Isometric Tensor Network States

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EQUAHUMO Efficient Quantum Algorithms for the Hubbard Model

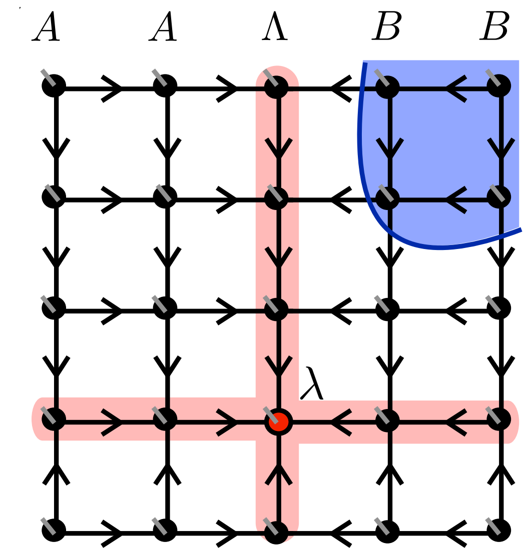
Munich Quantum Valley

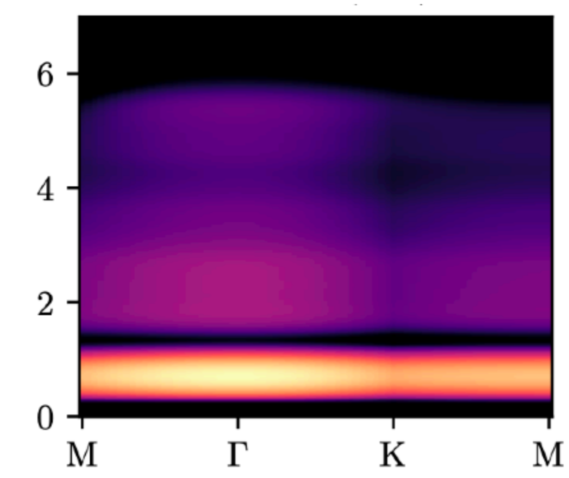
Tensor Networks: Mathematical Structures and Novel Algorithms
Mar. 8th 2023

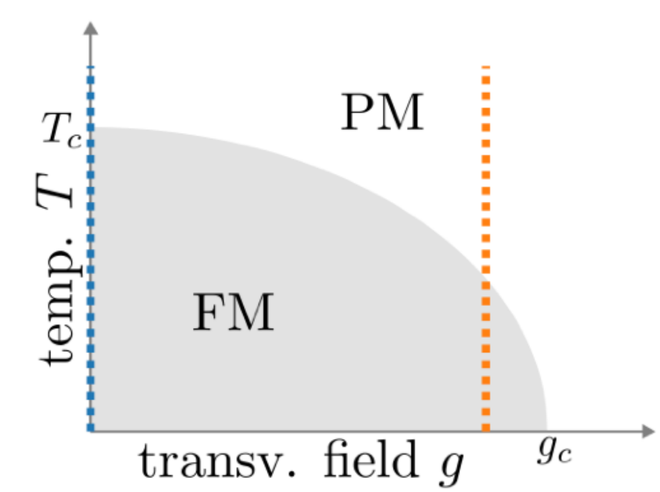
Outline

2D Tensor-Network State ansatz that allows for efficient contractions: isoTNS

- TEBD² to perform time evolution
- DMRG² to obtain ground states
- Purification of isoTNS for thermal states







Matrix-Product States in 1D

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

$$\psi_{j_1,j_2,j_3,j_4,j_5} = \sum_{\alpha_1,\alpha_2,\ldots,\alpha_4}^{\chi} M^{j_1}_{\alpha_1} M^{j_2}_{\alpha_1,\alpha_2} M^{j_3}_{\alpha_2,\alpha_3} M^{j_4}_{\alpha_3,\alpha_4} M^{j_5}_{\alpha_4}$$

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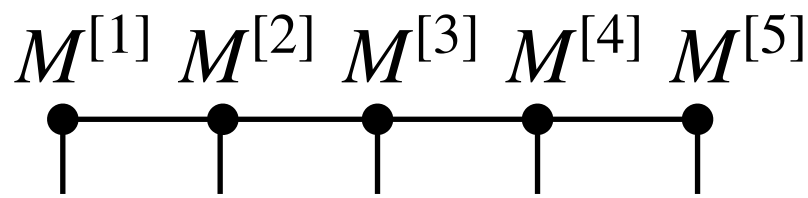
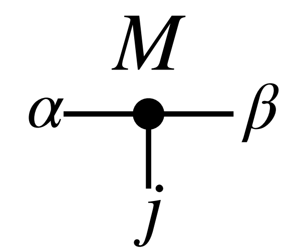


$M^j_{\alpha,\beta} =$



$\alpha, \beta = 1 \ldots \chi$

$j = 1 \ldots d$

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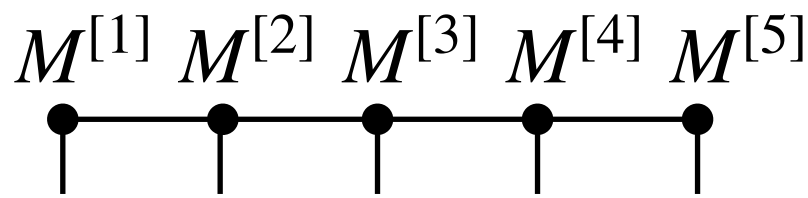

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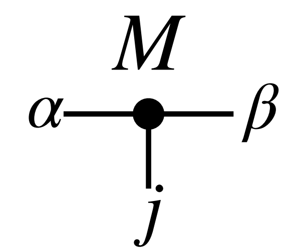

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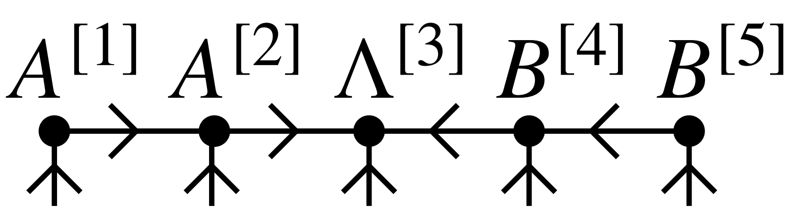
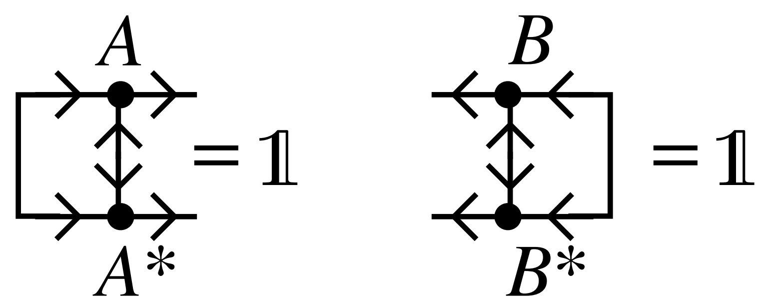
Isometric form: Use the gauge degree of freedom ($A^j = XM^jX^{-1}$) to find a convenient representation





(Isometries)

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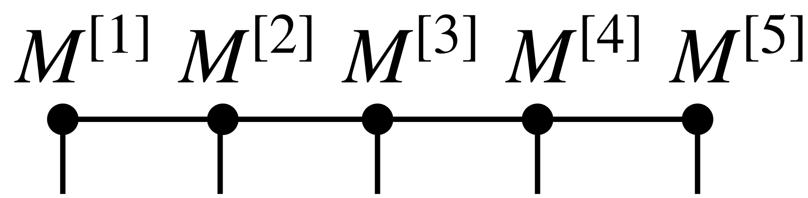
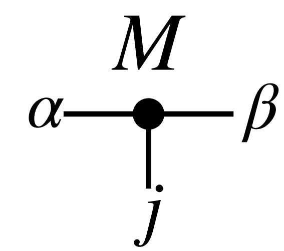
$\psi_{j_1,j_2,j_3,j_4,j_5} =$ 

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

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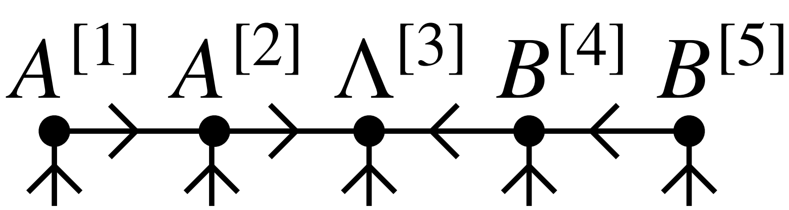
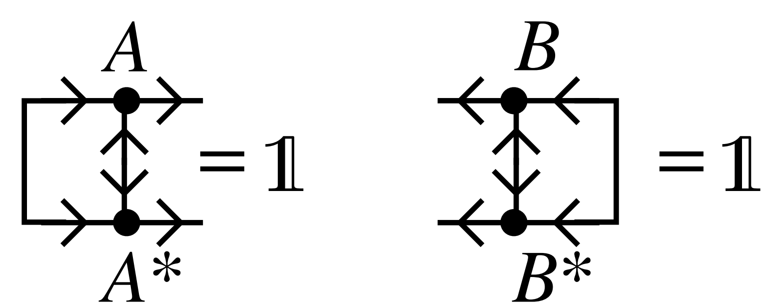




(Isometries)

Center matrix Λ represents wave function

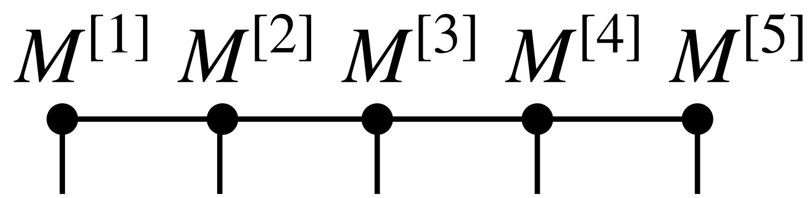
$$|\psi\rangle = \sum_{\alpha,\beta,j} \Lambda^j_{\alpha,\beta} |\alpha\rangle |j\rangle |\beta\rangle$$

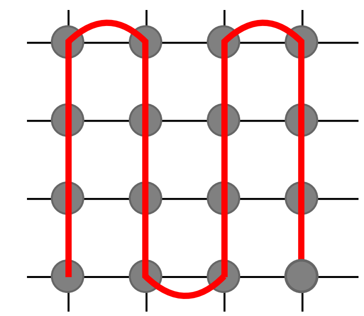
(orthogonal states $|j\rangle$, $|\alpha\rangle$, $|\beta\rangle$)

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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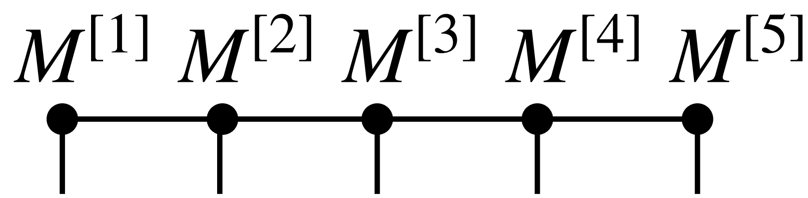

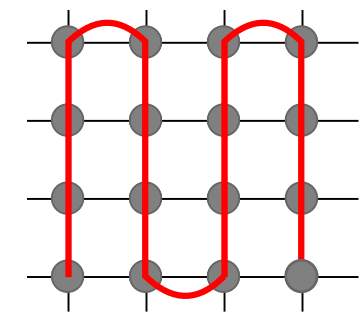

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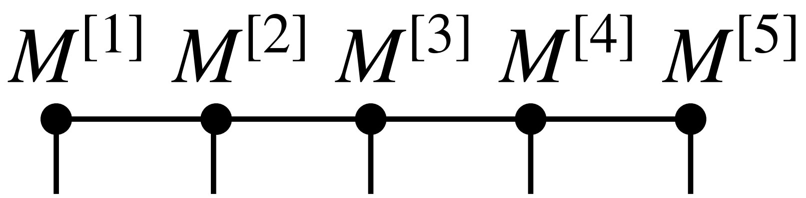
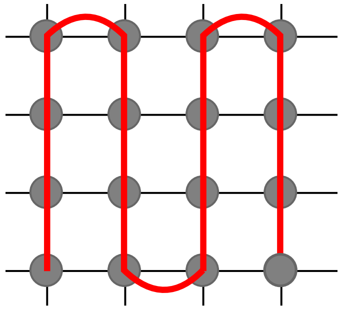
$\psi_{j_1,j_2,j_3,j_4,j_5} \approx$ 



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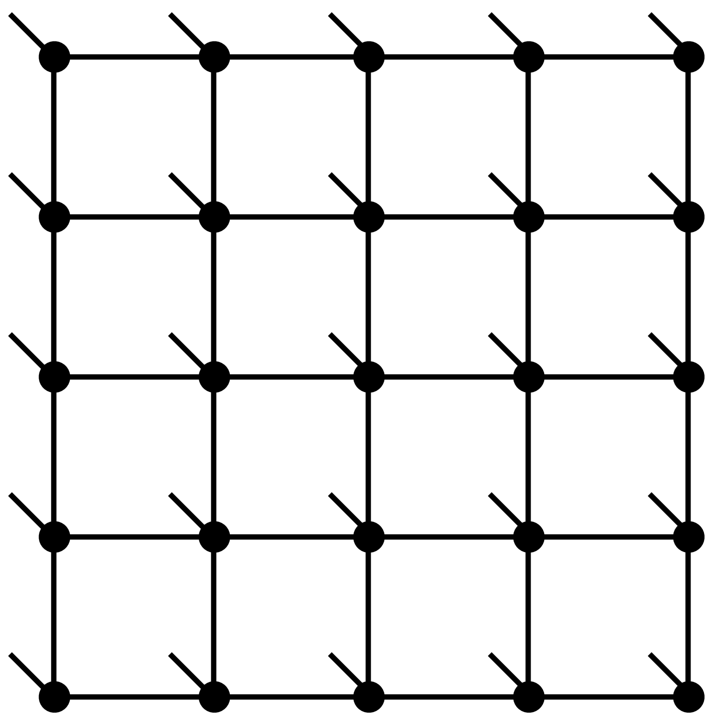
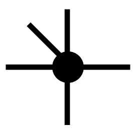


$T^{j}_{\alpha,\beta,\gamma,\delta} =$ 

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

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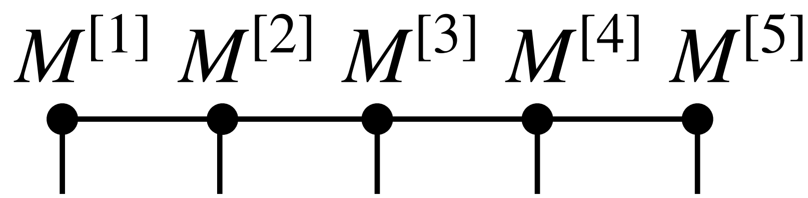

