Isometric Tensor Network States

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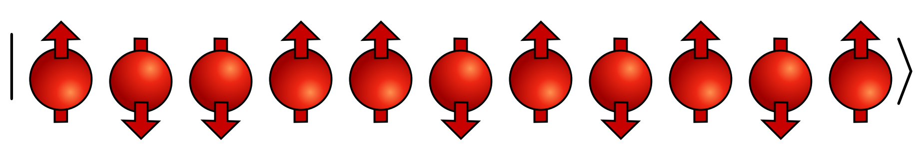
Technische Universität München

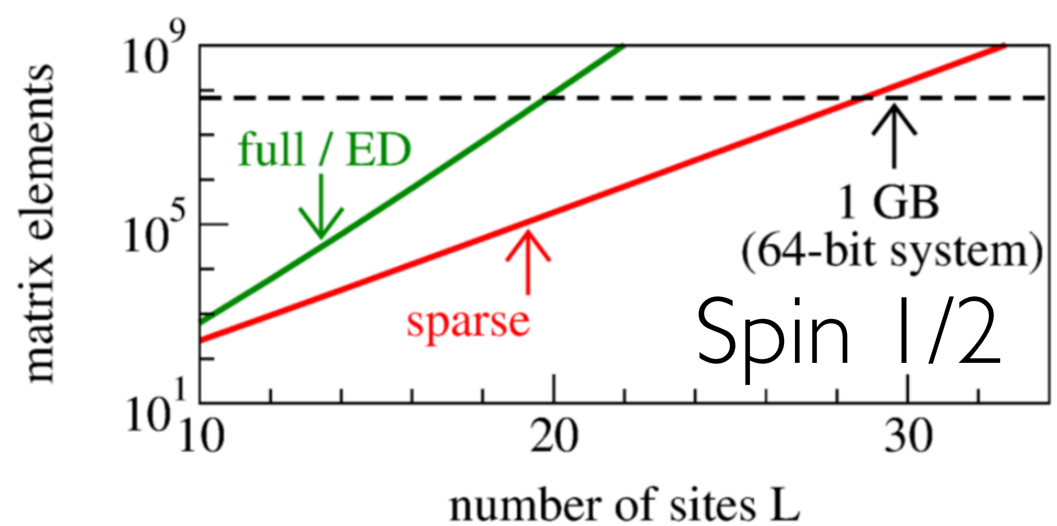
Zeuthen, Mar 4 2019

Complexity of a quantum many-body problem

Diagonalize a Hamiltonian in the full many-body Hilbert space

$$|\psi\rangle = \sum_{j_1, j_2, \ldots, j_L} \psi_{j_1, j_2, \ldots, j_L} |j_1\rangle |j_2\rangle \ldots |j_L\rangle \ , \ j_n = 1 \ldots d$$



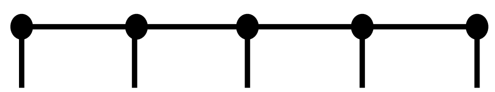


- ➡ Full diagonalization up to ~20 sites
- ➡ Sparse methods up to ~30 sites

Outlook

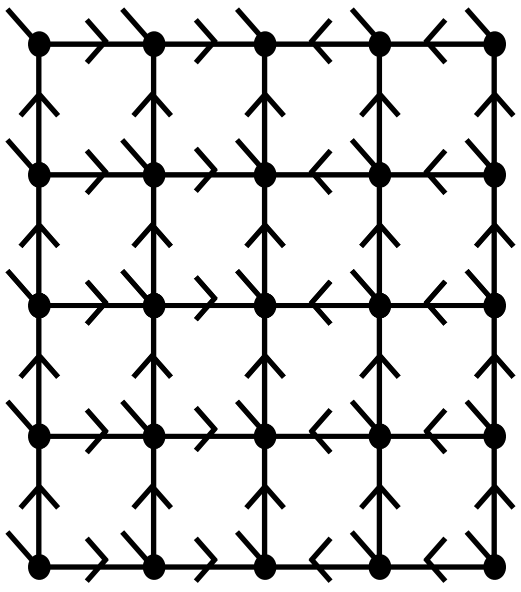
Efficient representation of quantum many-body states

- Brief review of **Matrix-Product States**



- **Isometric Tensor Network States in 2D:** Tensor-network state ansatz that allows for efficient contractions

  [Zaletel and FP; arXiv:1902.05100]



Entanglement

Generic quantum state has a d^L dimensional Hilbert space

$$|\psi\rangle = \sum_{j_1, j_2, \ldots, j_L} \psi_{j_1, j_2, \ldots, j_L} |j_1\rangle |j_2\rangle \ldots |j_L\rangle \ , \ j_n = 1 \ldots d$$

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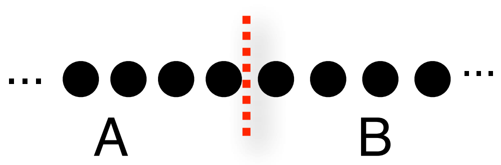
Decompose a pure state into a superposition of product states (**Schmidt decomposition**)



$$|\psi\rangle = \sum_{i,j} C_{i,j} |i\rangle_A \otimes |j\rangle_B = \sum_{\alpha} \Lambda_\alpha |\alpha\rangle_A \otimes |\alpha\rangle_B$$

with $\langle \alpha | \alpha' \rangle = \delta_{\alpha\alpha'}$

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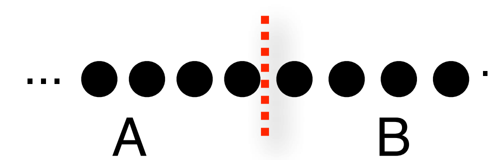

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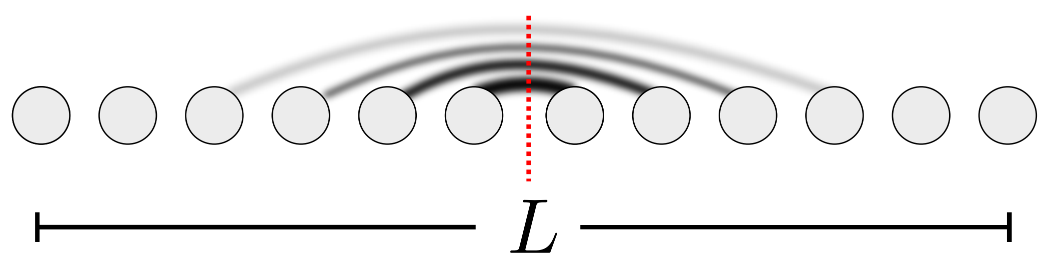
Entanglement entropy as a measure for the amount of entanglement $S = -\sum_\alpha \Lambda_\alpha^2 \log \Lambda_\alpha^2$

Entanglement

Area law for ground states of local (gapped) Hamiltonians in 1D systems

$S(L) = \text{const.}$ [Srednicki '93, Hastings '07]



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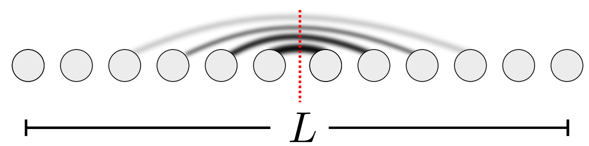

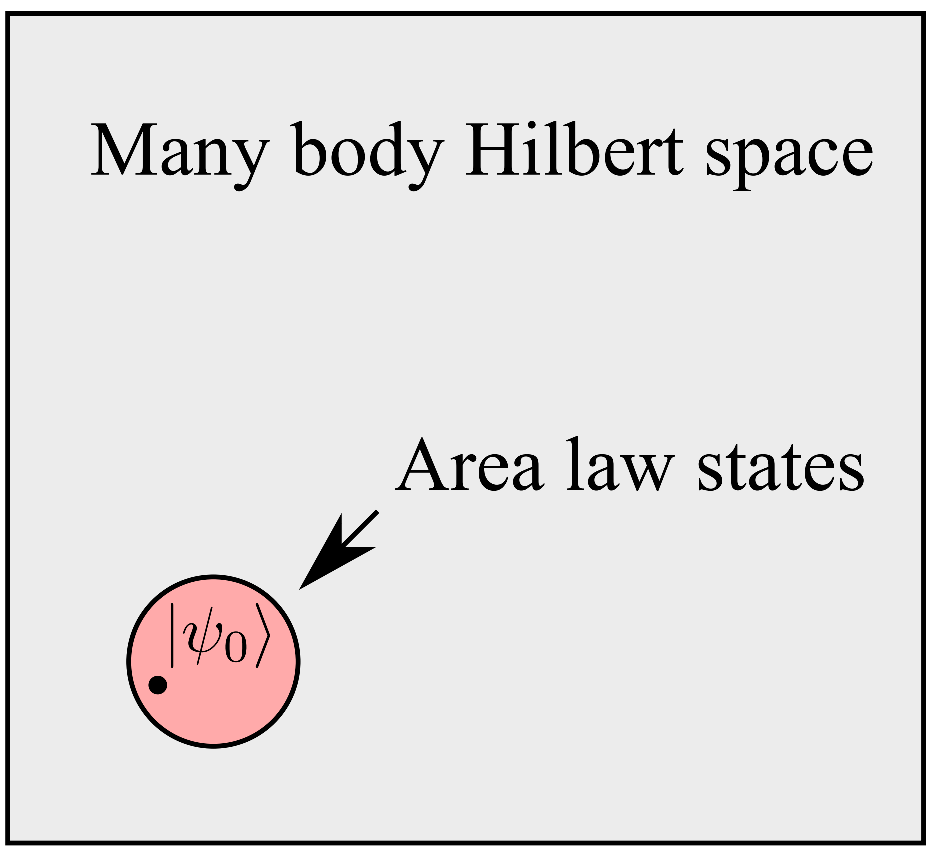

All ground states live in a tiny corner of the Hilbert space!

