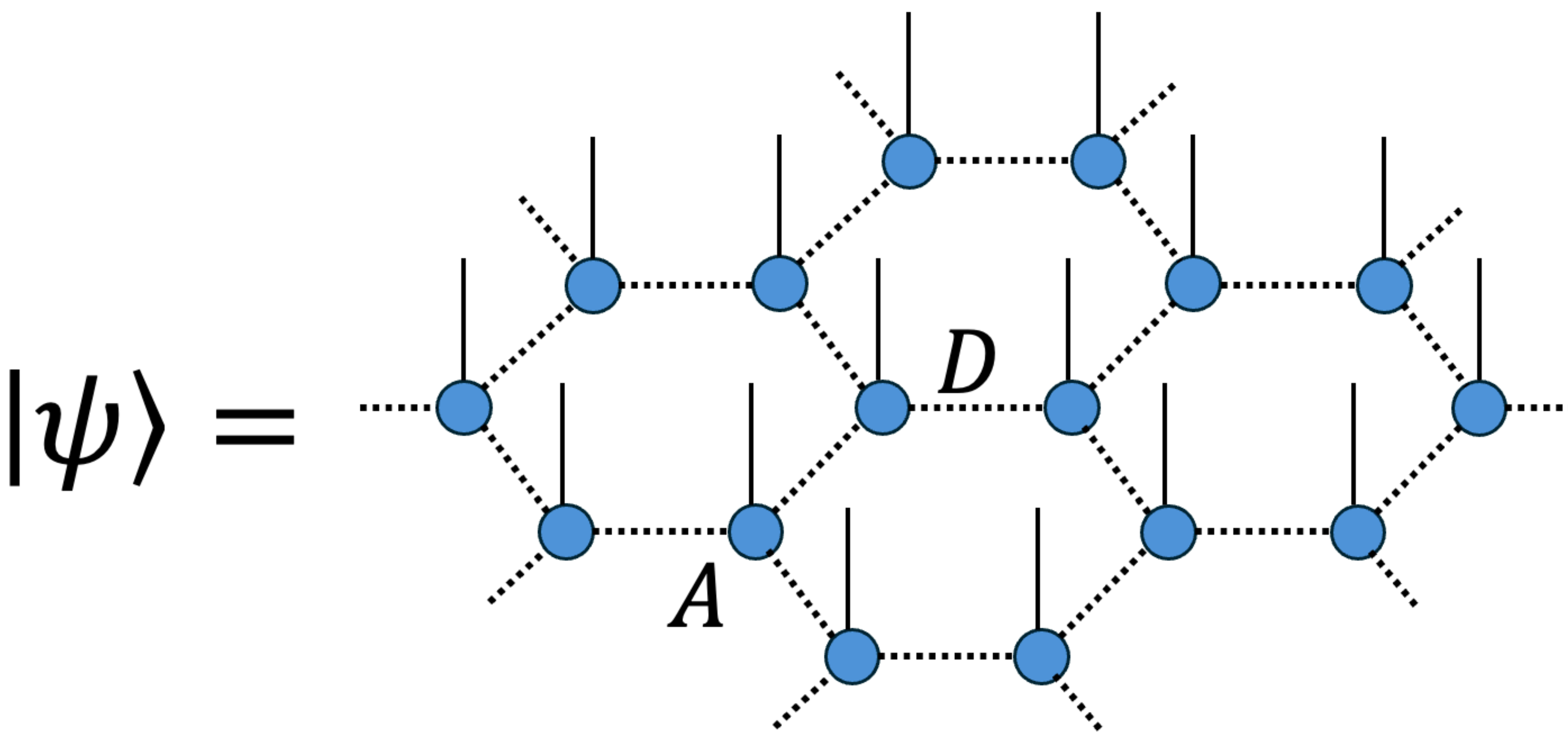
QR-based CTMRG on Honeycomb Lattice

Qi Yang



Philippe Corboz
Qi Yang
Yining Zhang

Jutho Haegeman
Yuchi He
Xingyu Zhang

UNIVERSITY OF AMSTERDAM
GHENT UNIVERSITY

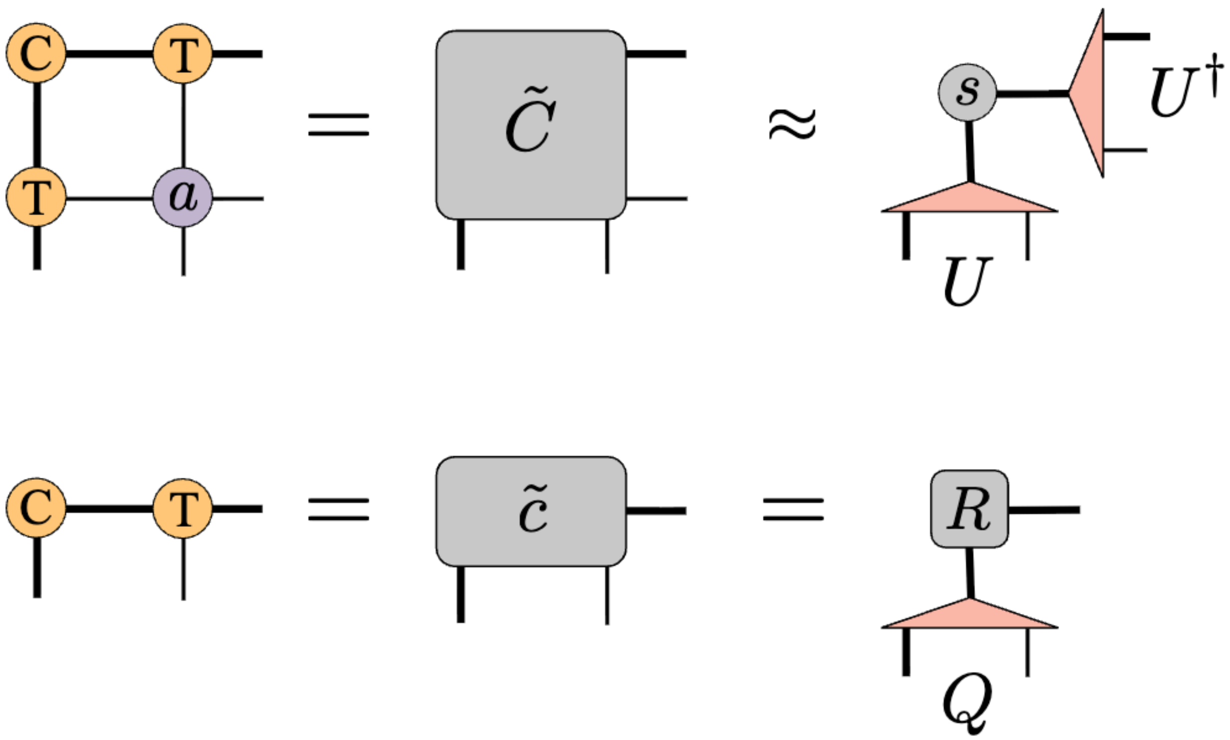
1. QRCTM C4v
2. QRCTM C3v
3. Higher Spin Kitaev