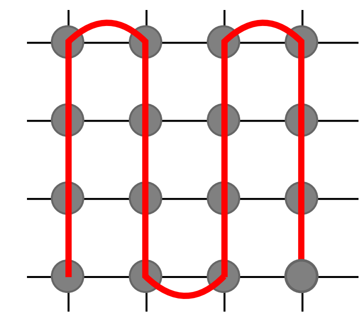

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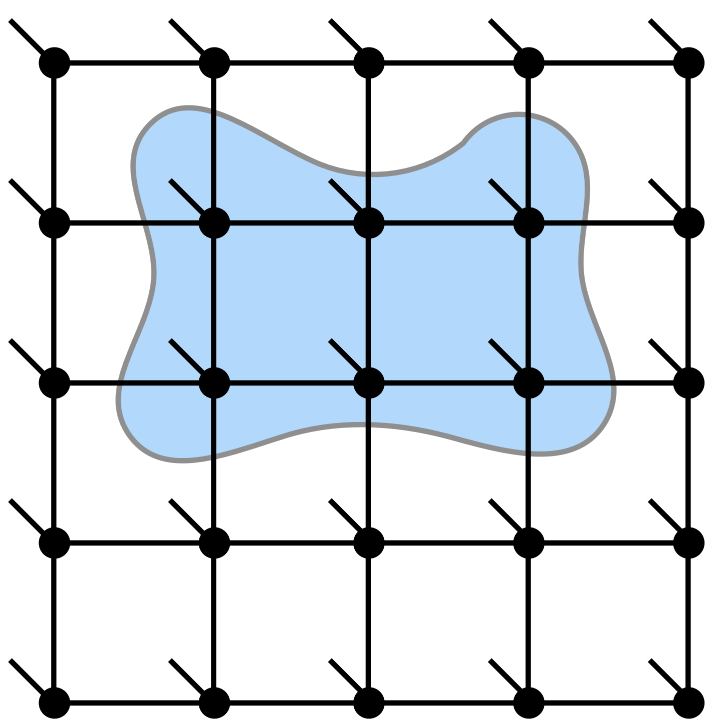
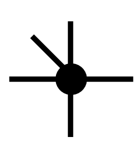
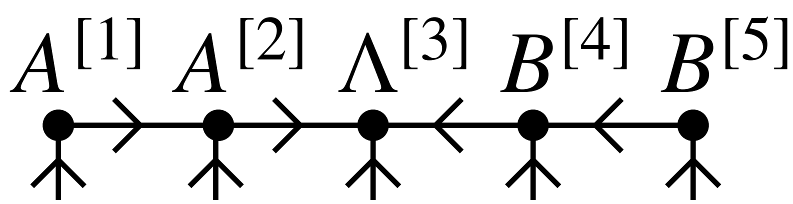


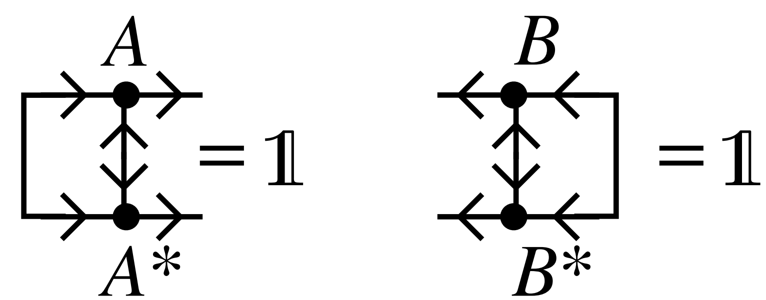
$T^{j}_{\alpha,\beta,\gamma,\delta} =$ 

- 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

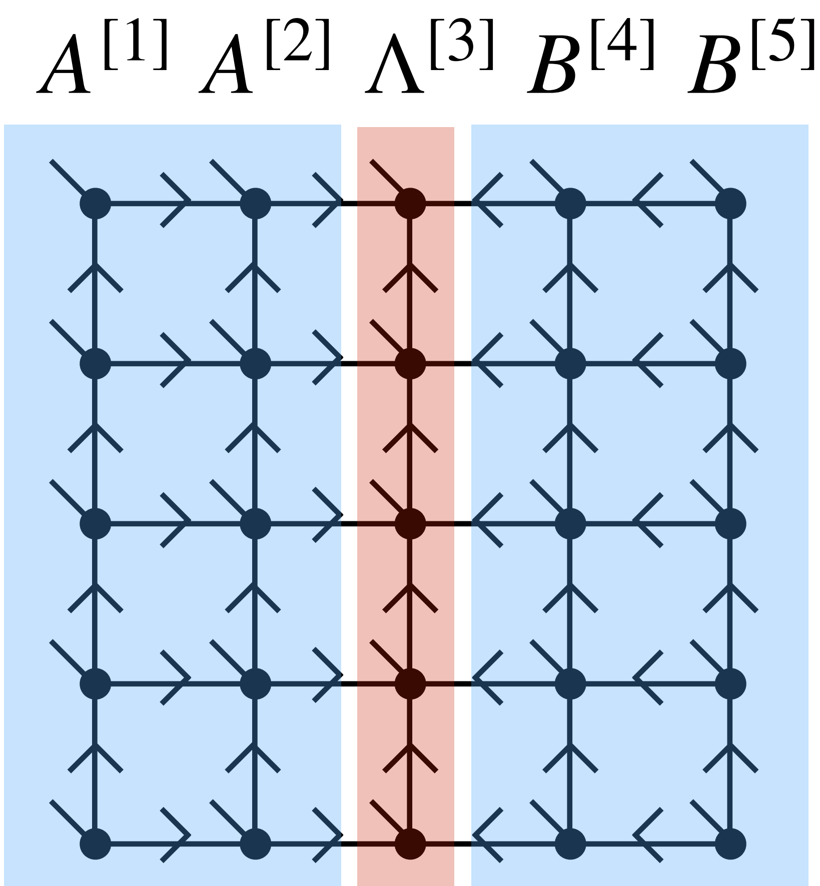
Recall: Canonical form of 1D MPS





(Isometries)

Isometric TNS



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

see also: Bañuls, Perez-García, Wolf, Verstraete, Cirac '08
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[Zaletel and FP, PRL **124**, 037201 (2020)]

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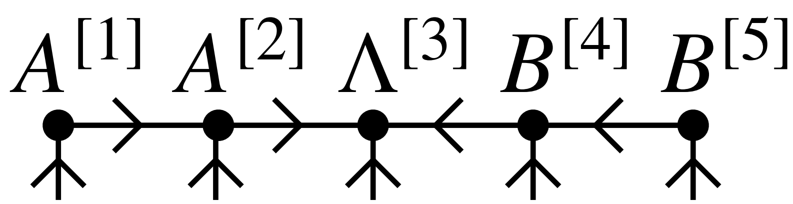

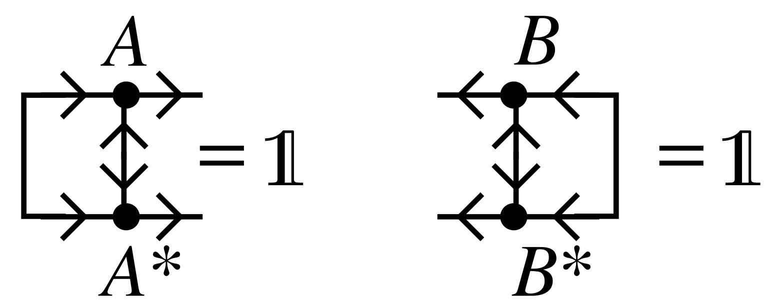

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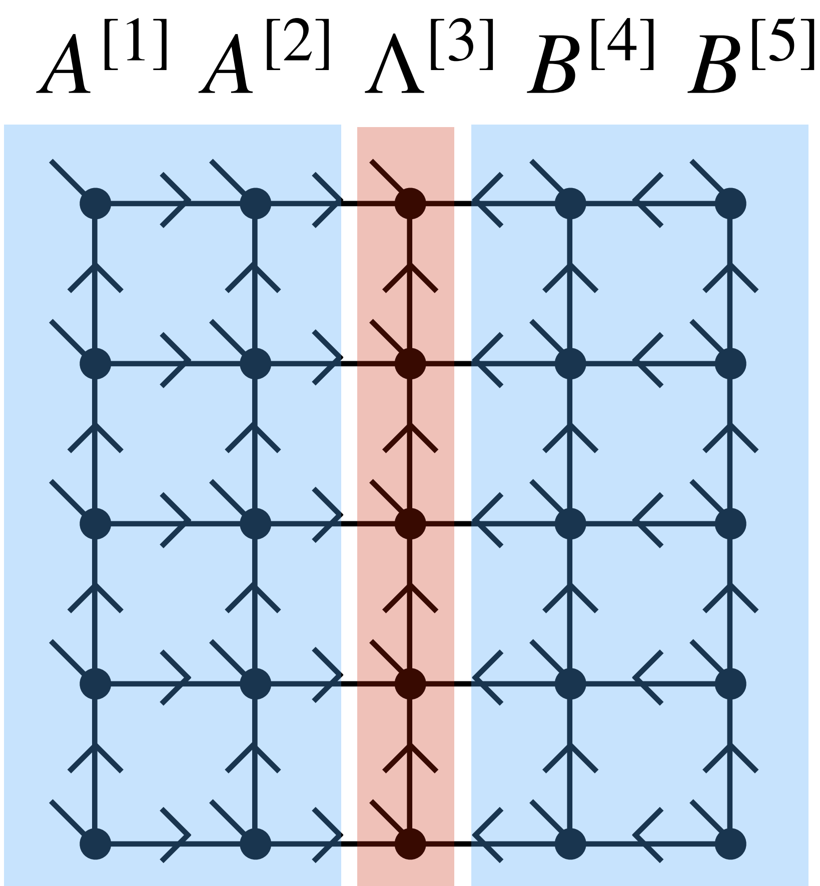

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- Orthogonality center column is a **1D MPS**: Standard DMRG techniques
- **Subset of TNS: Unclear what its variational power is!**

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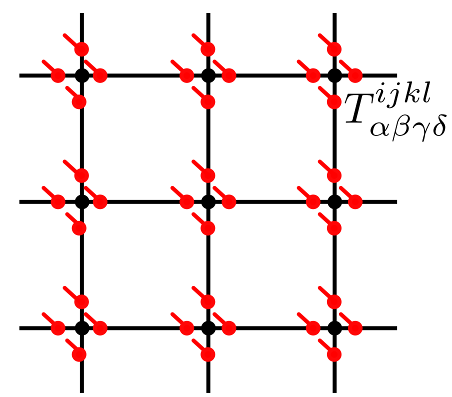
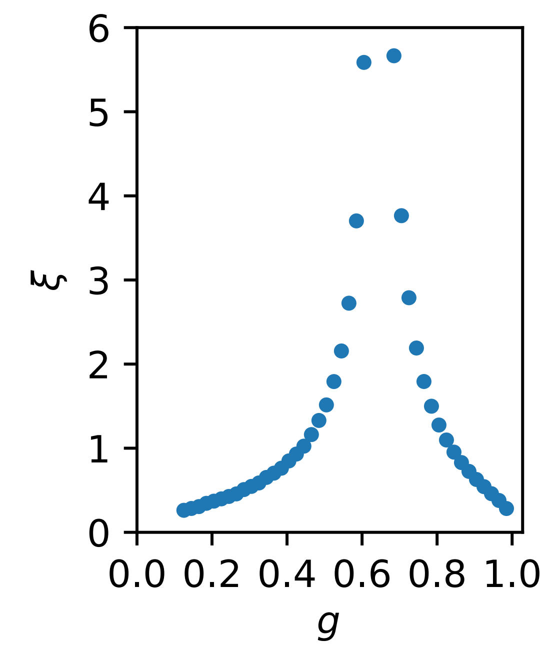
[Zaletel and FP, PRL **124**, 037201 (2020)]

Which states ca be represented as isoTNS?

All **string net states** can be represented exactly as isoTNS

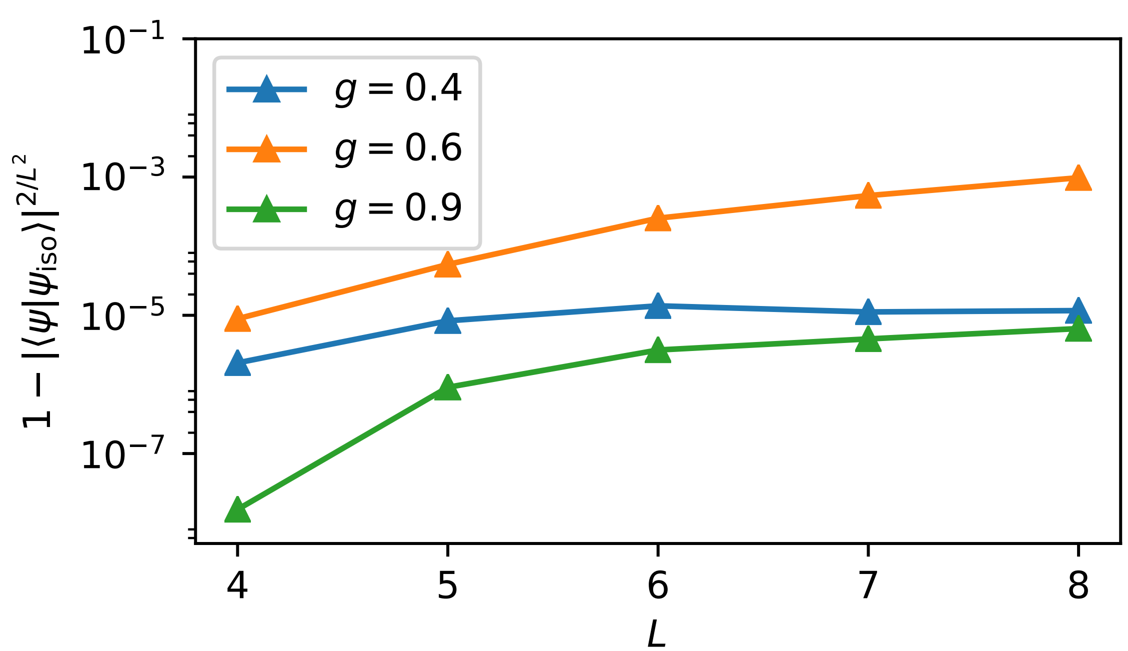
$$H = -\sum_s \sigma^z\sigma^z\sigma^z\sigma^z - \sum_p \sigma^x\sigma^x\sigma^x\sigma^x,$$





$$T^{ijkl}_{\alpha\beta\gamma\delta}(g) = \begin{cases} g^{i+j+k+l}\delta_{i,\alpha}\delta_{j,\beta}\delta_{k,\gamma}\delta_{l,\delta}, & \text{if } i+j+k+l = 0 \bmod 2 \\ 0, & \text{otherwise.} \end{cases}$$

- Error density becomes independent of the system size when $L \gg \xi$



[Soejima, Siva, Bultinck, Chatterjee, FP, Zaletel, PRB **101**, 085117 (2020)]

