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DMRG APPROACH TO OPTIMIZING TWO-DIMENSIONAL TENSOR NETWORKS

TNSAA 7

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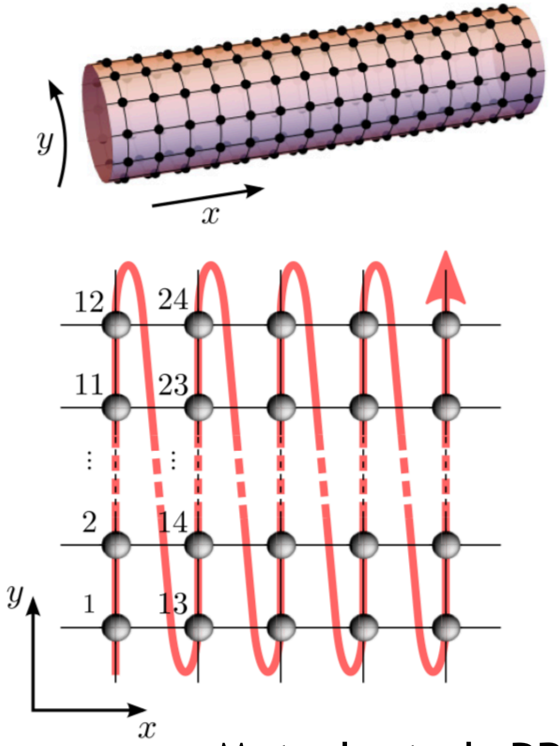
Dec 6, 2019

DMRG is extremely successful in (quasi)-1D

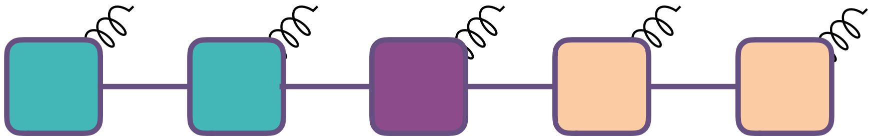


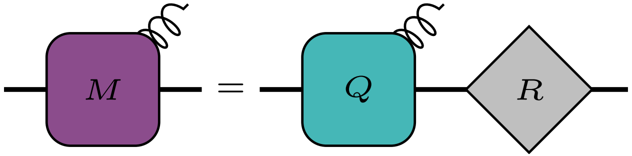
- Gold standard for gapped and even some gapless/critical models
- Time evolution through TEDB/t-DMRG
- Can simulate systems where one dimension is much longer than the other — infinite cylinders

Motruk et al. PRB 93(15) 155139

Canonical Form Through Matrix Decomposition

Left-canonical: $\hat{A}^\dagger \hat{A} = \mathbb{I}$ Right-canonical: $\hat{B}\hat{B}^\dagger = \mathbb{I}$





- Split single tensor into unitary Q and residual R
- Can also use SVD decomposition, allowing truncation of bond dimension χ

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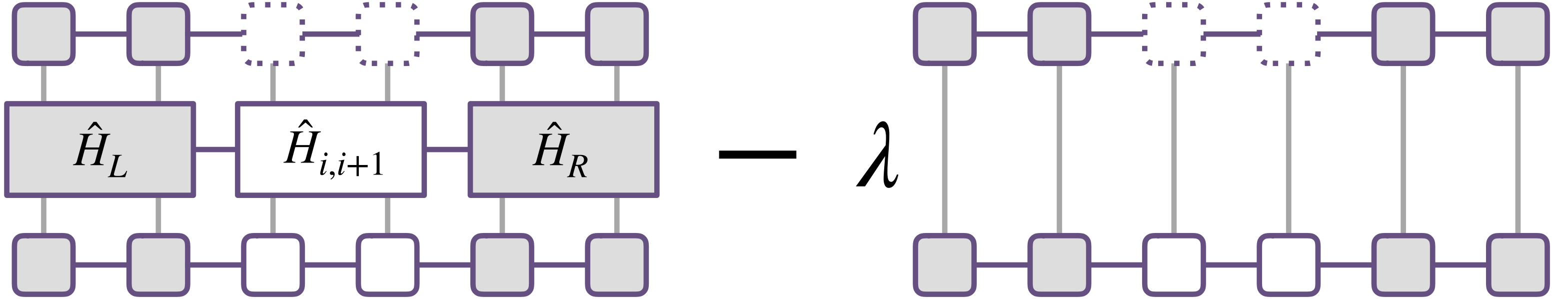
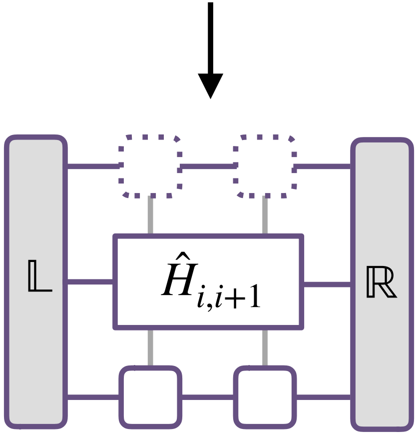
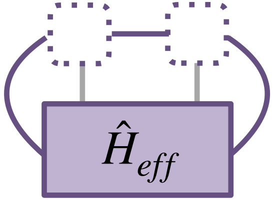
Canonical Form Makes DMRG Fast