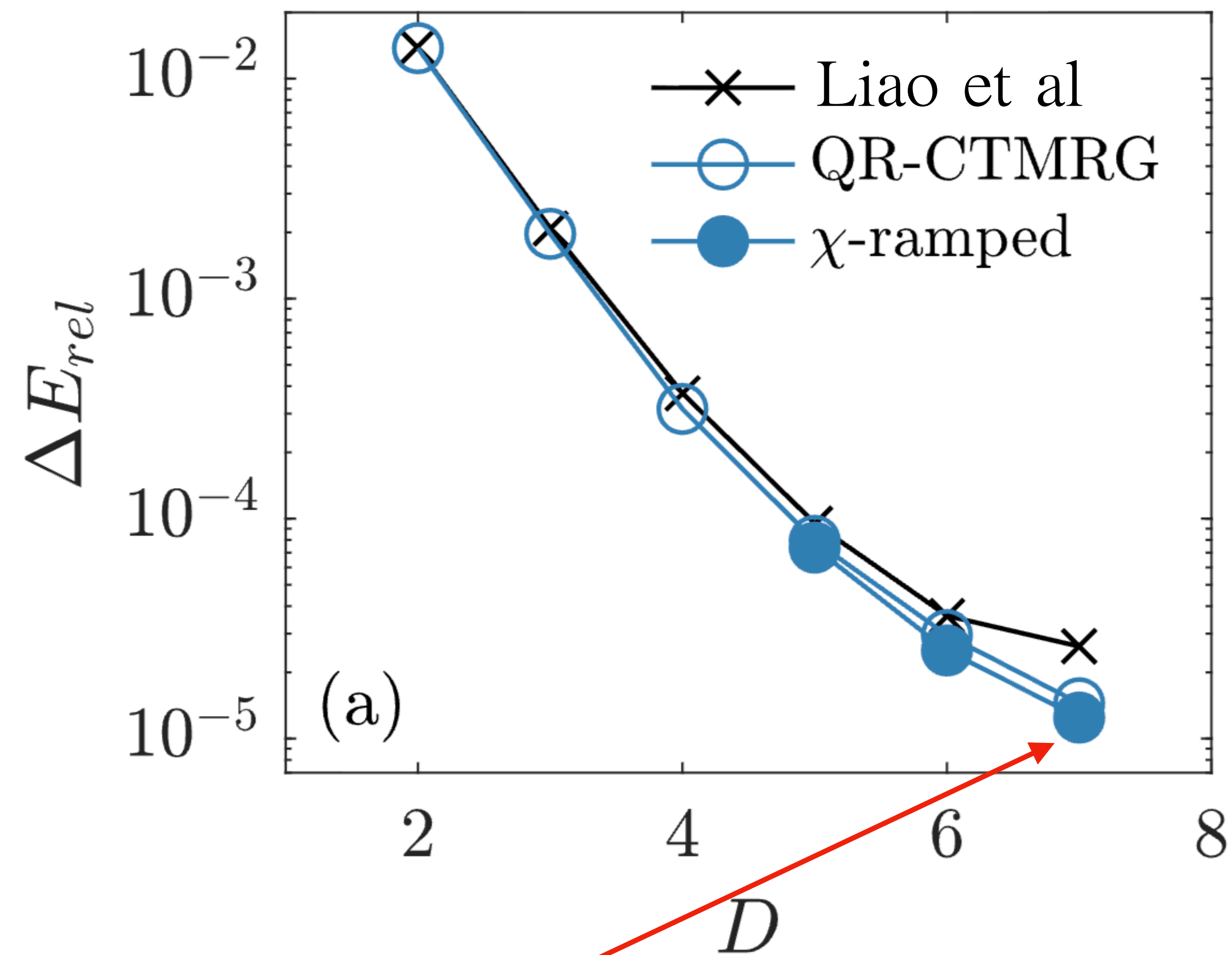
erc
EuroHPC Joint Undertaking

QRCTM facilitates large-D iPEPS

arXiv:2505.00494

PhysRevX.9.031041





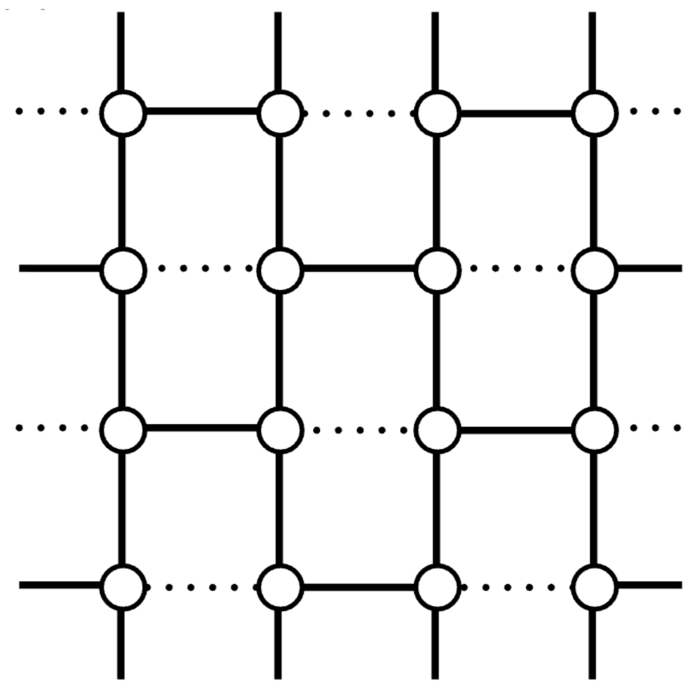
$D = 7, \chi = 300$ **AD+iPEPS less than one hour! (H100)**

But limited to C_{4v} **where VUMPS is also efficient, since transfer matrix (MPO) is Hermitian**

Where is the true Killing app for QRCTM?