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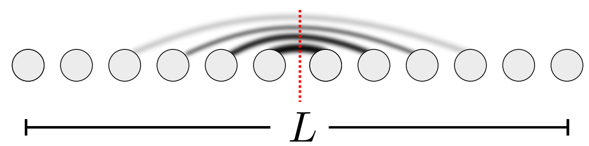
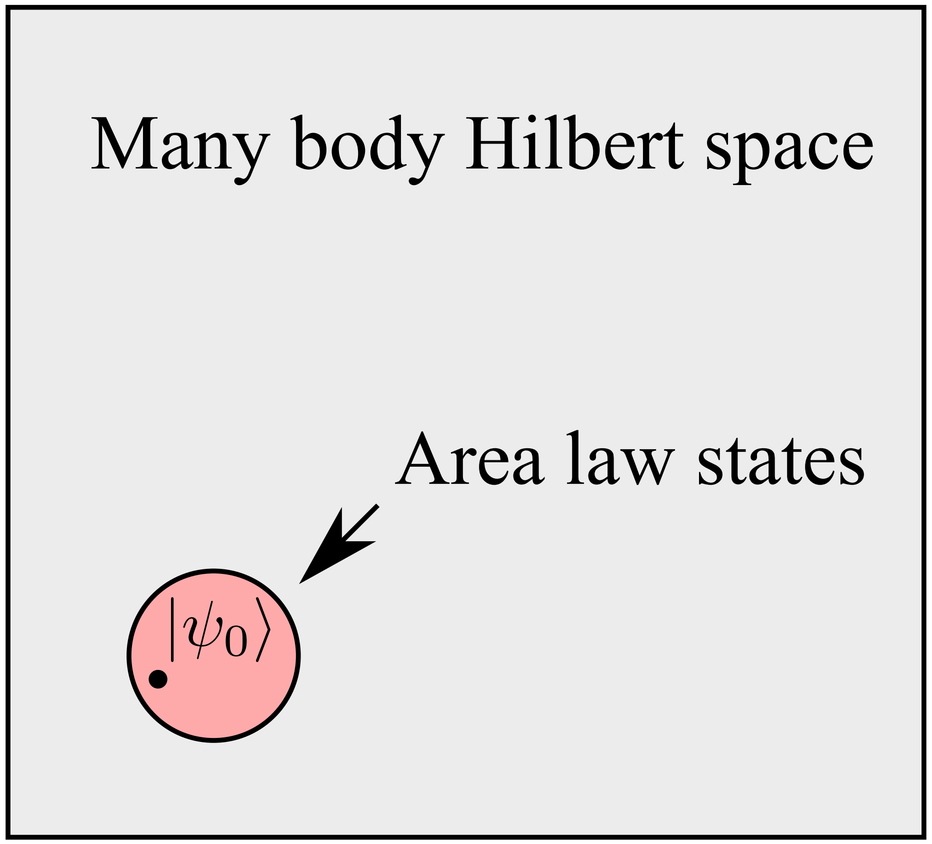
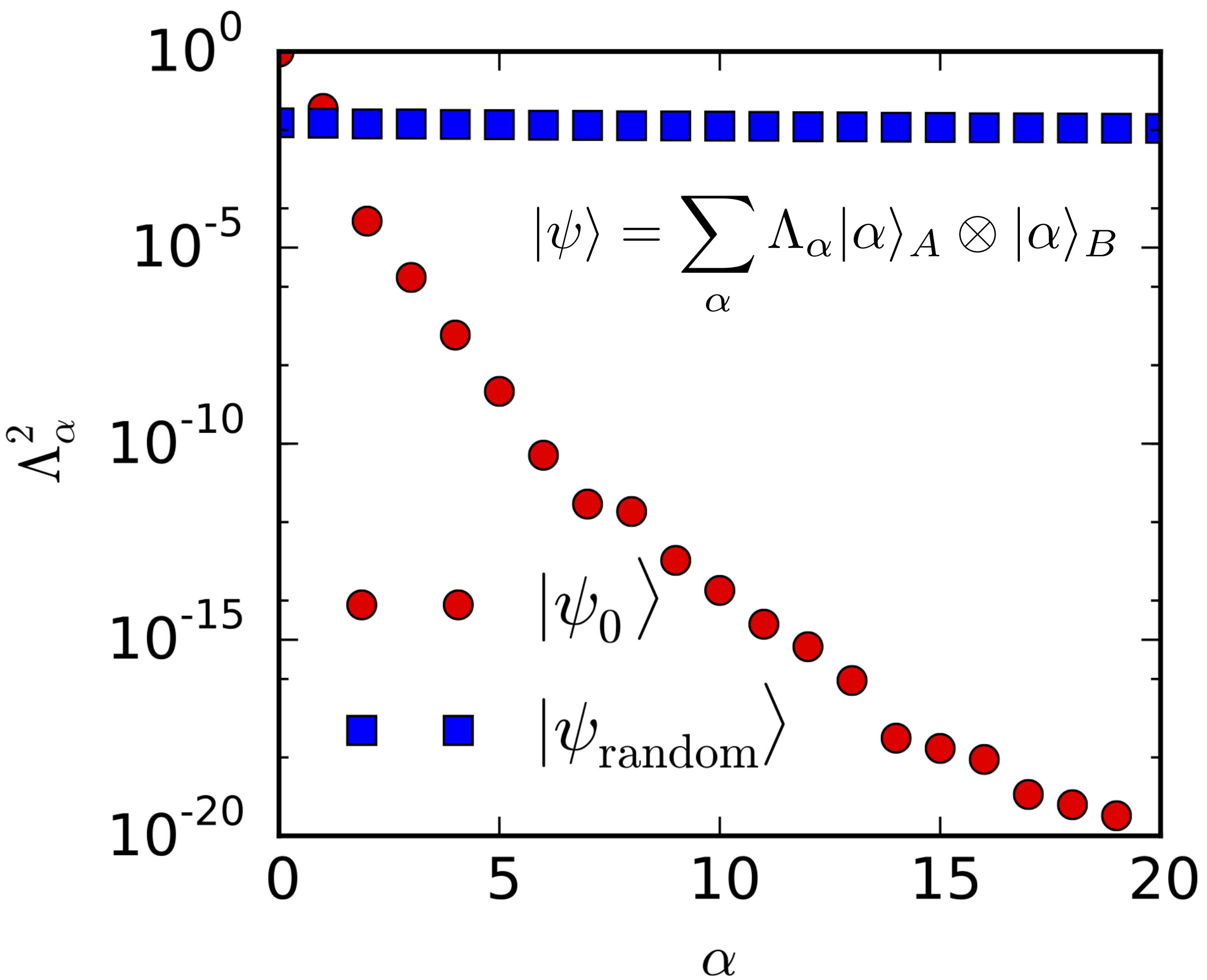




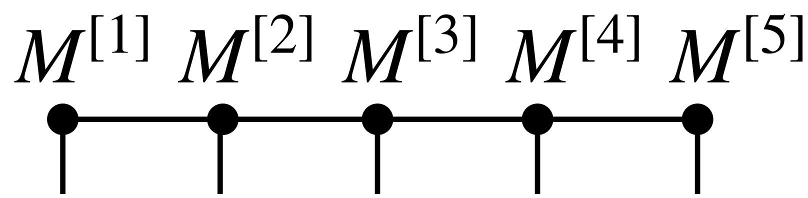


All ground states live in a tiny corner of the Hilbert space!

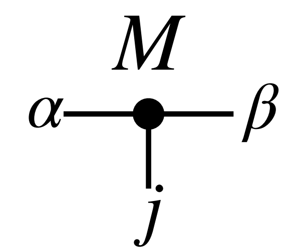
Matrix-Product States

Matrix-product states (MPS): Reduction of the number of variables: $d^L \to Ld\chi^2$ [M. Fannes et al. 92]

$\psi_{j_1,j_2,j_3,j_4,j_5} =$



$M^j_{\alpha,\beta} =$



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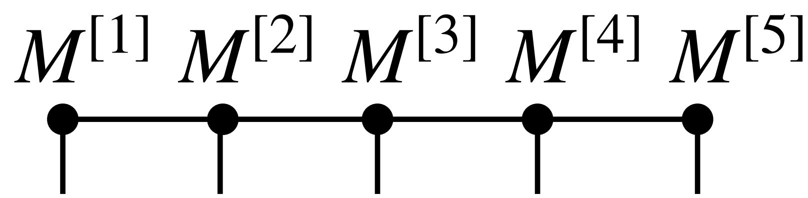

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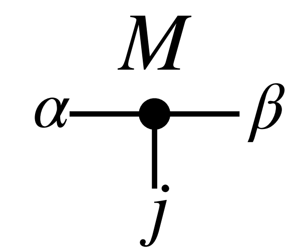

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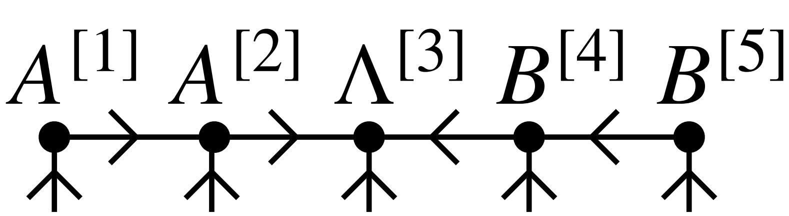
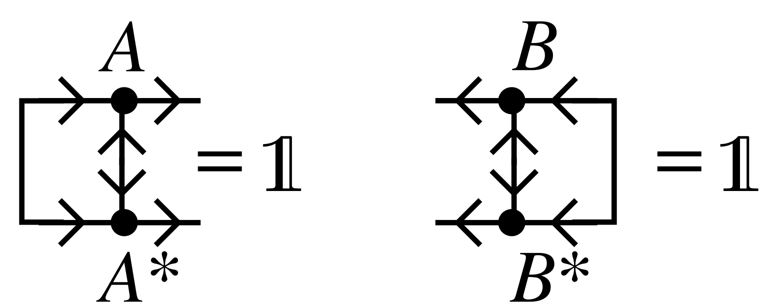
Canonical form: Use the gauge degree of freedom ($A^j = XM^jX^{-1}$) to find a convenient representation





(Isometries)

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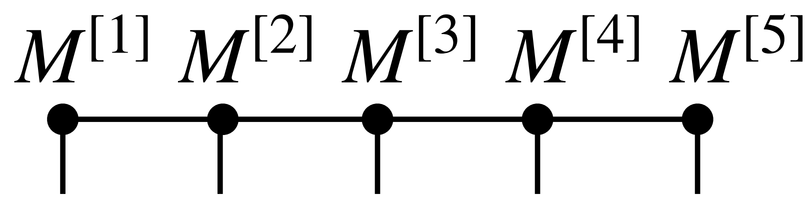

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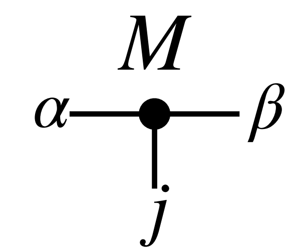

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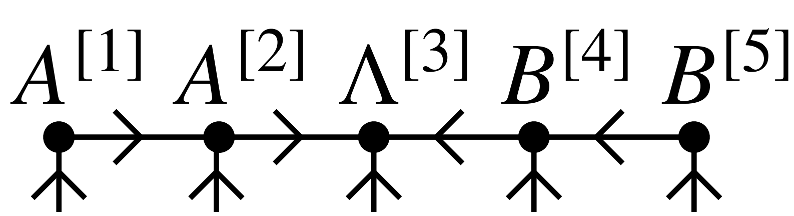
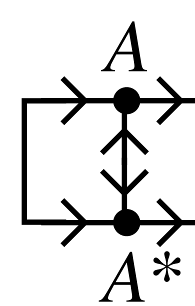
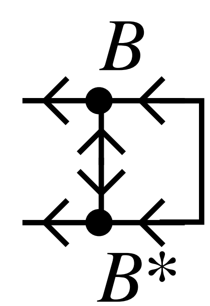




$= \mathbb{1}$



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(Isometries)

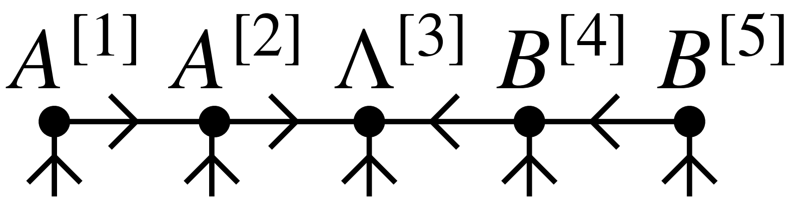
Center matrix Λ represents wave function

$$|\psi\rangle = \sum_{\alpha,\beta,j} \Lambda^j_{\alpha,\beta} |\alpha\rangle |j\rangle |\beta\rangle$$

(orthogonal states $|j\rangle$, $|\alpha\rangle$, $|\beta\rangle$)

Density Matrix Renormalization Group

Moving the center matrix: $\Lambda^{\ell} B^{[\ell+1]} = A^{[\ell]} \Lambda^{[\ell+1]}$ accomplished by an **orthogonal factorization** (e.g. QR or SVD)



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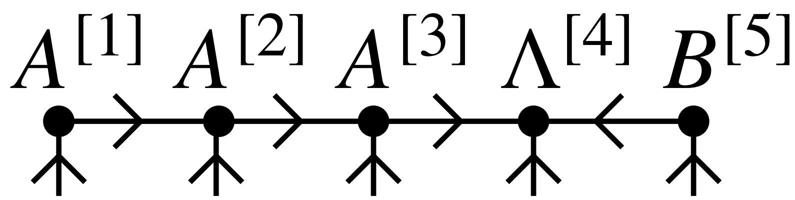

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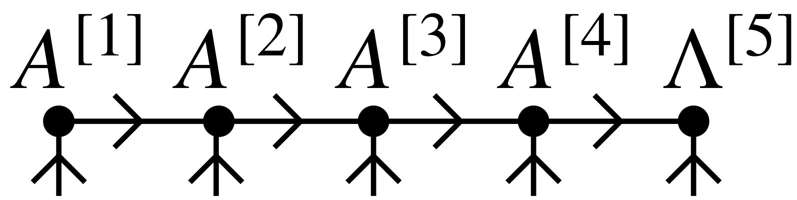

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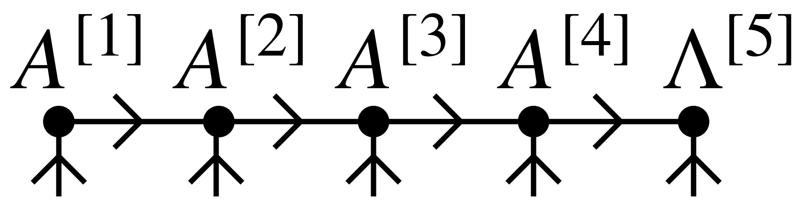
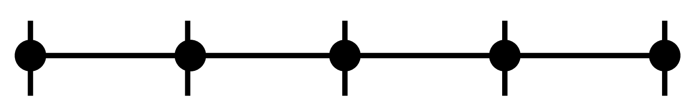


Find the **ground state** iteratively



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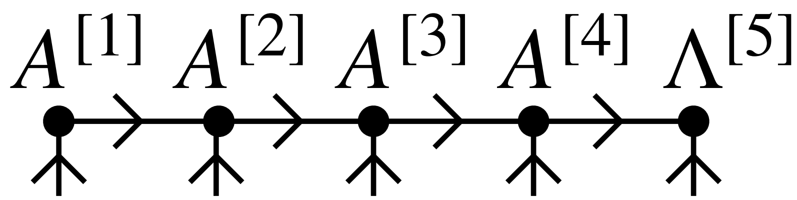