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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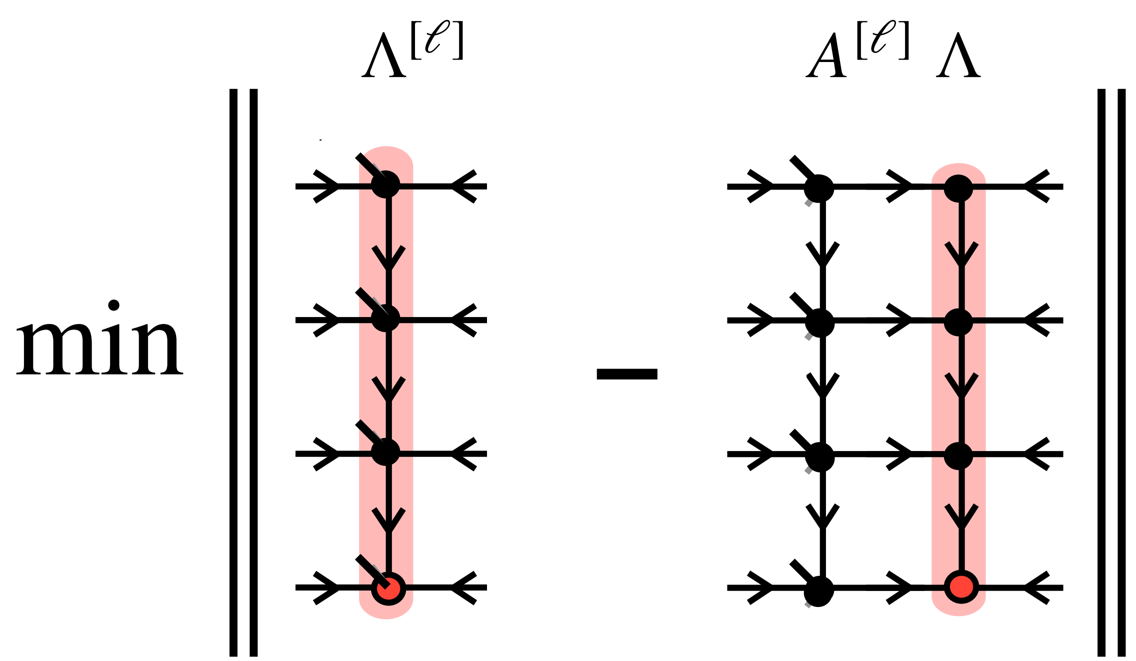
Solve the variational problem:

$$\min \left\| \Lambda^{[\ell]} - A^{[\ell]} \Lambda \right\|$$



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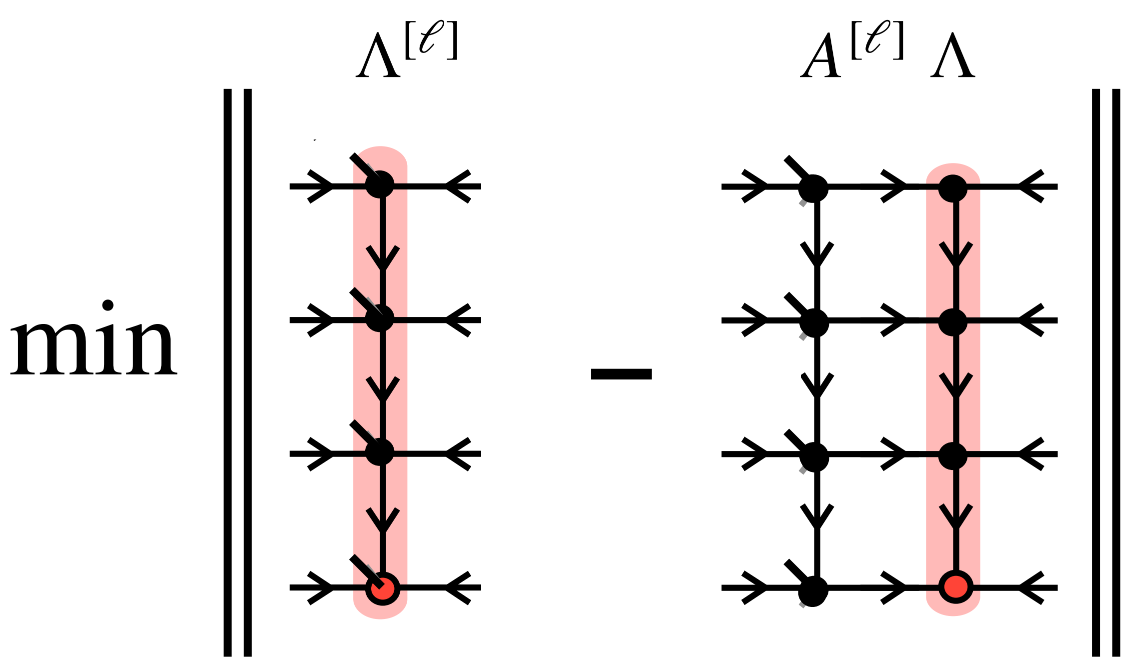

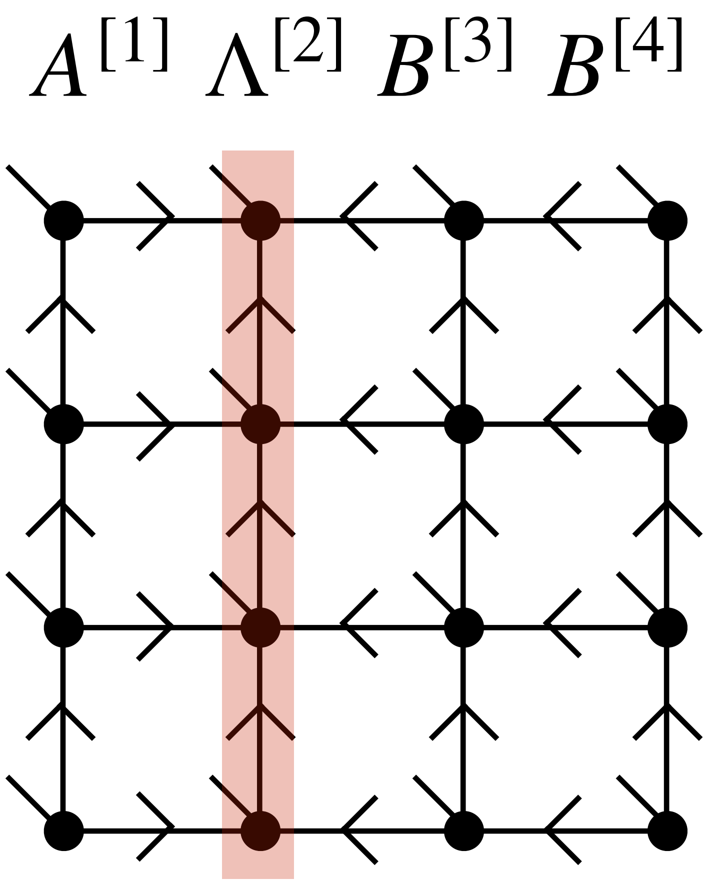

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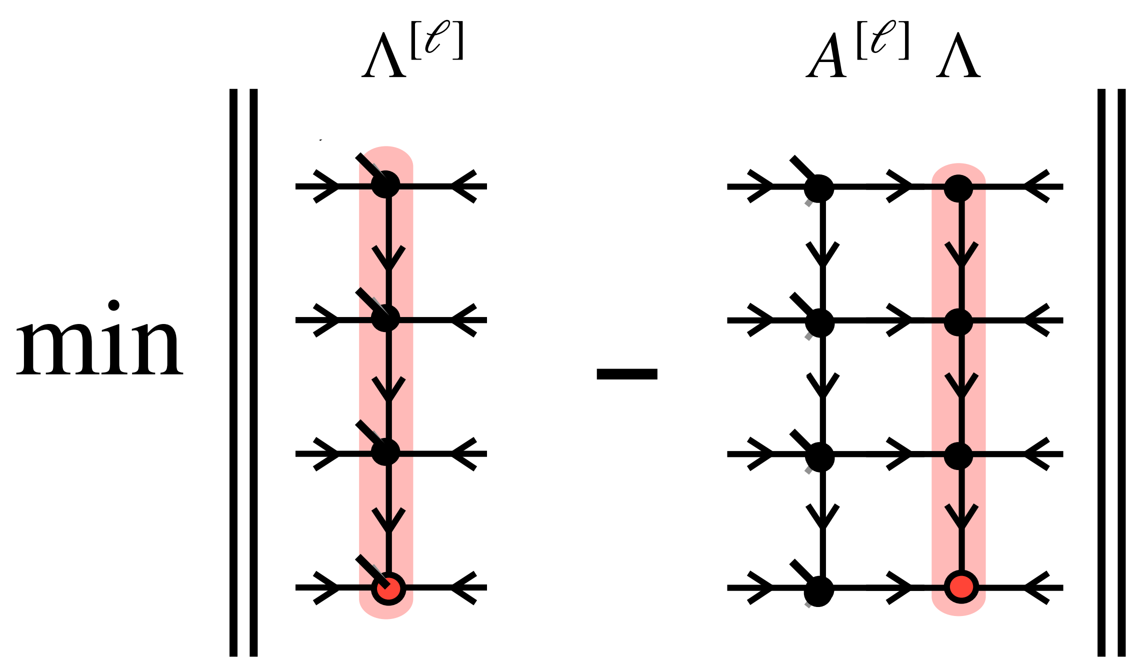
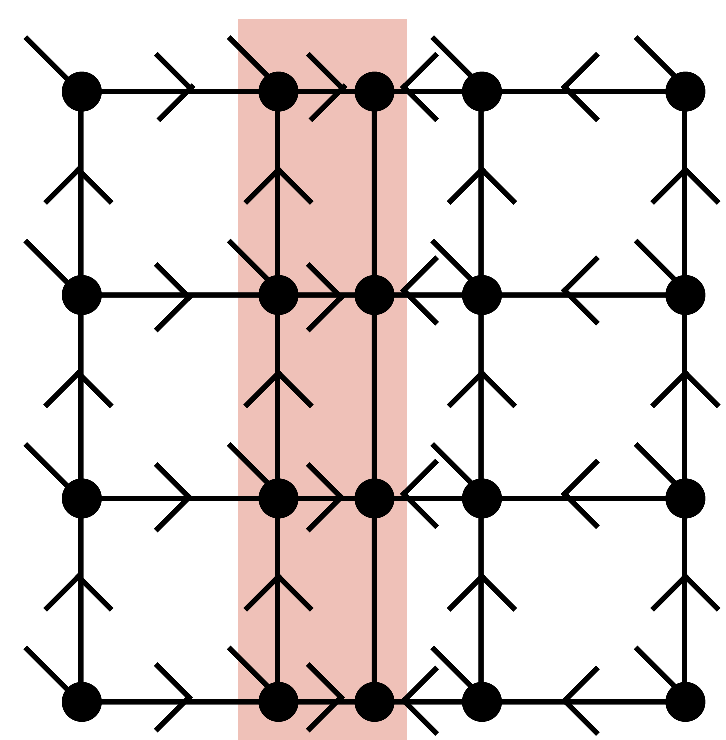


$A^{[1]}\ A^{[2]}\Lambda B^{[3]}\ B^{[4]}$



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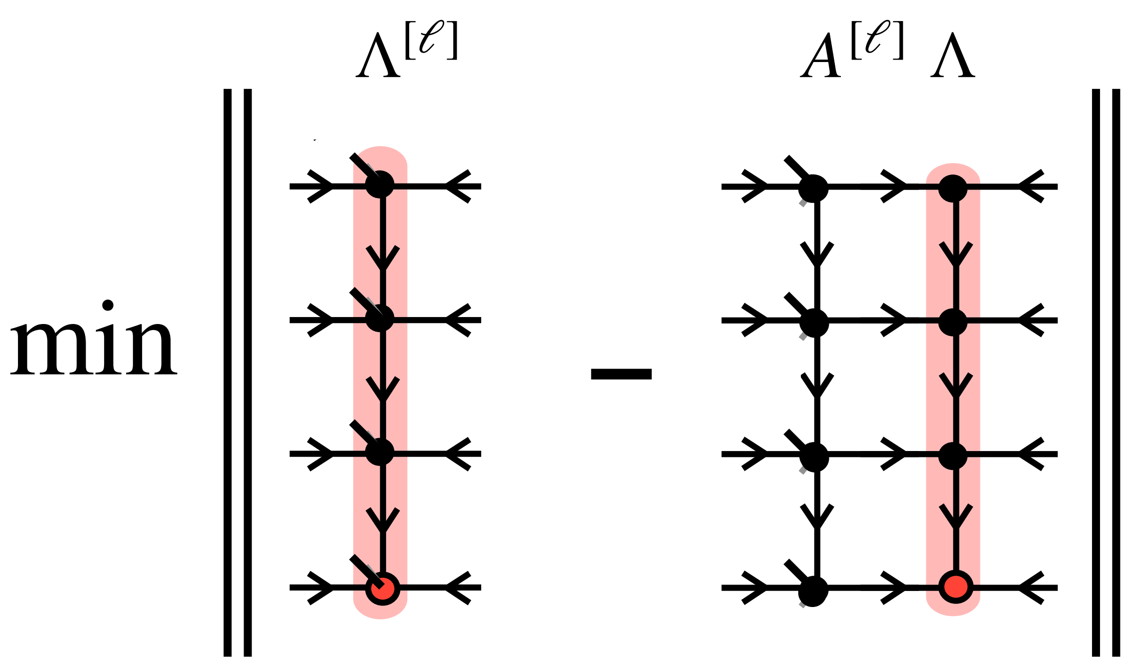