iPEPS on the Honeycomb Lattice: Brick-Wall Approach

Brick Wall



PhysRevX.2.041013

Large Unit Cell VUMPS

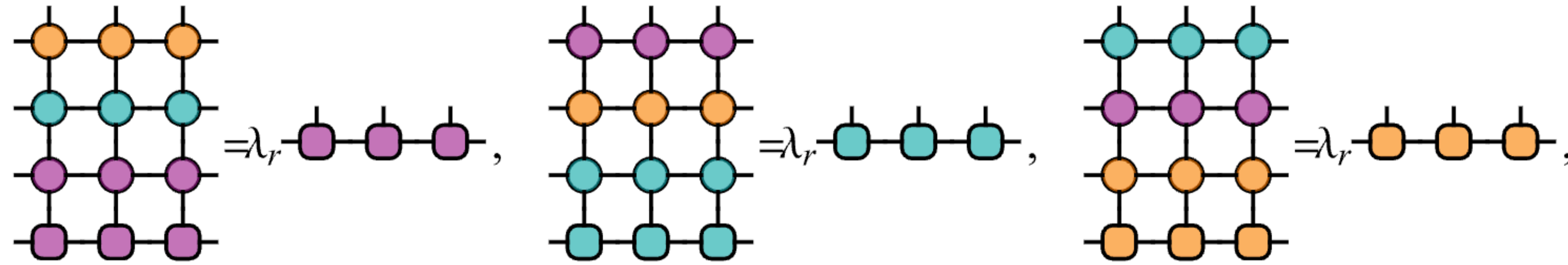


Fig: PhysRevB.108.085103

Large Unit Cell CTMRG

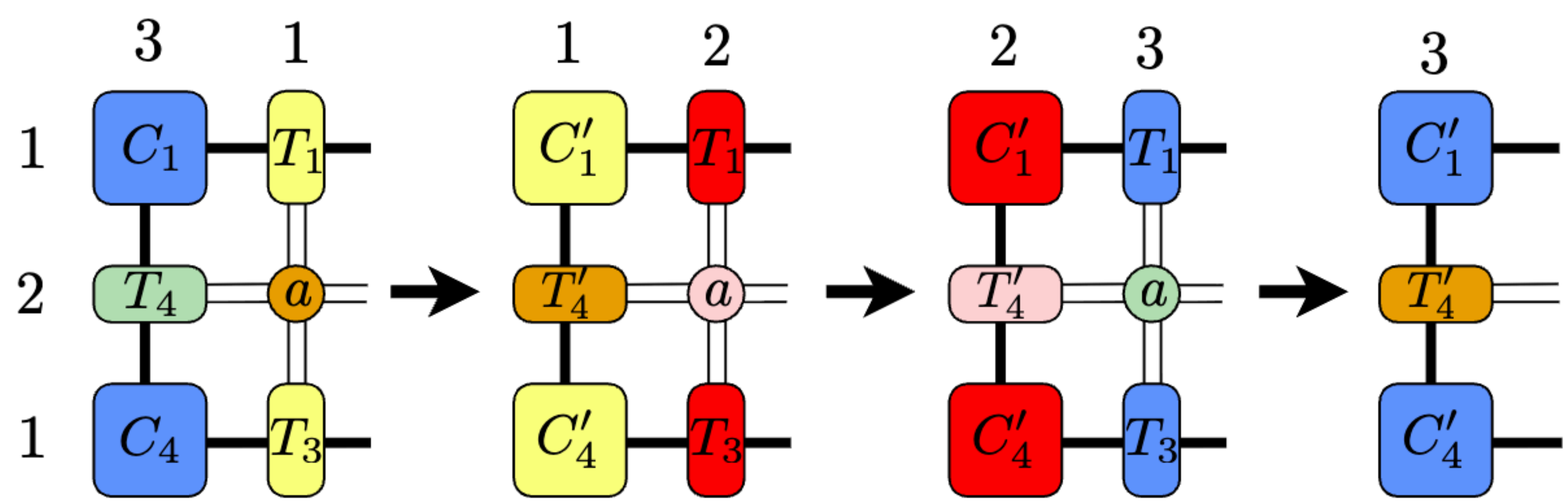
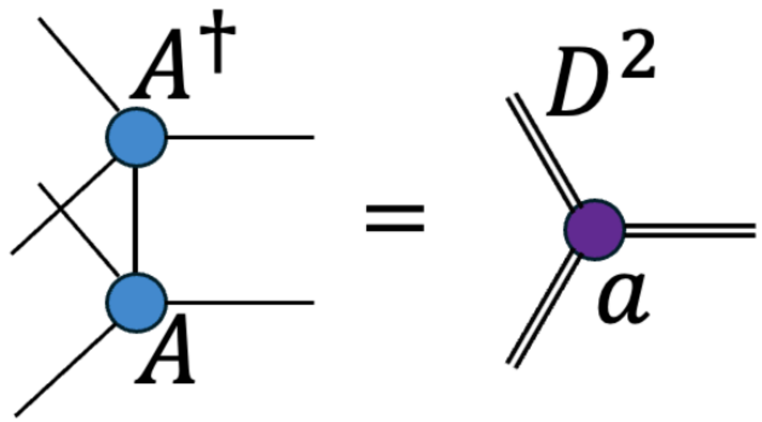


Fig: Philippe Corboz's slides@tnqmp2016

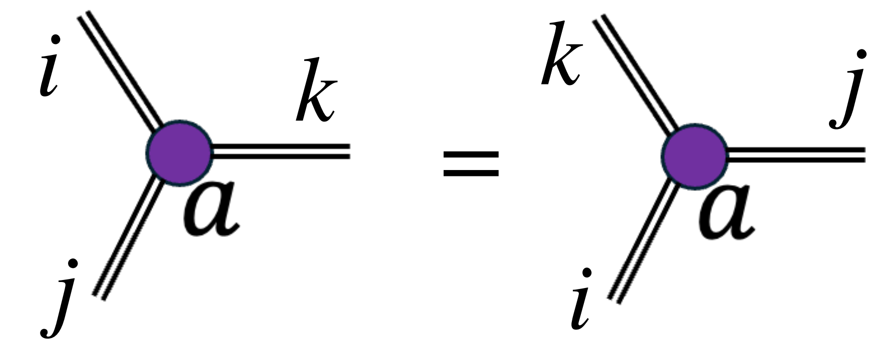
Coding complex, QR magic gone.

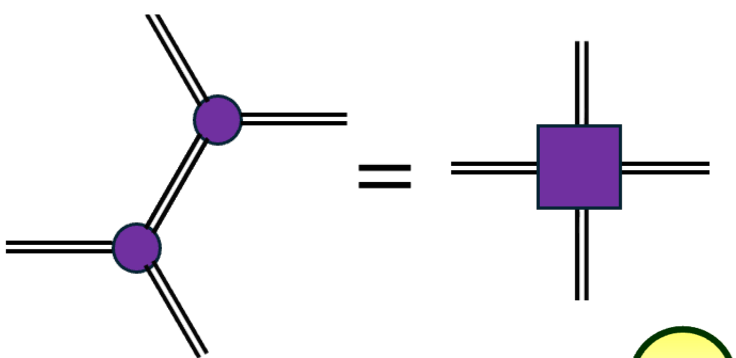
Figures shown for illustration only; credit for large–unit–cell algorithms goes to the original authors.

Uniform C_{3v} CTMRG on Honeycomb Lattice

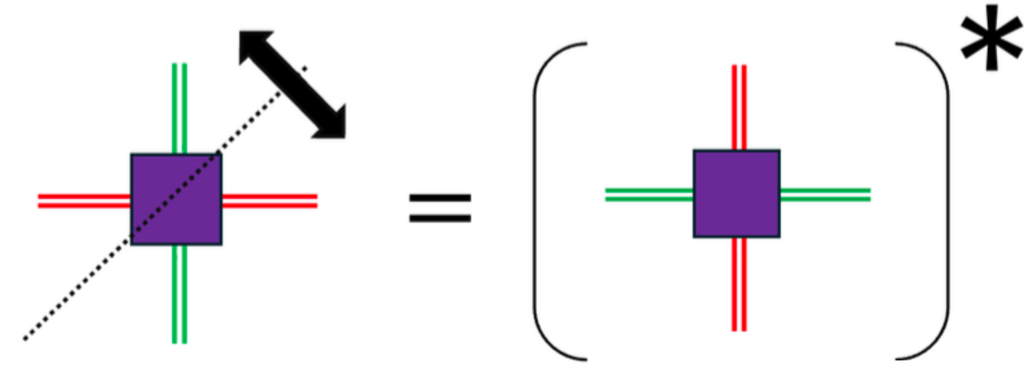


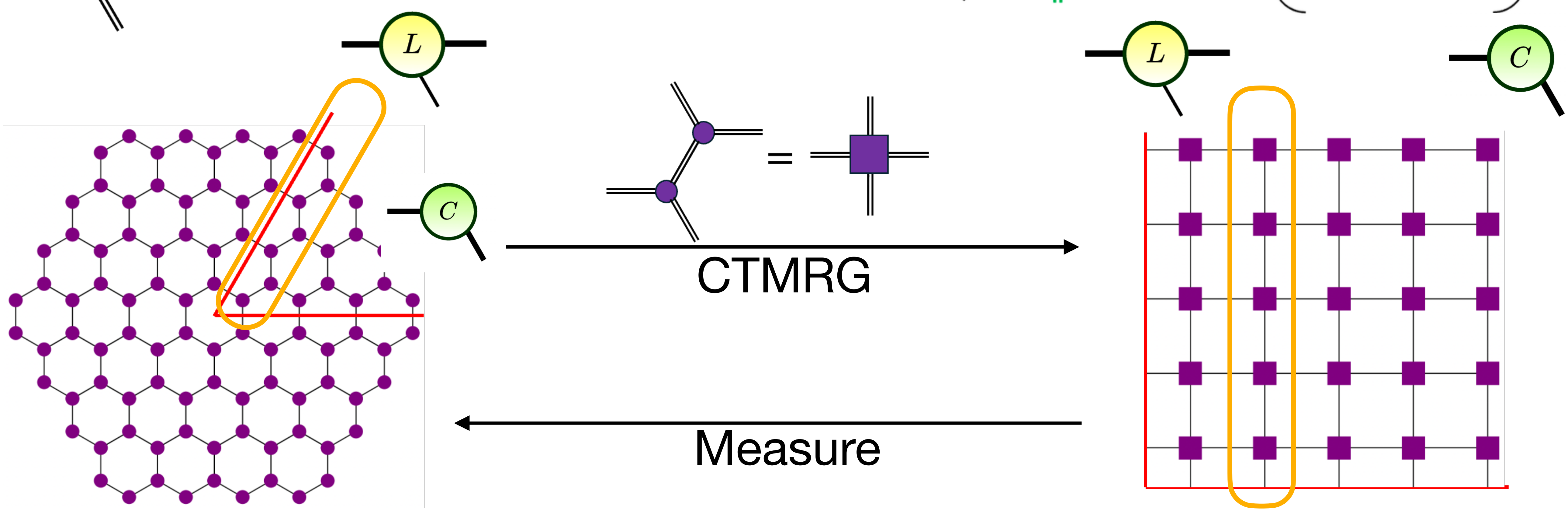
Rot. Symm. :





