Why not have a try to get a feeling?

GitHub: qiyang-ustc/QRCTM

All in one: 175 lines+PyTorch
D=4, chi=40,
a laptop,
1 minute,
error: 0.07%

```
18:07 › python3 <(curl -s https://raw.githubuserco
ntent.com/qiyang-ustc/QRCTM/main/heisenberg.py) --
chi 40 --D 4
```


Philippe Corboz
Qi Yang †*
Jutho Haegeman
Yuchi He
Xingyu Zhang*
Yining Zhang†

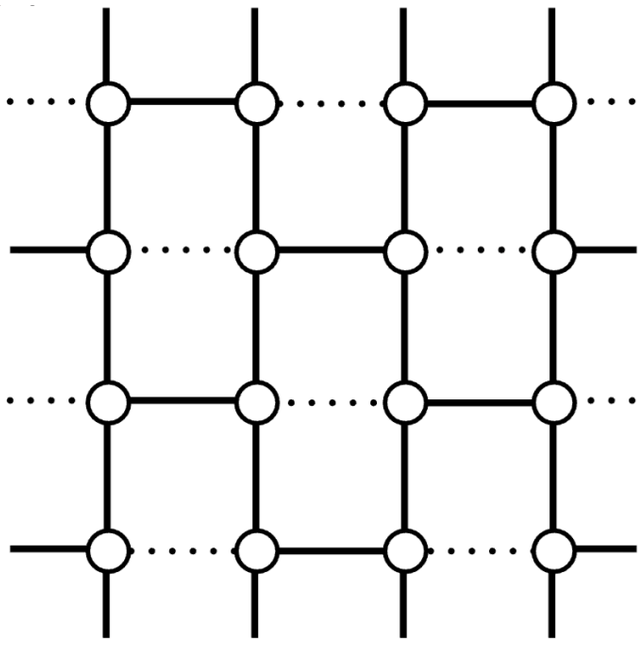
UNIVERSITY OF AMSTERDAM
GHENT UNIVERSITY
erc
EuroHPC Joint Undertaking

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

†*: equal

iPEPS on the Honeycomb Lattice: Brick-Wall Approach

Brick Wall



PhysRevX.2.041013

Large Unit Cell VUMPS

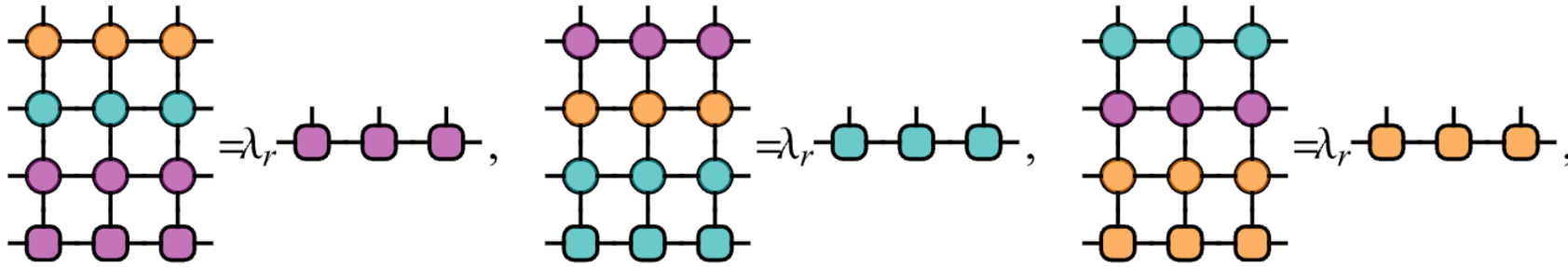


Fig: PhysRevB.108.085103

Large Unit Cell CTMRG

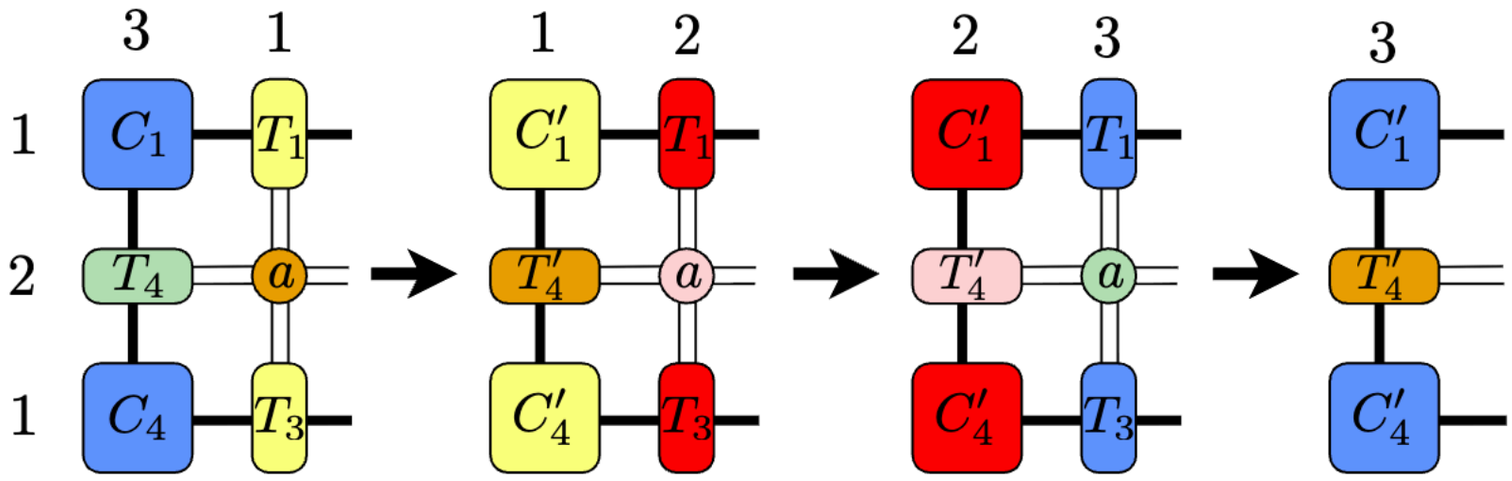
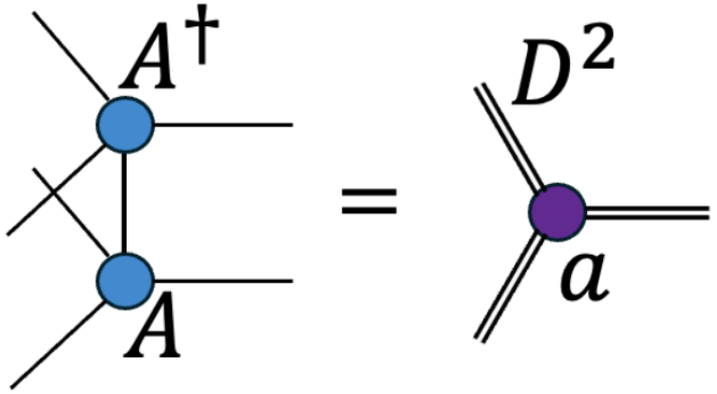


Fig: Philippe Corboz's slides@tnqmp2016

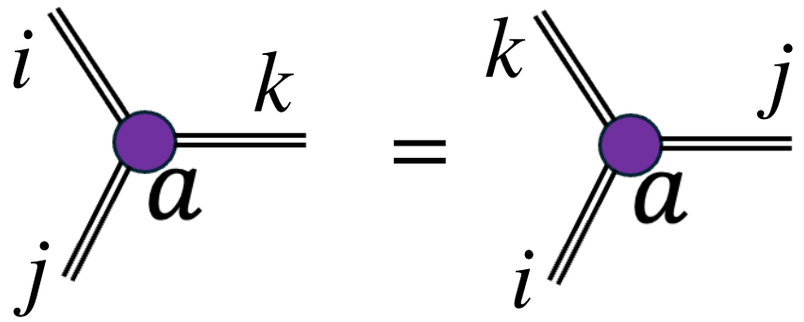
Complex Coding, QR magic lost.

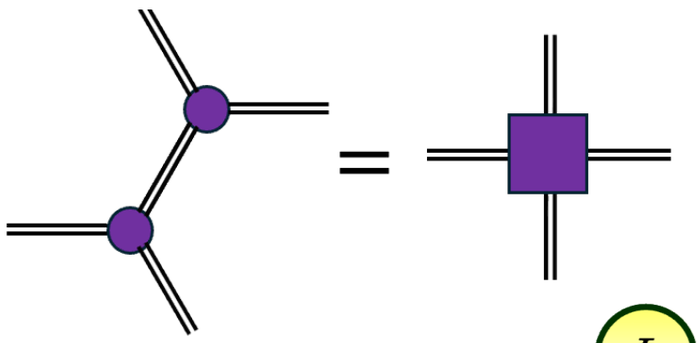
Figures shown for illustration only; credit for large–unit–cell algorithms goes to the original authors.