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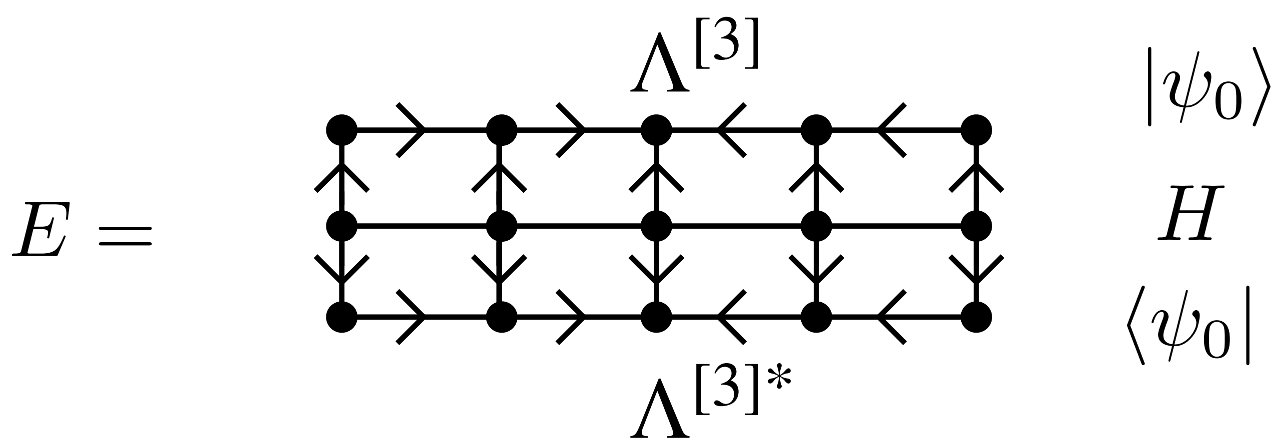

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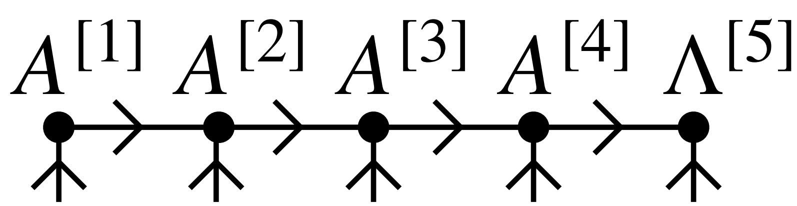

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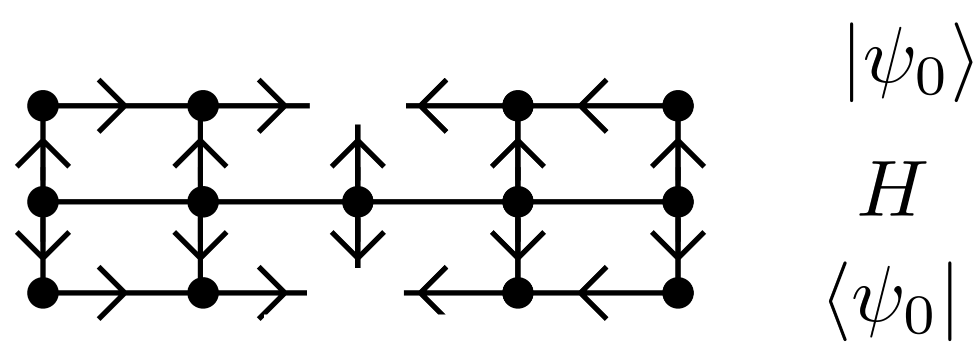
$$H_{\alpha i \beta;\alpha' i' \beta'} =$$



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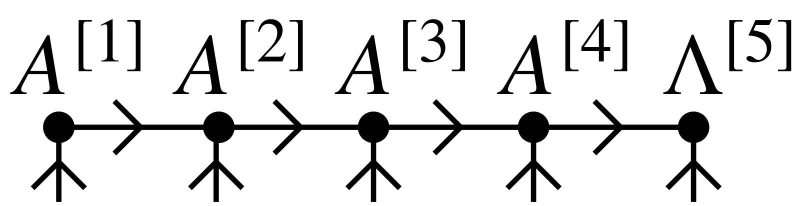

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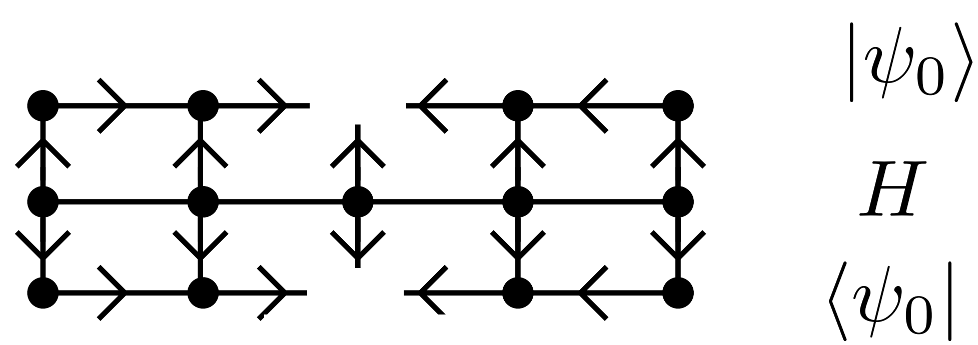


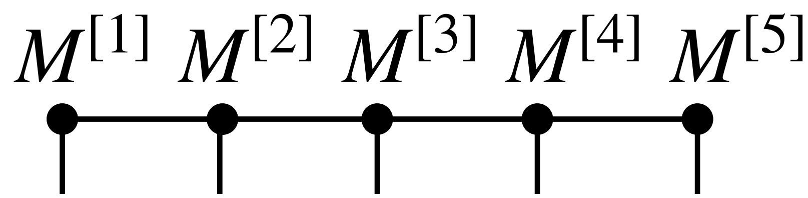
Locally minimize the energy of $H_{\alpha i \beta; \alpha' i' \beta'}$ (e.g., Lanczos)

Density matrix renormalization group (DMRG) [White '92, Schollwoeck '11]

Tensor Network States in 2D

MPS capture 1D area law → Exponential scaling in 2D

$$\psi_{j_1,j_2,j_3,j_4,j_5} \approx$$



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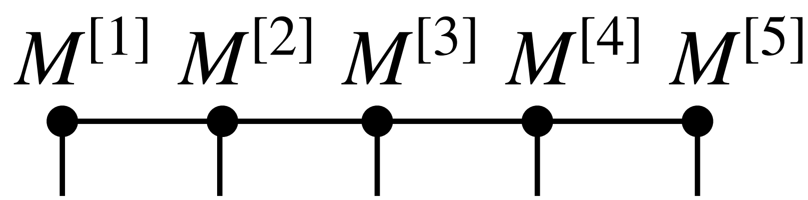

How to generalize the MPS approach to 2D?

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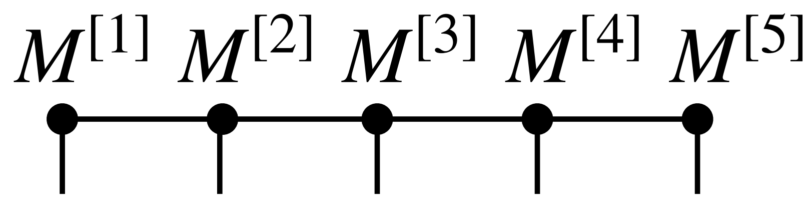

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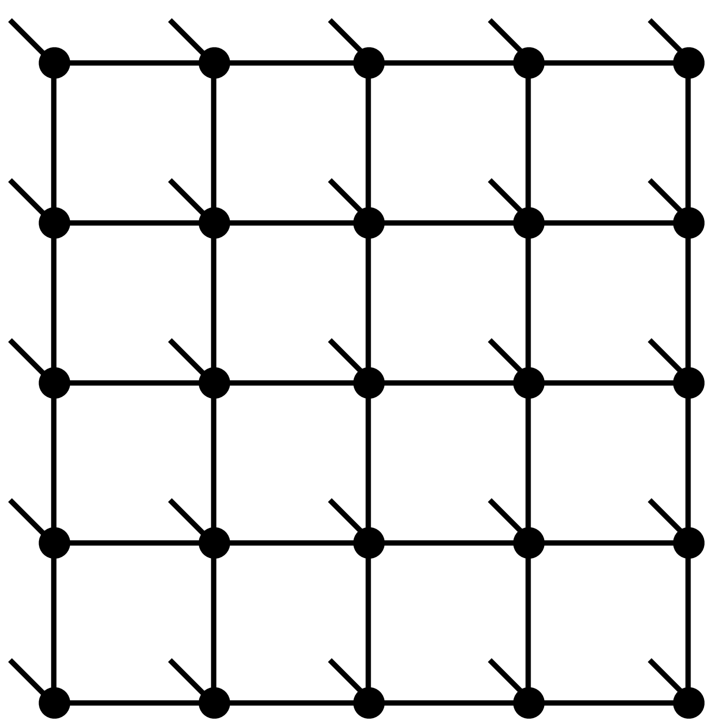
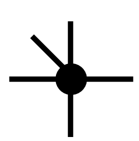


- Tensor Network States (TNS)
  [Maeshima et al. '01, Verstraete and Cirac '04]

$T^j_{\alpha,\beta,\gamma,\delta} =$



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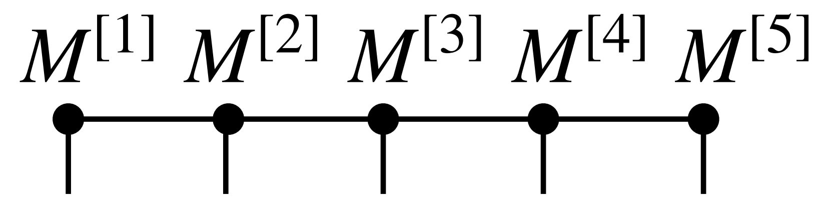

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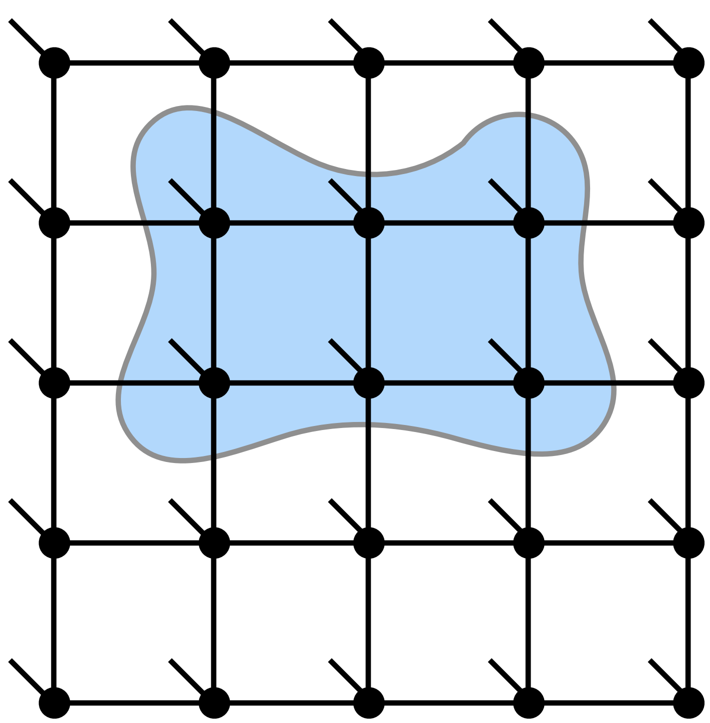

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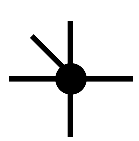
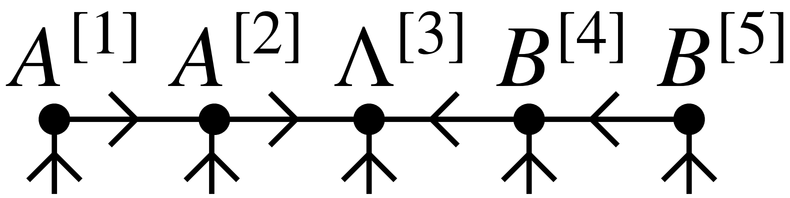
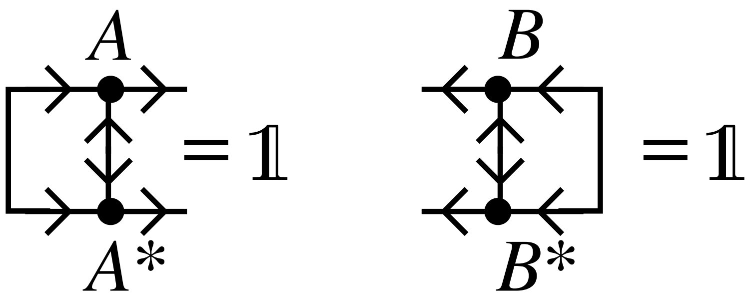


- **Tensor Network States (TNS)**
  [Maeshima et al. '01, Verstraete and Cirac '04]
- **Capture 2D area law** 😊
- Difficult to handle numerically:
  Exact contraction of the 2D network is still **exponentially hard** 🙁

Isometric Tensor Network States in 2D

Recall: Canonical form of 1D MPS





(Isometries)

[Zaletel and FP; arxiv:1902.05100]

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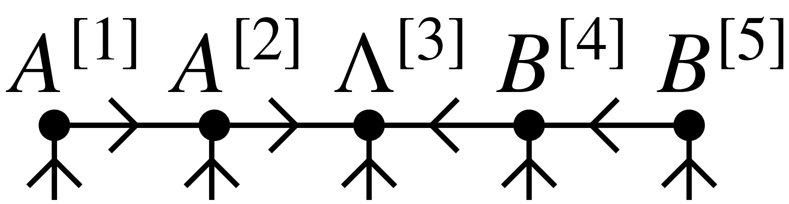