$$\hat{H}_{eff} v = \lambda \hat{\mathcal{N}} v$$



$$\hat{\mathcal{N}} = \mathbb{I}$$



$$\lambda v = \hat{H}_{eff} v$$

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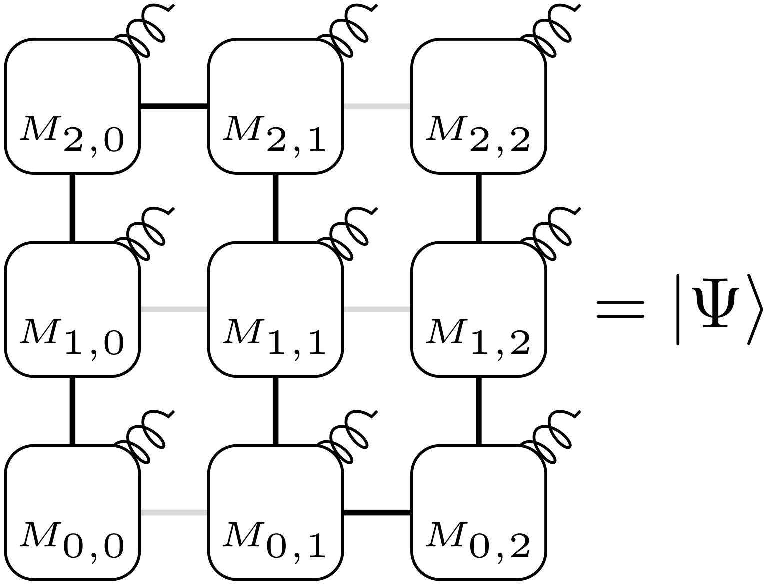
DMRG Will Never Be Able To Access Full 2D

- Size of virtual indices must grow exponentially in one of the dimensions
- Because of snaking, correlations become long distance in the MPS, which inflates χ



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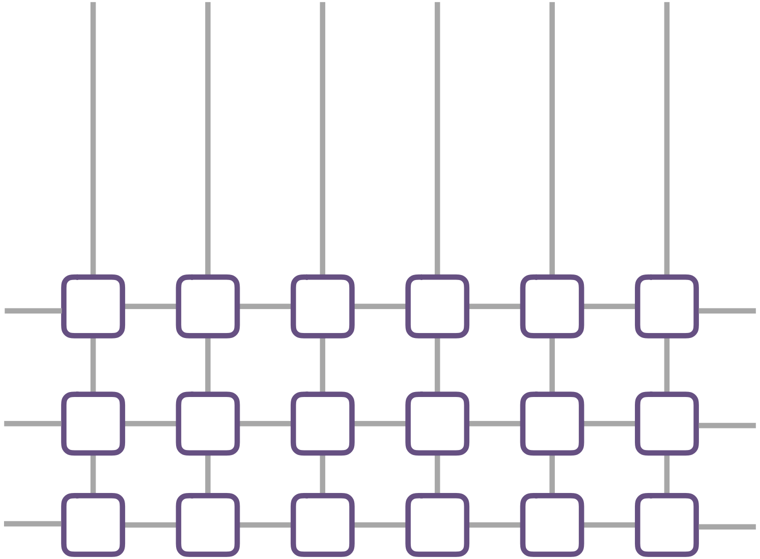
Our Goal: Extend To Full Two Dimensions



- Interesting physics in 2D
- Time evolution in 2D
- DMRG for critical models can stall out at 4-6 ladder legs
- Many interesting models have “fermion sign problem”
- Exact diagonalization cannot reach large sizes