Uniform C_{3v} CTMRG on Honeycomb Lattice

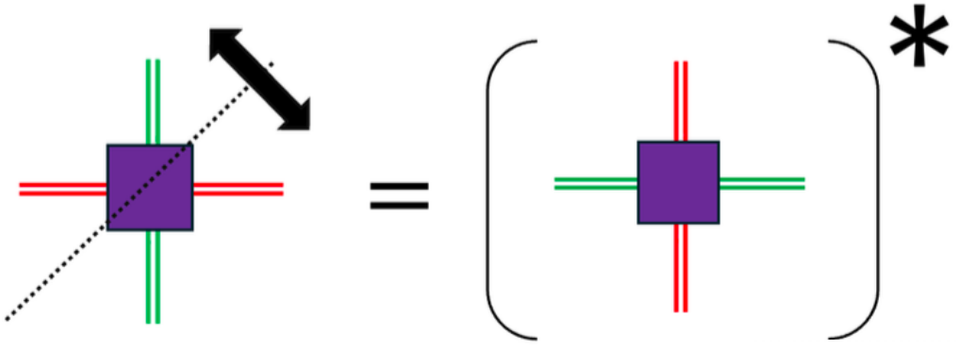


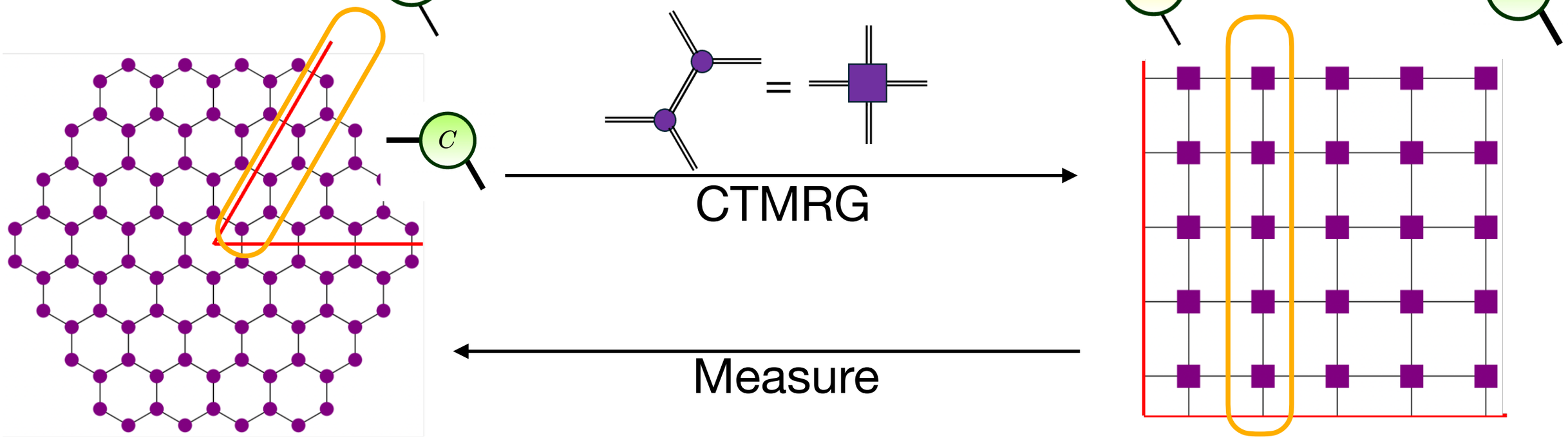
Rot. Symm. :





Refl. Symm. :





Thanks to our Ukrainian colleagues—their work paved the way

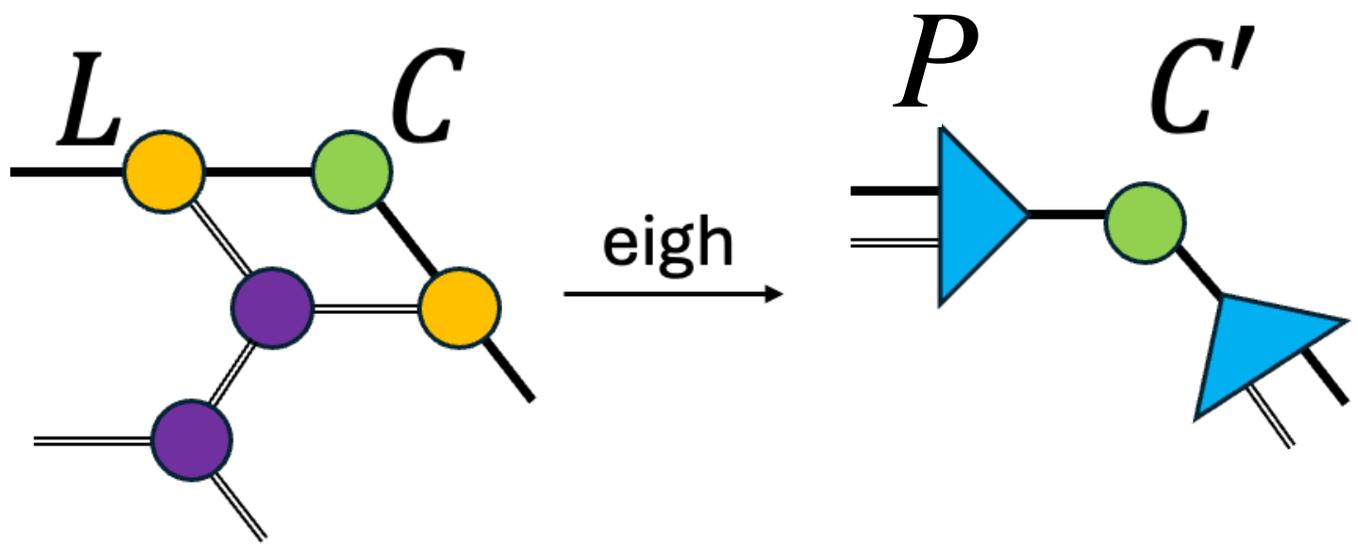
Lukin et al., PhysRevB.107.054424(2023)

CTMRG for uniform C_{3v} iPEPS

Lukin et al., PhysRevB.107.054424(2023)

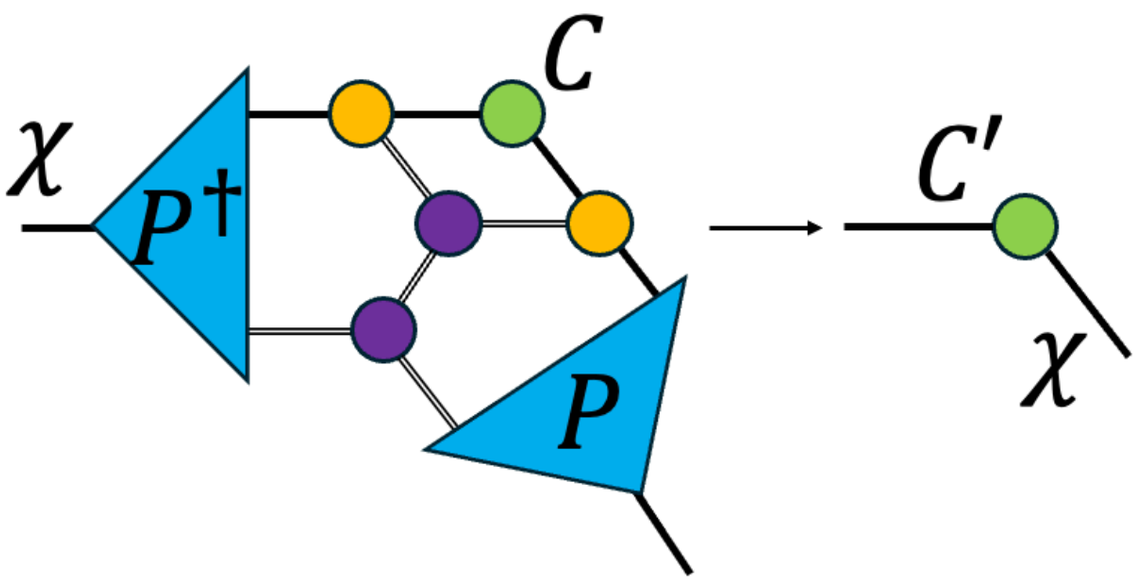
Step 1: Build projector. (expensive EVD)