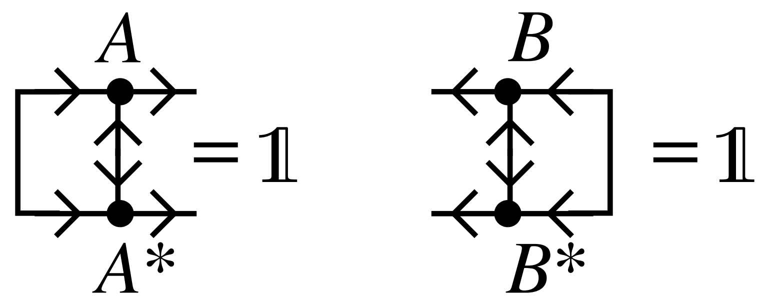

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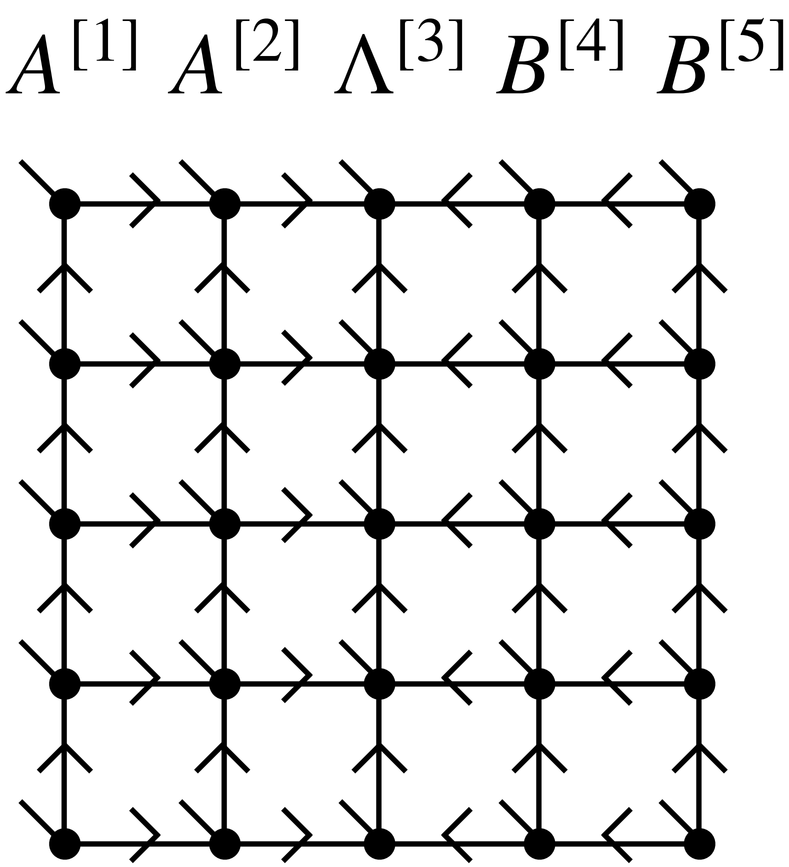
Isometric TNS



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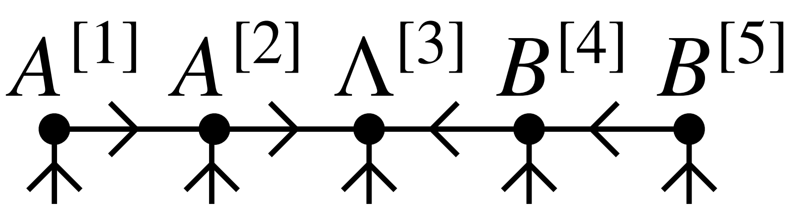

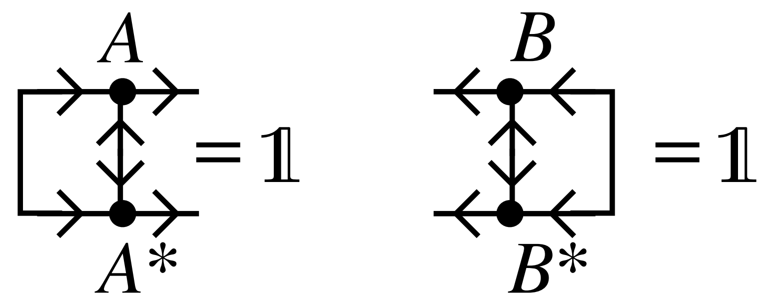

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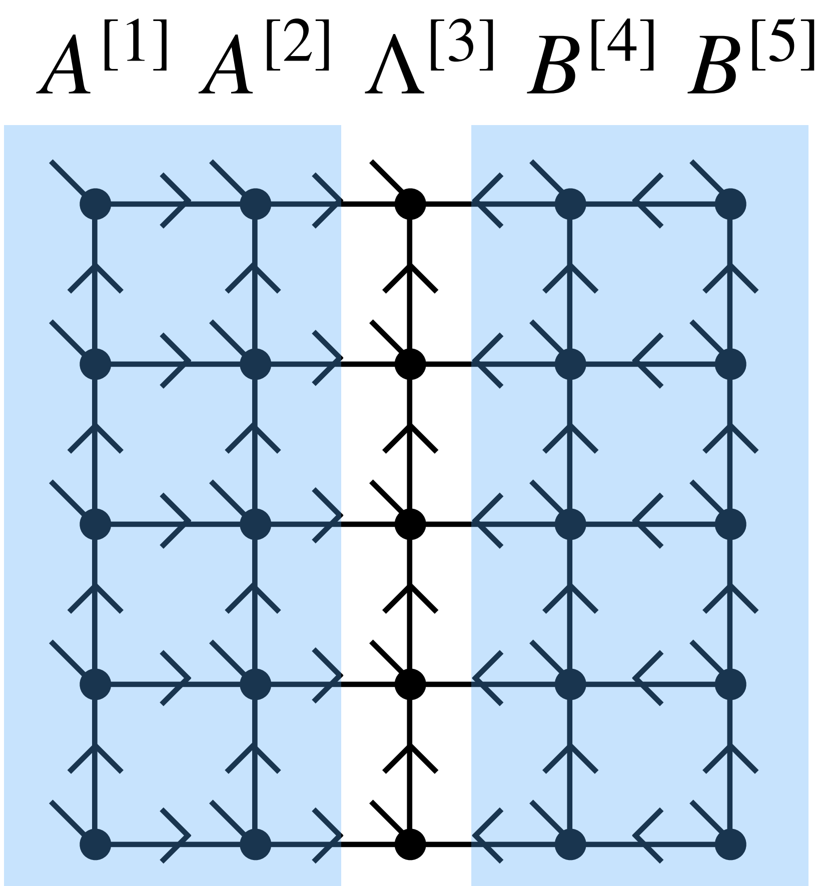
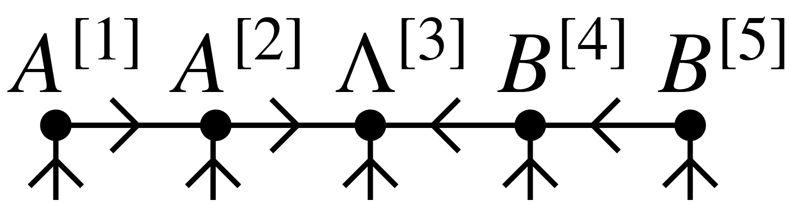


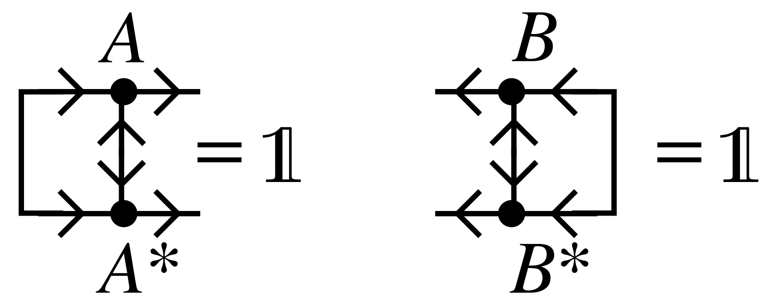
- Isometric tensors are **efficiently contractable**

[Zaletel and FP; arxiv:1902.05100]

Isometric Tensor Network States in 2D

Recall: **Canonical form of 1D MPS**





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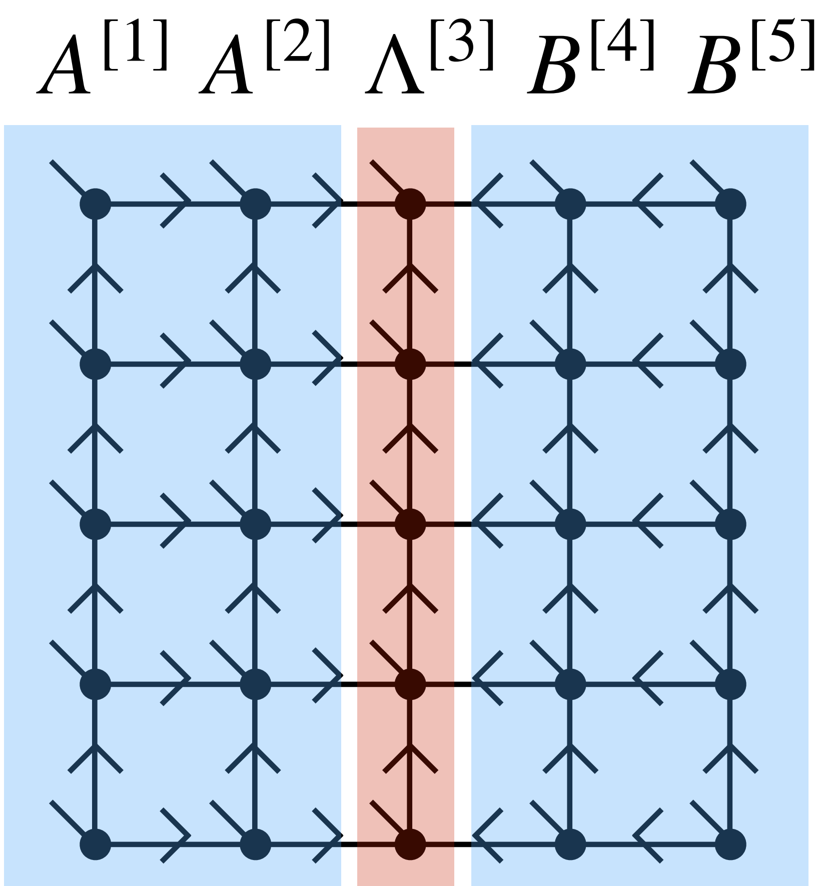
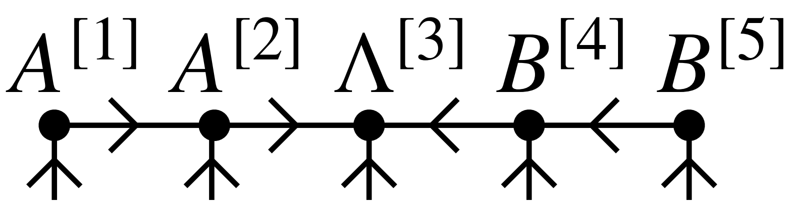


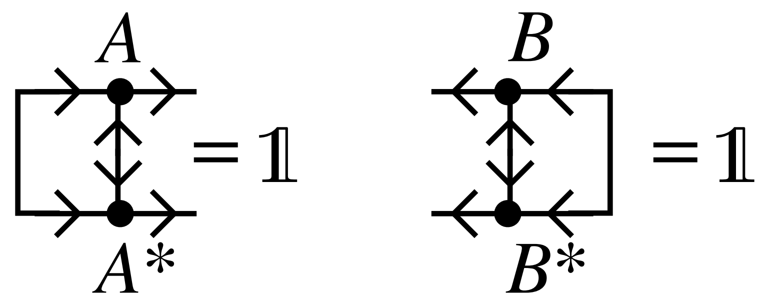
- Isometric tensors are **efficiently contractable**
- Orthogonality center column is a **1D MPS**: Standard DMRG techniques

[Zaletel and FP; arxiv:1902.05100]

