Towards Next-Generation iPEPS algorithms

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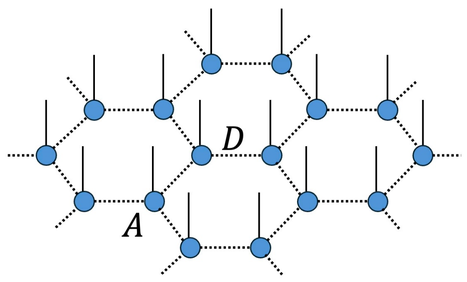
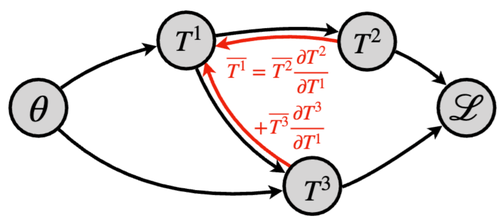
Next-Generation iPEPS Toolbox

Tensor Network Ansatz

$|\psi\rangle =$ 

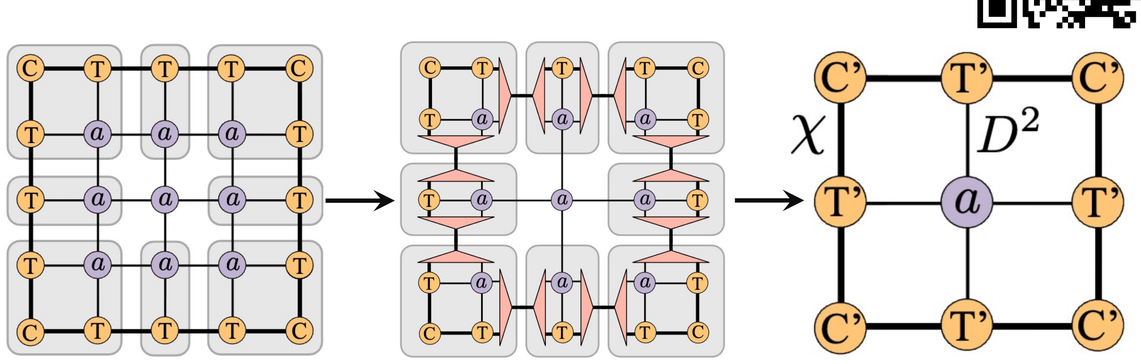
Automatic Differentiation(AD)



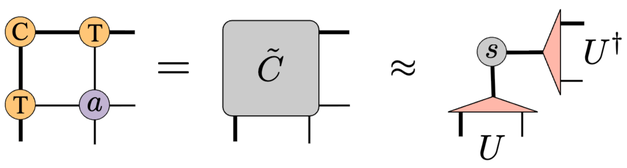
Background: Automatic differentiation enables high-precision iPEPS studies of 2D quantum many-body systems.

QRCTM

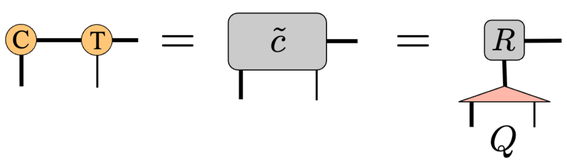
Scan me for code demos:



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

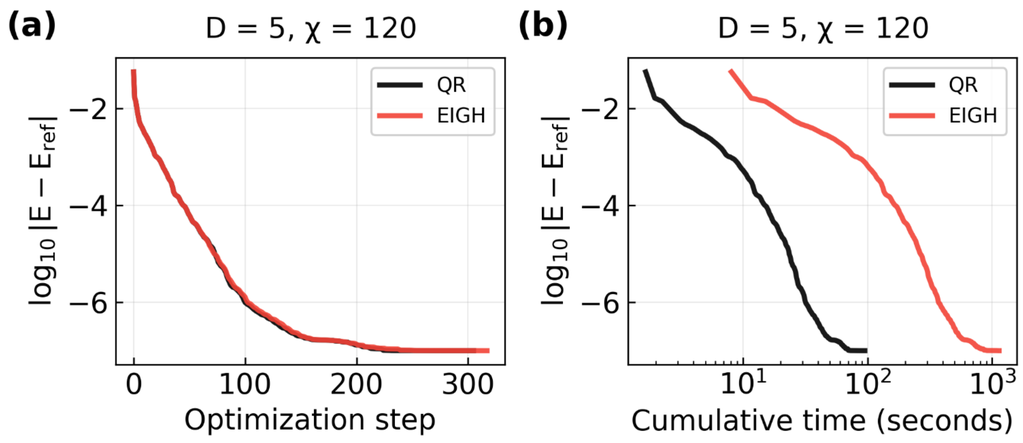


Traditional approach:
eigenvalue decomposition (or SVD) of **enlarged** corner tensors.