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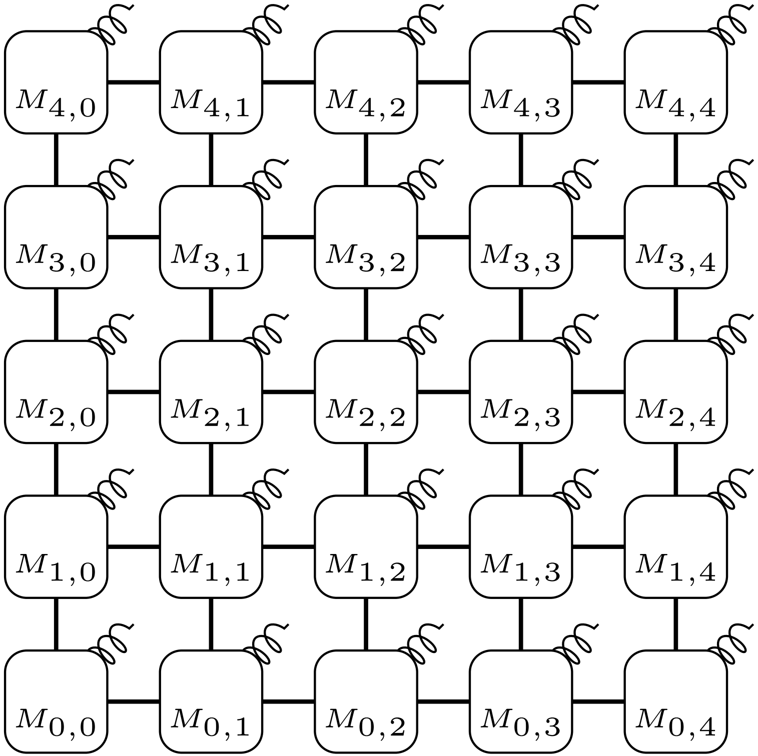
PEPS is the 2D Analogue of MPS



- "**P**rojected **E**ntangled **P**air **S**tates"
- Originally developed by F. Verstraete and J. I. Cirac in arXiv:cond-mat/0407066
- Each tensor has virtual indices connecting it to all its neighbors
- PEPS can efficiently represent area-law and critical states in 2D

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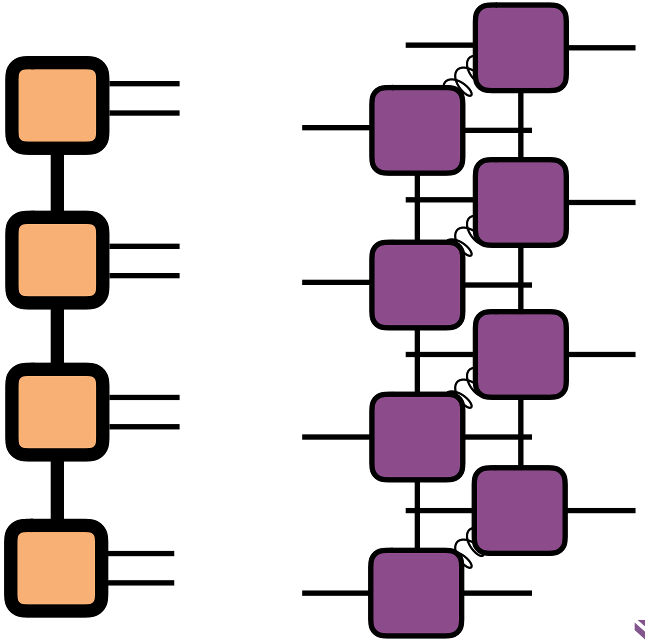
Calculating Observables is Hard

- Performing exact contraction of the entire PEPS is exponentially hard in bond dimension
- Instead, treat contractions as iterative MPO-MPS products and truncate after each
- Lose some accuracy, but hopefully not too much



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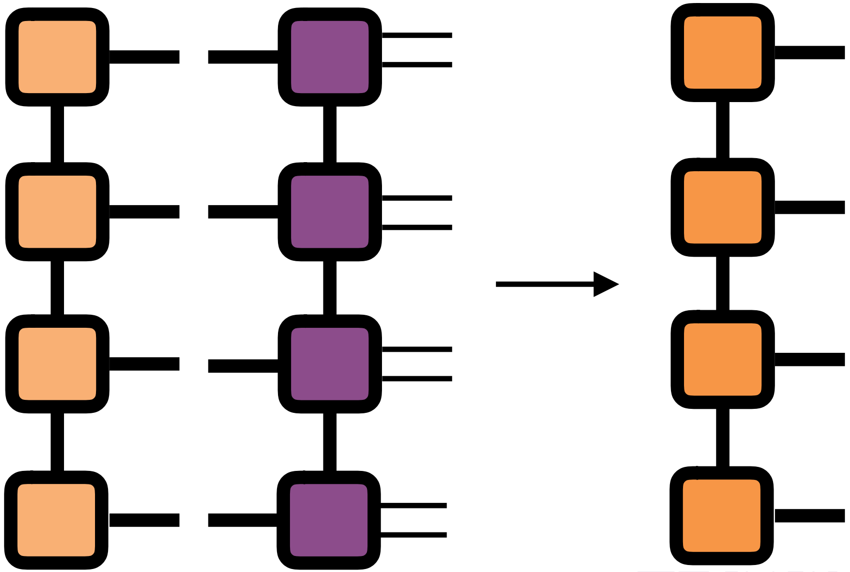

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“Why not use iPEPS?”