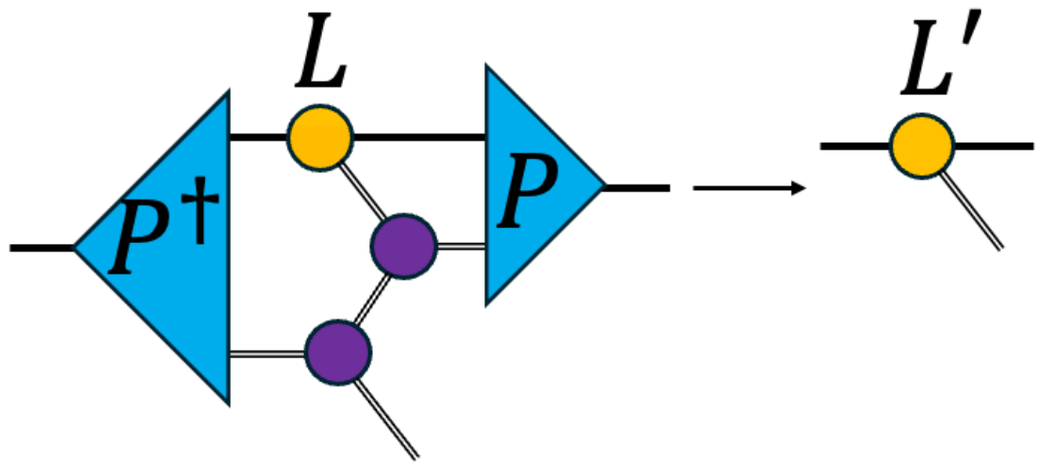
~95% time



Step 2: Update edge and corner tensors.

