Coding Session: Numerical Simulations of Quantum Many-Body Systems

A ~~Brief~~ full-speed Introduction to MPS and DMRG

Johannes Hauschild

Technical University Munich

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Outline

Simulation of quantum many-body systems

Goal

numerically solve

$$\hat{H} |\psi_0\rangle = E_0 |\psi_0\rangle$$

$$i\hbar\partial_t |\psi(t)\rangle = \hat{H} |\psi(t)\rangle$$

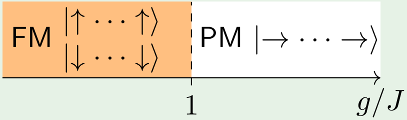
on classical computers

$$|\psi\rangle \in \mathcal{H} = \bigotimes_{i=0}^{N} \mathbb{C}^d$$

Example (Transverse Field Ising Model)

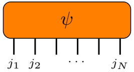
$$\hat{H} = -J \sum_{i=1}^{N-1} \hat{Z}_i \hat{Z}_{i+1} - g \sum_{i=1}^{N} \hat{X}_i$$

$$\hat{X} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{Z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$



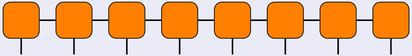
$\Rightarrow$ challenge: exponentially big $\dim \mathcal{H} = d^N$

Tensor Networks

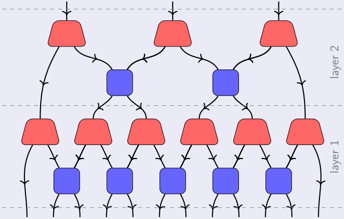
variational ansatz $|\psi\rangle = \sum_{j_1 \dots j_N}$ 

$|j_1, \dots, j_N\rangle$ with ψ tensor network

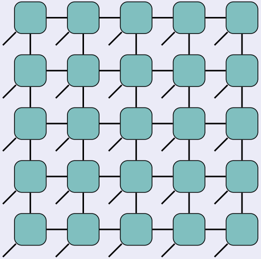
MPS (here)



MERA



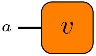
PEPS



and infinite versions

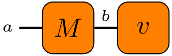
and more ...

Graphical Notation

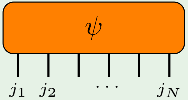
$v_a =$ 

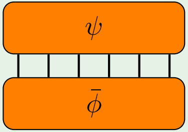
$M_{ab} =$ 

$$\Rightarrow \quad M \cdot v = \sum_b M_{ab} v_b =$$

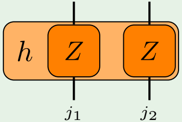


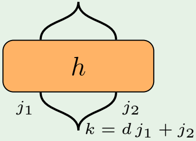
Example (overlap)

$|\psi\rangle = \sum_{j_1 \ldots j_N}$  $|j_1, \ldots, j_N\rangle$

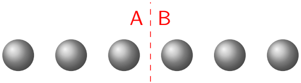
$\Rightarrow \langle \phi | \psi \rangle =$ 

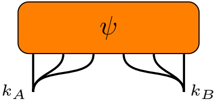
Example (reshape)

$h := \hat{Z}_1 \hat{Z}_2 =$ 

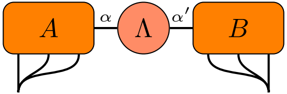
$\underset{\texttt{reshape}}{\simeq}$ 

Schmidt decomposition

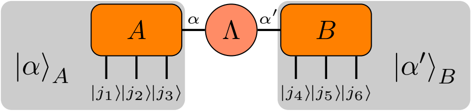


$$|\psi\rangle = \sum_{k_A,k_B}$$


$$|k_A\rangle\,|k_B\rangle$$

$$\underset{\text{SVD}}{=} \sum_{k_A,k_B}$$


$$|k_A\rangle\,|k_B\rangle$$

$$=$$


with diagonal $\Lambda_{\alpha,\alpha'} = \underbrace{\lambda_\alpha}_{\geq 0} \delta_{\alpha,\alpha'}$

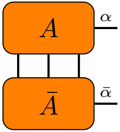
SVD Singular Value Decomposition

matrix decomposition

$$M = USV^\dagger$$

with diagonal $S \geq 0$ and isometries

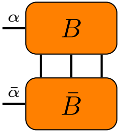
$$U^\dagger U = \mathbb{1} \qquad V^\dagger V = \mathbb{1}$$

$${}_A\langle\bar{\alpha}|\alpha\rangle_A =$$


$$=$$

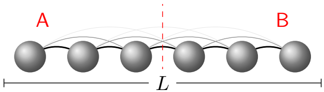

$$= \delta_{\alpha,\bar{\alpha}}$$

$$\delta_{\alpha',\bar{\alpha}'} =$$


$$=$$


$$= {}_B\langle\bar{\alpha}'|\alpha'\rangle_B$$

Area Law for Entanglement Entropy



Entanglement entropy

$$S = -\mathrm{Tr}\, \varrho_A \log(\varrho_A) = -\sum_\alpha \lambda_\alpha^2 \log \lambda_\alpha^2$$