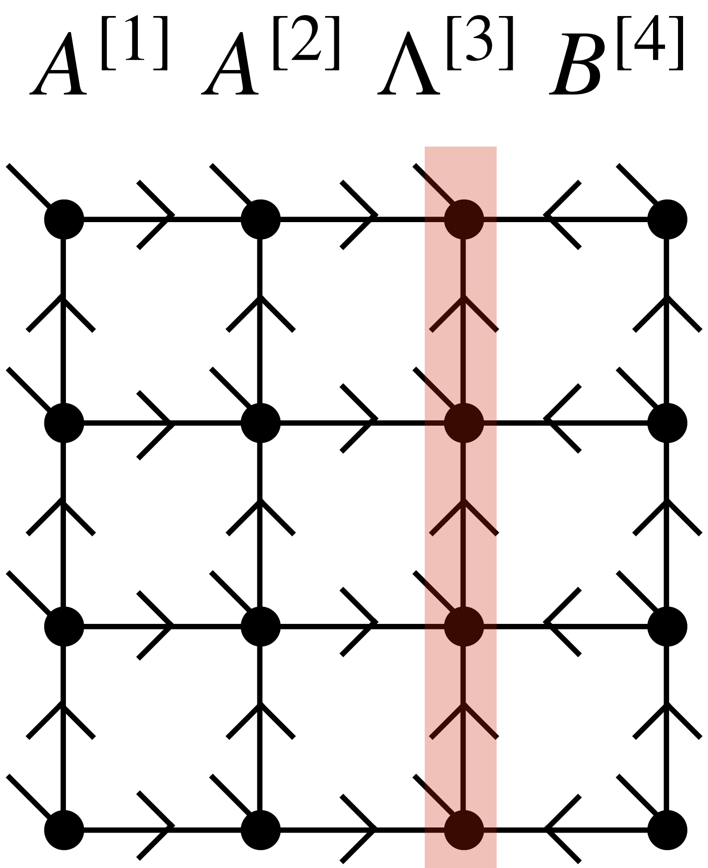

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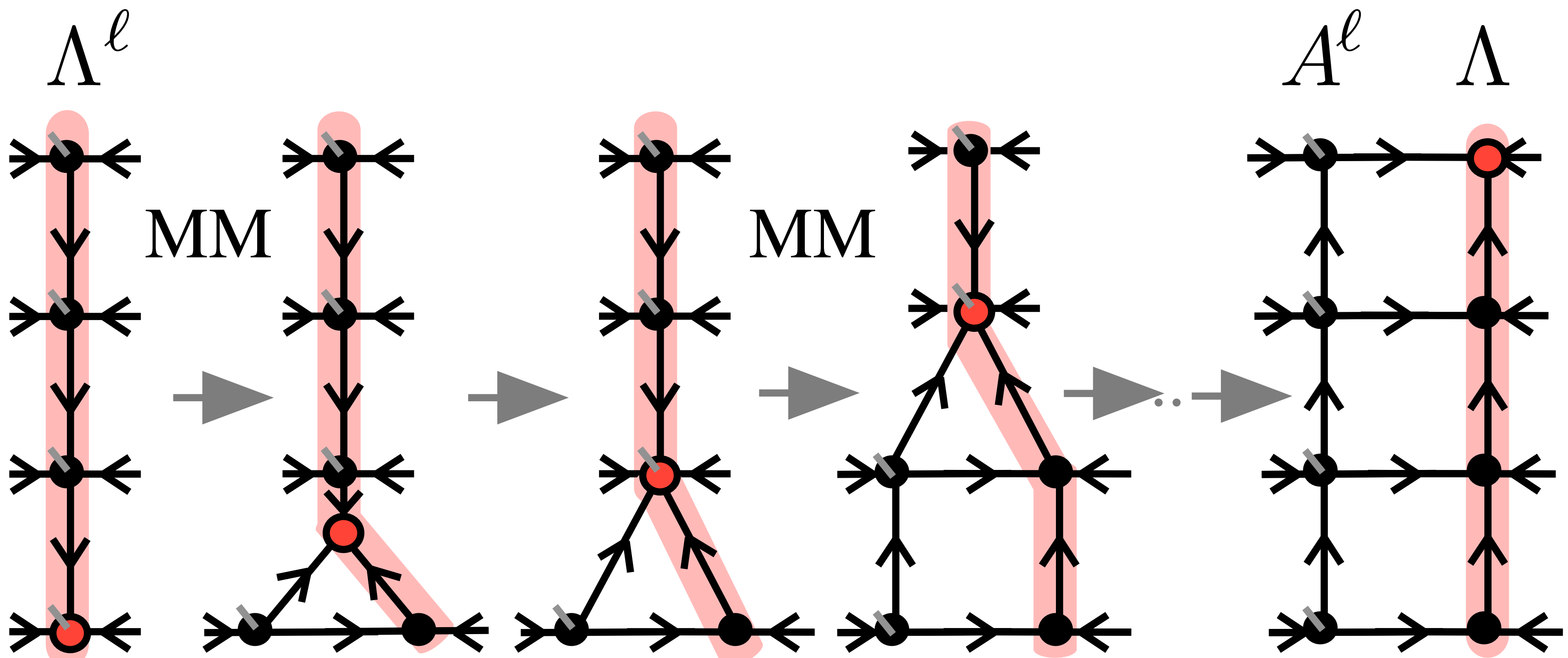
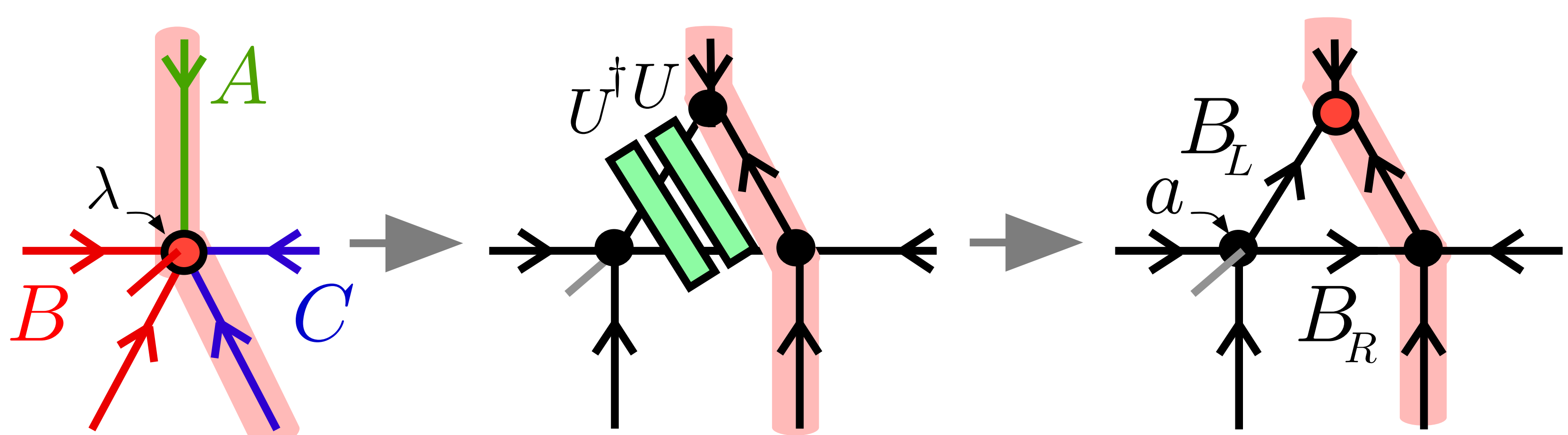
Isometric Tensor Network States in 2D

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





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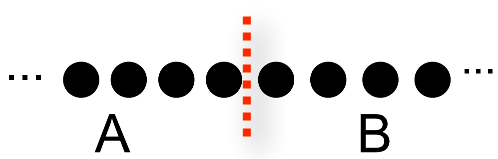
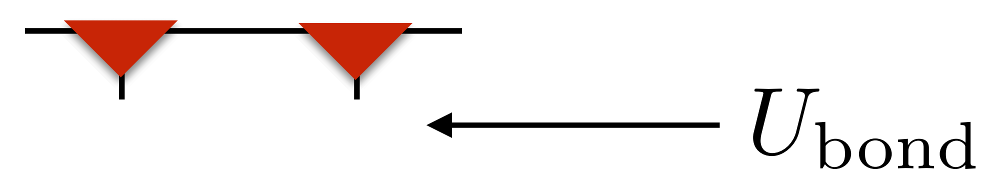
Finding the disentangler

Variationally disentangle the state: **minimize the Renyi entanglement entropy** $S_2 = -\ln \mathrm{Tr} \rho^2_{\mathrm{red.}}$ on each bond



$|\tilde{\psi}\rangle$:



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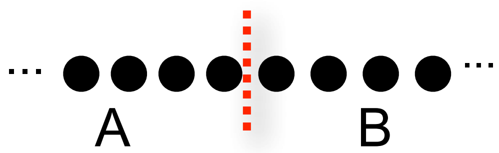

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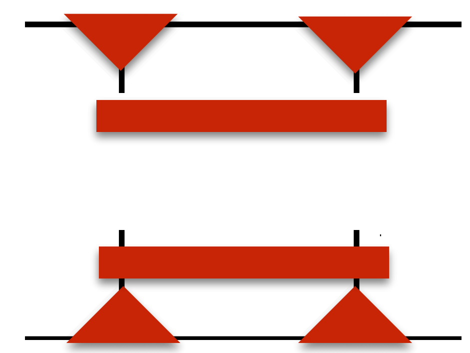

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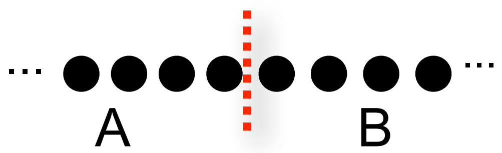

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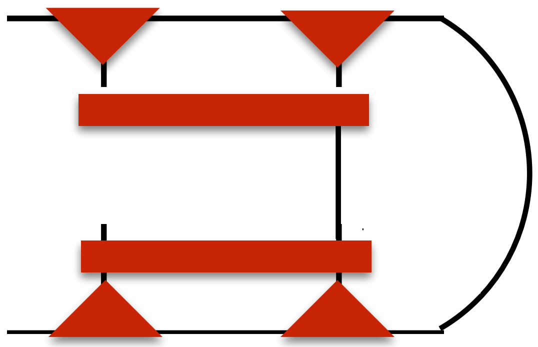

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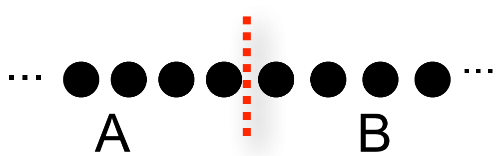

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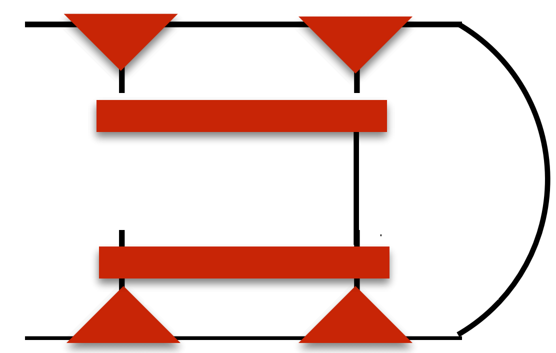

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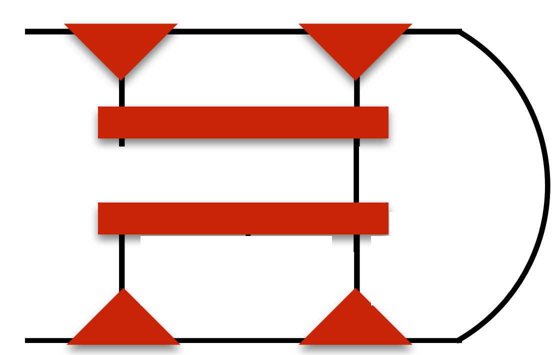

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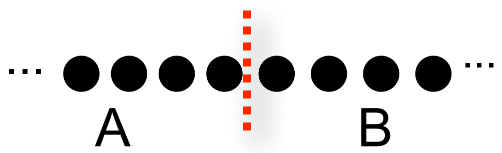
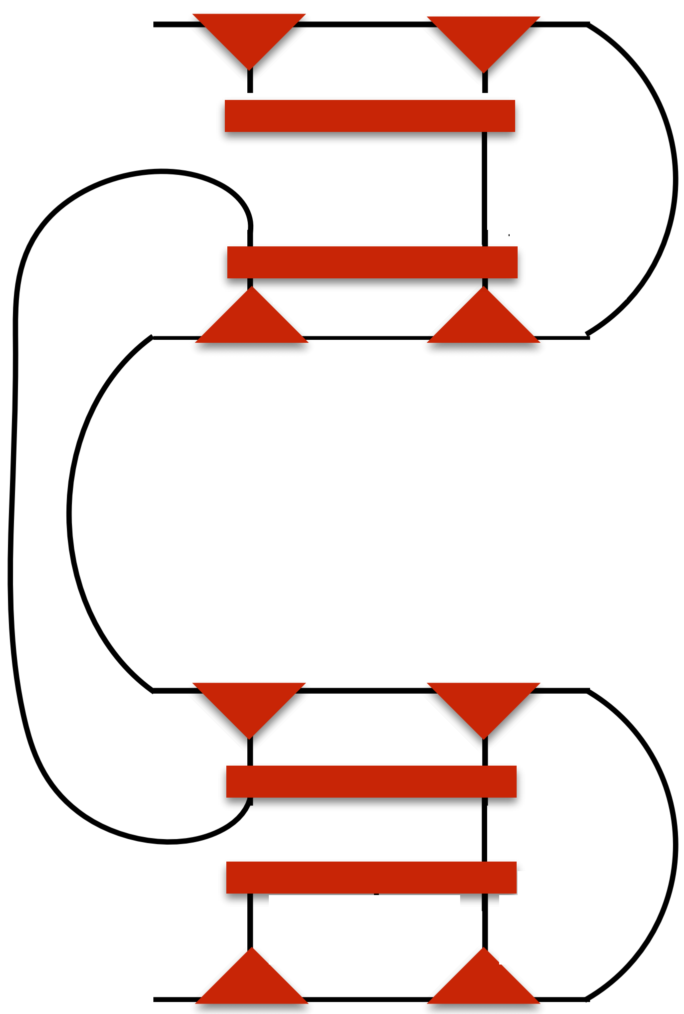


$\tilde{\rho}^2_{\mathrm{red.}}$:



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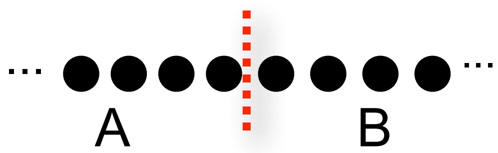
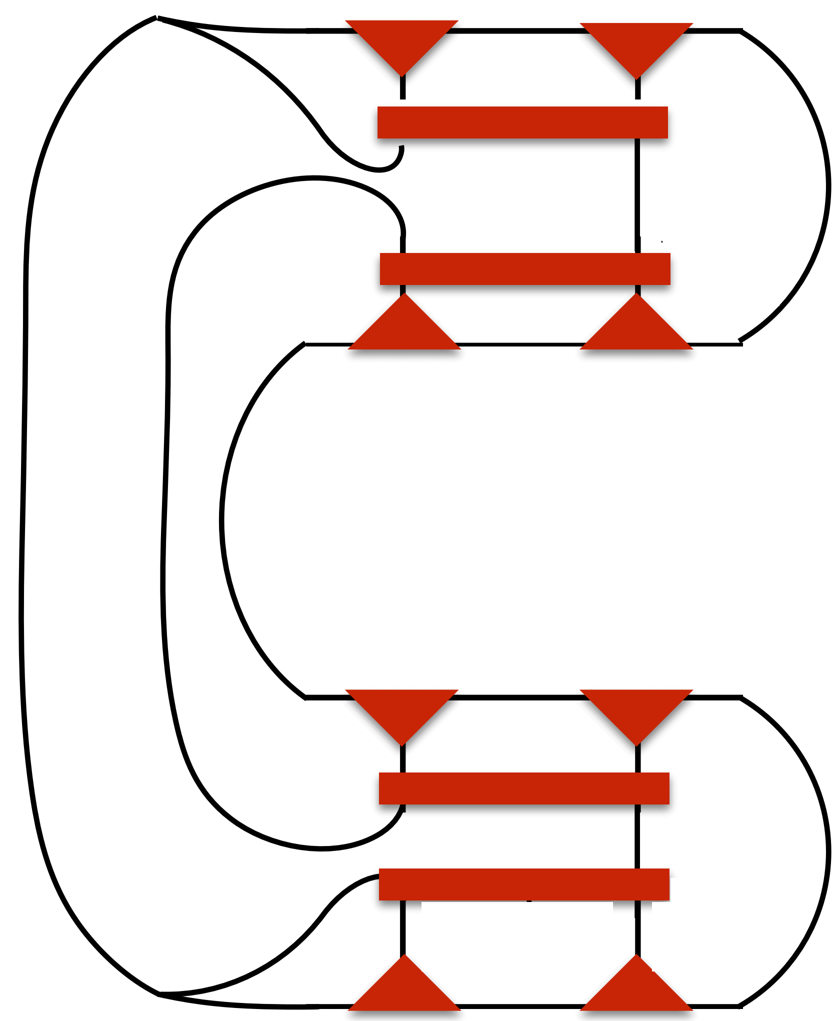


$\mathrm{Tr}\tilde{\rho}^2_{\mathrm{red.}}$:



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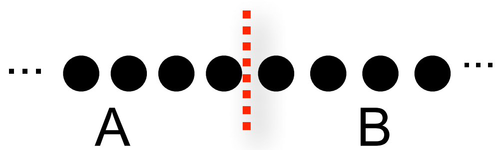
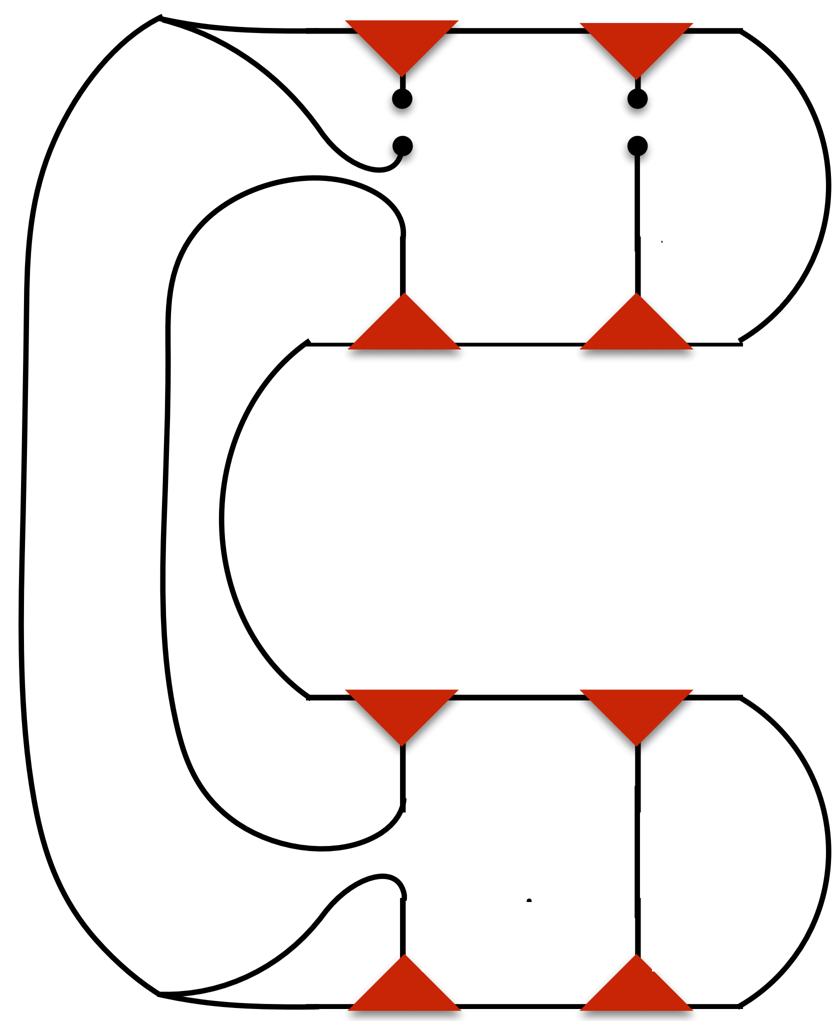