Isometric Tensor Network States in 2D

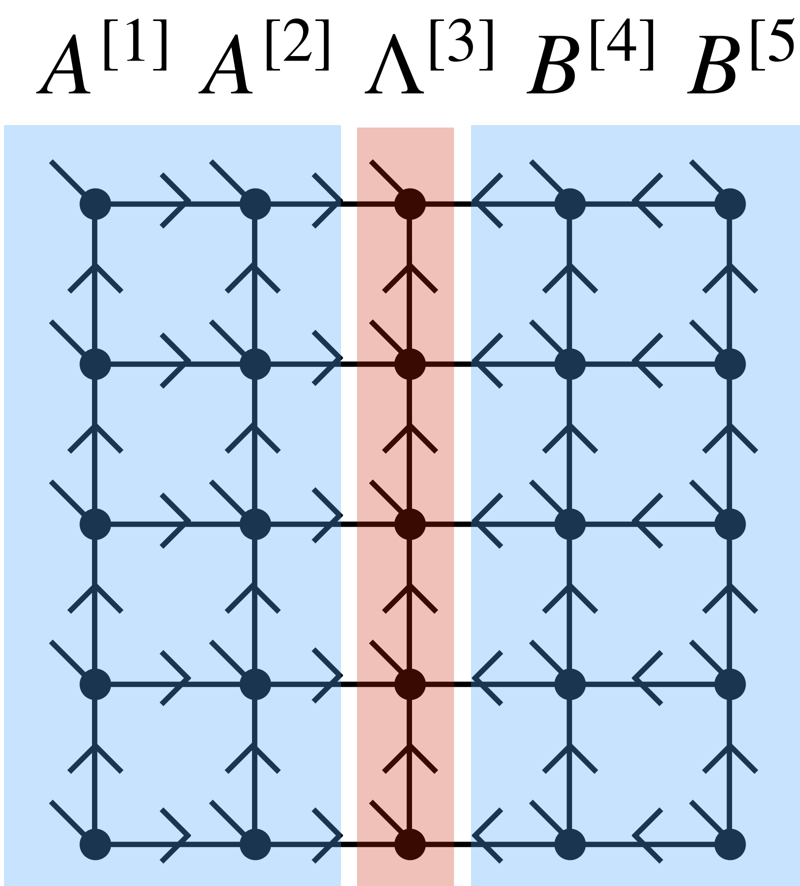
Recall: **Canonical form of 1D MPS**





(Isometries)

Isometric TNS



- Isometric tensors are **efficiently contractable**
- Orthogonality center column is a **1D MPS**: Standard DMRG techniques
- **Subset of TNS: Unclear what its variational power is!**

[Zaletel and FP; arxiv:1902.05100]

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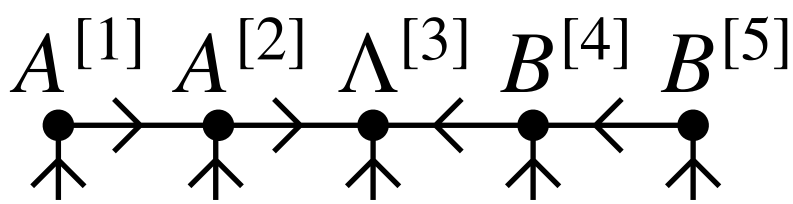

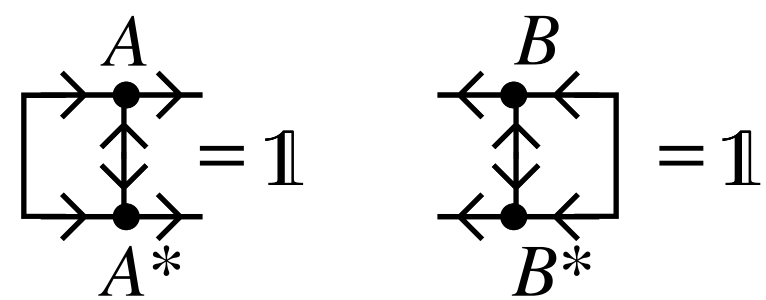

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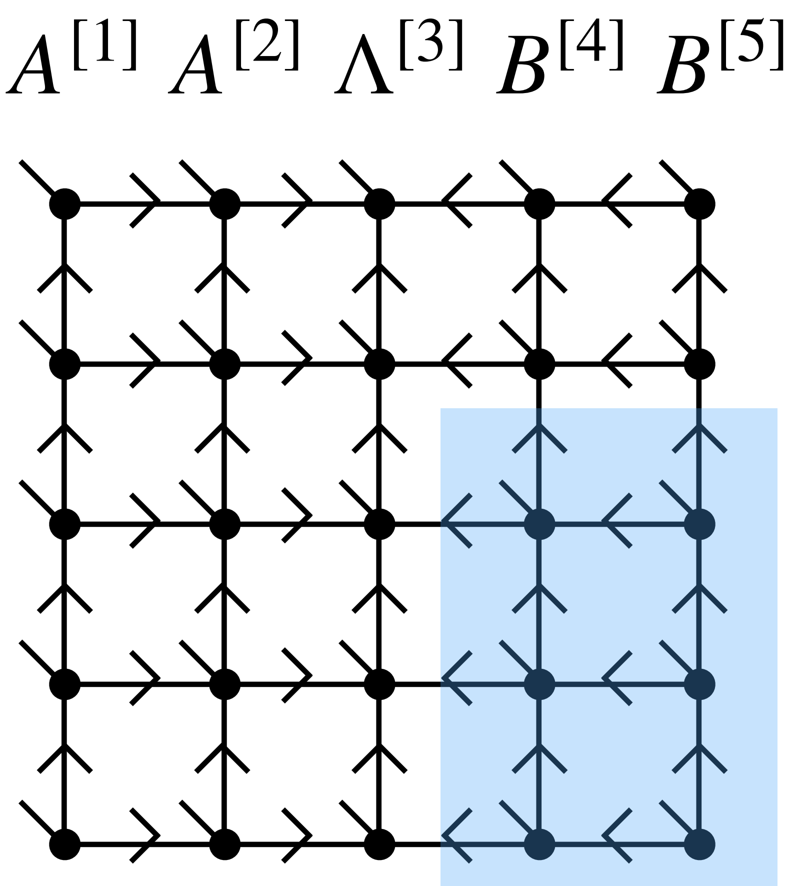

- **Subregions** with only outgoing arrows have isometric boundary maps
- **Causal structure**: time flows opposite to the direction of the arrows

[Zaletel and FP; arxiv:1902.05100]

Isometric Tensor Network States in 2D

How to shift the orthogonality center?

Recall: 1D MPS $\Lambda^{\ell} B^{[\ell+1]} = A^{[\ell]} \Lambda^{[\ell+1]}$ solved by QR or SVD

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Not possible for 2D TNS as it would destroy the locality of Λ

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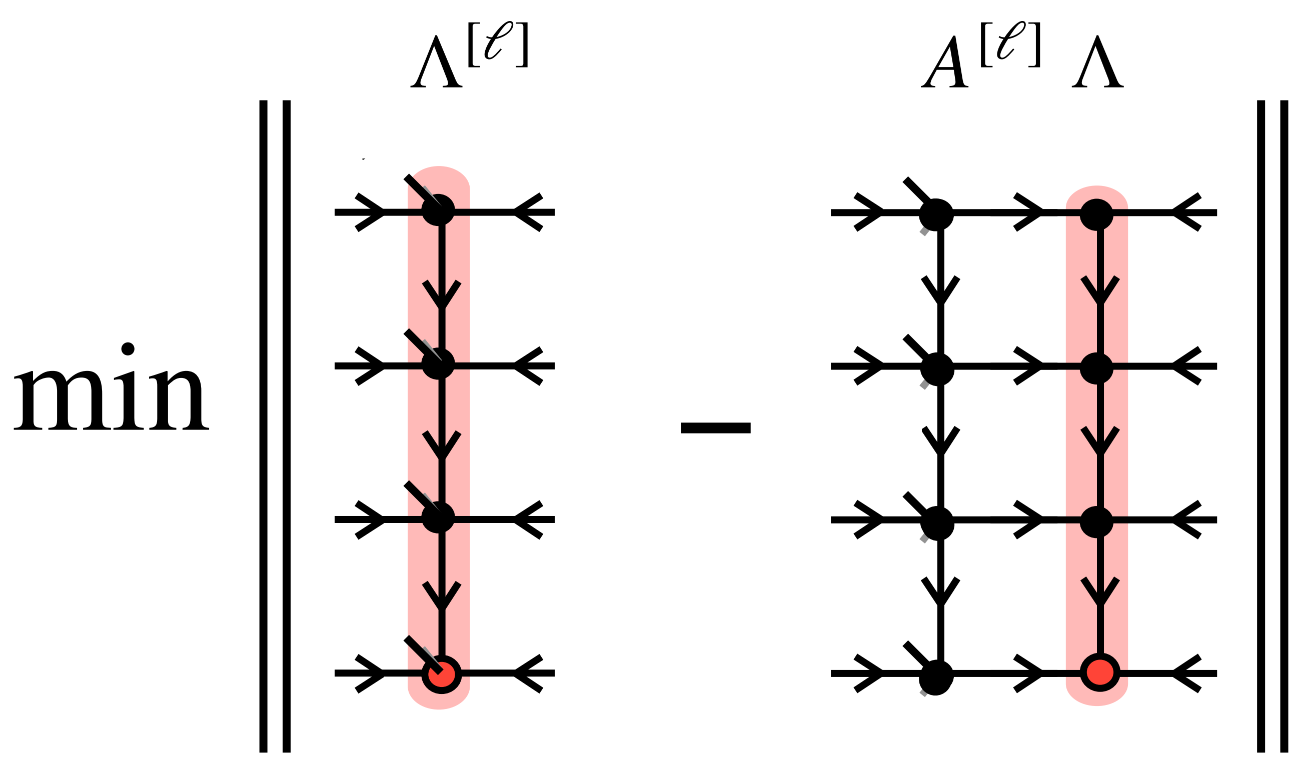

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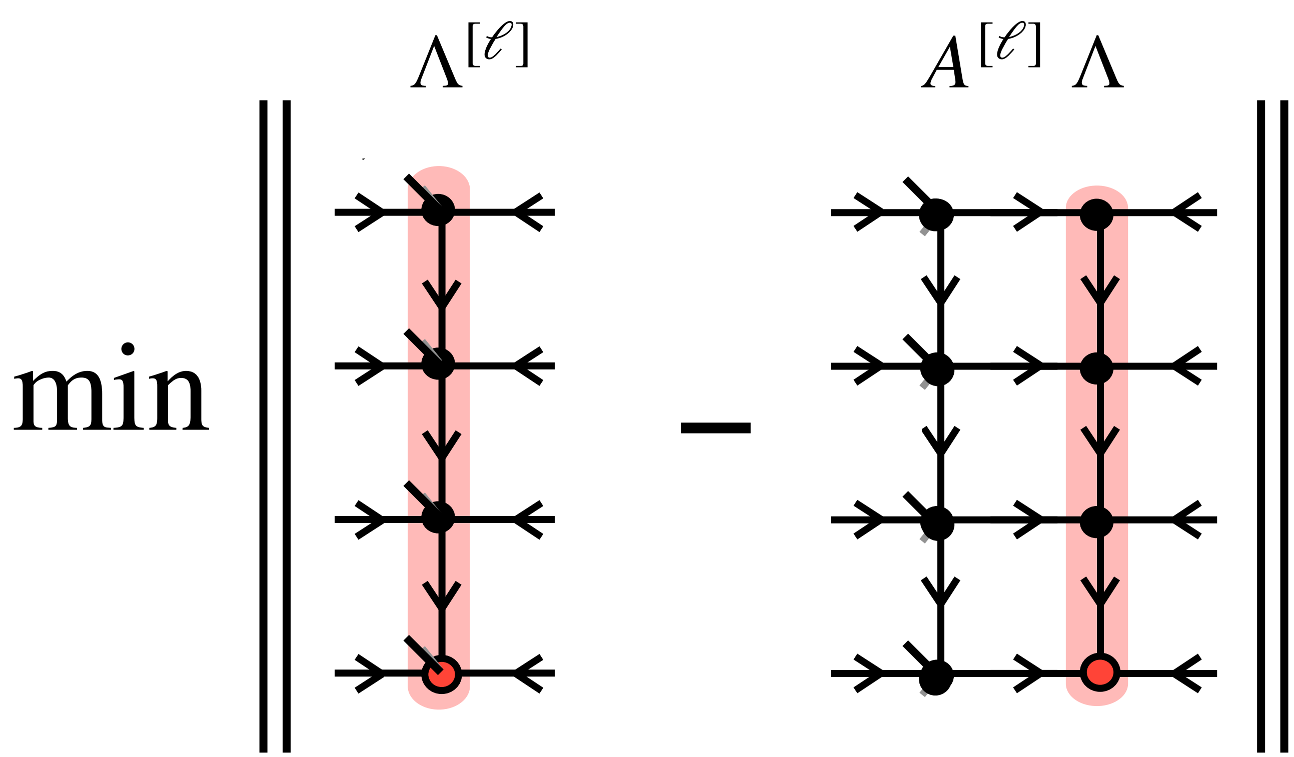