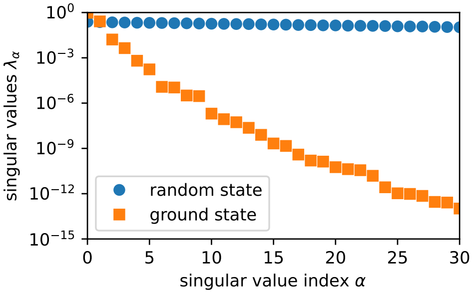
where $\varrho_A = \mathrm{Tr}_B \left|\psi\right\rangle \left\langle\psi\right| = A\Lambda^2 A^\dagger$

Area law

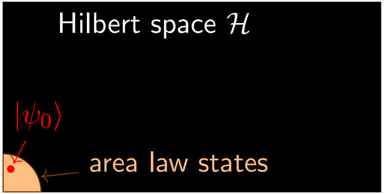
for ground states of gapped Hamiltonians

$$S \propto \text{area of cut} \underset{\text{in 1D}}{=} \mathcal{O}(L^0)$$

Hastings (J.Stat.Mech. 2007)



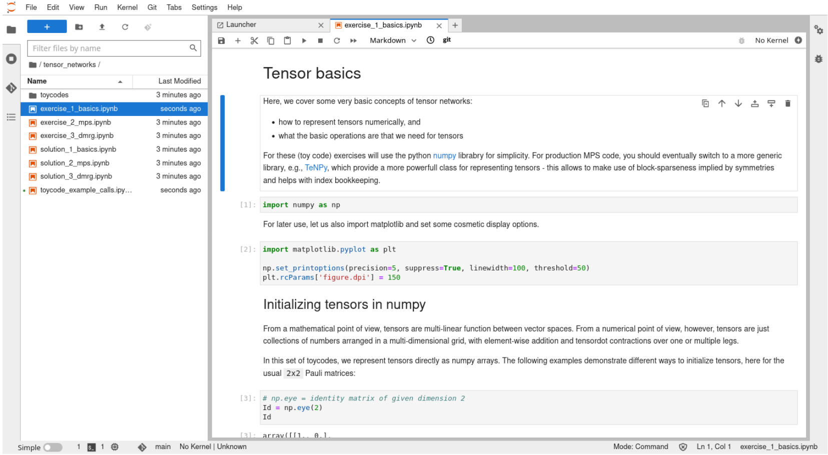
$\Rightarrow$ can truncate: only keep χ largest λ_α



Exercise 1: Tensor Basics

`https://quanthub.pks.mpg.de`, Login and Passwort same as for WiFi

also `https://github.com/mgbukov/quant22_notebooks`

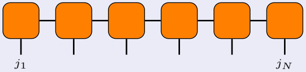


Matrix Product States (MPS)

Definition (MPS)

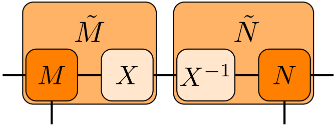
Variational Ansatz

$$|\psi\rangle = \sum_{j_1 \dots j_N}$$



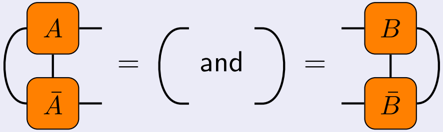
$$|j_1, \dots, j_N\rangle$$

gauge freedom on contracted legs:

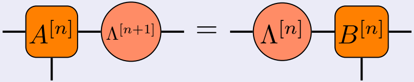


Canonical Form

ONB of Schmidt states



in canonical form with



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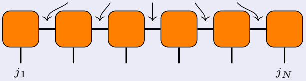
$|\psi\rangle = \sum_{j_1 \dots j_N}$  $|j_1, \dots, j_N\rangle$

free parameters $\mathcal{O}(d^N) \to \mathcal{O}(N\chi^2)$

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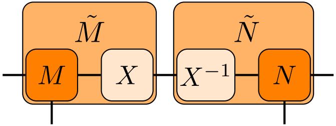

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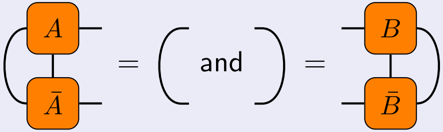

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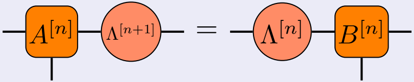

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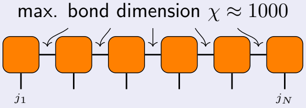
$|\psi\rangle = \sum_{j_1 \dots j_N}$ 

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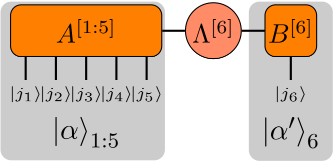

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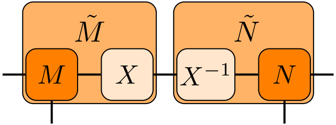