~ 5% time



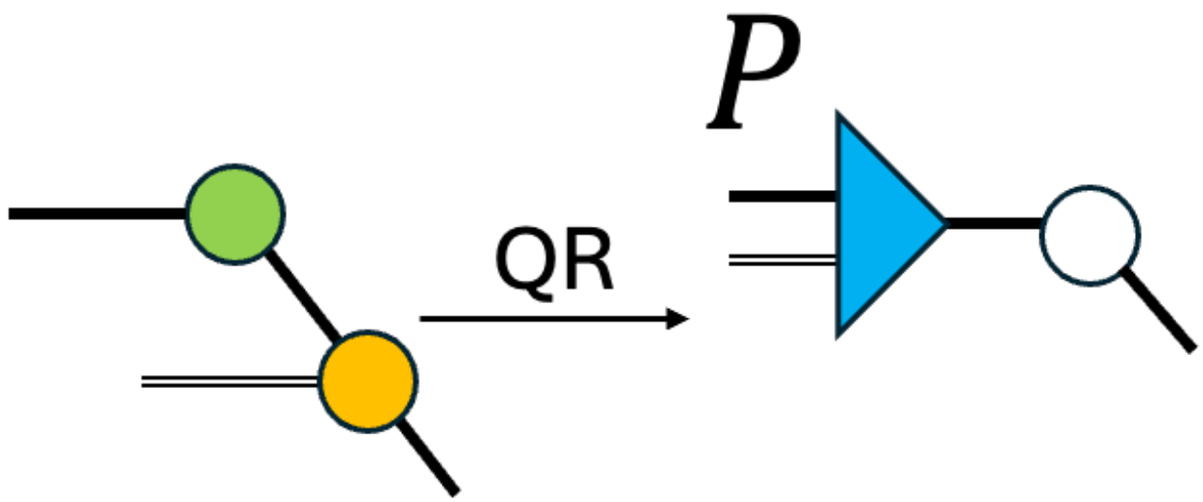


H100, double, very large D>6 and chi>600

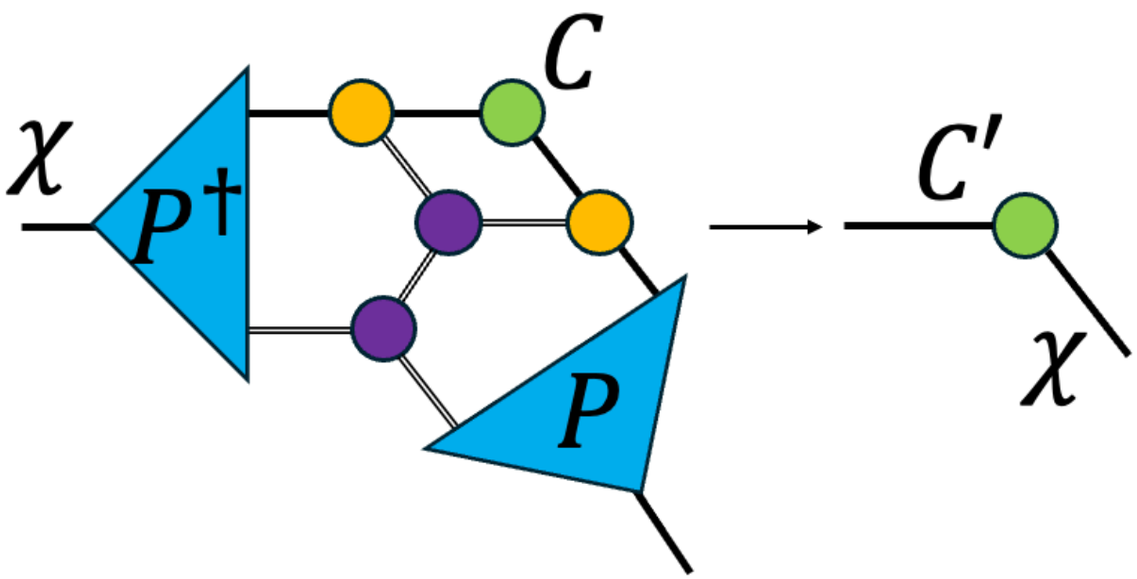
QRCTM for uniform C_{3v} iPEPS

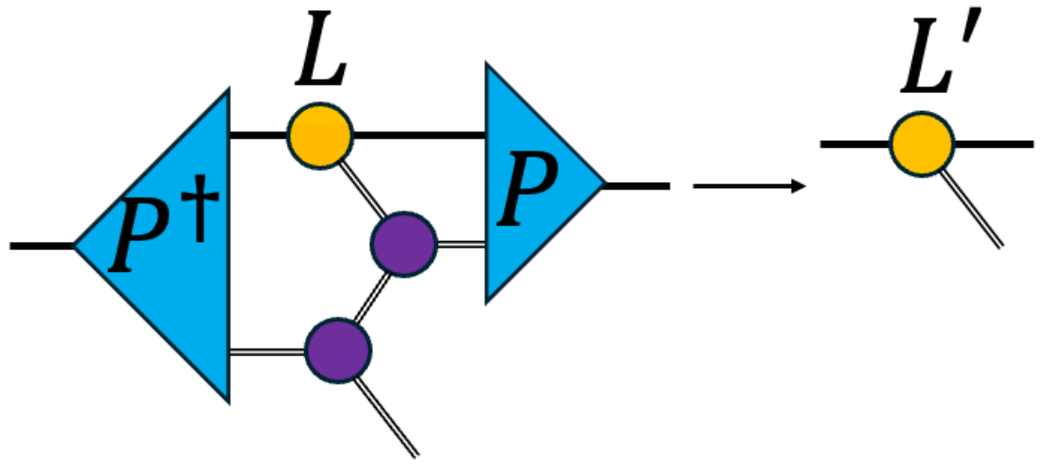
arXiv:2509.05090

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



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





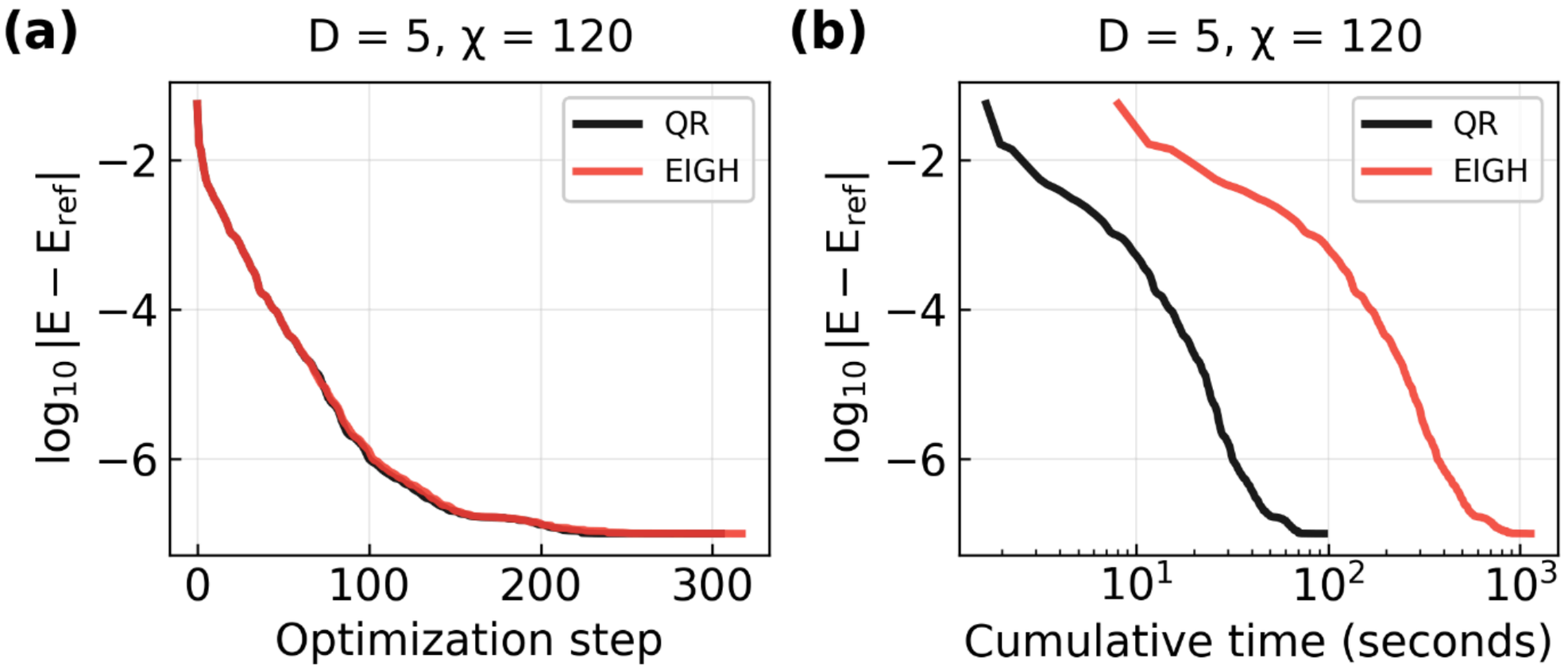
H100, double, D=6 and chi=600

AFM Heisenberg on the Honeycomb Lattice

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

Training Dynamics

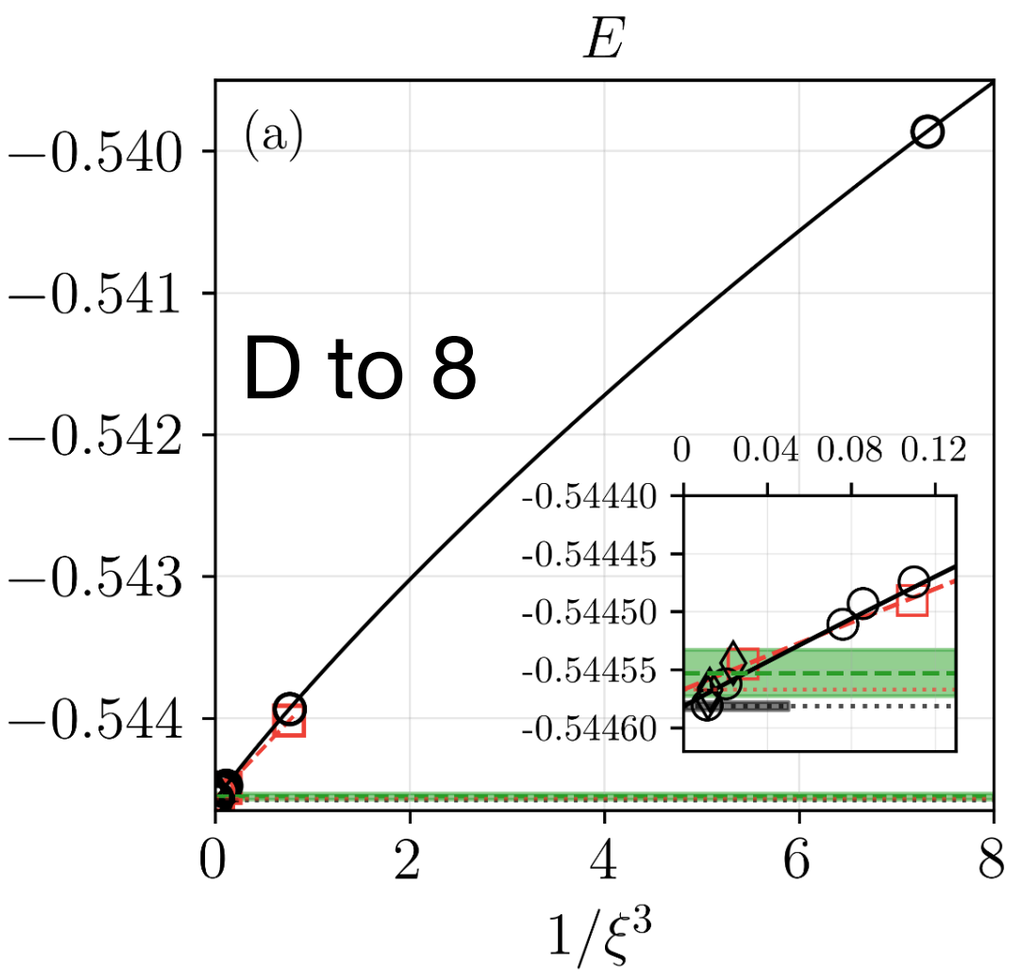
Speed up

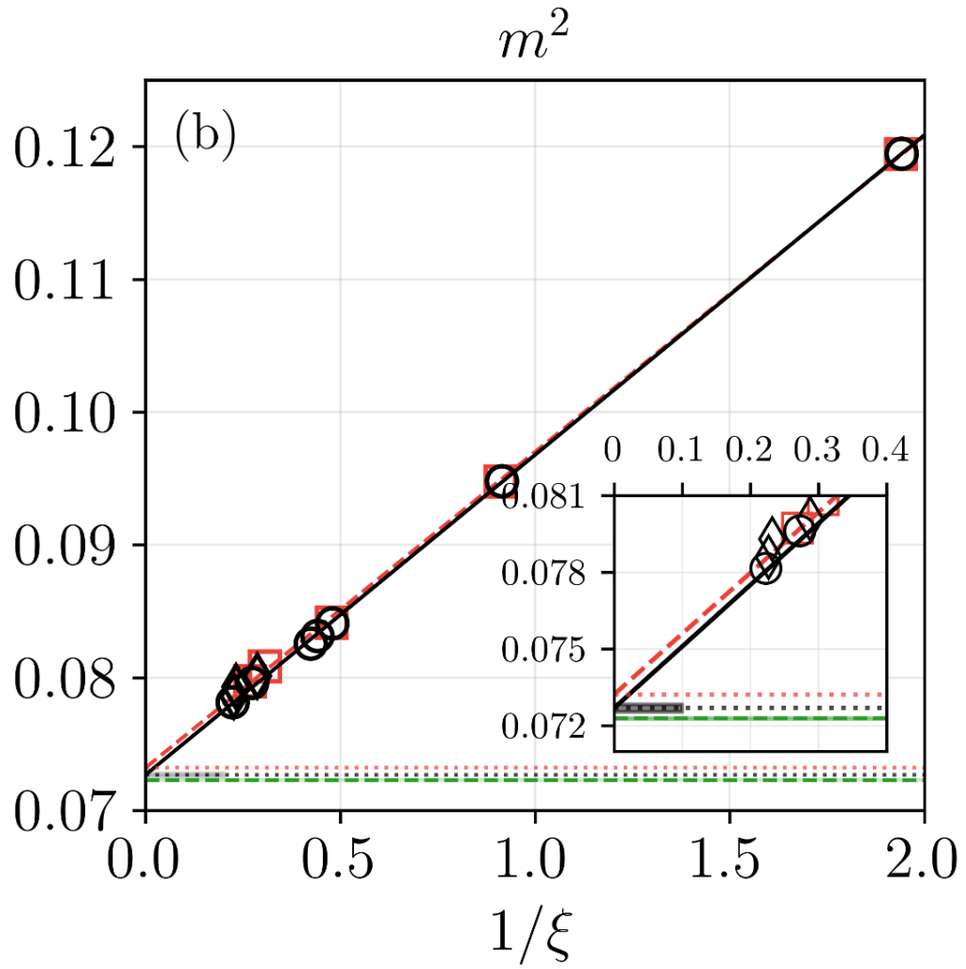


Similar training dynamics, SUPER FAST!