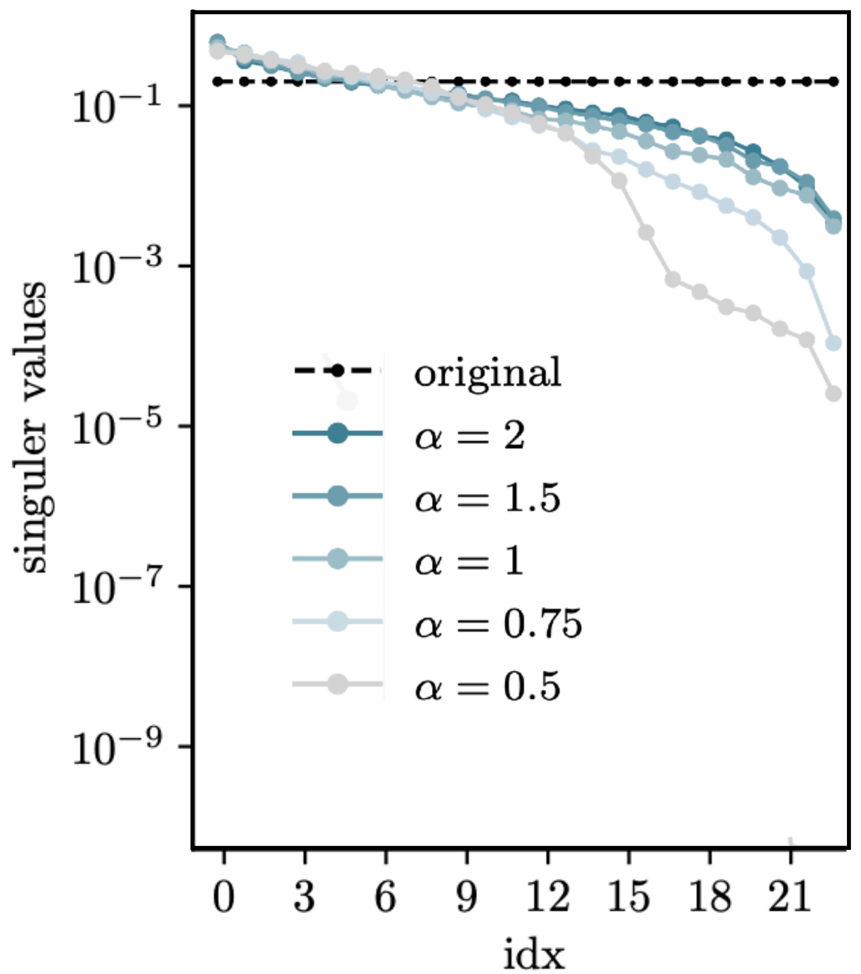
$$\frac{\partial}{\partial U}\left(\mathrm{Tr}\tilde{\rho}_{\mathrm{red}}\right)_{U=1} =$$



- Polar decomposition to minimize S_2 [Evenbly & Vidal '09]

Finding the disentangler

Role of the disentangler:



[Zaletel and FP, PRL **124**, 037201 (2020)]

Finding the disentangler

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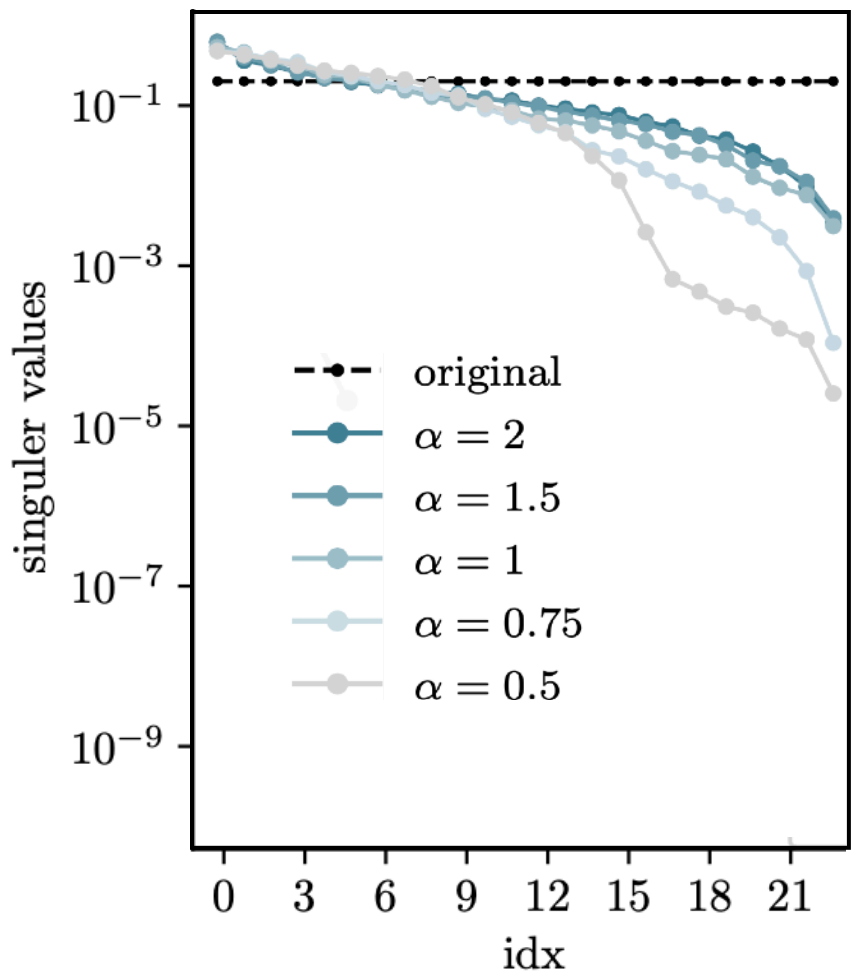
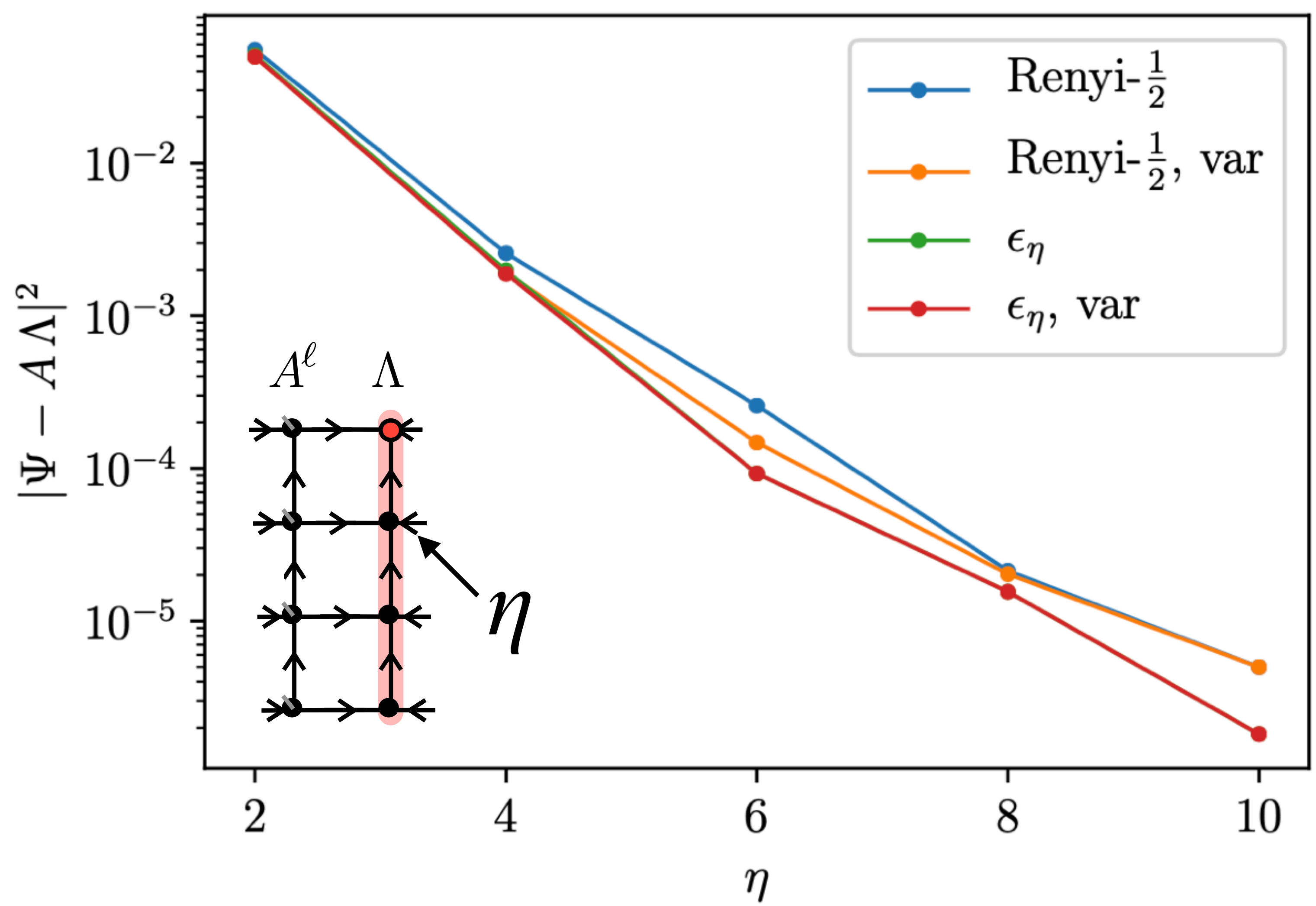


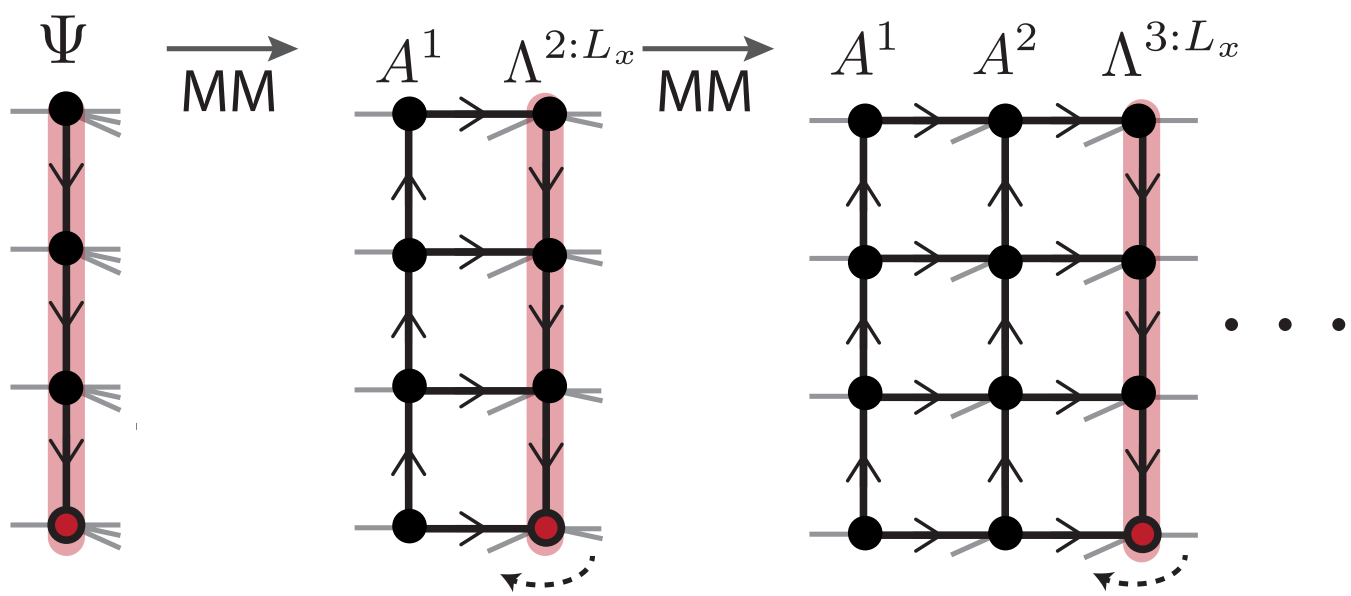
Variational vs. Moses Move:



[Zaletel and FP, PRL **124**, 037201 (2020)]

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, PRL **124**, 037201 (2020)]