Refl. Symm. :





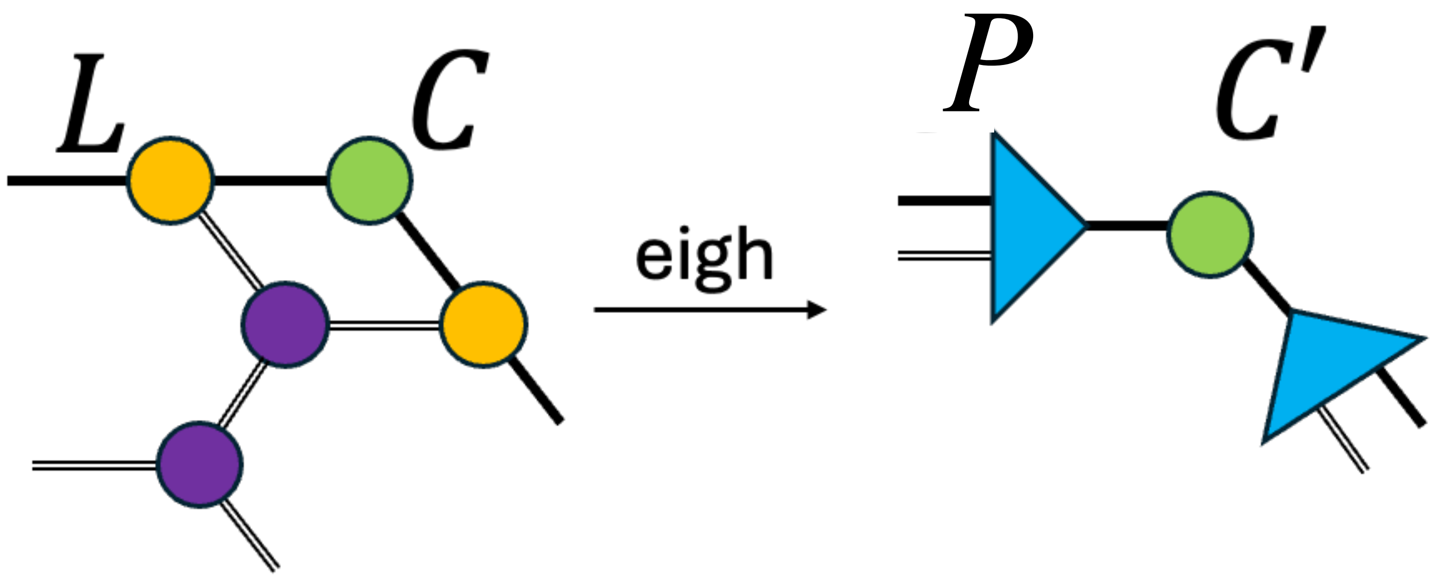
Thanks to our Ukrainian colleagues—their work paved the way

Lukin et al., PhysRevB.107.054424(2023)

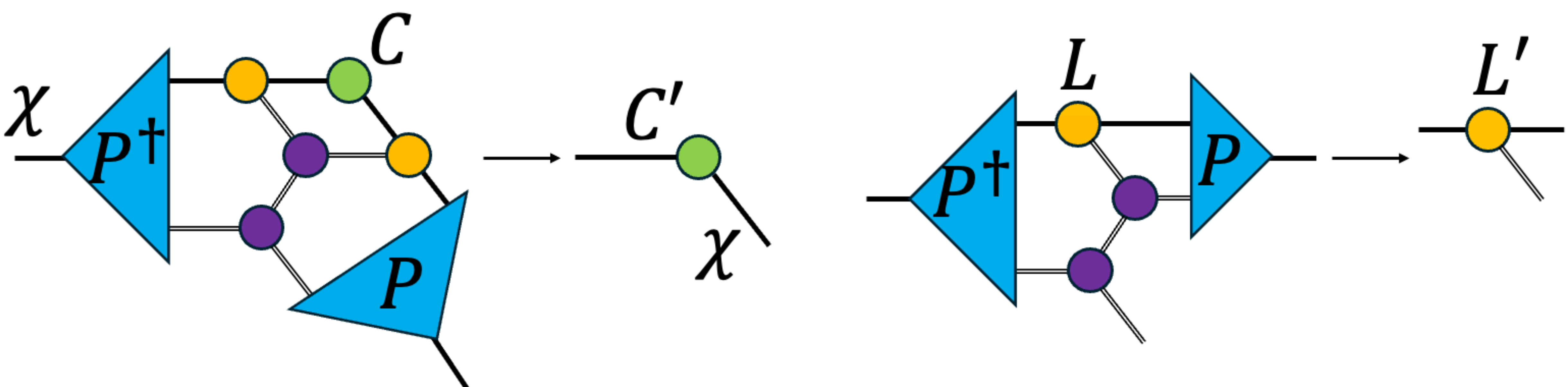
CTMRG for uniform C_{3v} iPEPS

Lukin et al., PhysRevB.107.054424(2023)