- iPEPS optimizes a “representative” tensor which is infinitely tiled
- Requires a system with translation invariance — what about disorder?
- Can be difficult to handle non-square geometries
- iPEPS and finite PEPS both have their strengths, and both are interesting

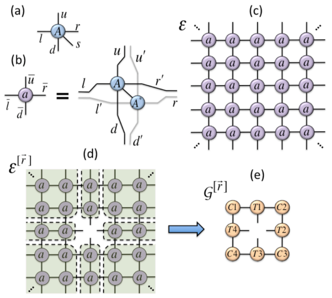

FIG. 1: (color online) Diagrammatic representation of (a) infinite PEPS tensor A with physical index s and bond indices u, r, d and l; (b) reduced tensor a; (c) infinite 2D tensor network $\mathcal{E}$; (d) environment $\mathcal{E}^{[\vec{r}]}$ for site $\vec{r}$; (e) eight-tensor effective environment $\mathcal{G}^{[\vec{r}]}$.

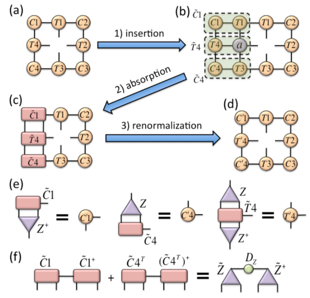

FIG. 2: (color online) (a)-(d) Main steps of a left move: insertion, absorption and renormalization; (e) the CTMs $\widetilde{C}_1$, $\widetilde{C}_4$ and the half-row transfer matrix $\widetilde{T}_4$ are renormalized with isommetry Z; (f) eigenvalue decomposition for the sum of the squares of CTMs $\widetilde{C}_1$ and $\widetilde{C}_4$.

Orus & Vidal, PRB 80(9), 094403

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Must Develop Canonical Form for PEPS

- Because of loop structure of PEPS, it's **impossible** to **exactly** represent $|\psi\rangle$ with a **perfect** unitary at fixed bond dimension
- If you can cope with infinite bond dimension, the world is your oyster
- Our approach approximates $|\psi\rangle$ while enforcing unitarity
- There are many possible canonization schemes for PEPS

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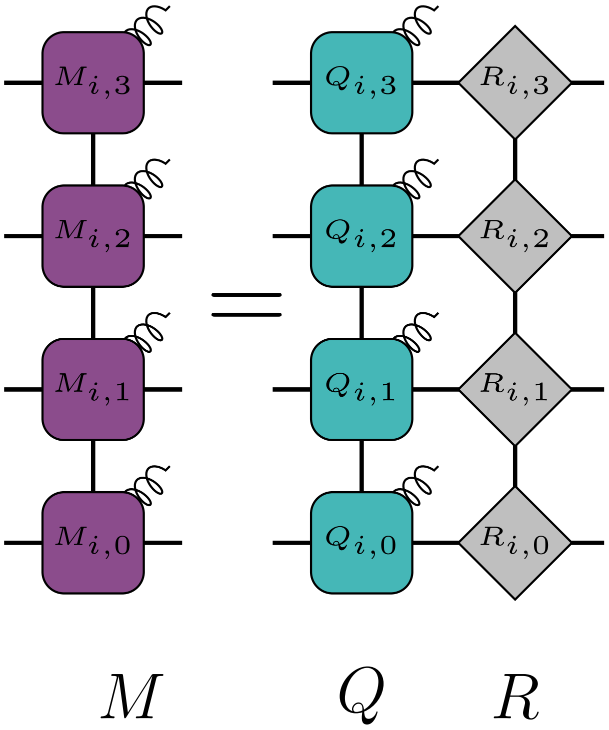
Our Approach: Analogy of QR decomposition



- Treat column of PEPS as “MPO”
- Split into:
    - unitary “Q”-like MPO which carries physical degrees of freedom
    - remainder “R”-like MPO which is multiplied into the next column
- We do not actually perform a QR decomposition!