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

AFM Heisenberg on the Honeycomb Lattice





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

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

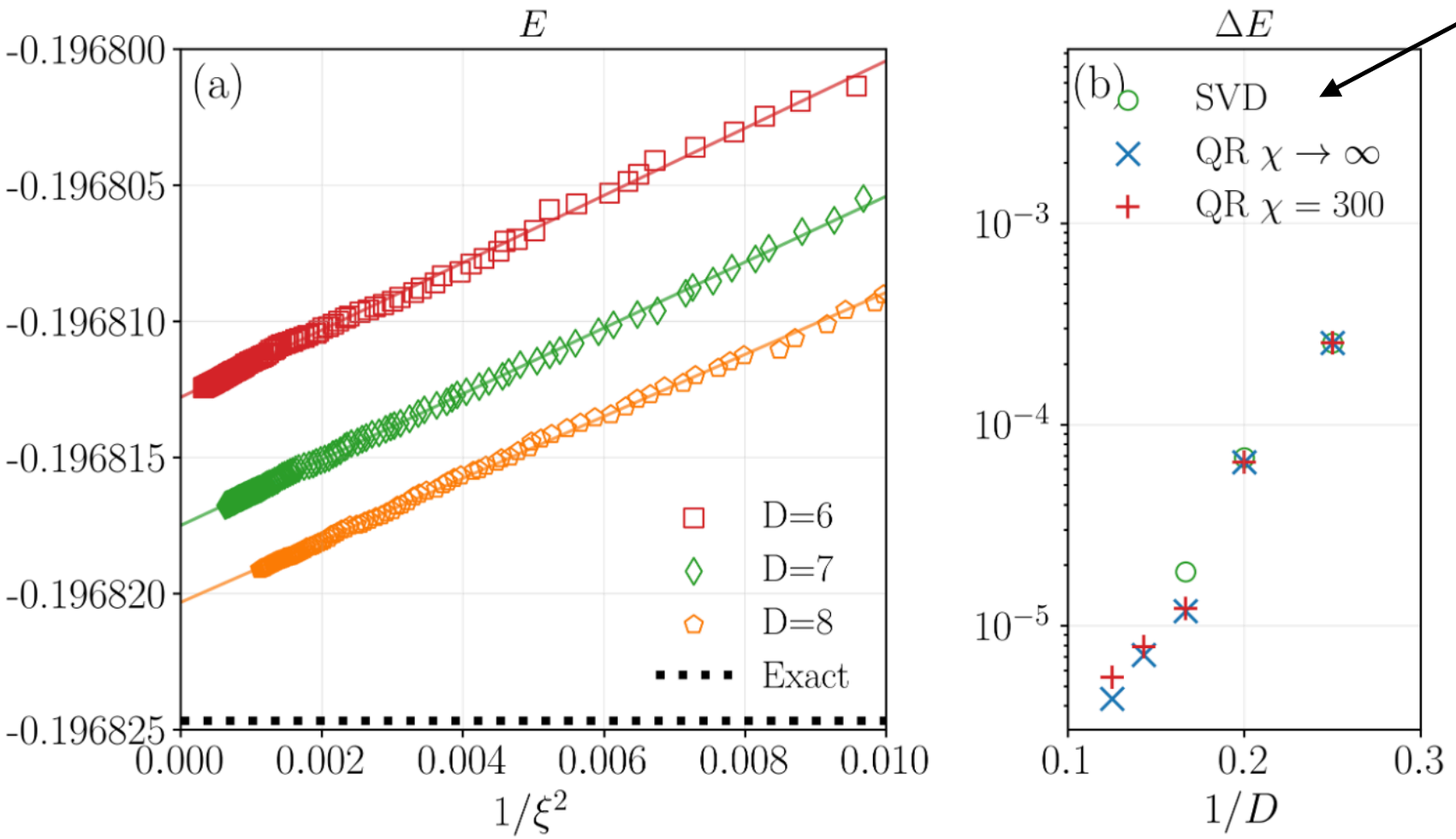
D=8, accurate results—consistent with QMC

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)



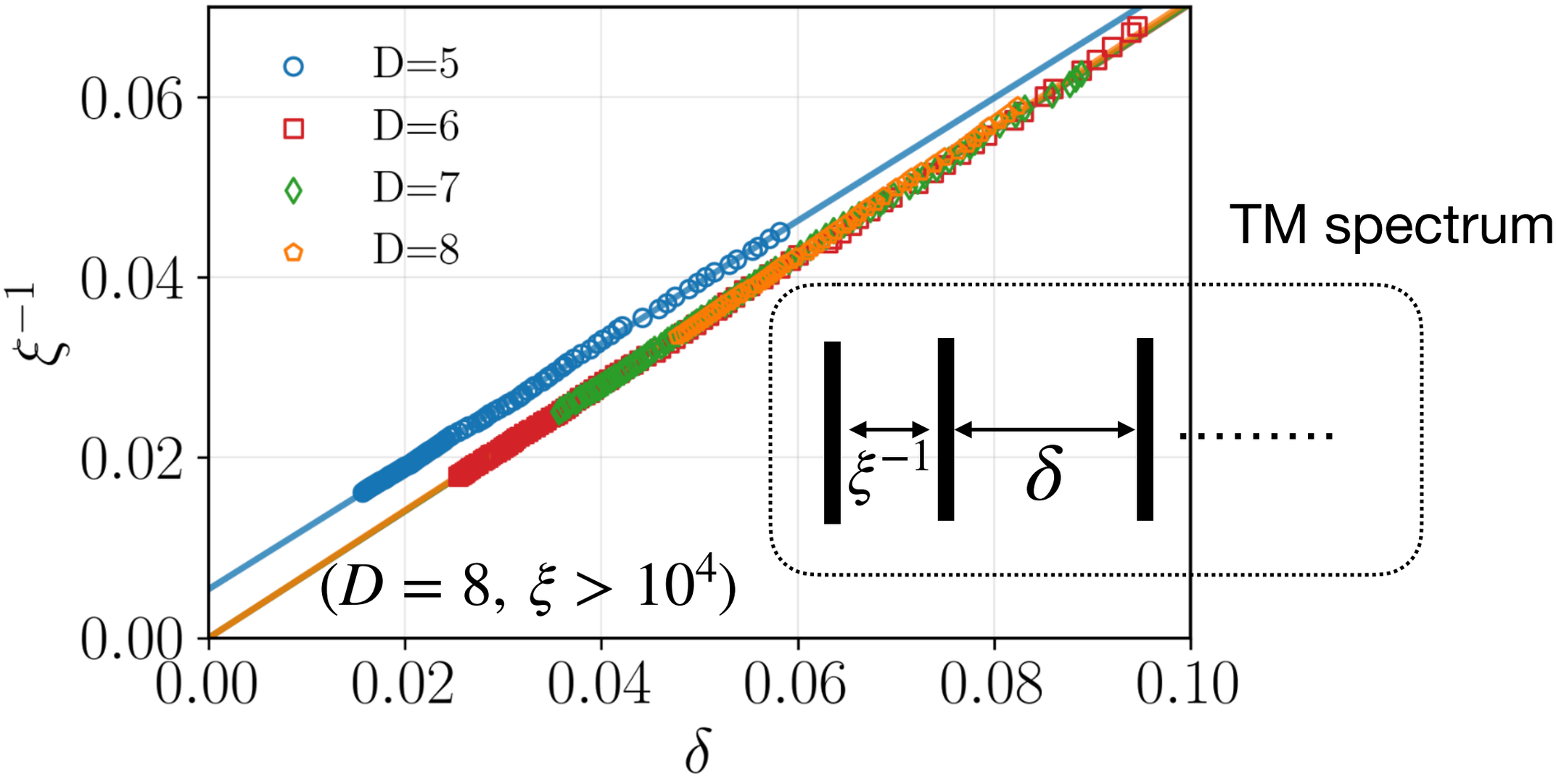
Critical SG	$D = 8,\ \|\|\Delta E/E\|\| = 7 \times 10^{-5}$	PhysRevLett.123.087203(2019)
AD+CTMRG	$D = 6,\ \|\|\Delta E/E\|\| = 9 \times 10^{-5}$	PhysRevB.107.054424(2023)
AD+QRCTM	$D = 8,\ \|\|\Delta E/E\|\| = 2 \times 10^{-5}$	

SOTA reported energy with AD+iPEPS

Not extrapolated, energy per sites.