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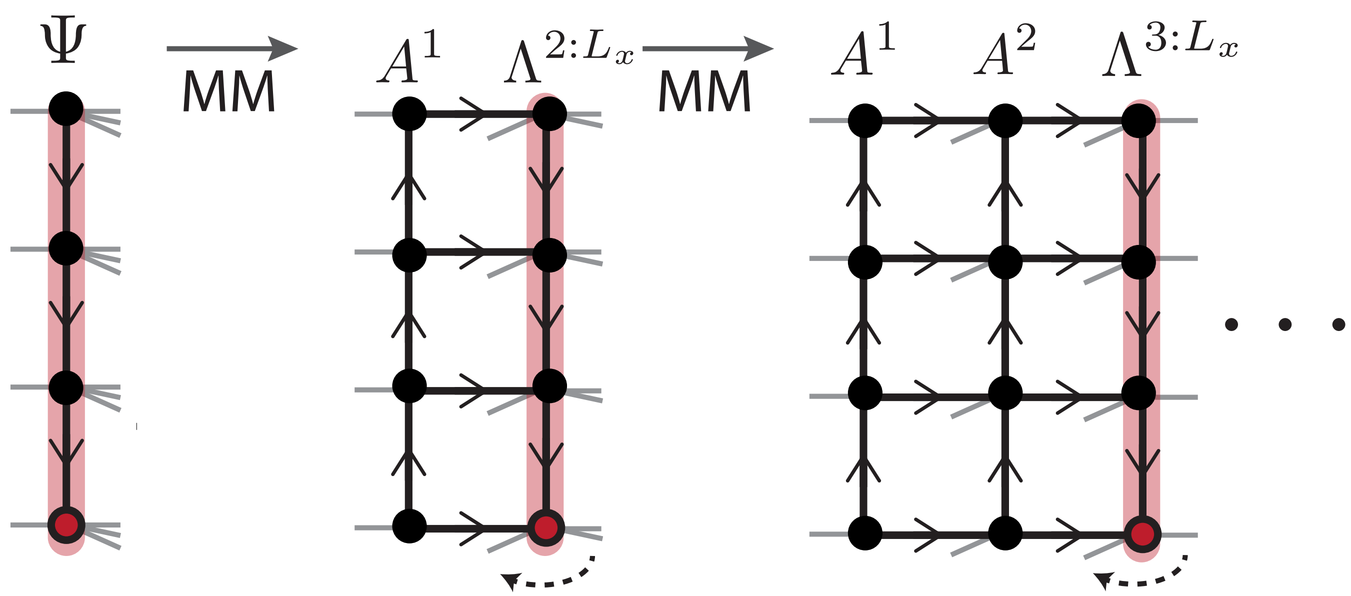
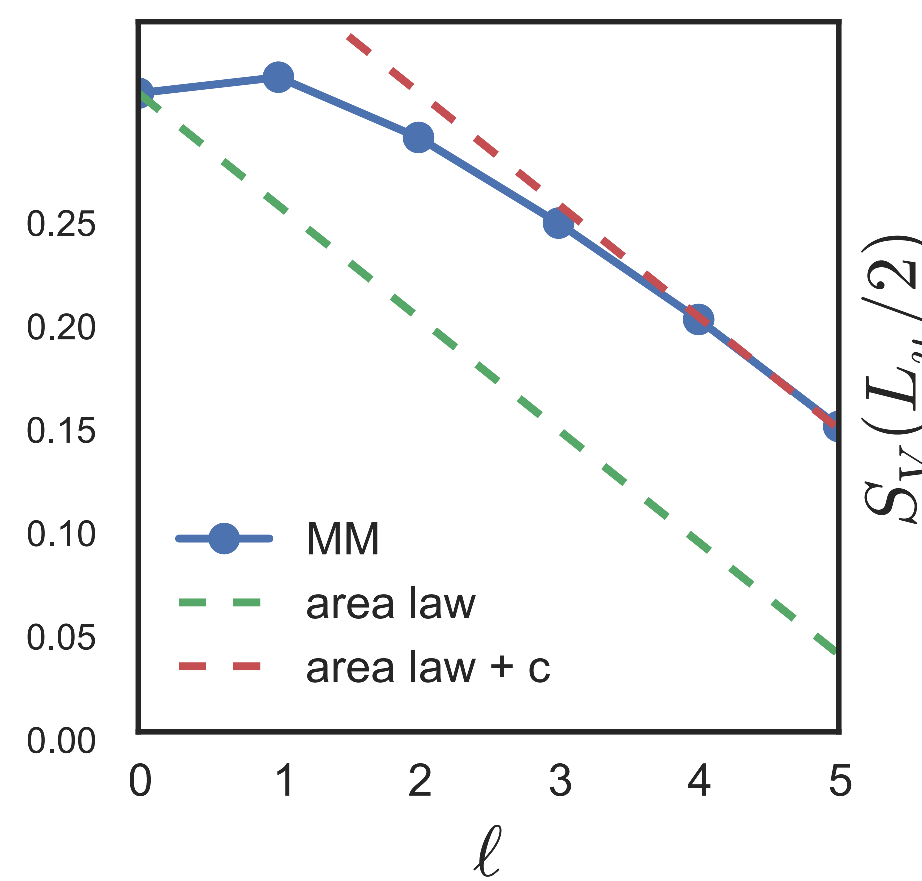


- Sequentially disentangle the state
- Efficient compression

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

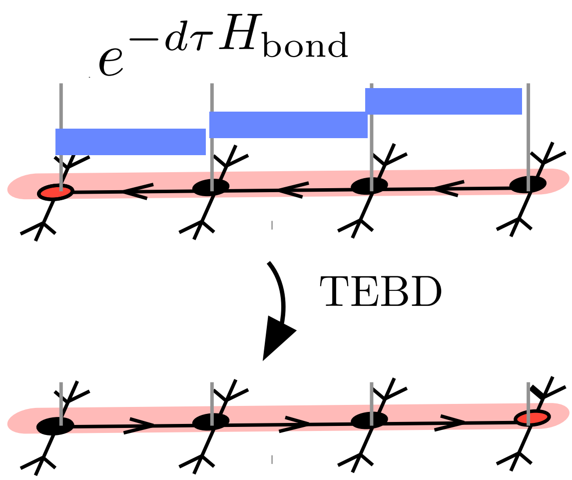
$$H = -\sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - g \sum_i \sigma^x$$

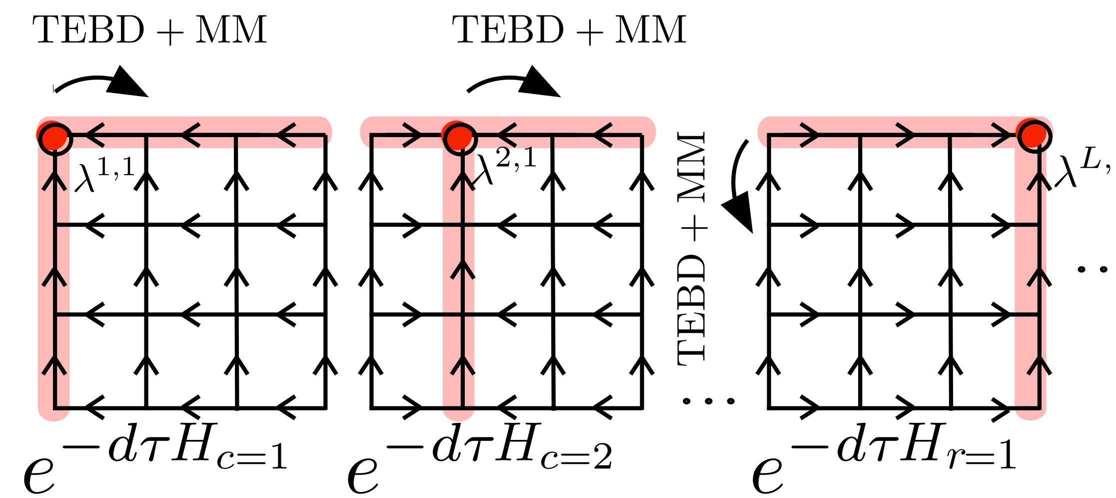


[Zaletel and FP, PRL **124**, 037201 (2020)]

Time evolution of 2D Hamiltonians (TEBD^2)

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





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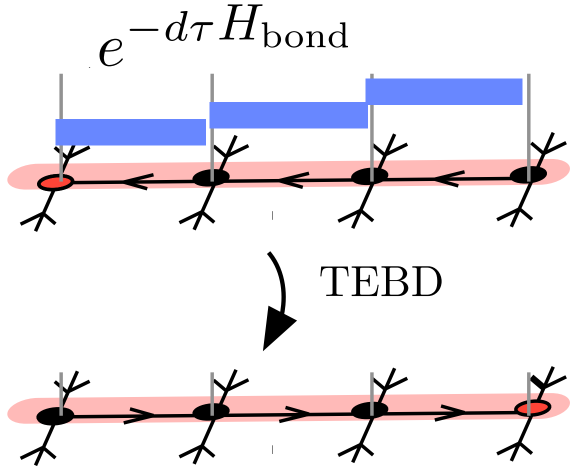
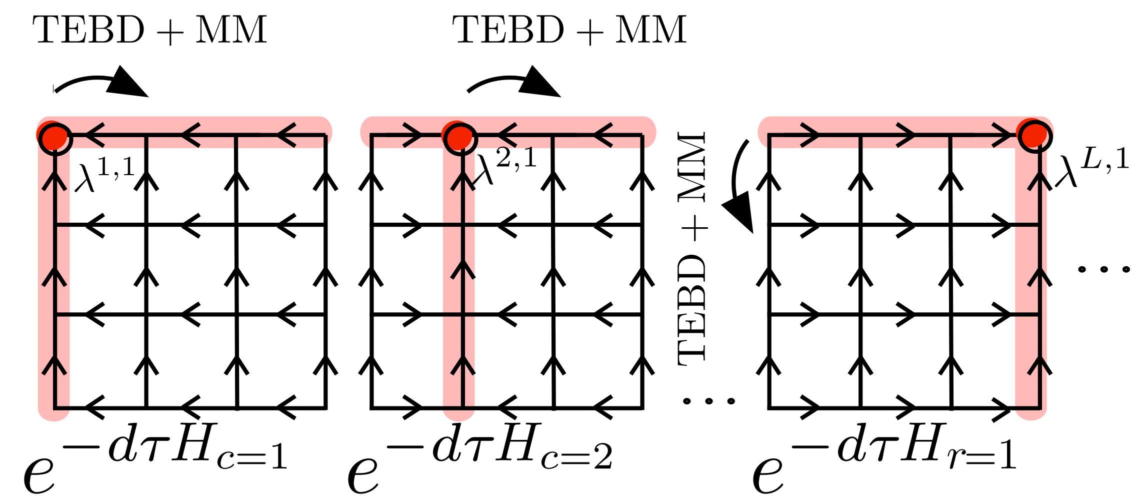
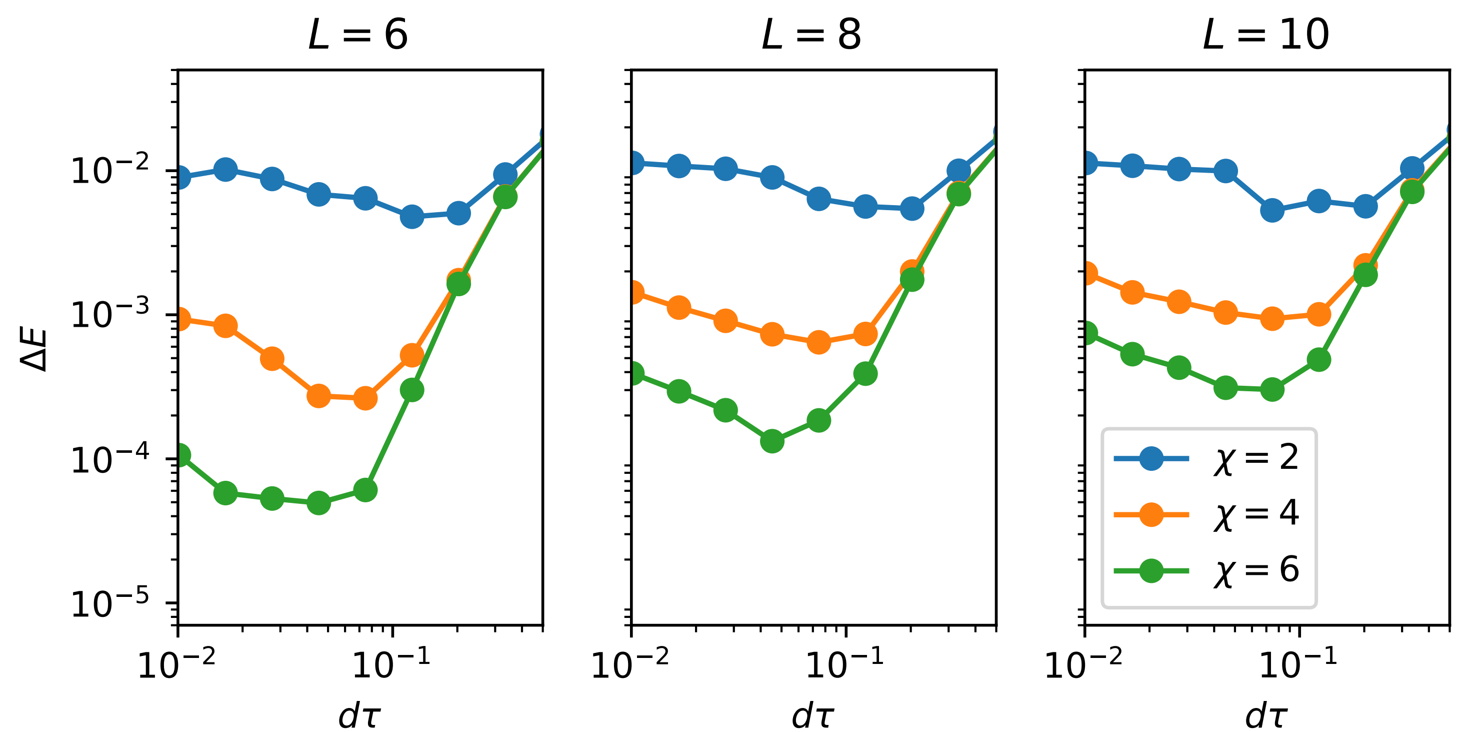




2D transverse field Ising Model ($g = 3.5$)

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

Imaginary time evolution: $|\psi_0\rangle$



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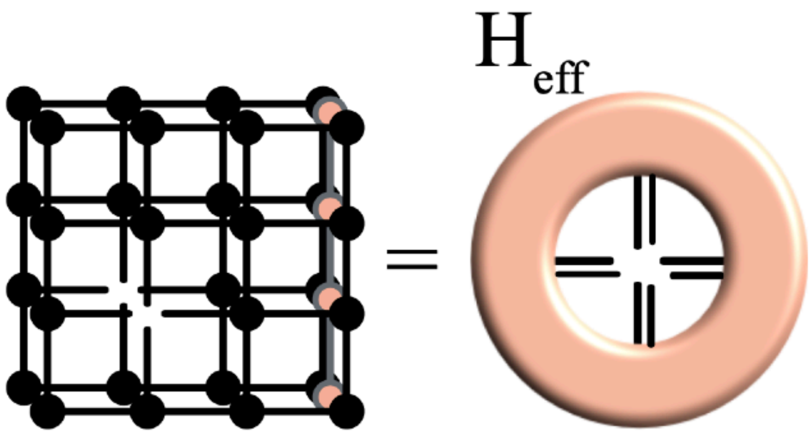
Variational optimization (DMRG²)

Iteratively minimize the energy by sequentially optimizing the isometries



[SH Lin, M Zaletel, FP, Phys. Rev. B **106**, 245102 (2022)]

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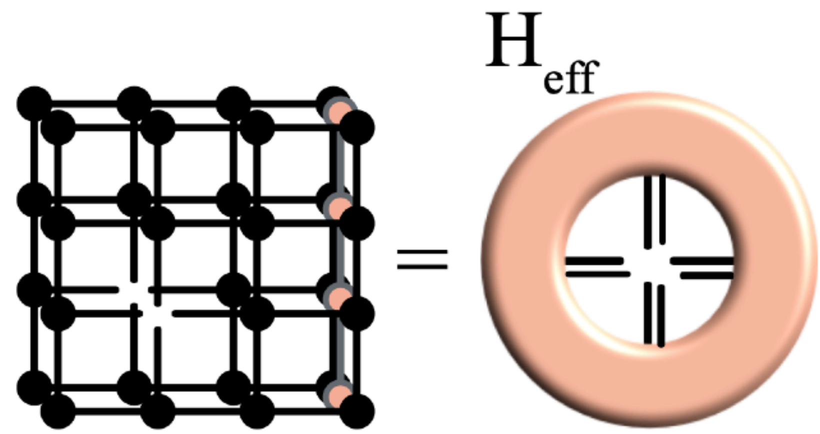