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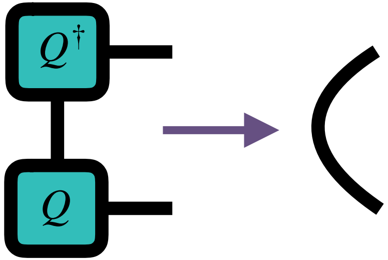
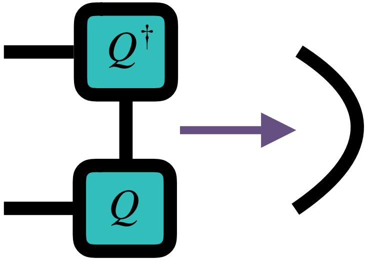
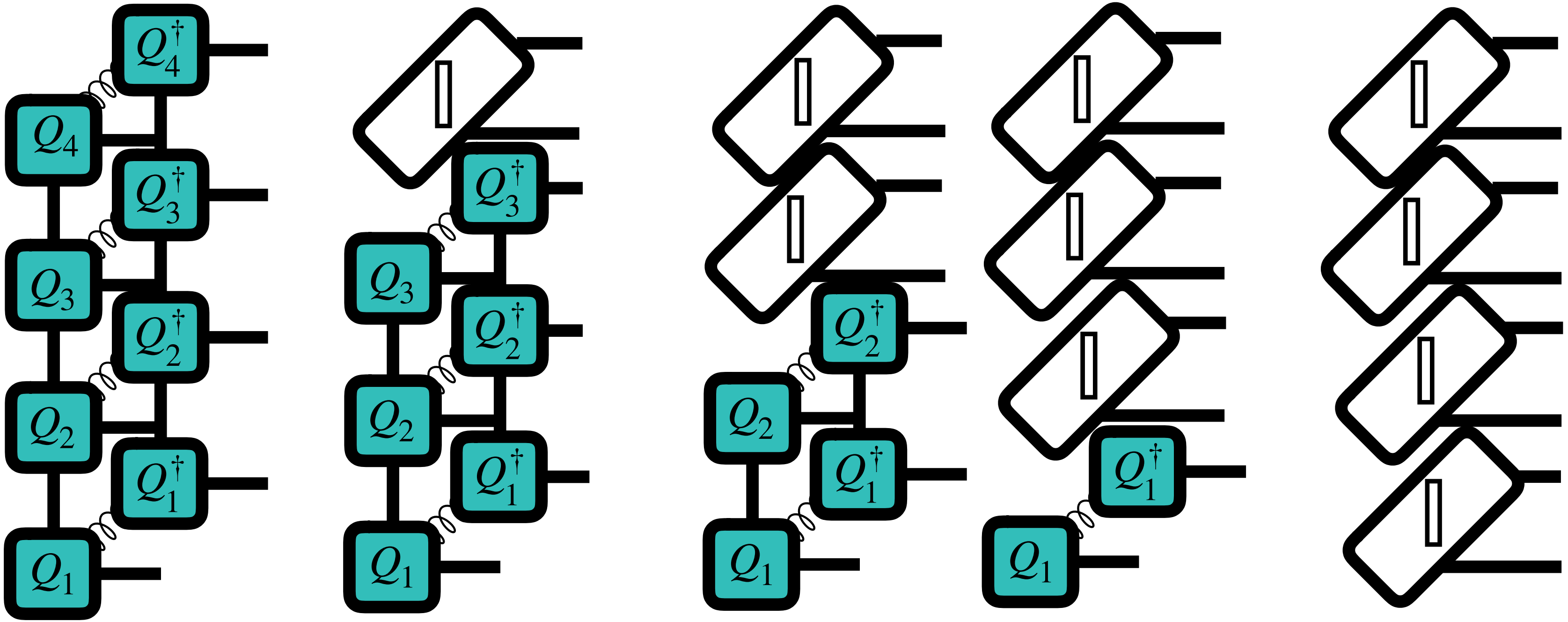
What Do We Mean By Unitary?
Simpler 1D Case:





What Do We Mean By Unitary?



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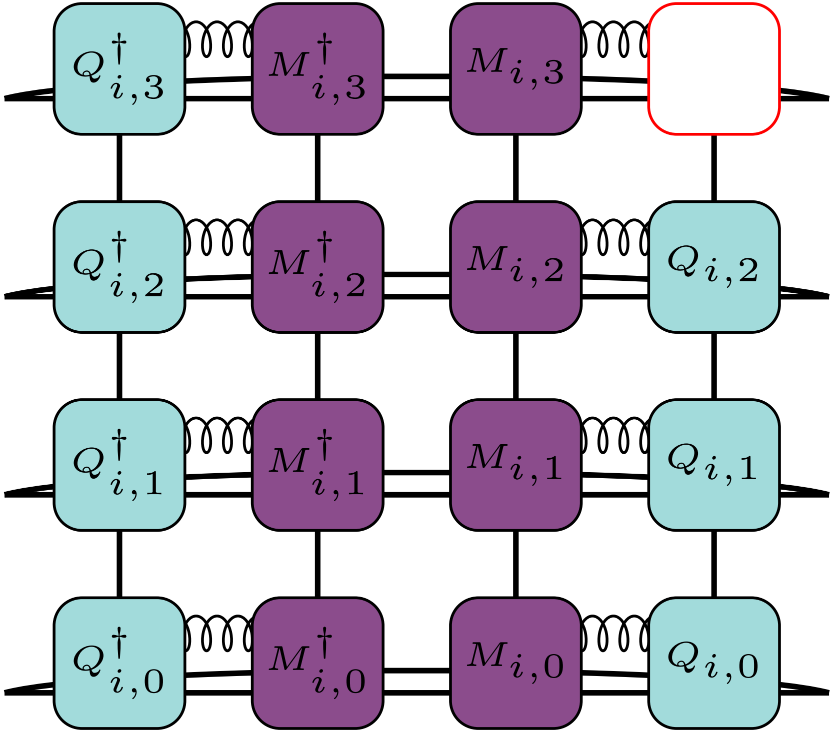
Construct environment for each element of Q