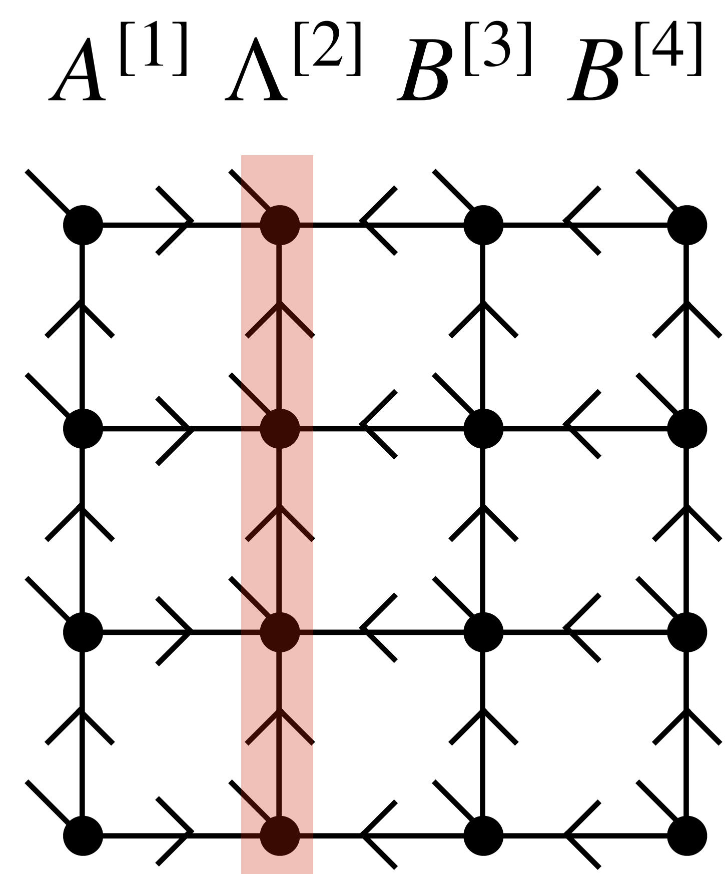

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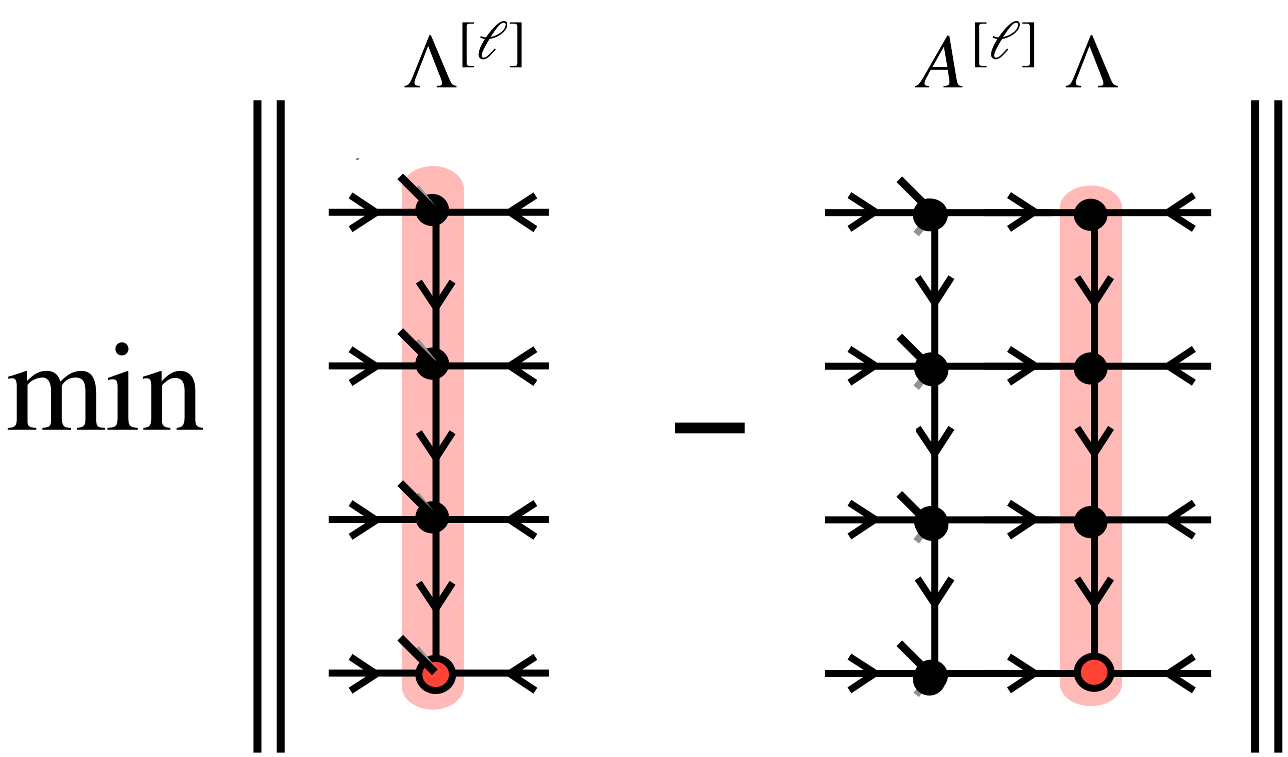
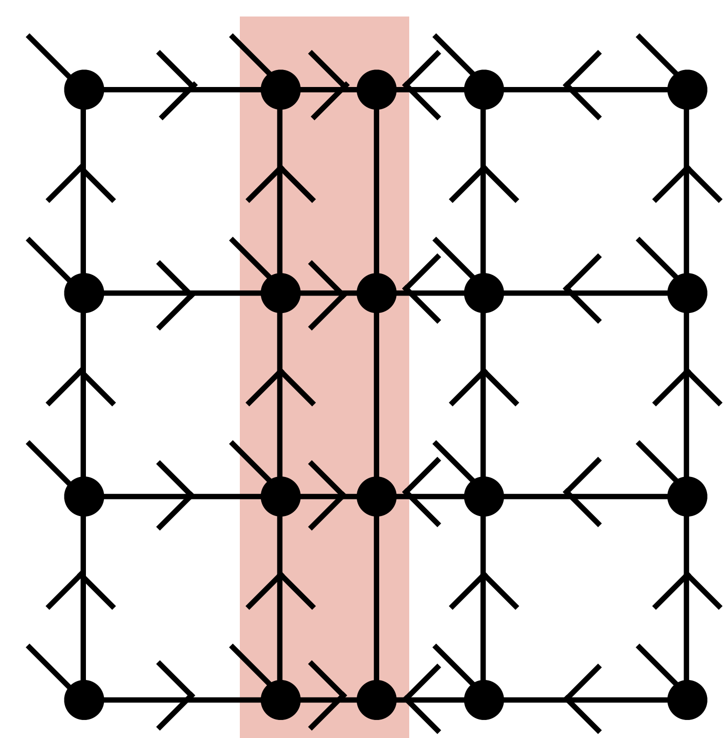


$A^{[1]} \; A^{[2]} \Lambda B^{[3]} \; B^{[4]}$



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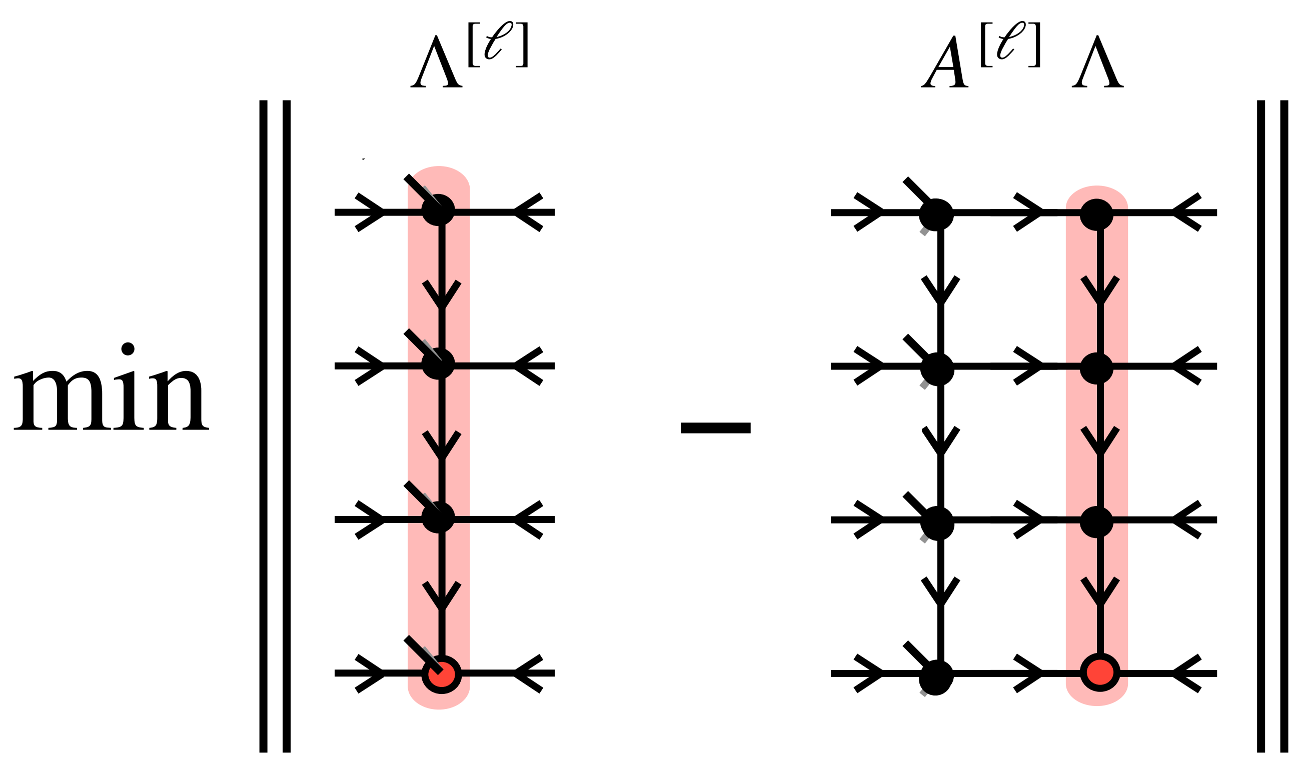
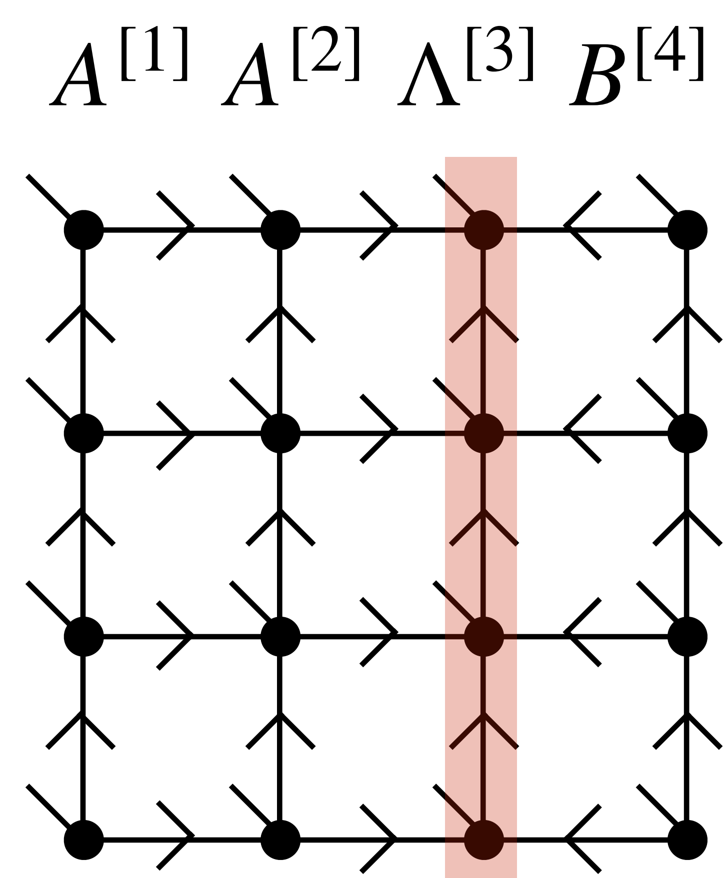
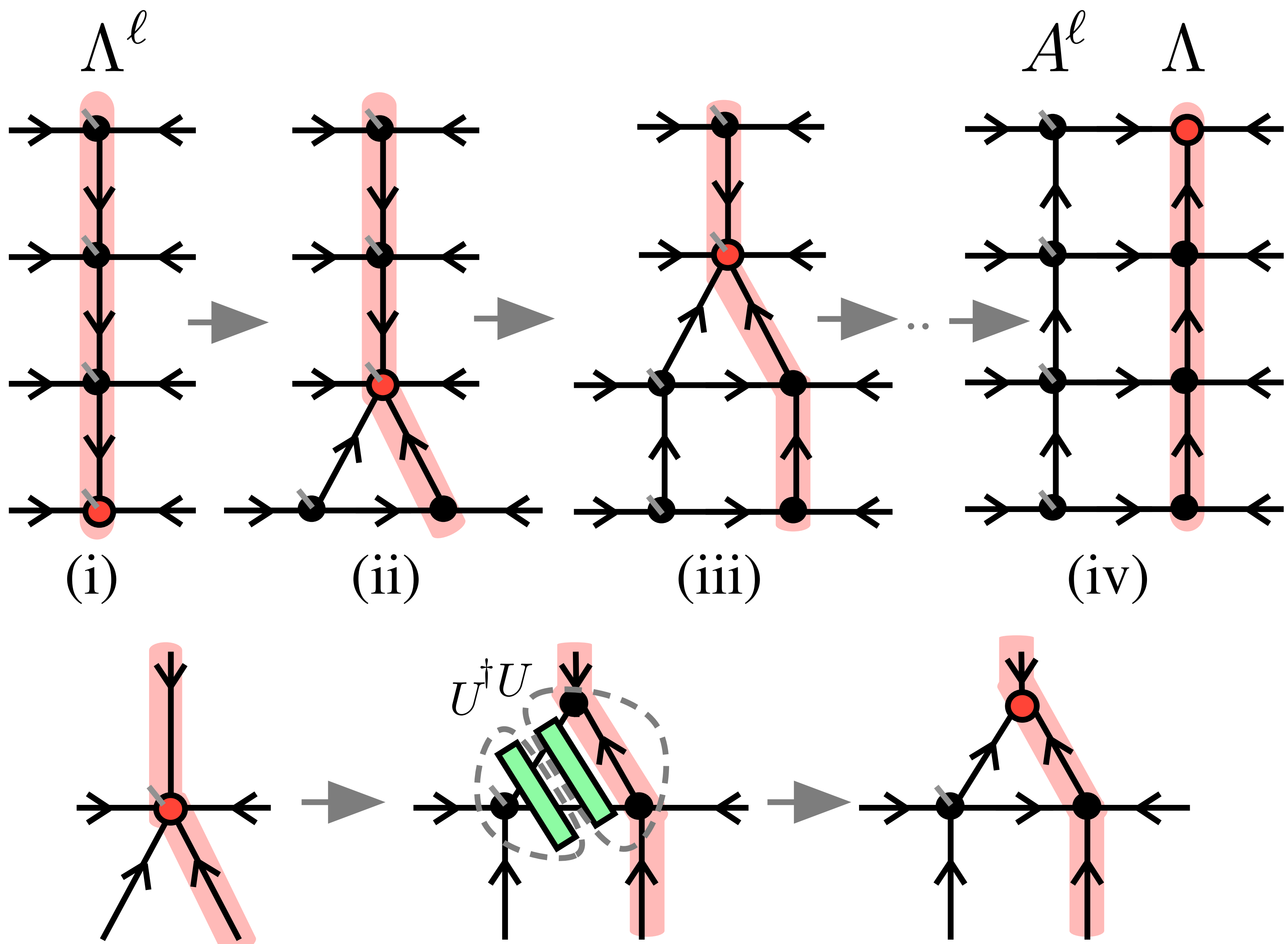