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



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

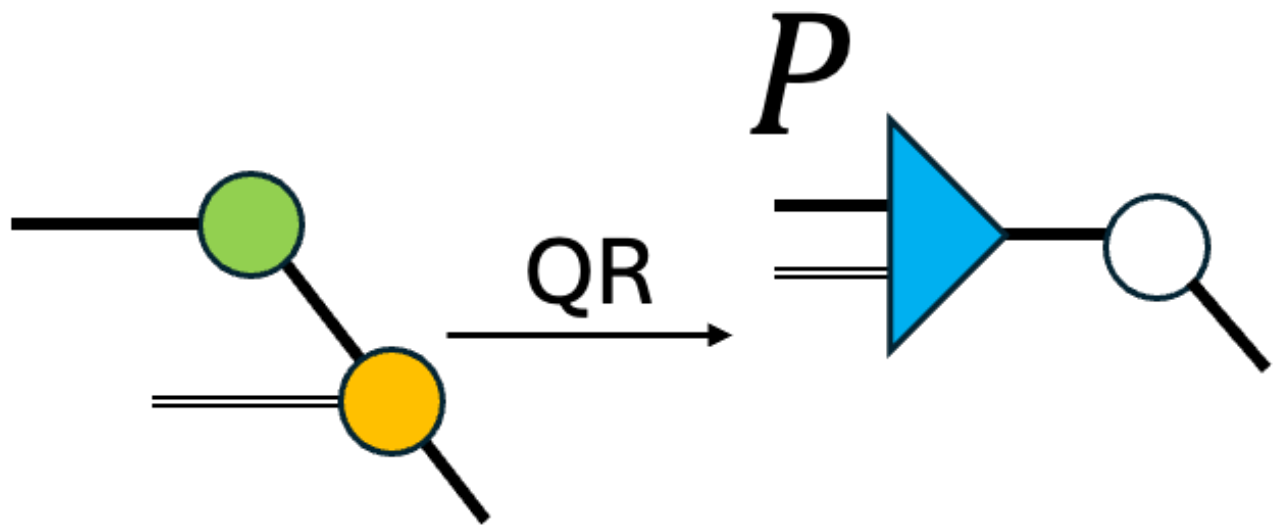


H100, double, very large D>6 and chi>600

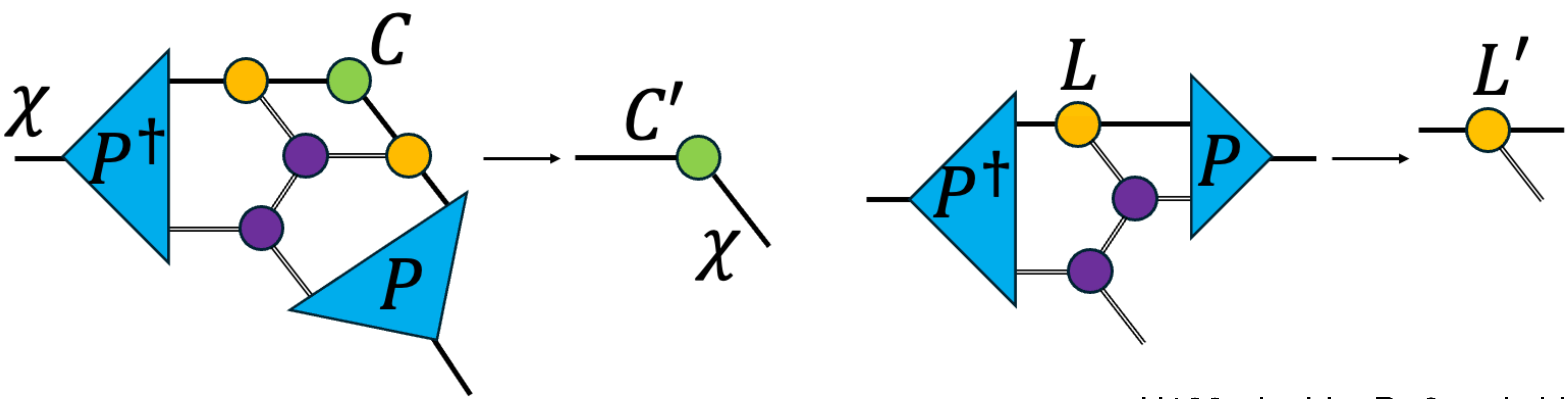
QRCTM for uniform C_{3v} iPEPS

arXiv:2509.05090

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



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



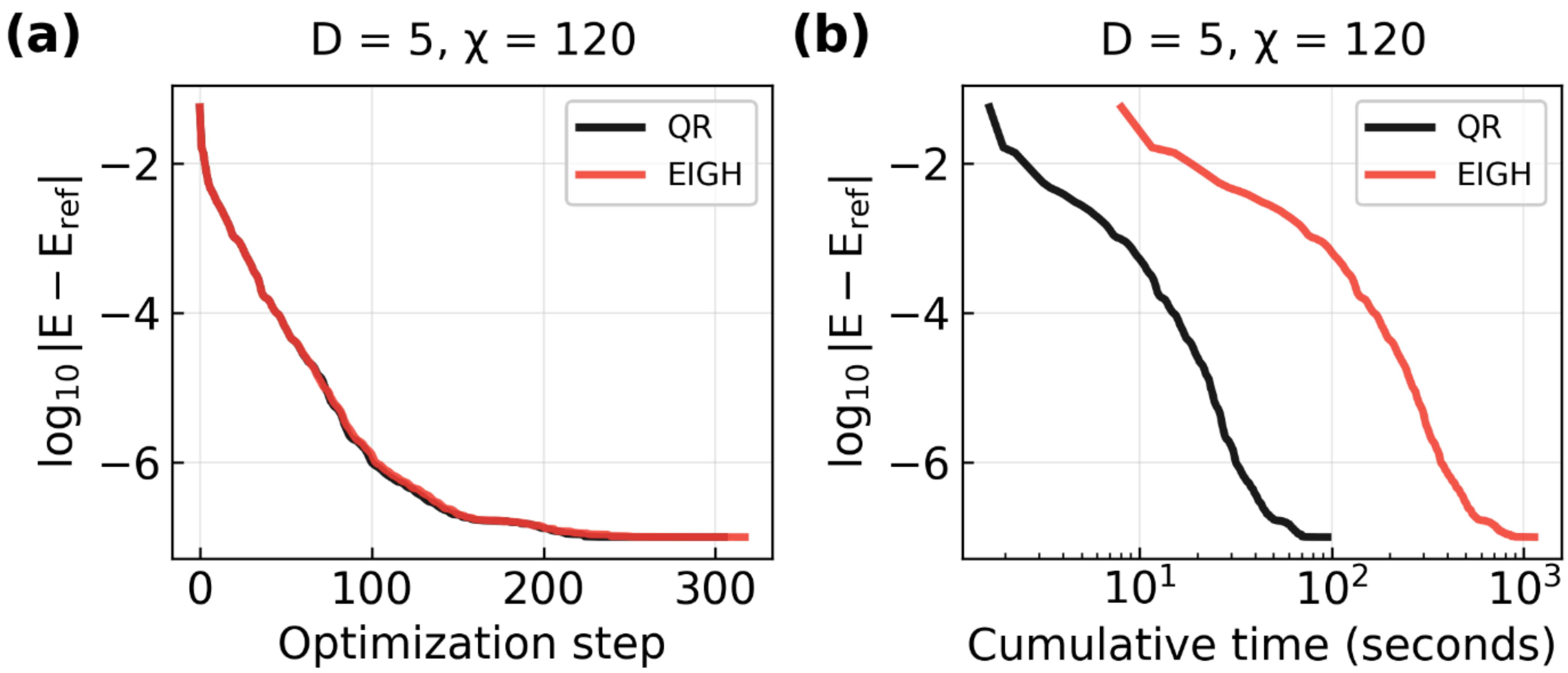
H100, double, D=6 and chi=600

AFM Heisenberg on the Honeycomb Lattice

$$H = \sum_{\langle ij \rangle} \vec{\mathbf{S}}_i \cdot \vec{\mathbf{S}}_j$$