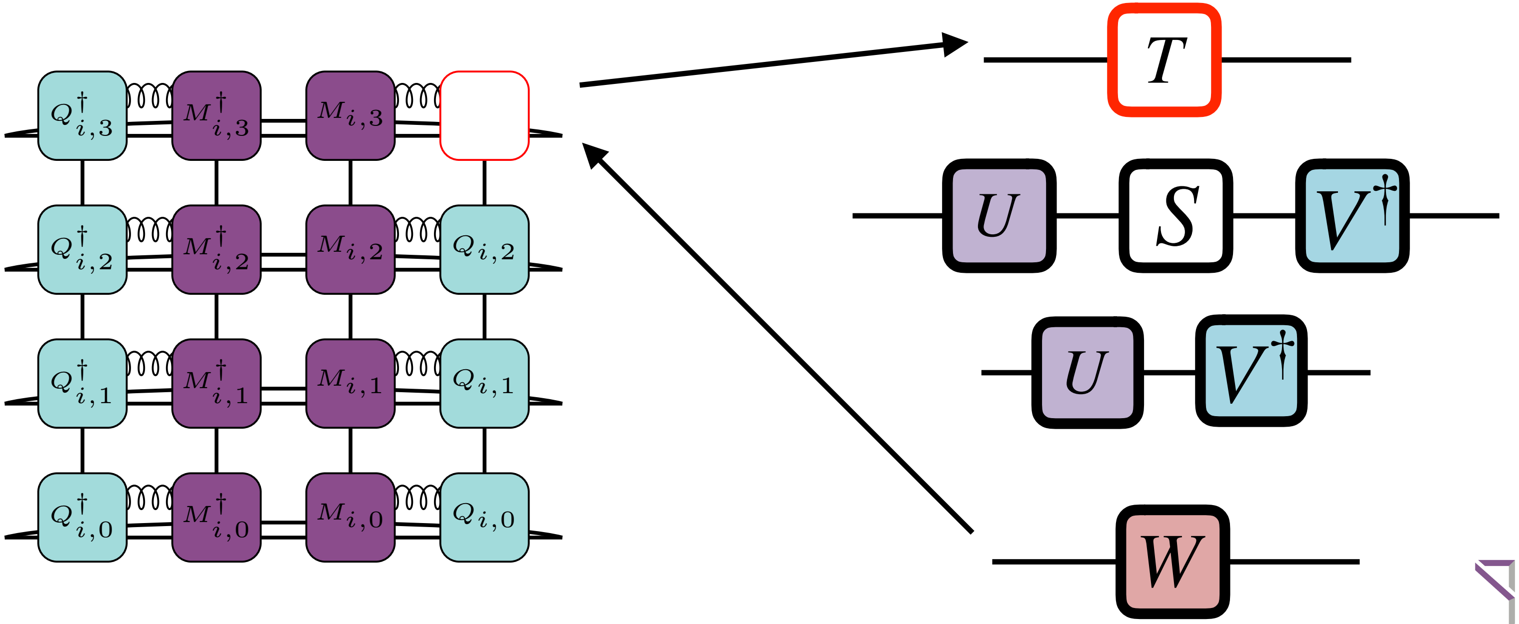


$$\langle MQ|MQ\rangle = (MQ)^\dagger(MQ)$$
$$= Q^\dagger M^\dagger MQ$$

Now compute at each row the unitary Q with best overlap with its environment. This Q then forces:

$$Q^\dagger M = R$$

Polar decomposition finds unitary with greatest overlap with Q_i



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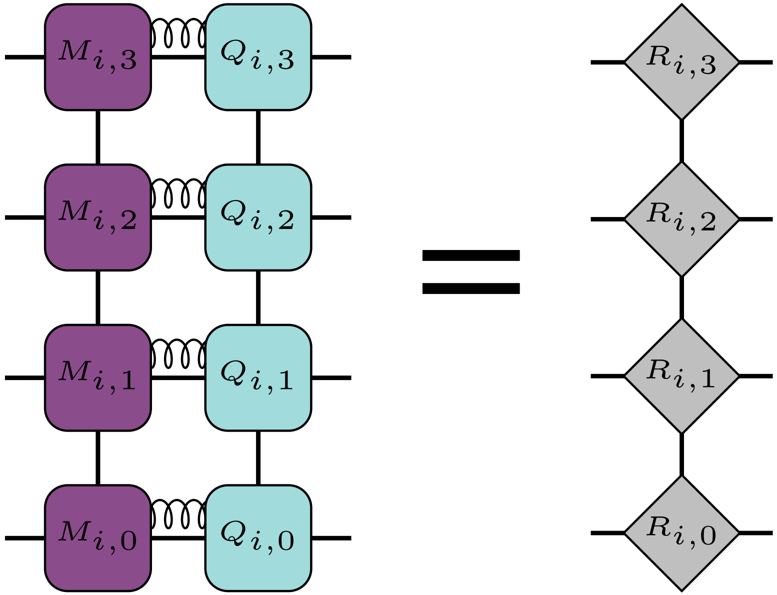
Generate R from Q and M