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

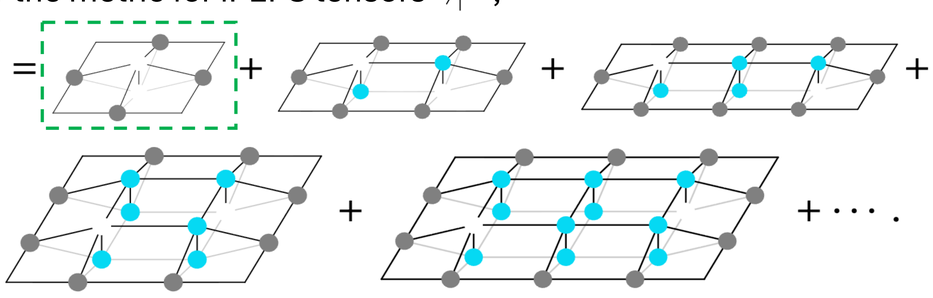
Benchmark: 2D AFM Heisenberg model on Honeycomb Lattice



Results: [1] 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  ,

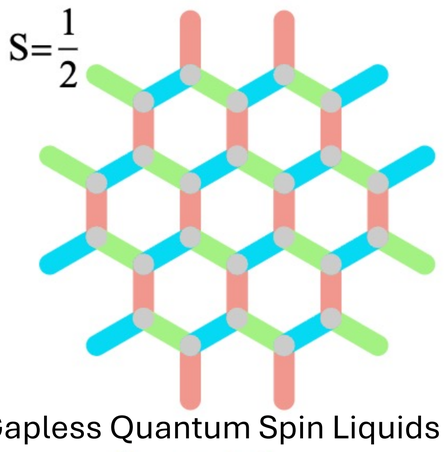
$\mathbf{N} =$ 

We use the leading term as an approximation of full metric for preconditioning the optimizer (L-BFGS) to speed up convergence.

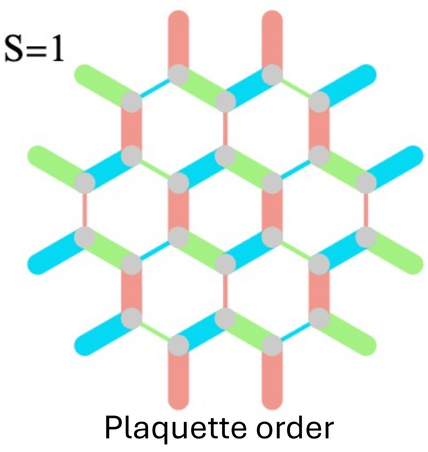
Results: Local preconditioning yields faster convergence.
More details in Ref.[3]

Physical Results for Kitaev-Type Models

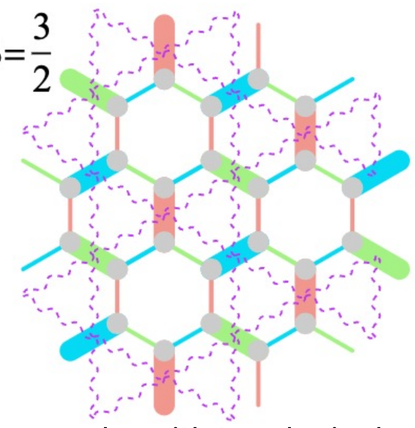
Ground states for Spin-S isotropic Kitaev model