Kitaev model: Finite Correlation Length Scaling

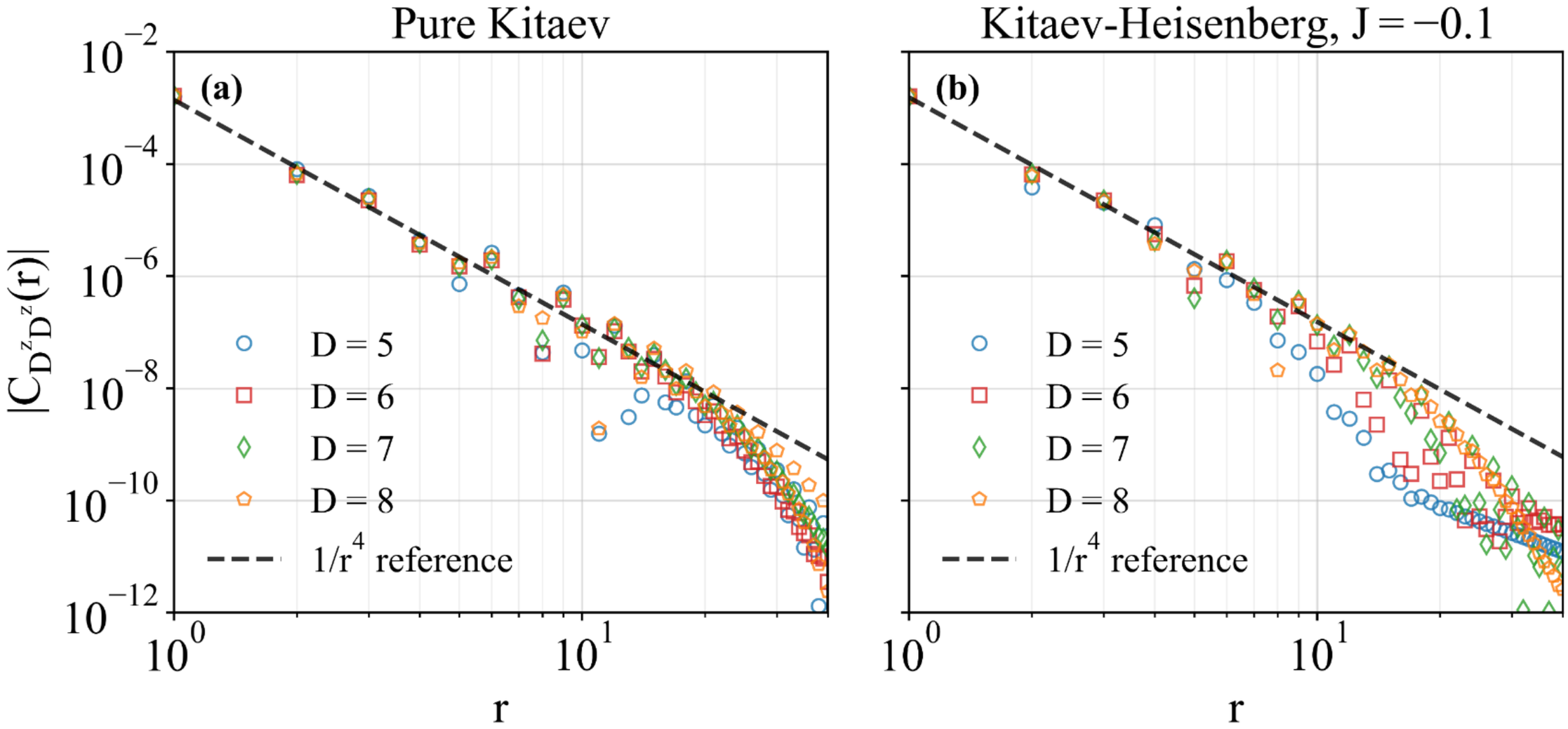
Phys. Rev. X 8, 031030 (2018)
Phys. Rev. X 8, 031031 (2018)



Finite D, infinite ξ !

Finite-correlation-length-scaling reveals gapless nature.

iPEPS evidence for Dimer-Dimer correlation decay



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

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

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

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)

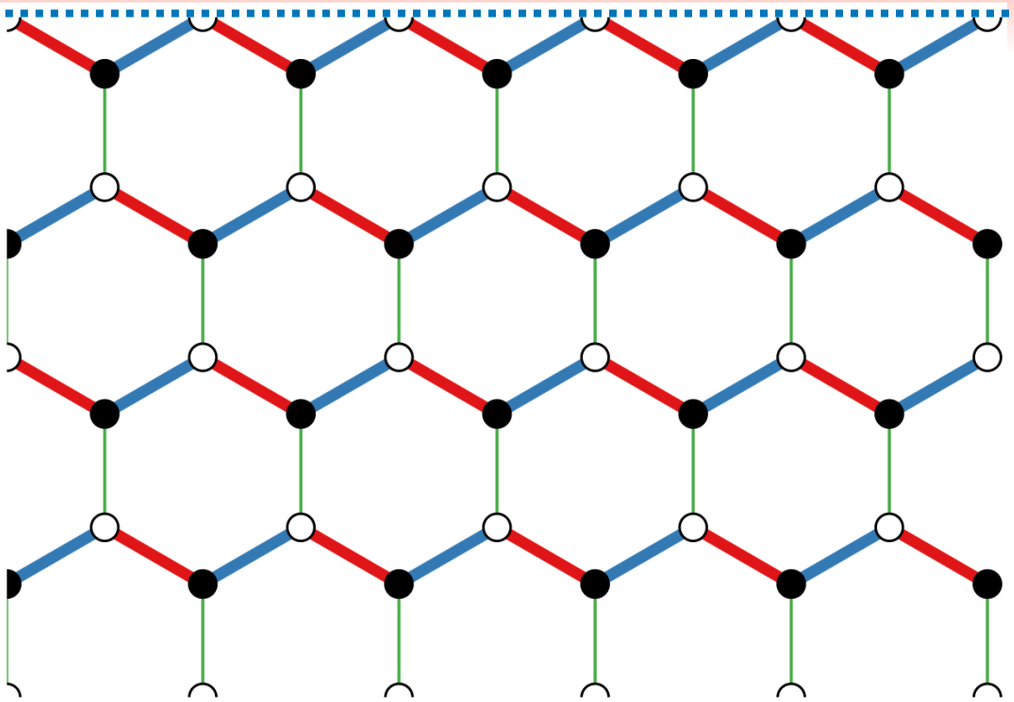
Quantum many-body methods

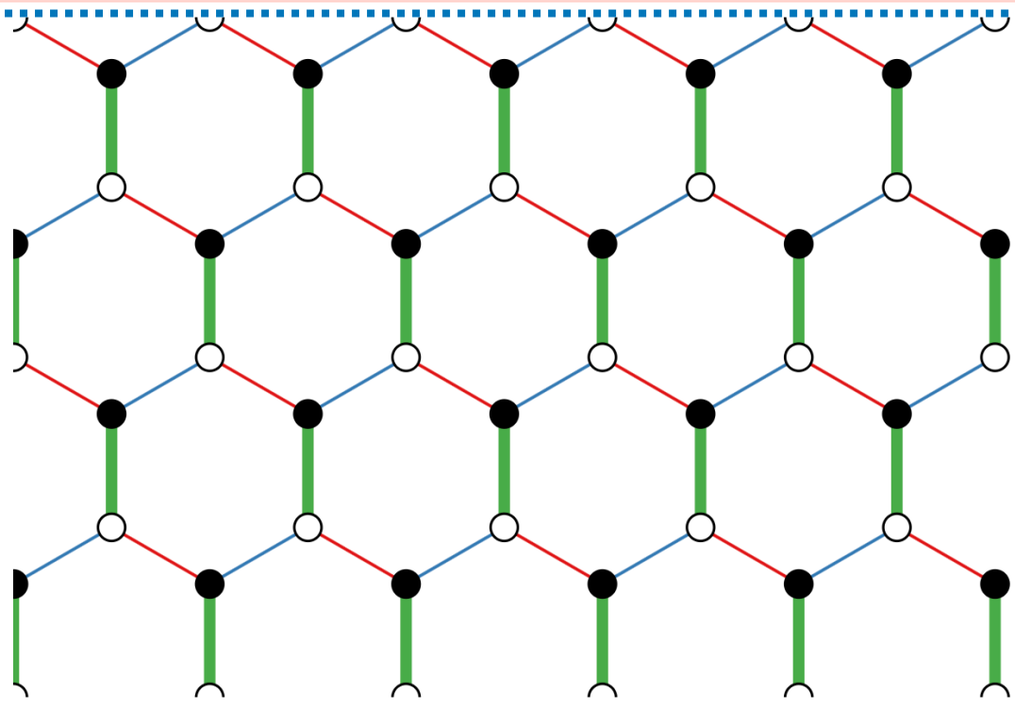
JPSJ 87, 063703 (2018)
PRR 2, 033318 (2020)
PRR 3, 013160 (2021)
PRB 105, L060403 (2022)
Nat. Commun. 13, 3813 (2022)
PRB 106, 174416 (2022)
SciPost Phys. 16, 100 (2024)
PRR 6, 033077 (2024)
PRB 110, 134402 (2024)
PRR 6, 033168 (2024)
arXiv:2503.24246 (2025)
…….
Results: **QSL, no symmetry breaking**