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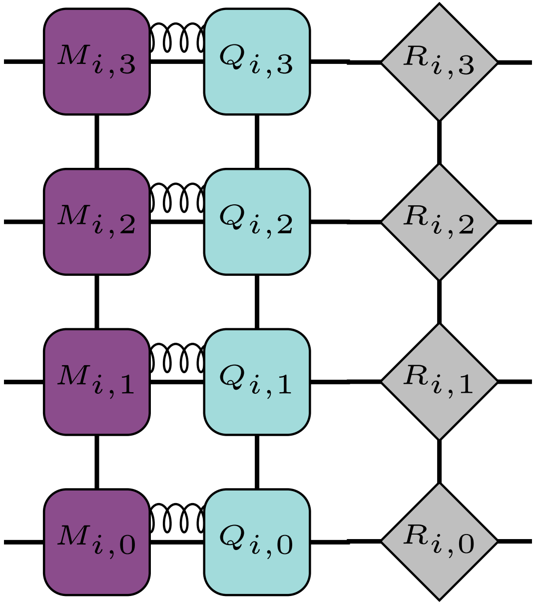
Repeat until $QRM/|M|^2$ > cutoff



$$= \langle QR|M\rangle$$

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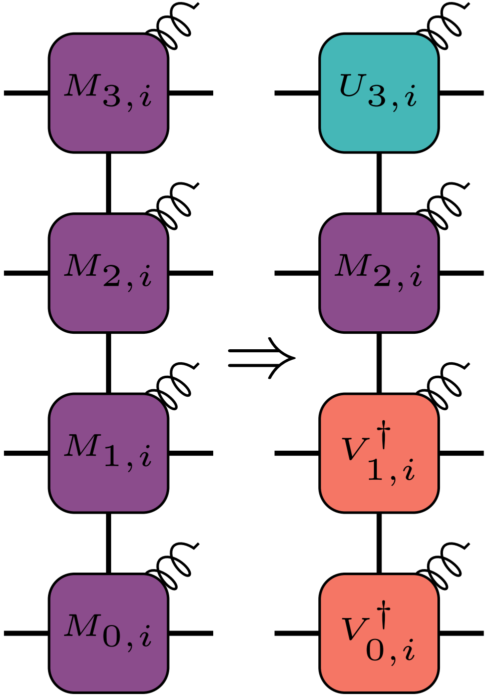
For Full Unitarity, Canonization Within A Column



- Simple SVD, as in 1D MPS case
- Norm at tensor to-be-optimized is exactly 1
- After each optimization, restore canonical form with SVD again as in DMRG

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Consequences Of Our Method For PEPS

- We can use an iterative regular eigensolver, rather than a general eigensolver or gradient descent
- Fast(er) computation of observables
- We broke translation invariance, but we are using finite PEPS anyway
- At fixed χ, can have inexact representation of $|\psi\rangle$ that is exactly unitary **or** exact representation of $|\psi\rangle$ that is not quite unitary
- Stopping canonization step early can undo optimization progress

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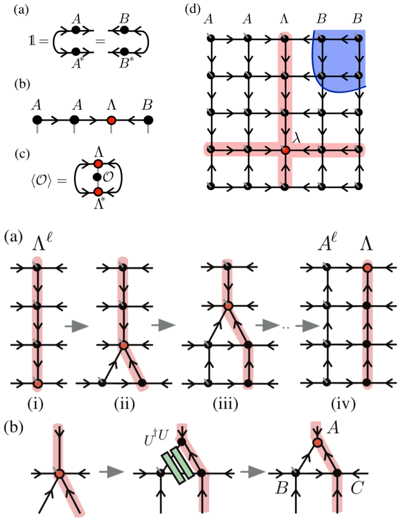
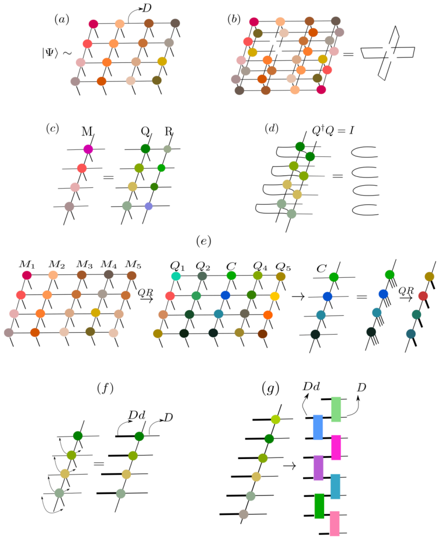
Some Other Strategies Exist