[Zaletel and FP; arxiv:1902.05100]

Isometric Tensor Network States in 2D

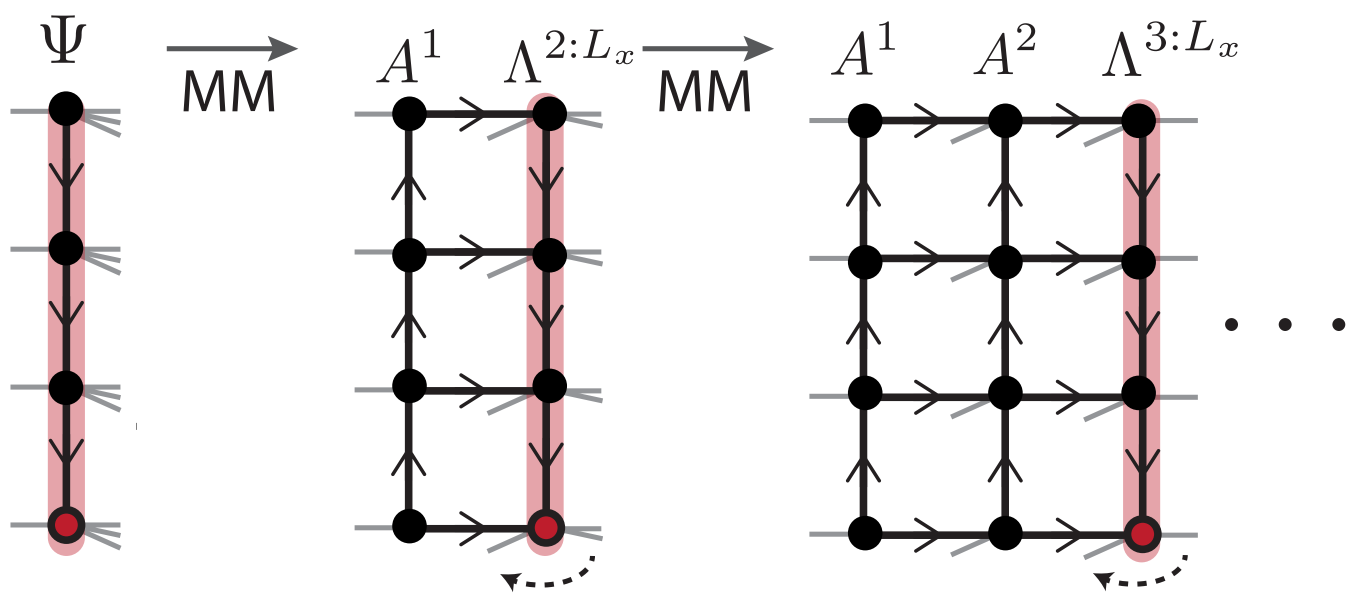
Sequential splitting based on disentangling: **"Moses Move" (MM)**



[Zaletel and FP; arxiv:1902.05100]

Convert quasi 1D MPS to isometric TNS

"Peel off" layers from MPS representation of 2D state



- Sequentially disentangle the state
- Efficient compression

[Zaletel and FP; arxiv:1902.05100]

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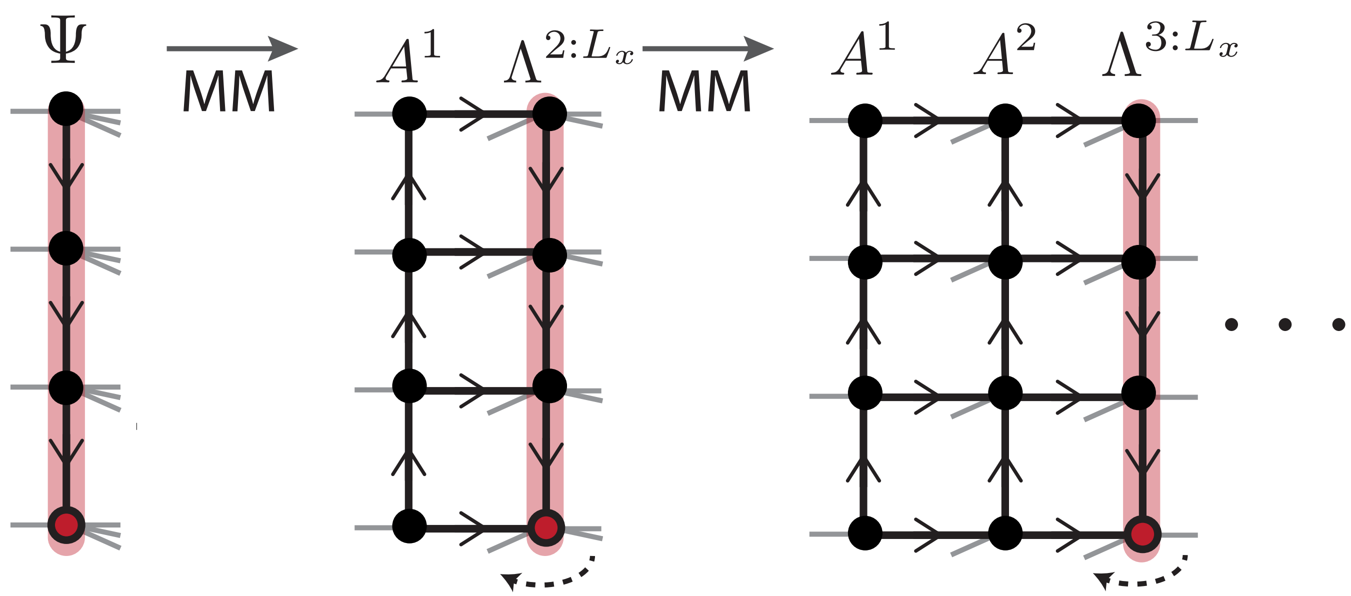
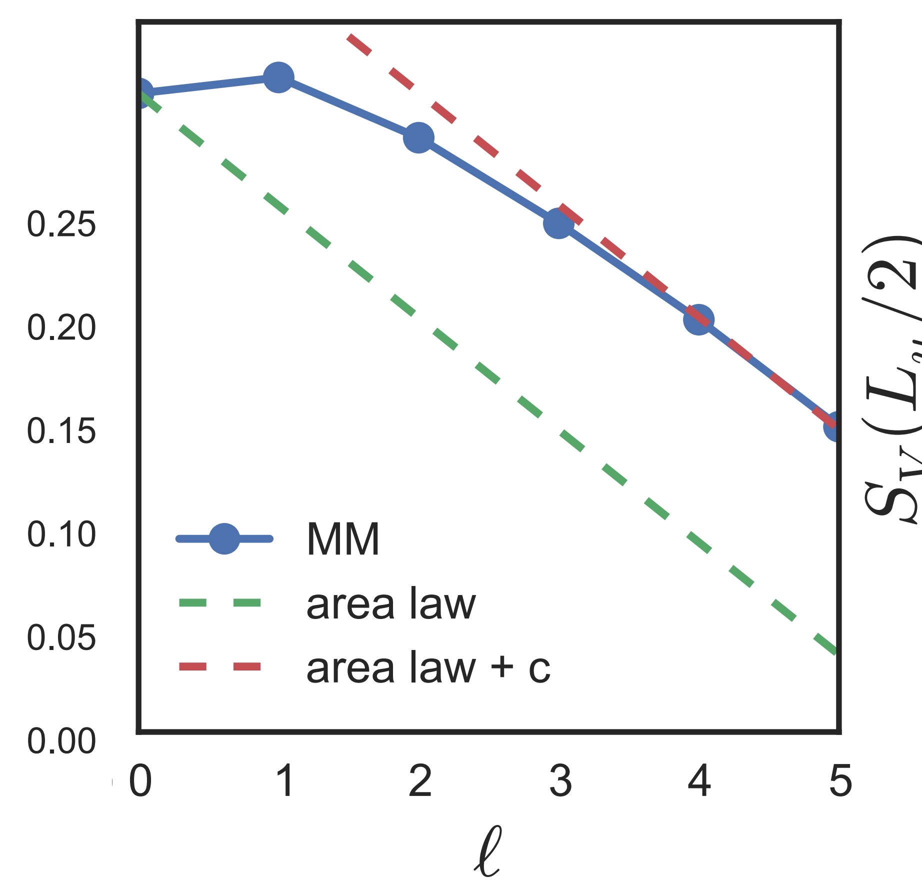


- Sequentially disentangle the state
- Efficient compression

2D transverse field Ising Model ($g = 3.5$)

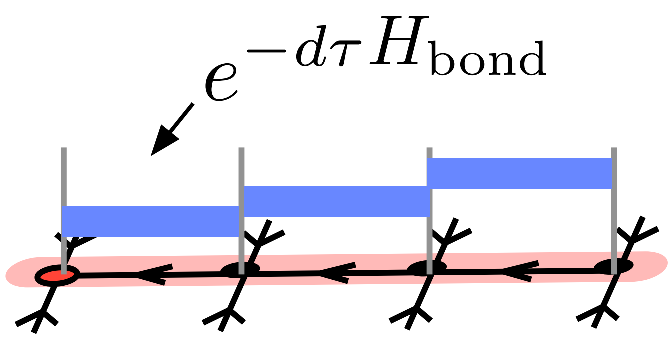
$$H = -\sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - g \sum_i \sigma^x$$

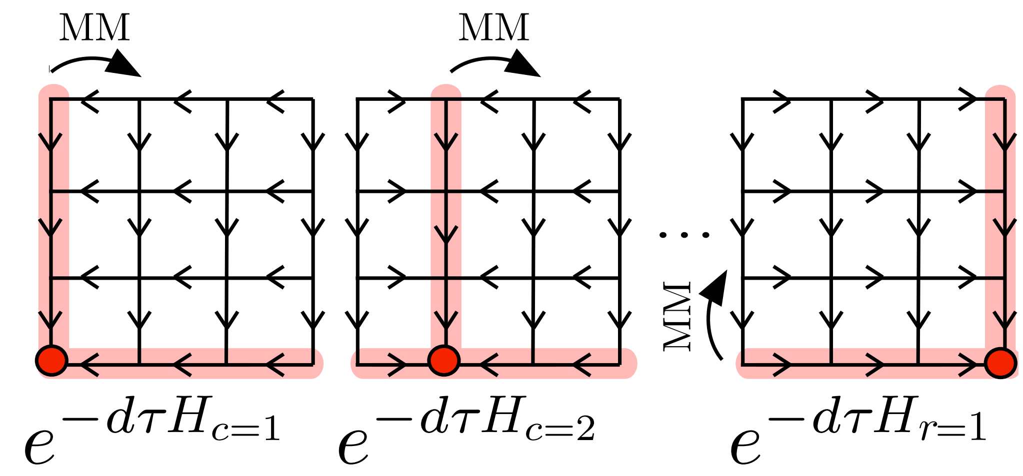


[Zaletel and FP; arxiv:1902.05100]