Training Dynamics

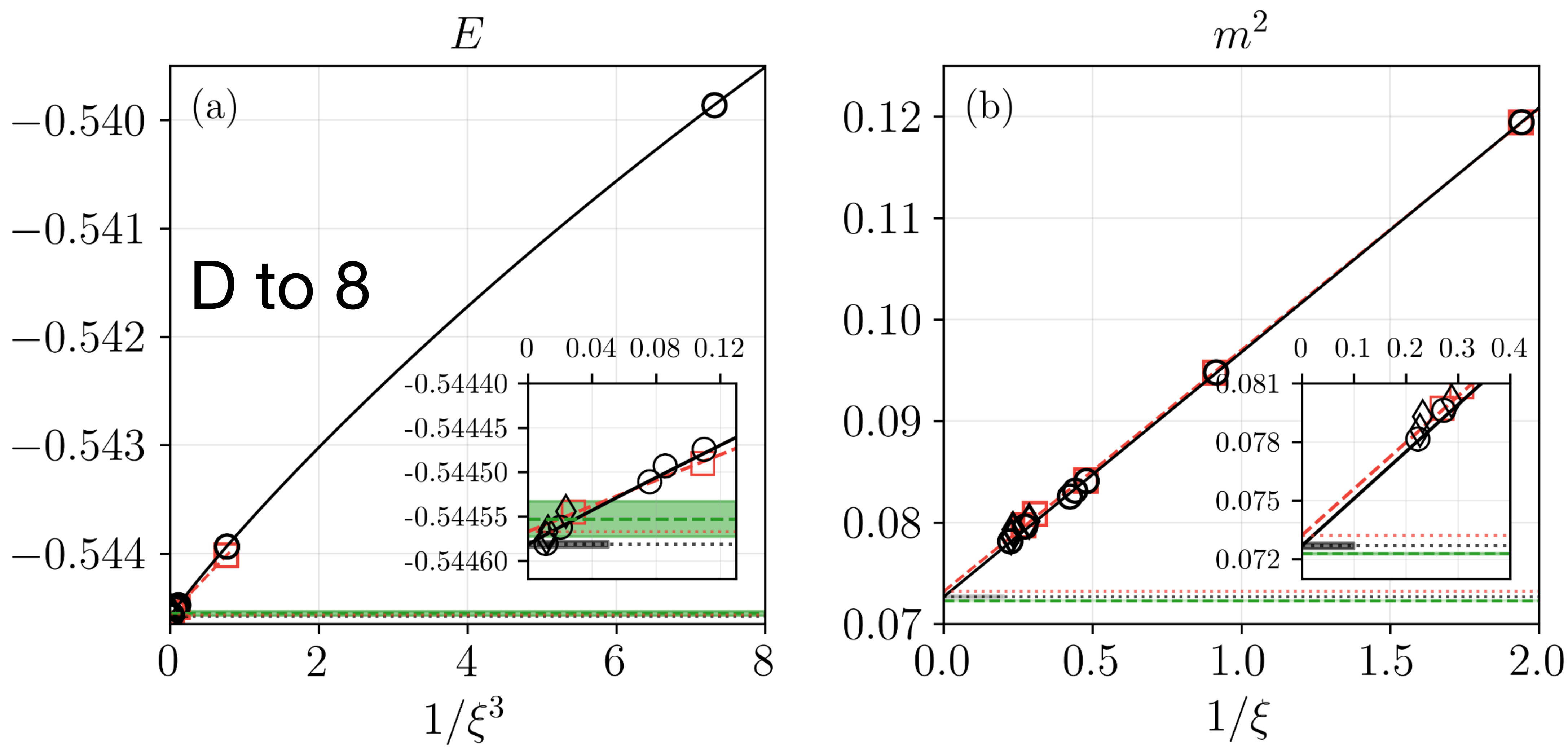
Speed up



Similar training dynamics, SUPER FAST!

H100, double, real, same initialization, Eref=Emin+1E-7

AFM Heisenberg on the Honeycomb Lattice



"Lower" ⟶ $E_0 = -0.544582(3)$ $\qquad$ $m_0 = 0.2696(3)$

$E_{QMC} = -0.544553(20)$ $\qquad$ $m_{QMC} = 0.26885(2)$

D=8, accurate results — consistent with QMC

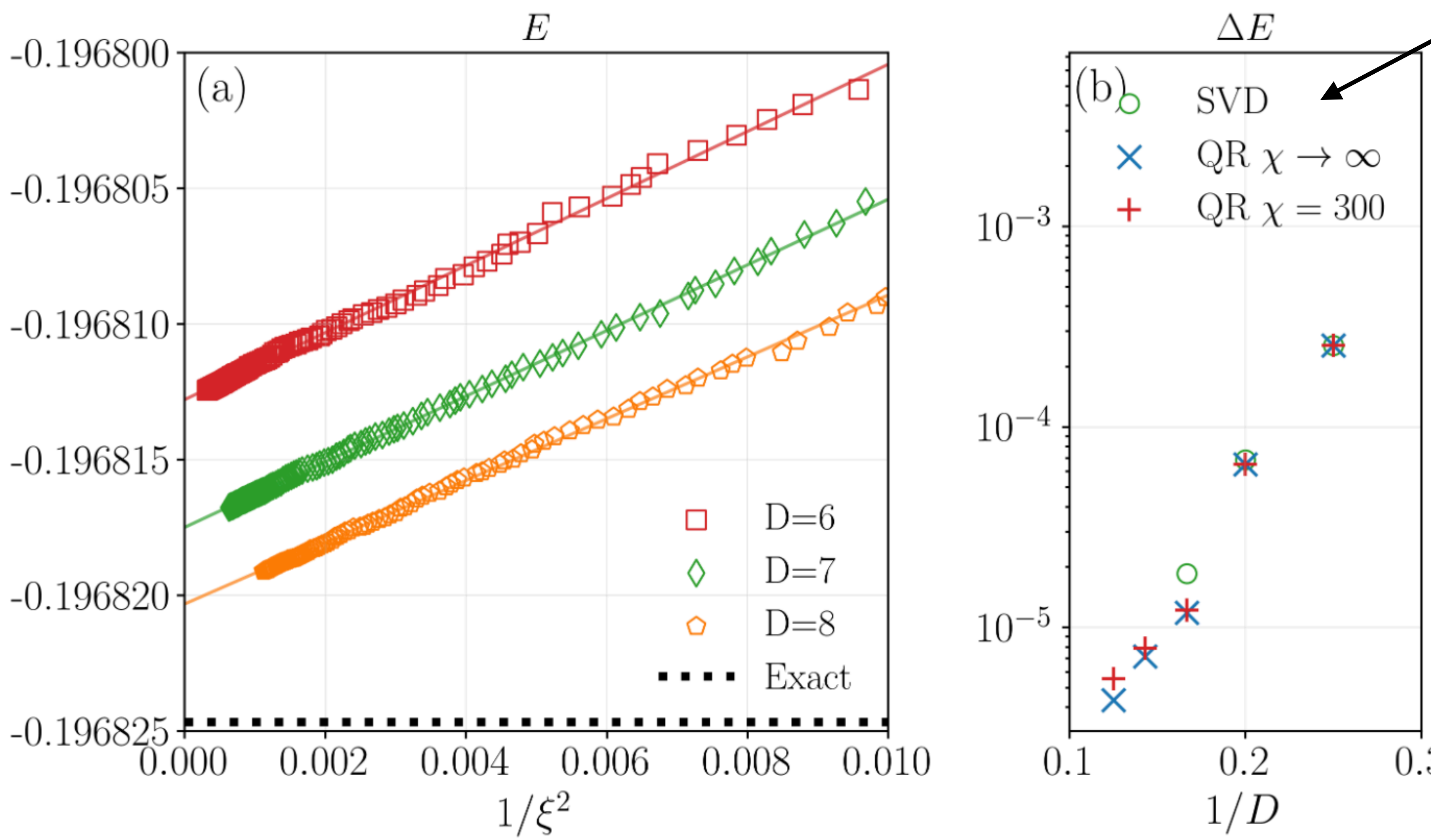
F. Jiang, Eur. Phys. J. B 85, 1(2012)
U. Low, Condens. Matter Phys. (2009)

Both QMC and our iPEPS results are extrapolated (FSS, FCLS)

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)