(a) S=$\frac{1}{2}$ 

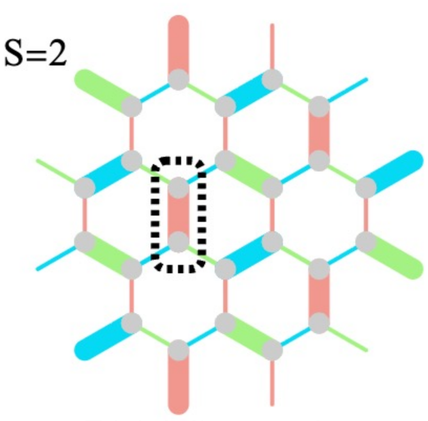
Gapless Quantum Spin Liquids

(b) S=1 

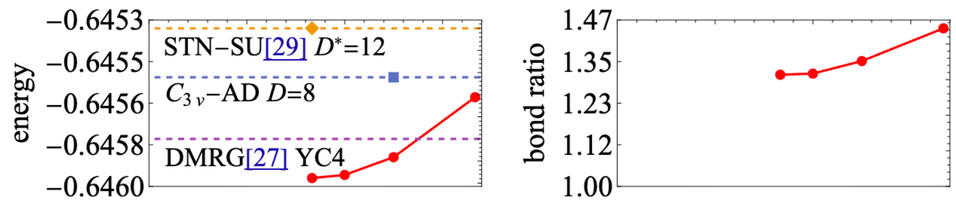
Plaquette order

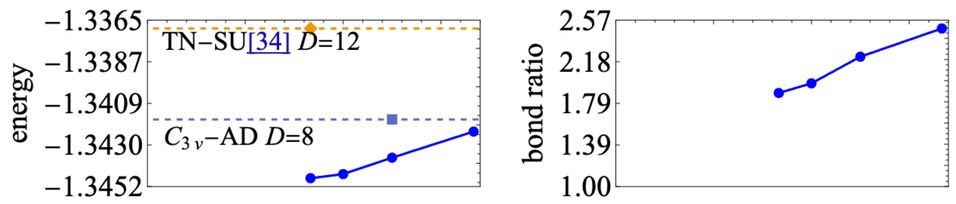
(c) S=$\frac{3}{2}$ 

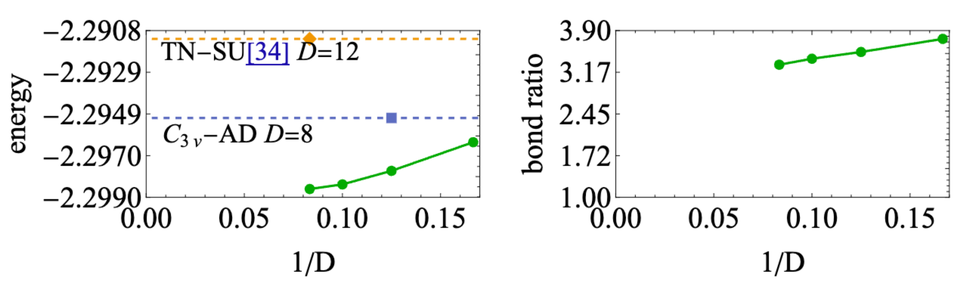
Dimer order with topological order

(d) S=2 

Trivial dimer order

S=1 

S=$\frac{3}{2}$ 

S=2 

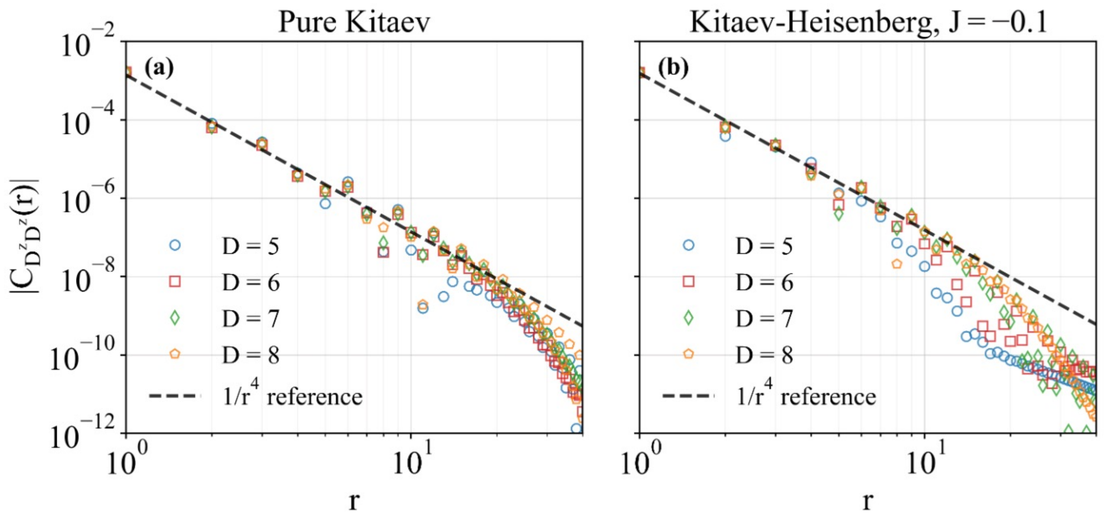
Results: [4] Up to S=2, ground states of higher-Spin Kitaev models break lattice symmetry.

Results for Spin-1/2 Kitaev-Heisenberg model

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

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

Dimer-dimer correlation with QSL regime:



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

* contributed equally.
[1] Y. Zhang*, **Q. Yang***, and P. Corboz. Accelerating two-dimensional tensor network contractions using QR-decompositions. arXiv: 2505.00494.
[2] **Q. Yang** and P. Corboz. Efficient iPEPS Simulation on the Honeycomb Lattice via QR-based CTMRG. arXiv: 2509.05090
[3] X.-Y. Zhang*, **Q. Yang***, P. Corboz, J. Haegeman, and W. Tang. Accelerating two-dimensional tensor network optimization by preconditioning. arXiv: 2511.09546
[4] X.-Y. Zhang*, **Q. Yang***, P. Corboz, J. Haegeman, and Y. He. Topological and Trivial Valence-Bond Orders in Higher-Spin Kitaev Models. arXiv: 2511 . 07415