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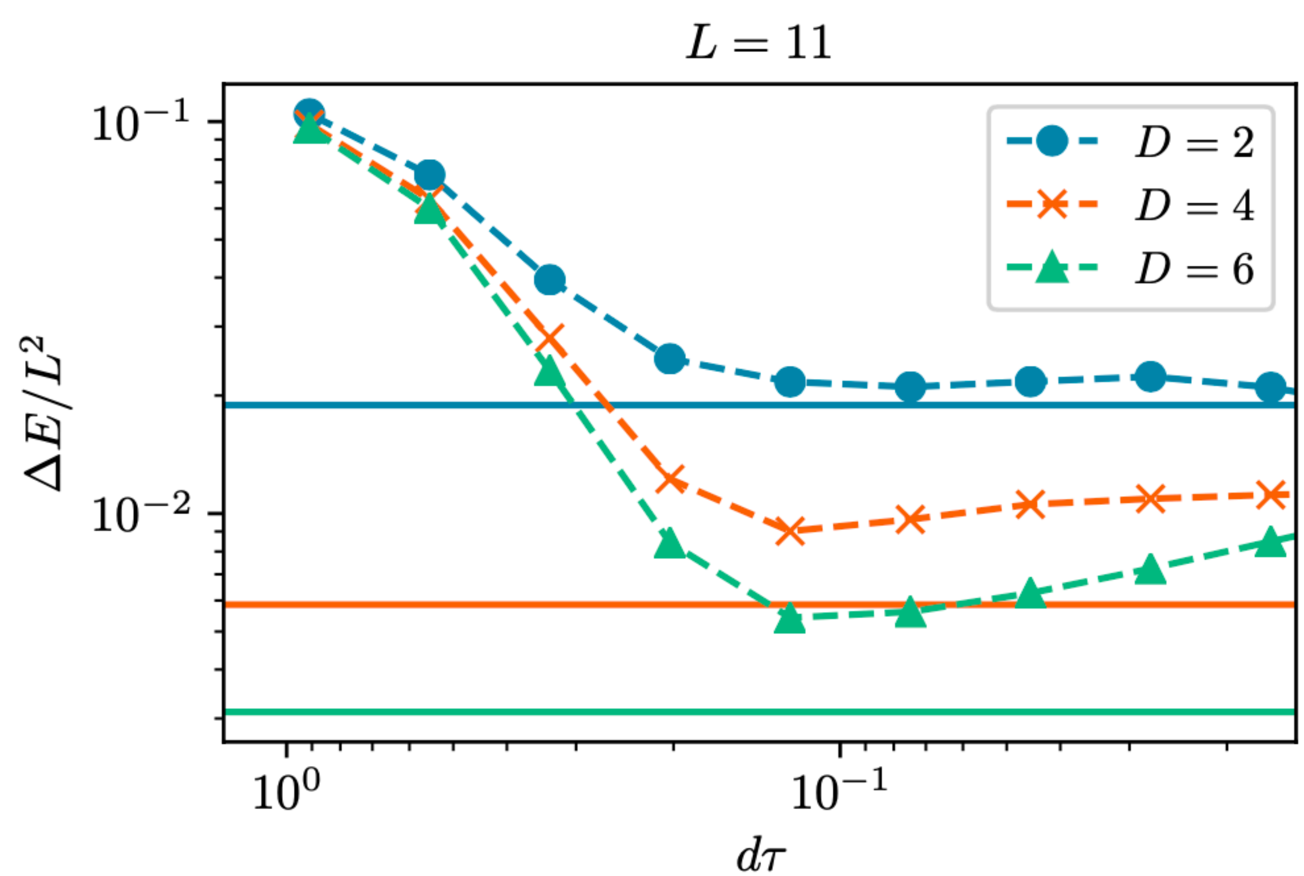
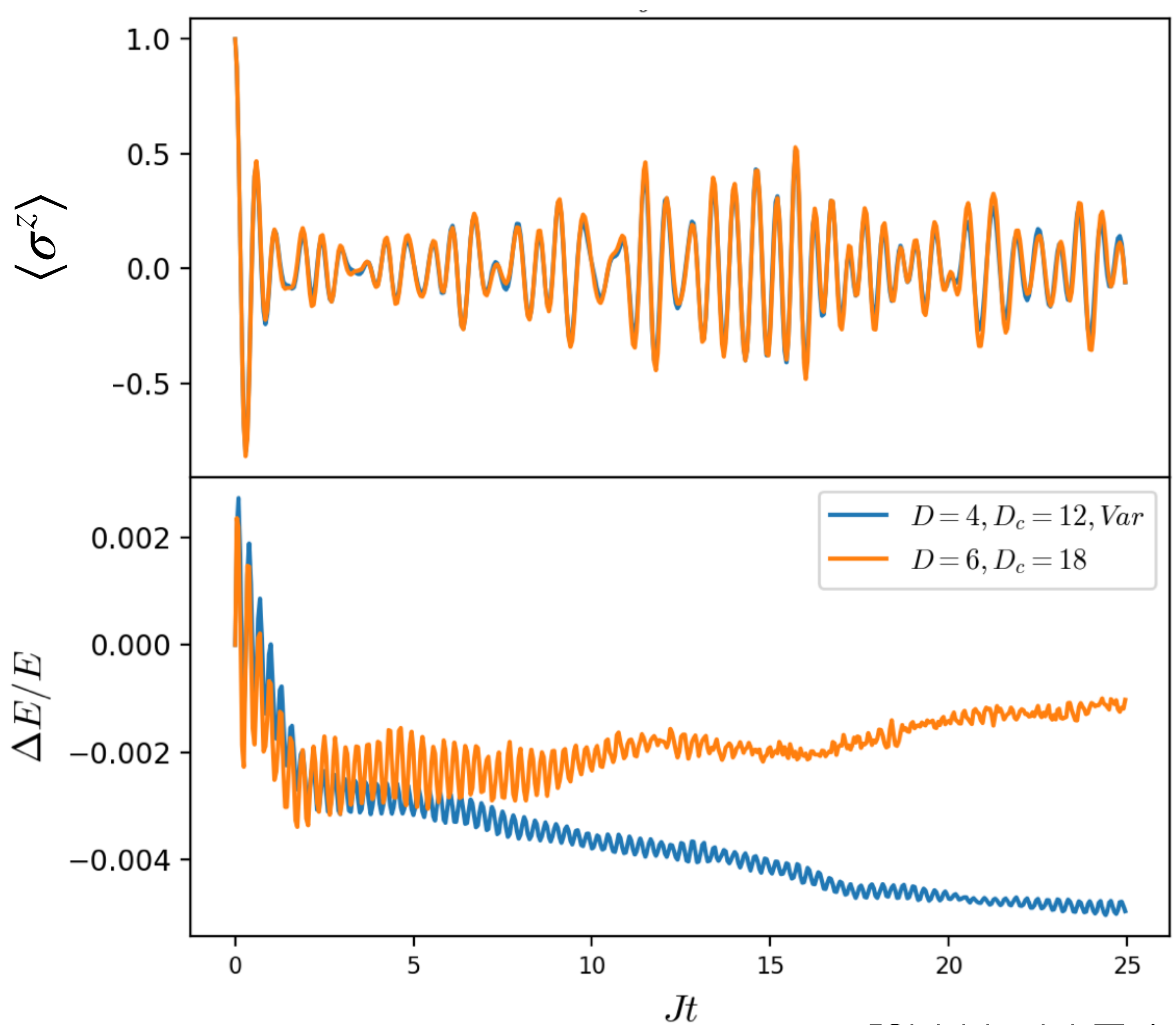
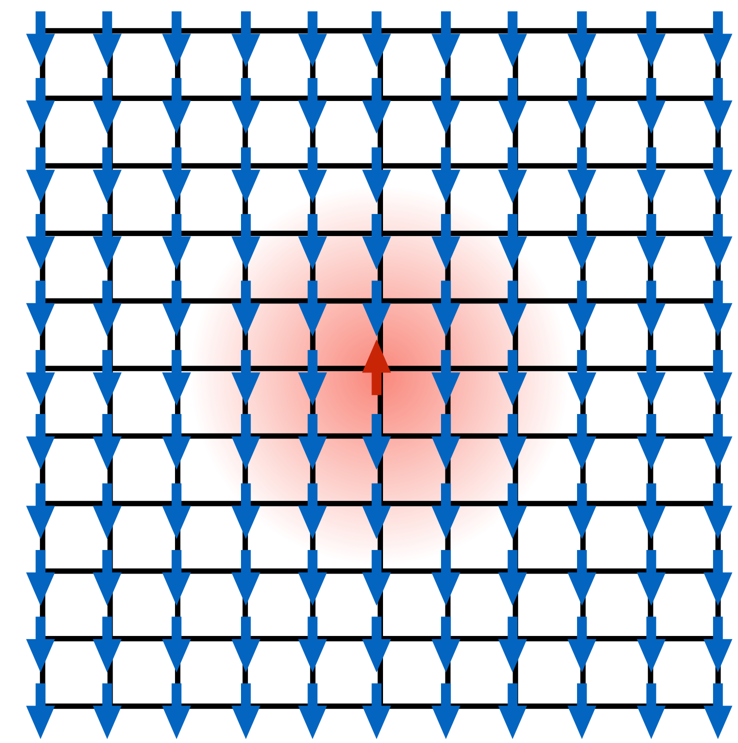


[SH Lin, M Zaletel, FP, Phys. Rev. B **106**, 245102 (2022)]

Dynamical spin structure factors from isoTNS

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





- Good convergence at small bond dimension χ

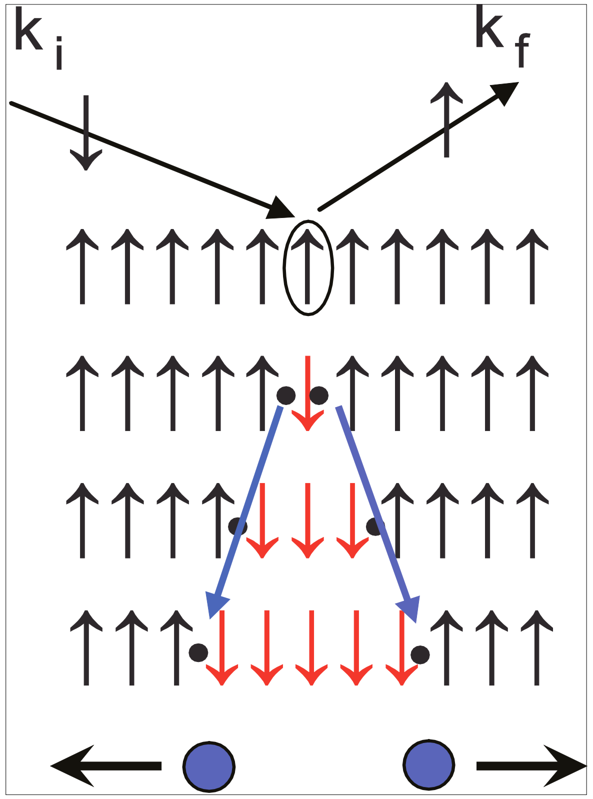
[SH Lin, M Zaletel, FP, Phys. Rev. B **106**, 245102 (2022)]

Dynamical spin structure factors from isoTNS

Numerical calculation of the **dynamical structure factor**

$$S(k,\omega) = \sum_x \int_{-\infty}^{\infty} dt\; e^{-i(kx+\omega t)} C(x,t)$$

with $C(x,t) = \langle \psi_0 | \sigma_x^y(t) \sigma_0^y(0) | \psi_0 \rangle$



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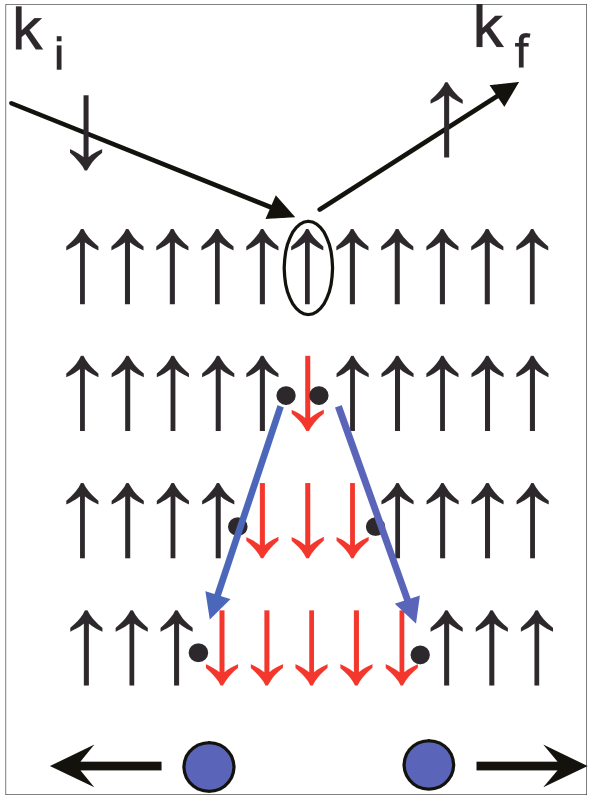

(1) Find the ground state $|\psi_0\rangle$: DMRG²

(2) Time evolve $\sigma_0^y |\psi_0\rangle$ to obtain $C(x,t)$

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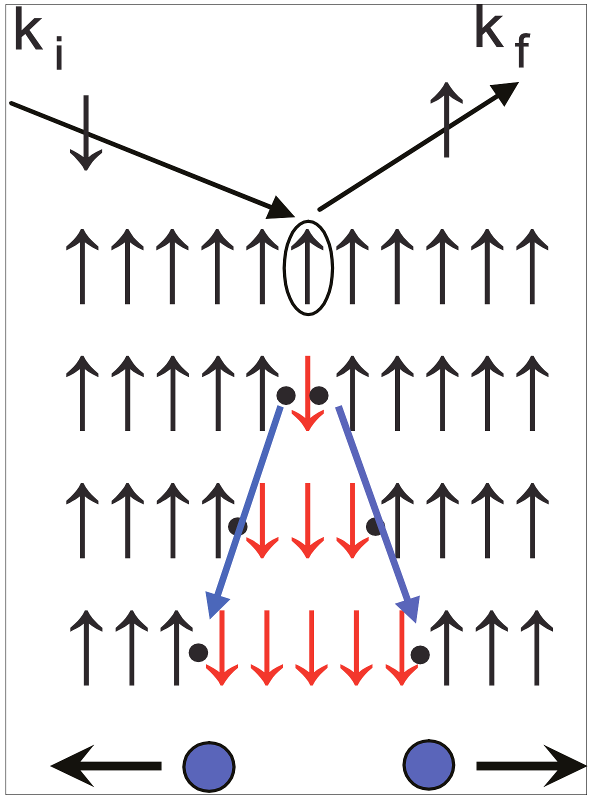


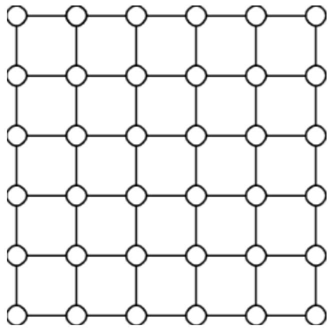
Slow growth of entanglement: Long times!