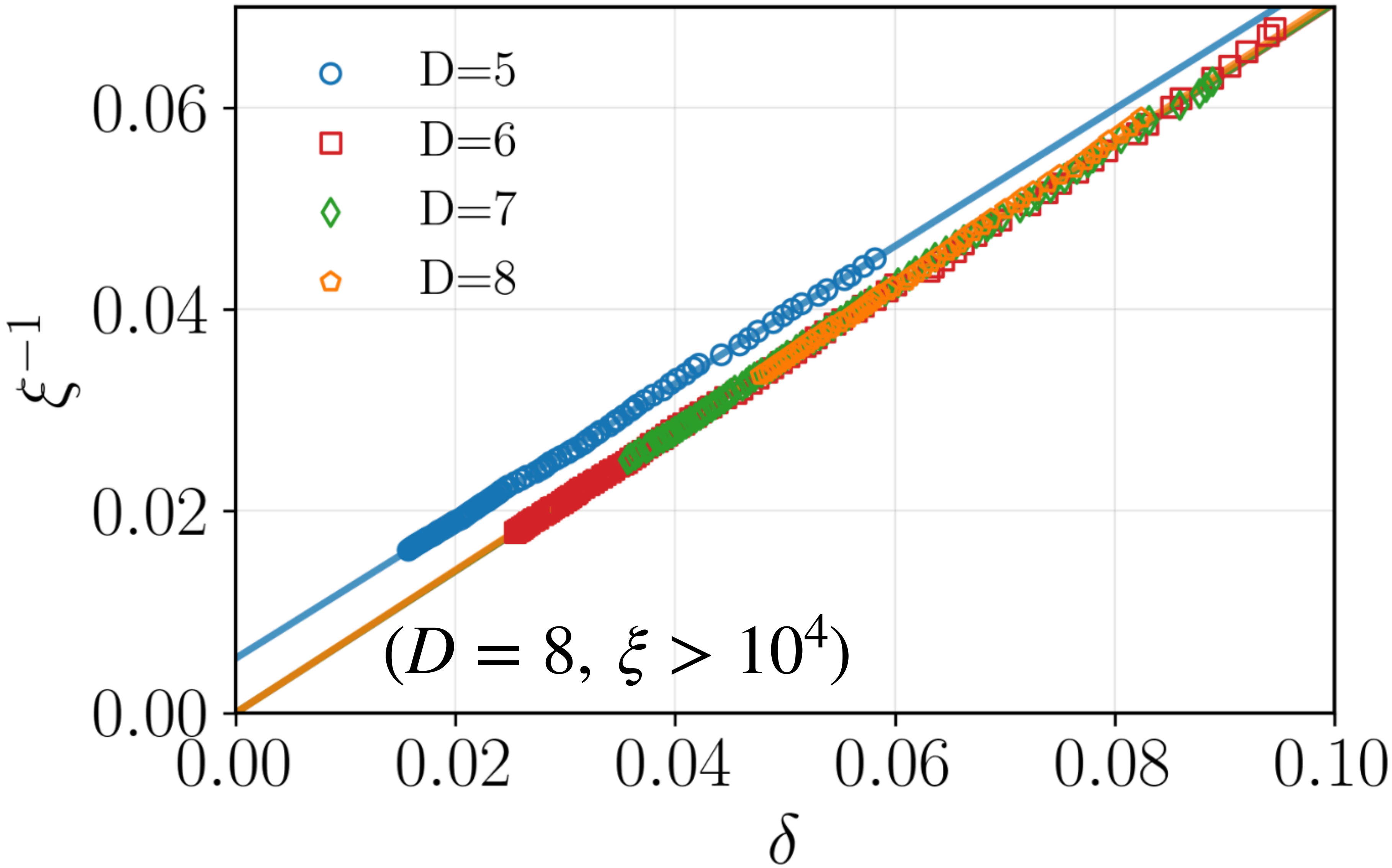
AD+CTMRG $D = 6,\ \|\Delta E/E\| = 9 \times 10^{-5}$ PhysRevB.107.054424(2023)

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

SOTA reported energy with AD+iPEPS

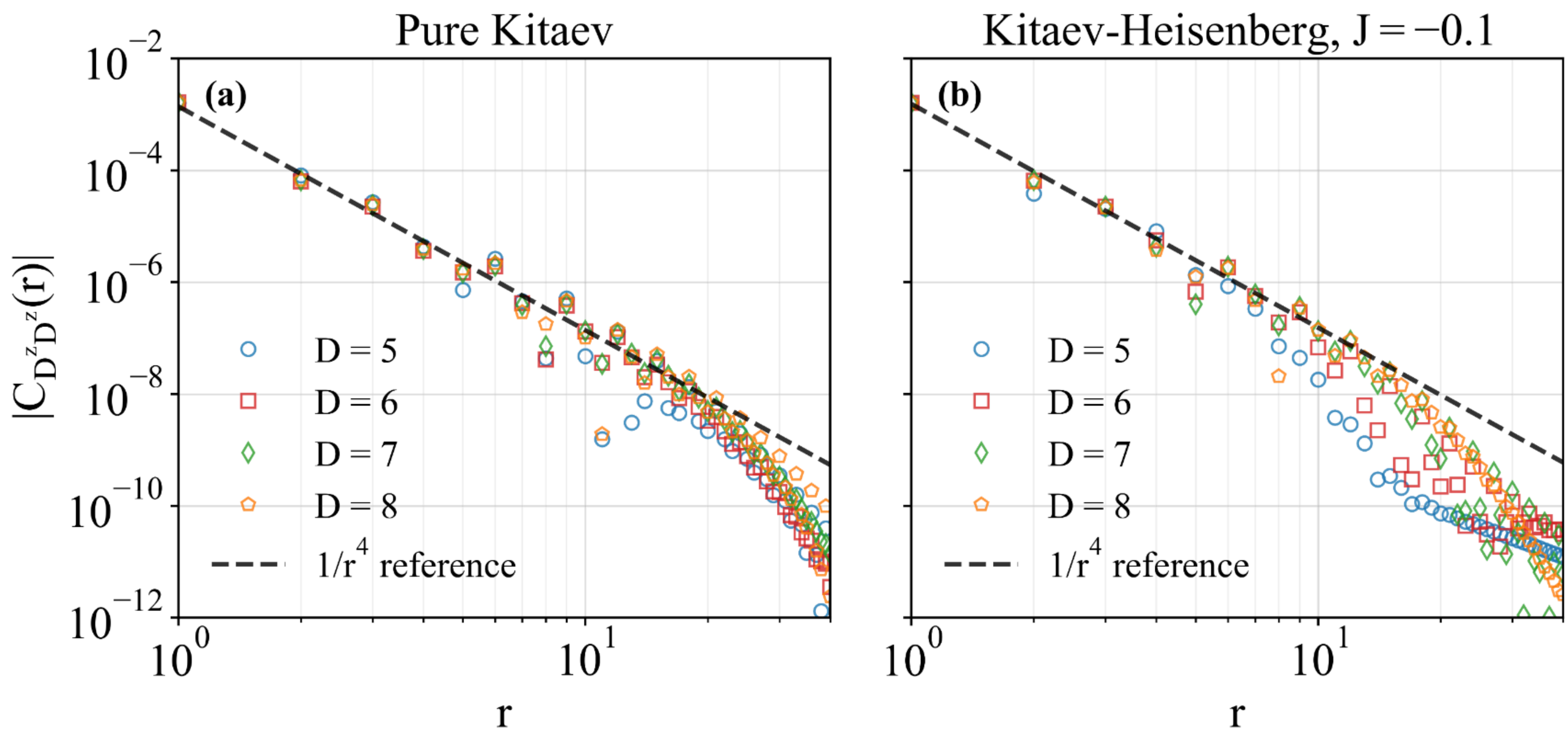
Not extrapolated, energy per sites.

Kitaev model: Finite Correlation Length Scaling



Finite-correlation-length-scaling reveals gapless nature.