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

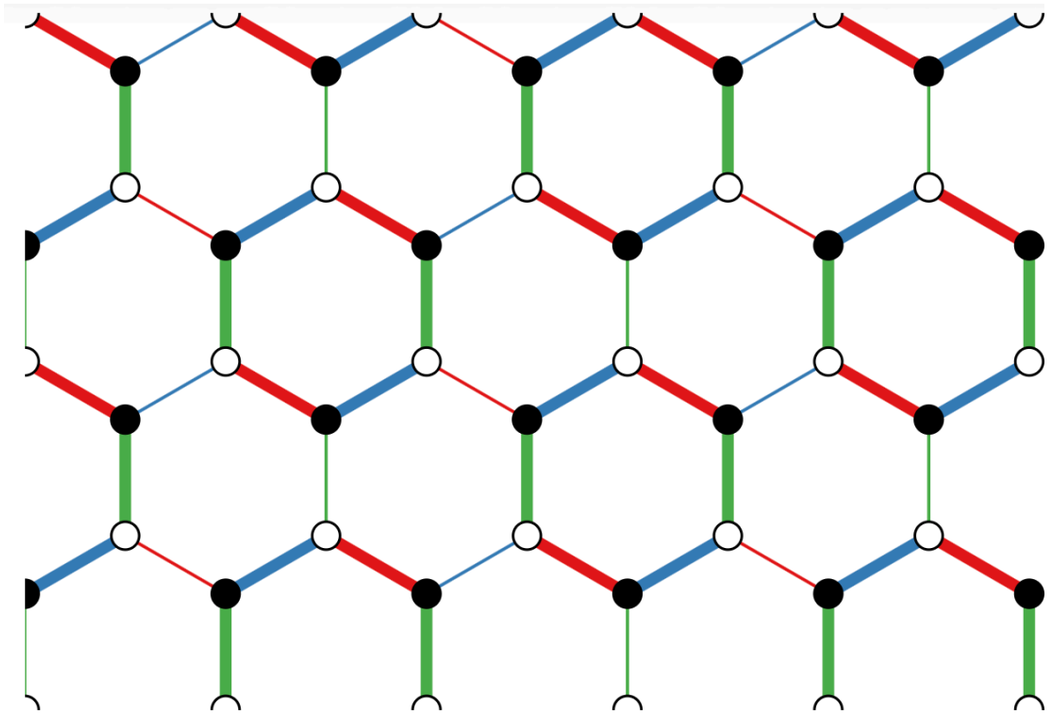
Collaboration with Xingyu Zhang*, Jutho Heageman, Yuchi He @Ghent

Ground states candidates from SU

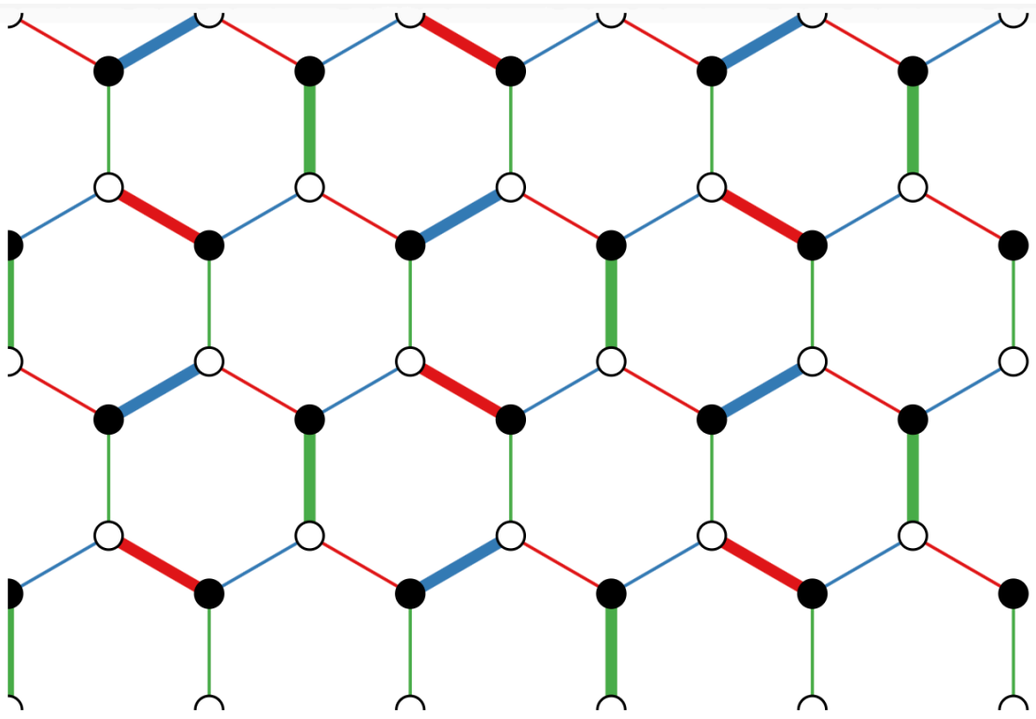




Uniform anisotropic, high E, 2x1 unit-cell



Plaquette

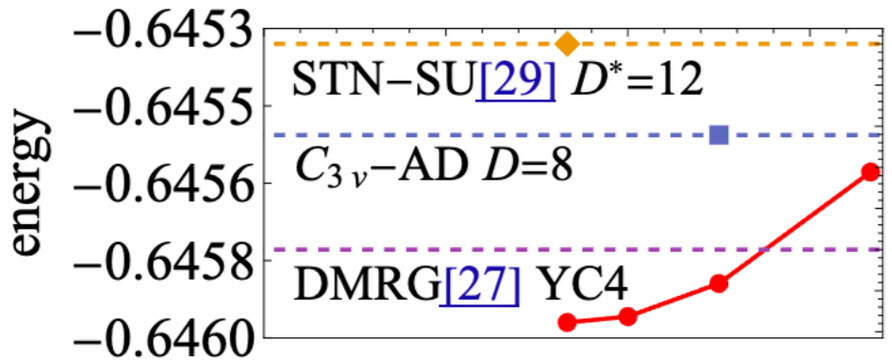


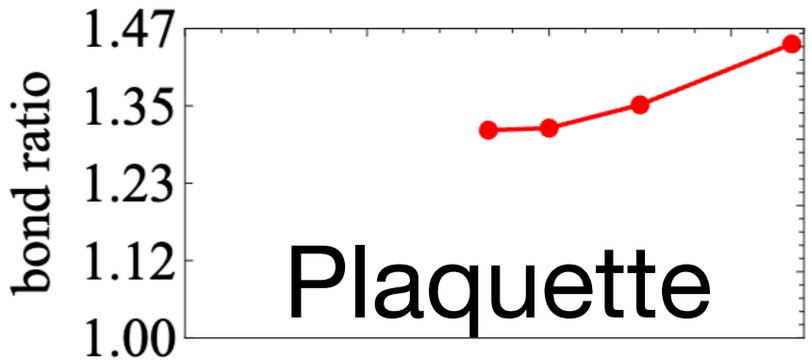
Dimer

Detect SSB: Energy comparison

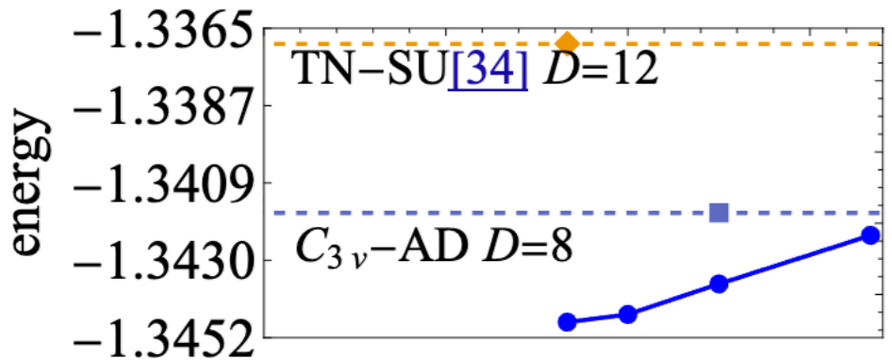
Comparing with AD+VUMPS, Precondition + multiple GPUs

