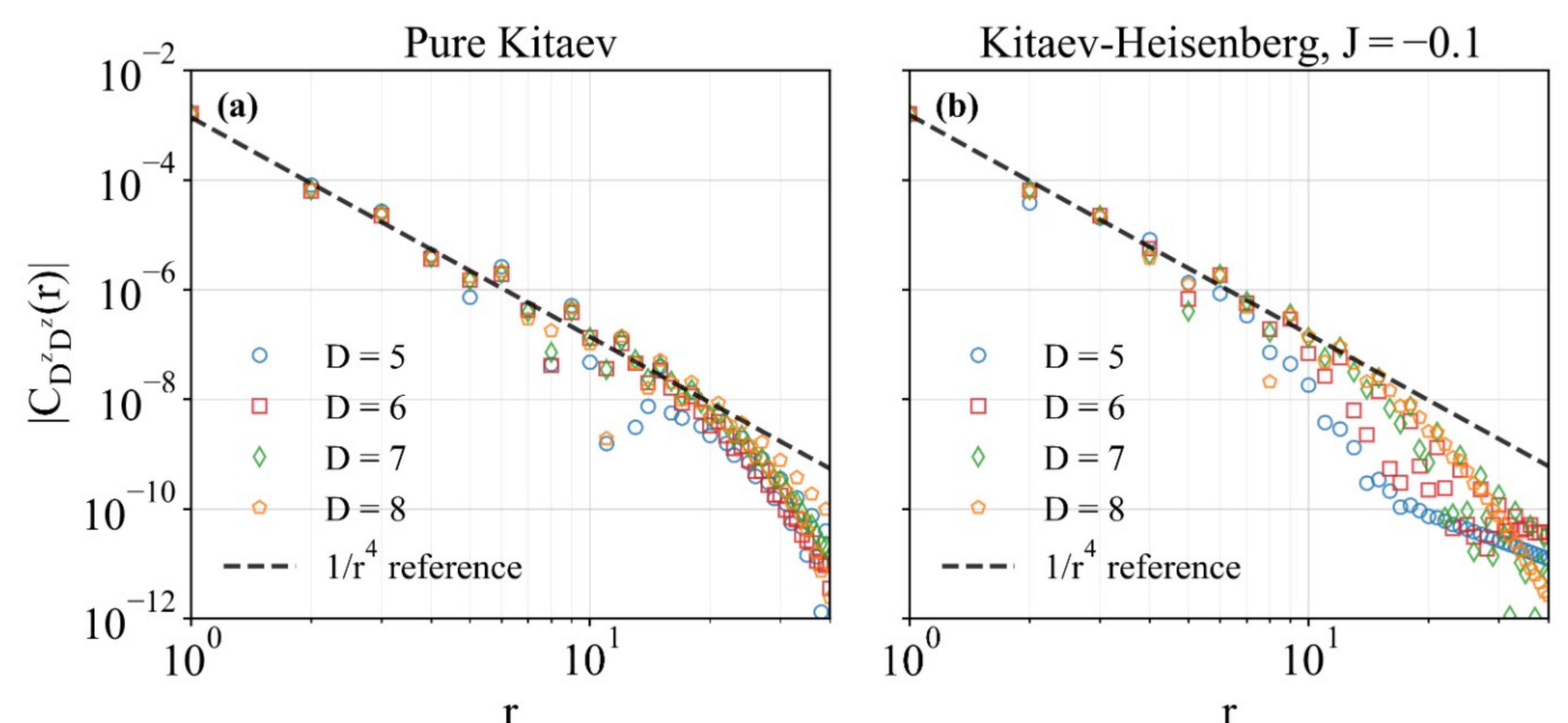
Results for spin-1/2 Kitaev-Heisenberg model

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

Dimer-dimer correlations:

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

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



* 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