iPEPS evidence for Dimer-Dimer correlation decay

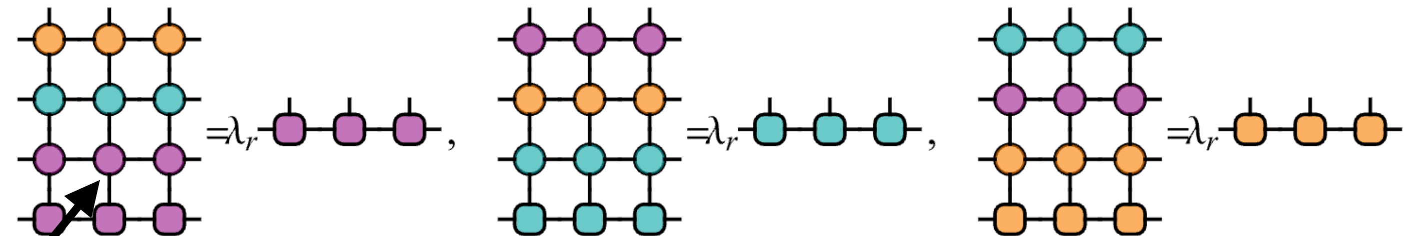


Dimer–Dimer r^{-4} tail persists in Kitaev-Heisenberg model

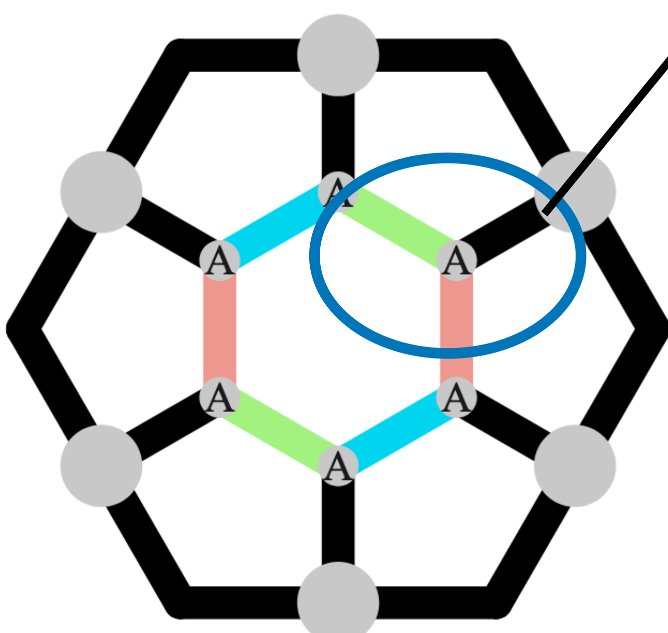
As predicted by field theory; to our knowledge, first confirmed using iPEPS

Env. SSB in S>1/2 Kitaev model via QRCTM

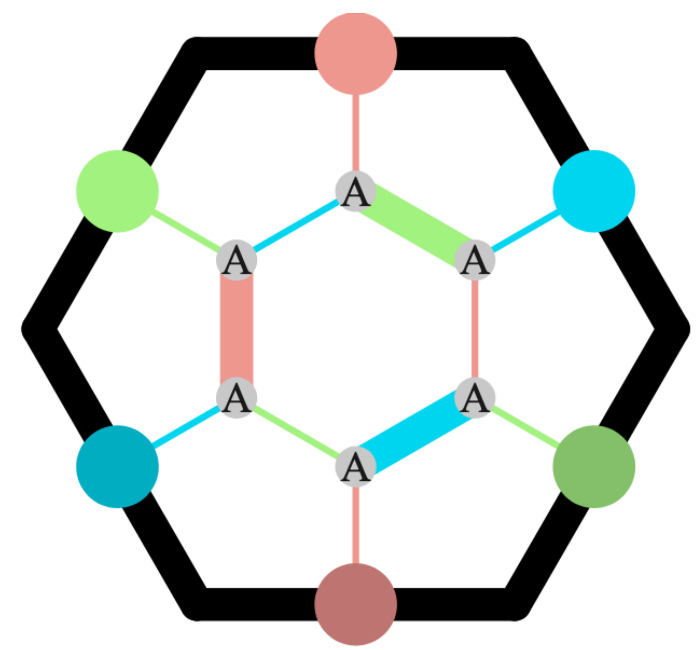
$$H = \sum_{\langle i,j \rangle_\gamma} K_\gamma S_i^\gamma S_j^\gamma$$

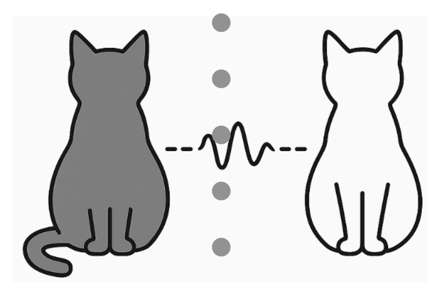


AD+QRCTM+ C_{3v}



Env. SSB





observables uniform ← observables non-uniform!

cat states

(one of) evidence to rule out QSL phase for S=1,3/2,2

Outlook and Thank you

Minimal Working Demos for interesting QRCTM applications

GitHub: qiyang-ustc/QRCTM (Classic 2DIsing $D = 10^4$)

All raw data and iPEPS tensors for comparison

Zenodo: 17093955 *Zenodo: 17107603*

Finely optimized code

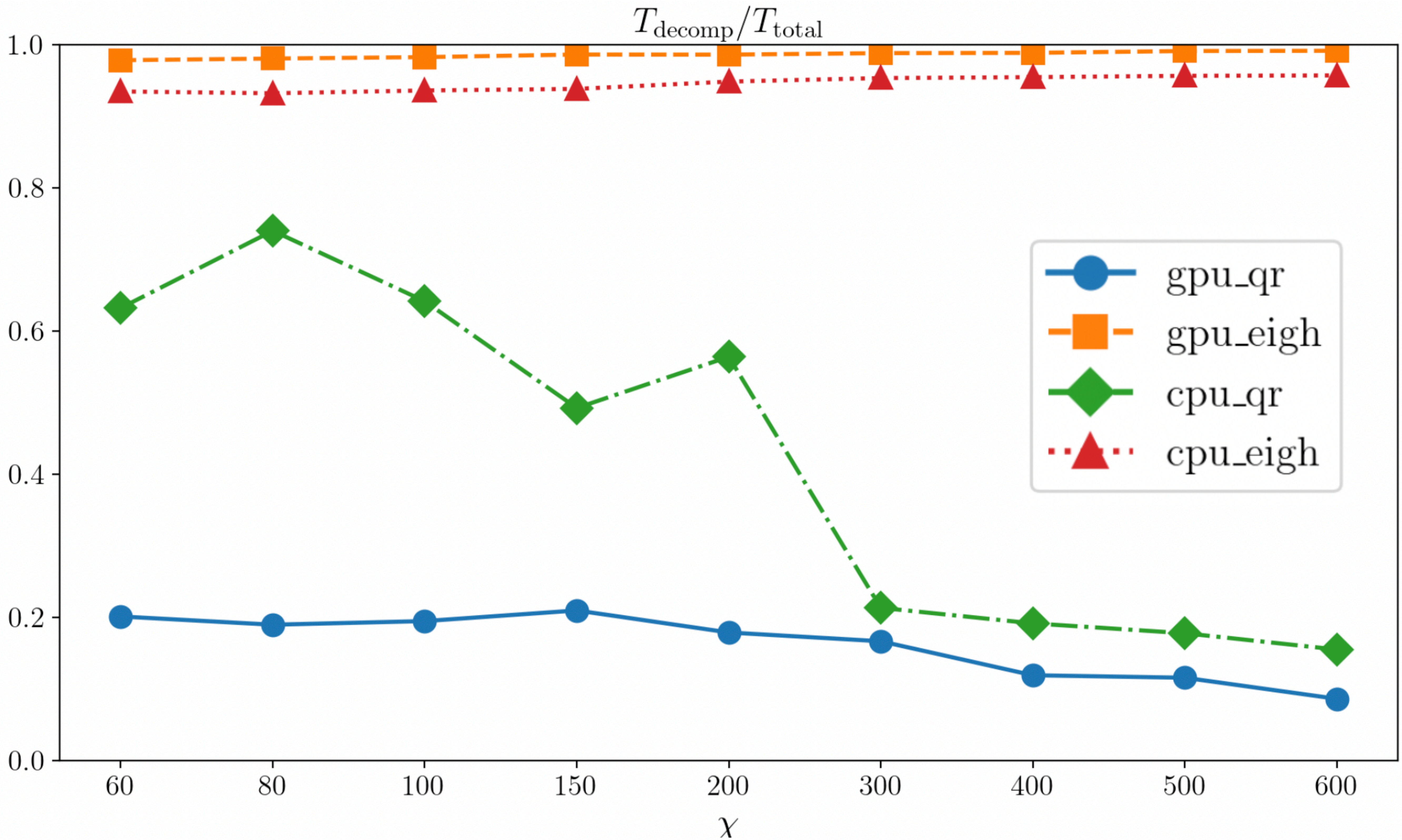
under active development and EuroHPC support

EuroHPC Joint Undertaking

How about more interesting models?

Let us enjoy what QRCTM can bring us!

Decomposition become cheaper



D=6, real, H100

Energy for S=1 Kitaev