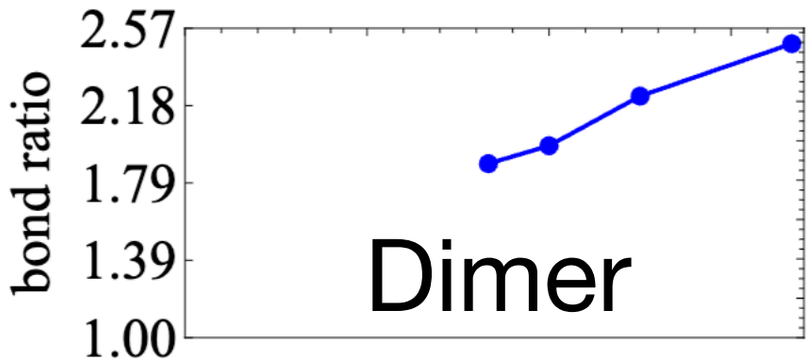
(a) S=1



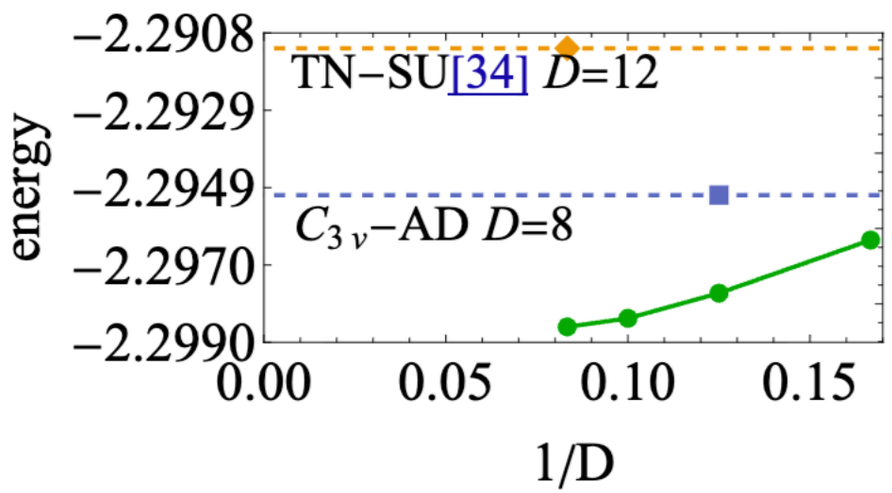


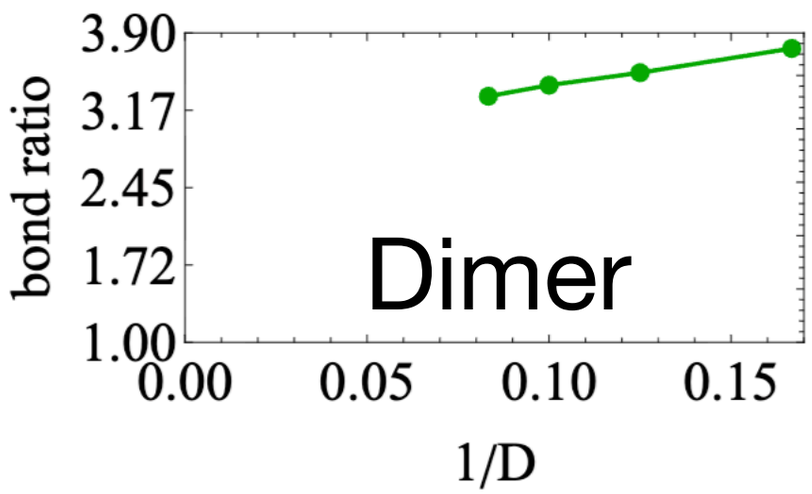
(b) S=$\frac{3}{2}$





(c) S=2

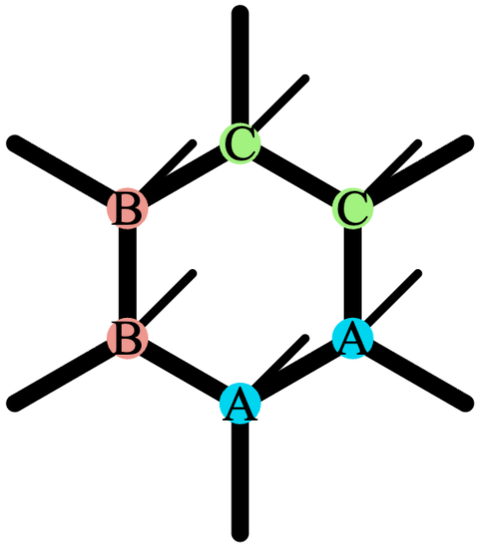


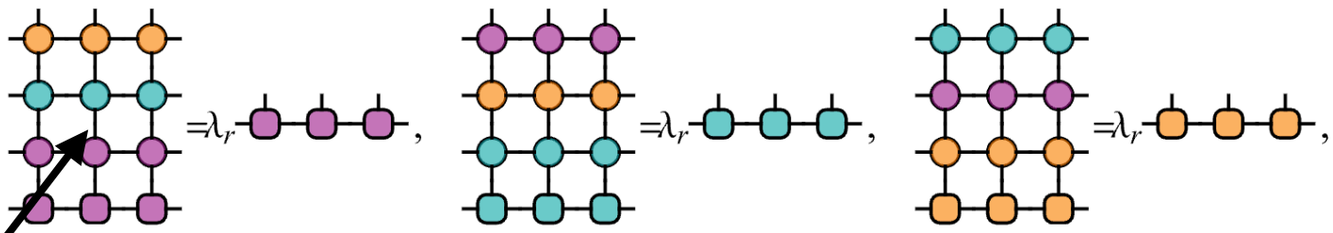


VUMPS: talk to Xingyu Zhang@Ghent

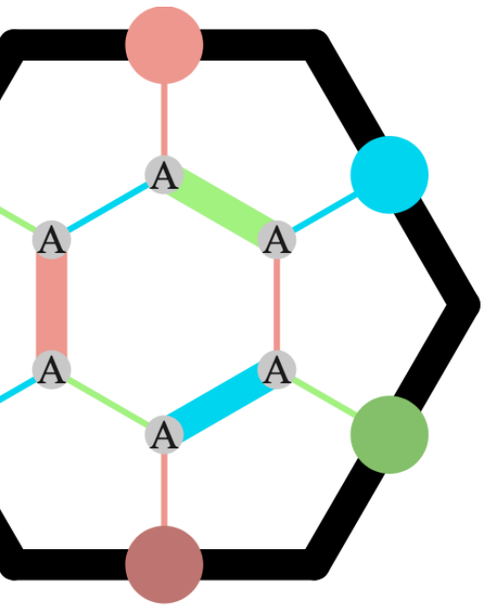
Detect SSB: A New Diagnostic

VUMPS

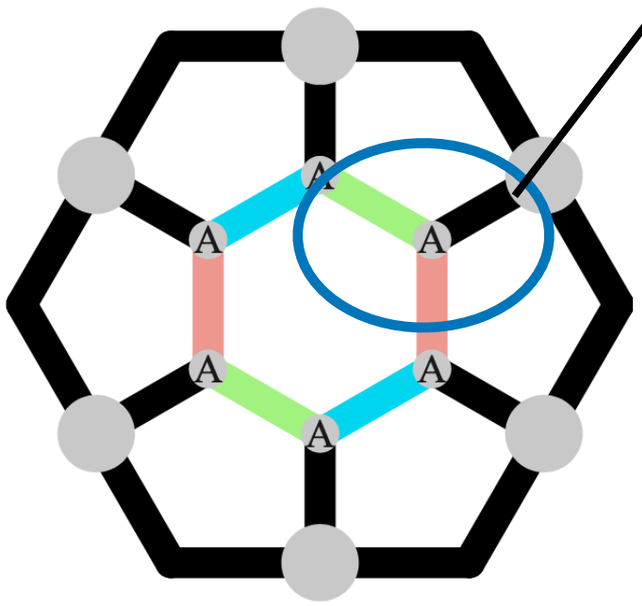


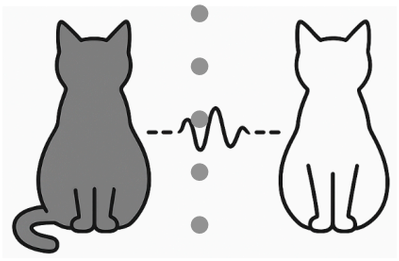


Env. SSB



QRCTM





observables uniform ← cat states → observables non-uniform!

Another evidence of SSB for S=1,3/2,2

Quantifying SSB: Energy and Scaling