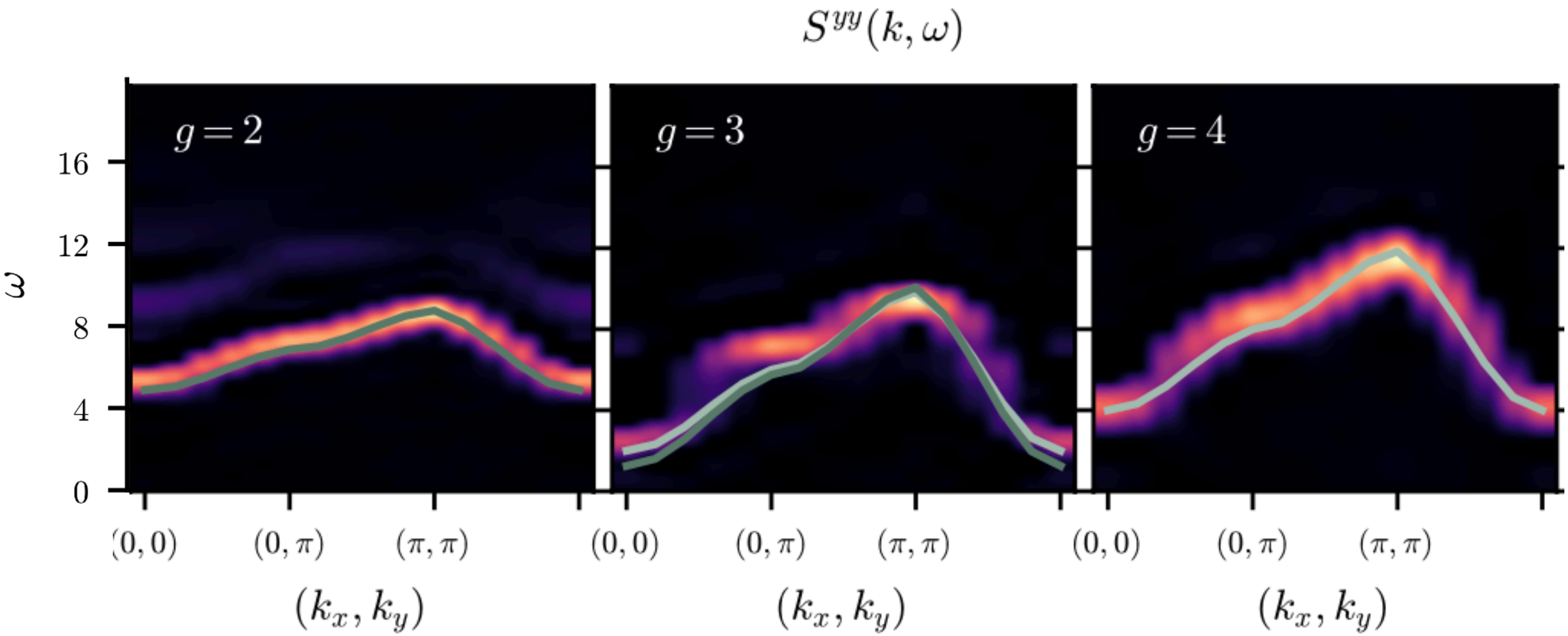
[SH Lin, M Zaletel, FP, Phys. Rev. B **106**, 245102 (2022)]

Dynamical spin structure factors from isoTNS

Dynamical structure factor: Transverse field Ising

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



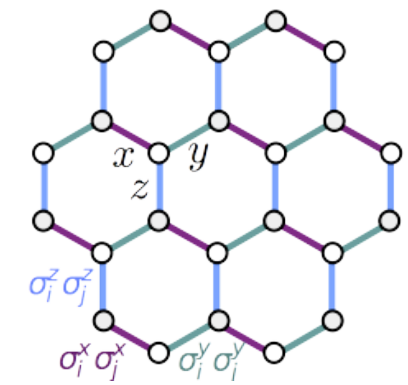


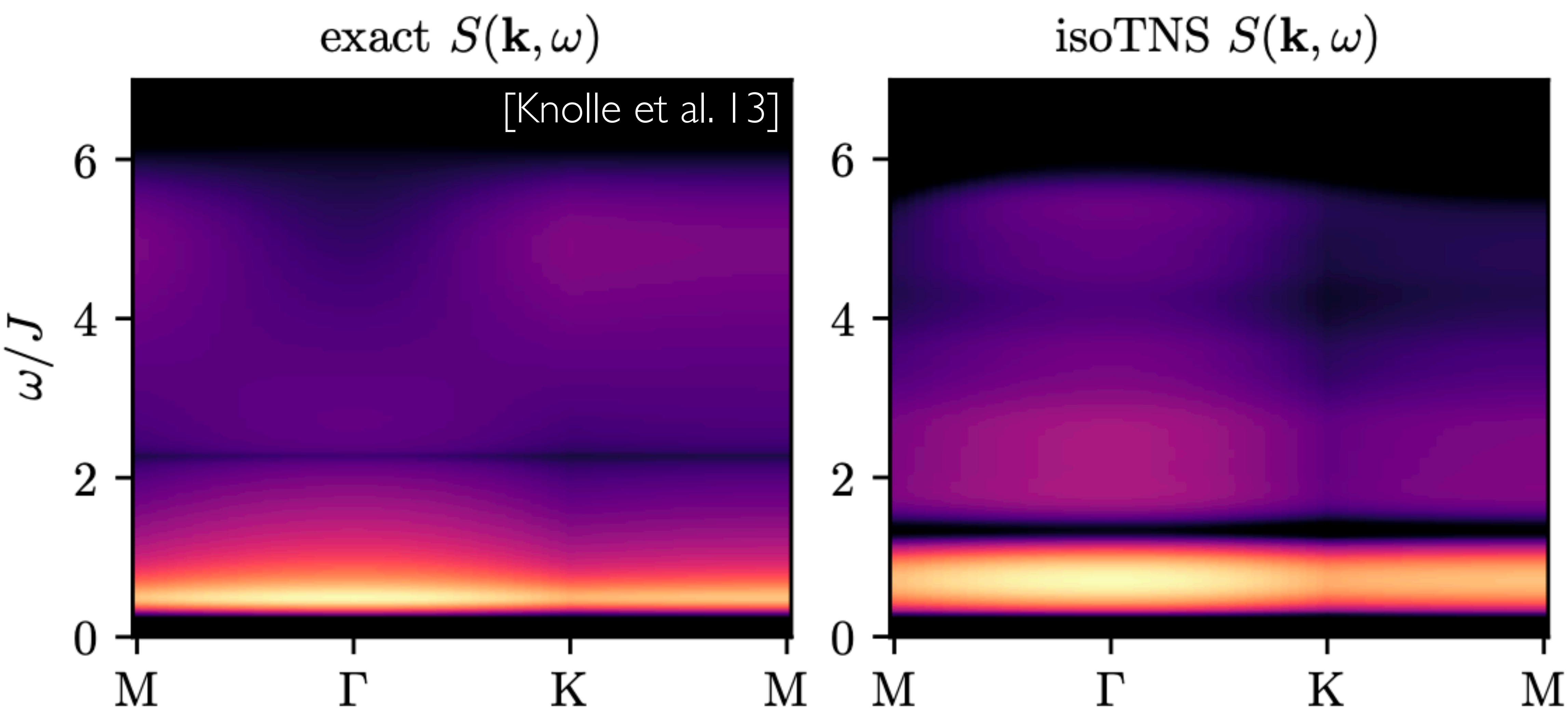
[SH Lin, M Zaletel, FP, Phys. Rev. B **106**, 245102 (2022)]

Dynamical spin structure factors from isoTNS

Dynamical structure factor: Kitaev model

$$H = J \sum_{\langle i,j \rangle_{\alpha=x,y,z}} \sigma_i^\alpha \sigma_j^\alpha$$





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isoTNS representations of thermal states

Purified isometric tensor networks

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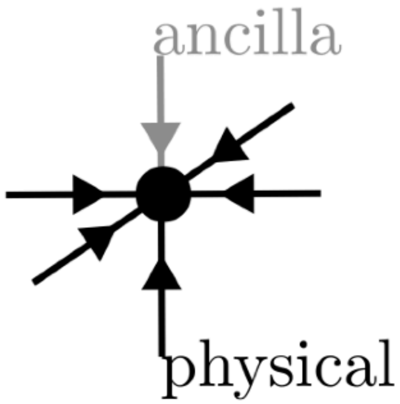

[Verstraete, Ripoll, Cirac '04]

[Kadow, FP, Knap, arXiv:2302.07905]

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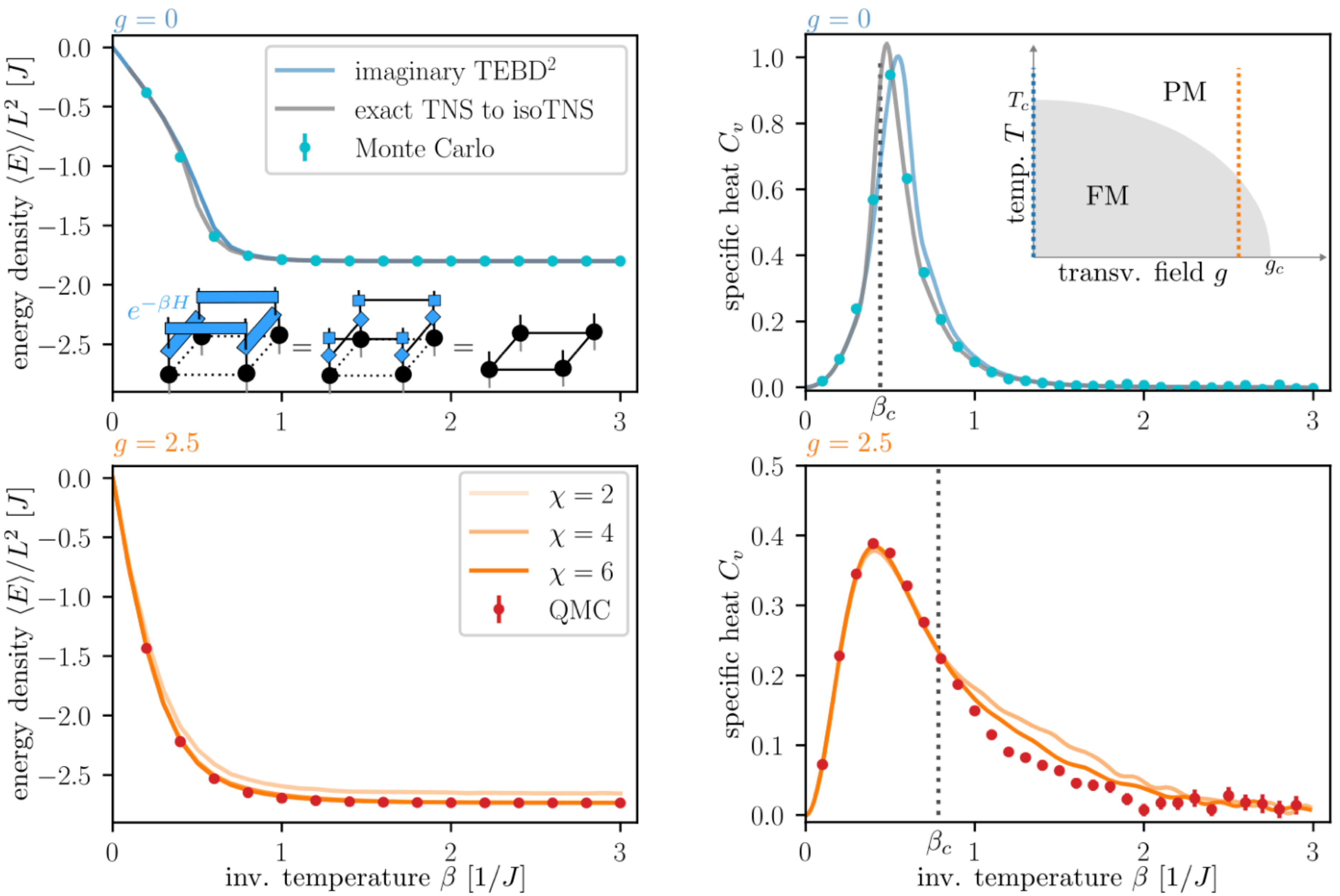

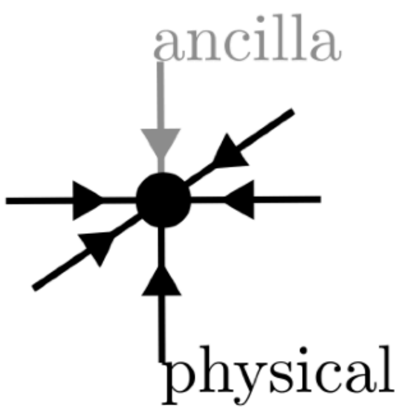

[Verstraete, Ripoll, Cirac '04]

$L = 10$

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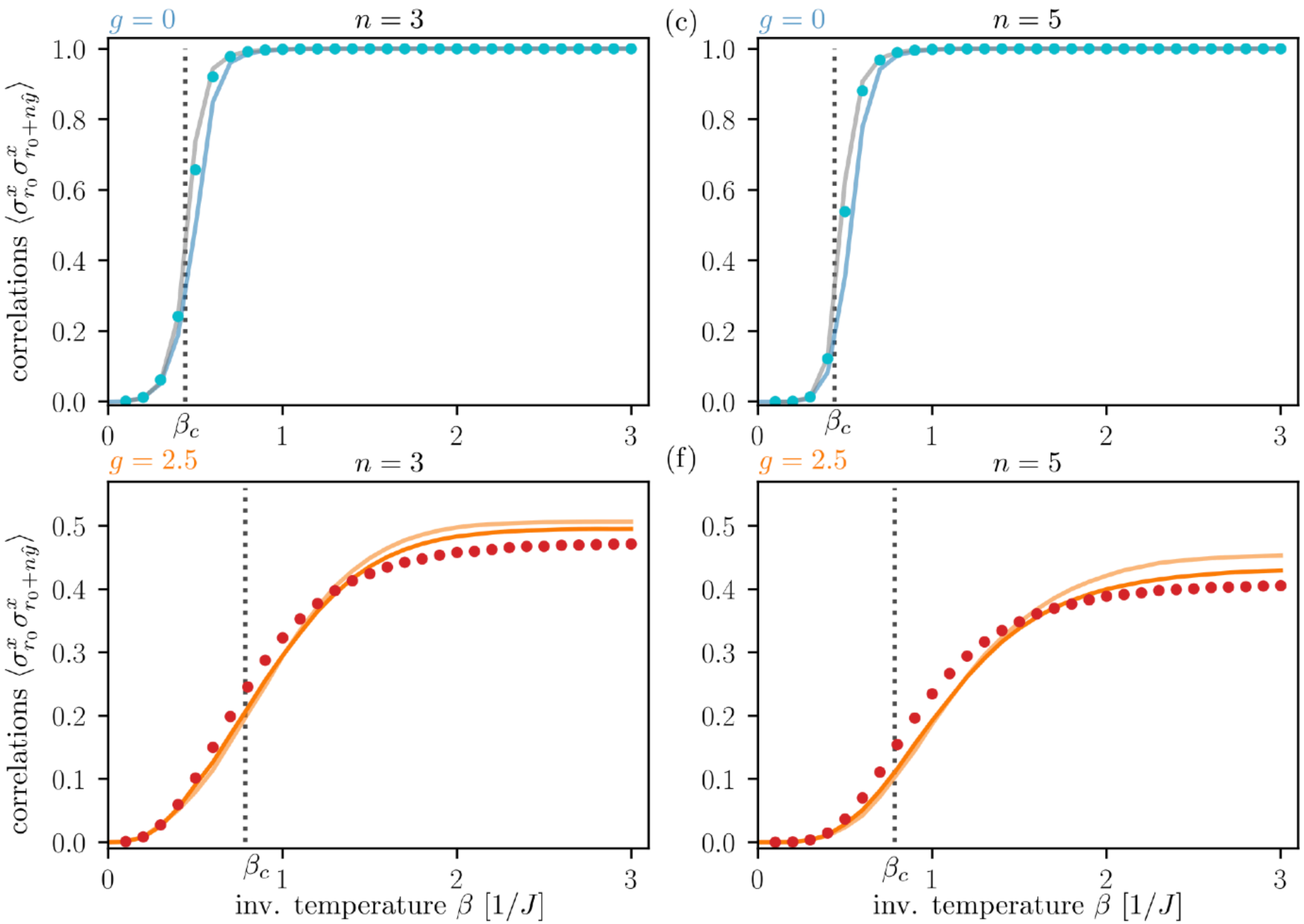

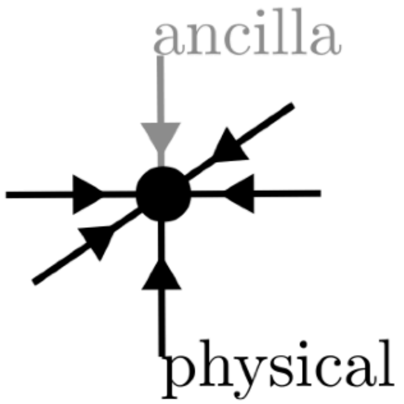

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[Kadow, FP, Knap, arXiv:2302.07905]

Outline

2D Tensor-Network State ansatz that allows for efficient contractions: isoTNS

- **TEBD²** to perform time evolution
- **DMRG²** to obtain ground states
- **Purification** of isoTNS

Mike Zaletel

Shenghsuan Lin

Wilhelm Kadow

Michael Knap