Ground states of 2D Hamiltonians

Sequentially apply **1D Time-Evolving Block Decimation (TEBD)** algorithm on the center columns/rows: 2nd order [Vidal '03]





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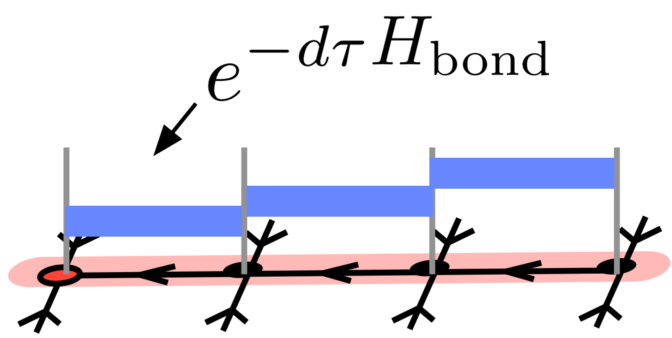

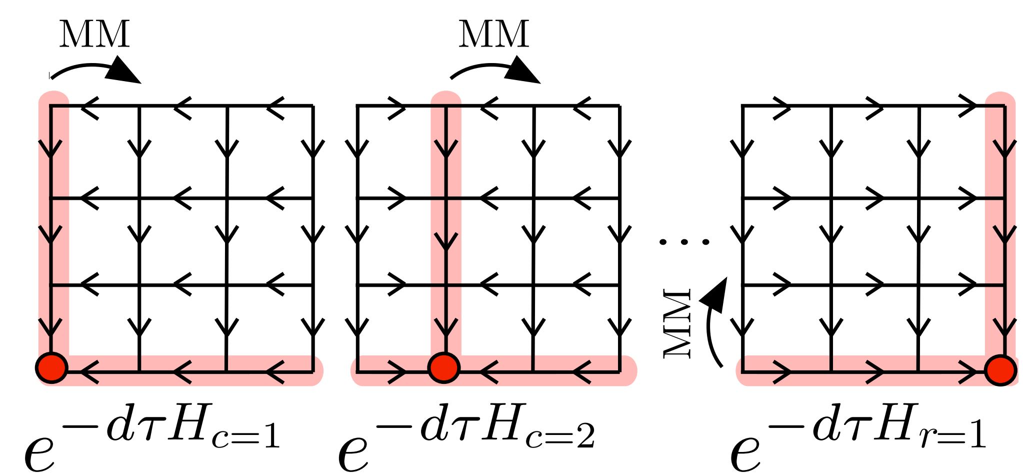

2D transverse field Ising Model ($g = 3.5$)

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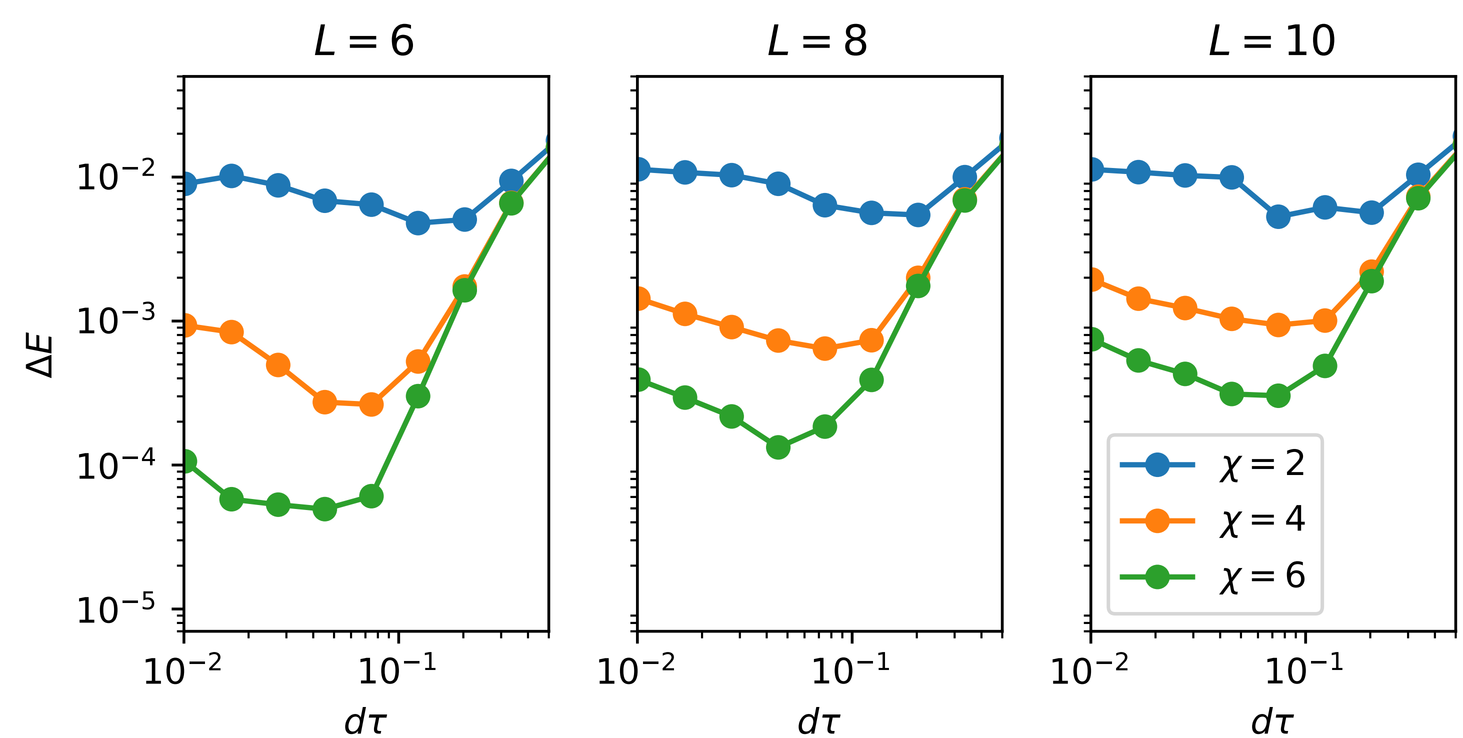
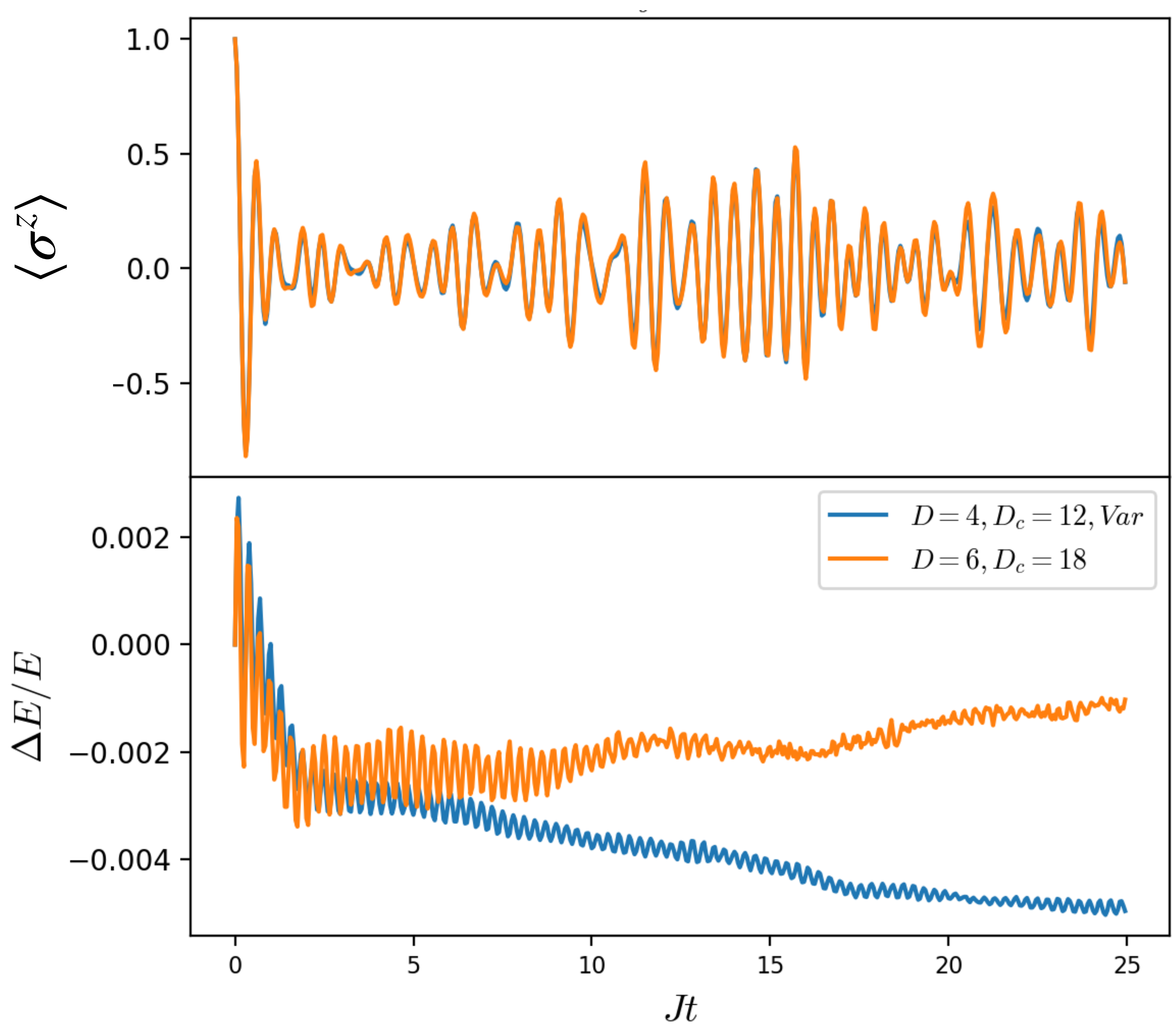
Imaginary time evolution: $|\psi_0\rangle$

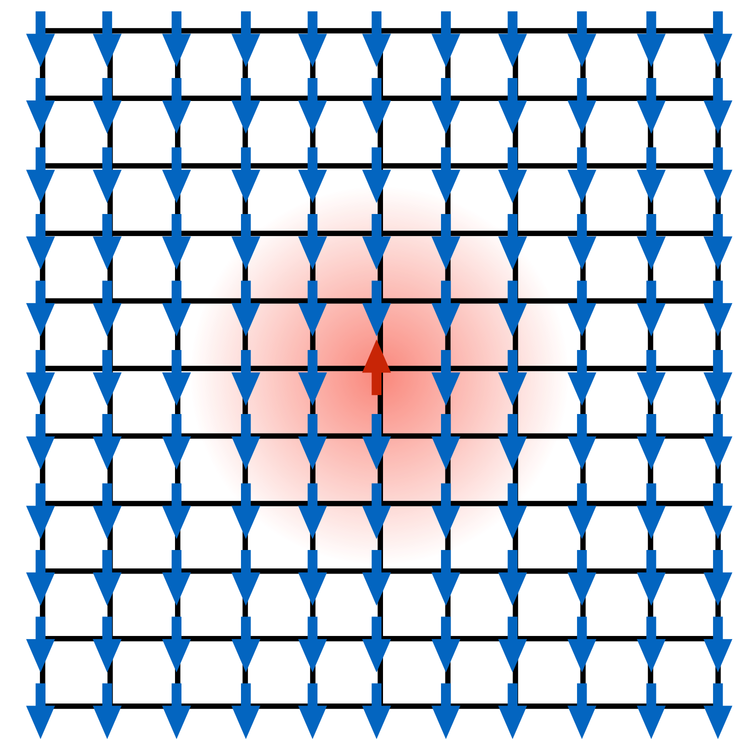


[Zaletel and FP; arxiv:1902.05100]

Real time evolution of 2D Hamiltonians

Real time evolution of $|\psi_0(t)\rangle = e^{-iHt}\,\sigma^+|\psi_0\rangle$ for the transverse field Ising model (paramagnetic phase)

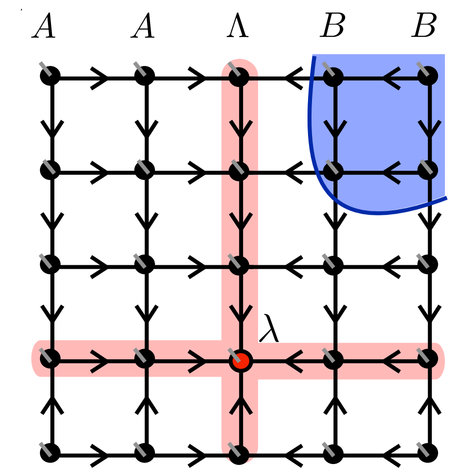




- Good convergence at small bond dimension χ

[**Lin**, Zaletel and FP; work in progress]

Summary



2D tensor-network state ansatz that allows for efficient contractions

- Subset of TNS: Variational power?
- Sequential splitting based on disentangling Moses Move
- TEBD^2 to obtain ground states and perform time evolution

[Zaletel and FP; arXiv:1902.05100]

Thank You!