- Zaletel & Pollmann, arXiv:1902.05100
- Haghshenas, O'Rourke, and Chan, arXiv:1903.03843





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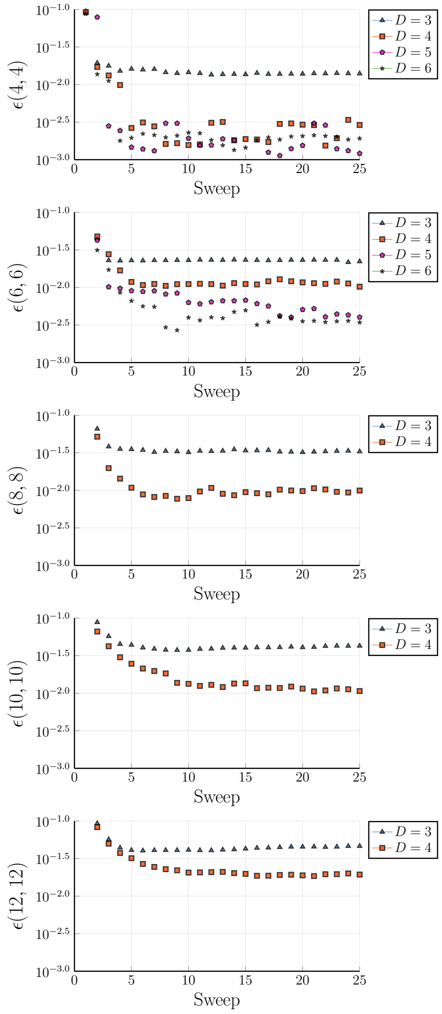

Case Study: Antiferromagnetic Heisenberg Model on Square Lattice

$$\hat{H} = \sum_{\langle i,j \rangle} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j$$

- Divergence of PEPS per-site energy from QMC goes **down** with increasing bond dimension
- No sign problem - compare to QMC SSE results
- Slight "jumps" in divergence due to less-faithful gauges, yet simulation recovers

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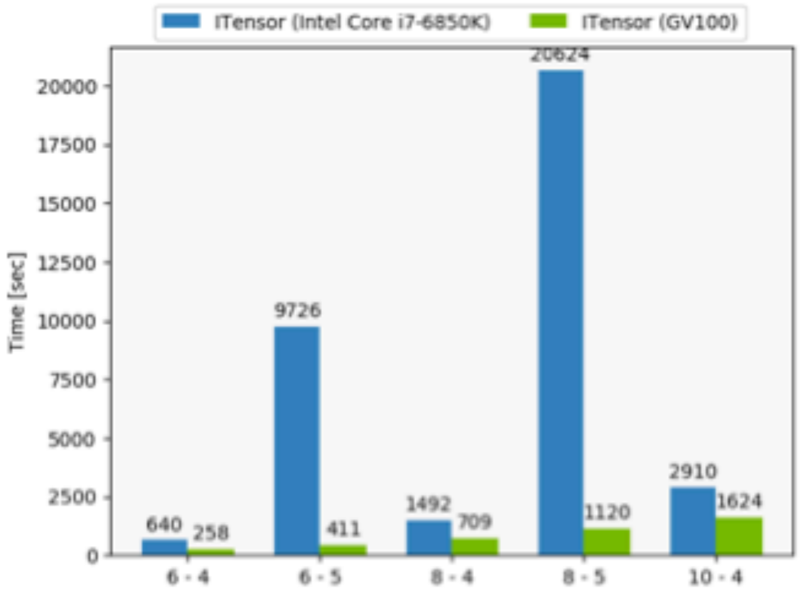
Reimplementation in Julia led to GPU speedups

ITENSOR



- Rewrote ITensor in Julia language, available to all at https://github.com/ITensor/ITensors.jl
- New GPU backend — huge speedup on PEPS code — available at https://github.com/ITensor/ITensorsGPU.jl
- GPU code is based on NVIDIA's CuTensor library

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There's Still Much Not Understood About PEPS

- Does the canonization restrict what states can be represented with PEPS?
- Recent paper by Zaletal et al. shows almost all gapped states can be represented by canonized PEPS
- Are there canonization schemes best suited to particular states?
- More efficient/faithful methods of performing canonization?

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Many Possible Improvements & Applications Exist

- Two-site optimization — could capture quantum fluctuations better?
- Long range interactions
- Geometries beyond the square lattice
- More interesting models: J1-J2, disordered systems, topological models…
- Quantum chemistry
- More inspiration from DMRG: growing, symmetries, time evolution, finite temperature

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