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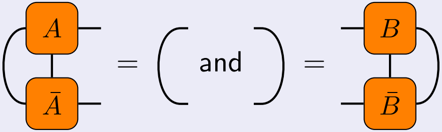

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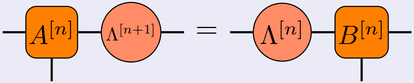

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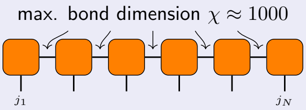
$|\psi\rangle = \sum_{j_1 \dots j_N}$  $|j_1, \dots, j_N\rangle$

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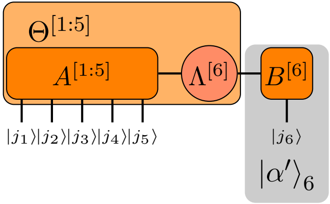

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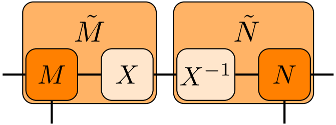

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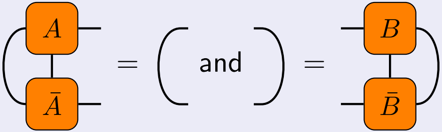

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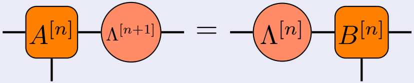

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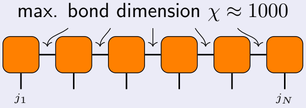
$$|\psi\rangle = \sum_{j_1 \dots j_N}$$ 

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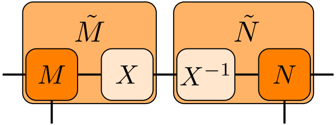

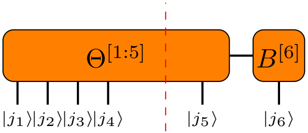

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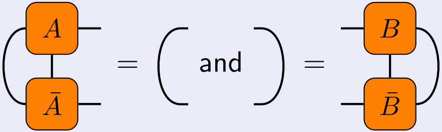

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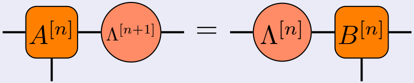

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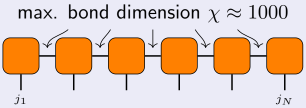
$$|\psi\rangle = \sum_{j_1 \dots j_N}$$ 

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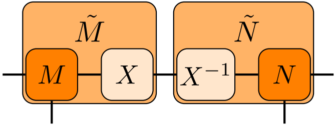

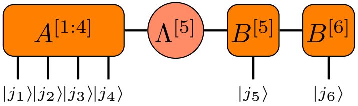

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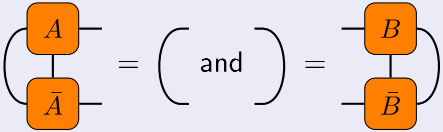

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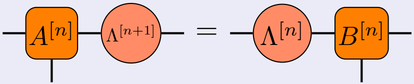

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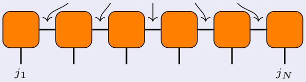
$$|\psi\rangle = \sum_{j_1 \dots j_N}$$  $$|j_1, \dots, j_N\rangle$$

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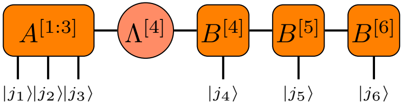

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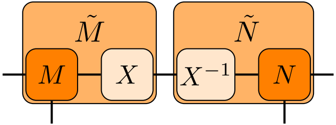

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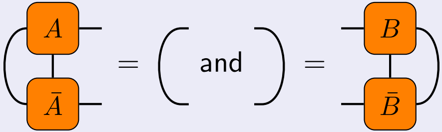

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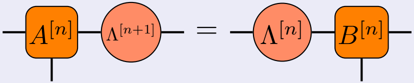

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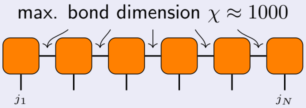
$|\psi\rangle = \sum_{j_1 \dots j_N}$  $|j_1, \dots, j_N\rangle$

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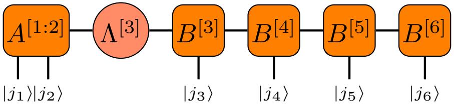

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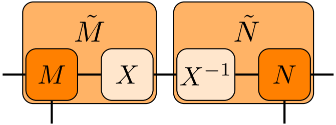

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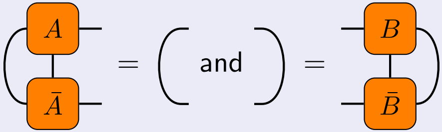

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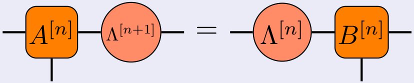

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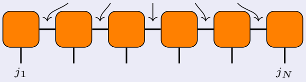
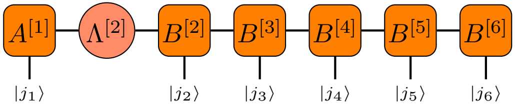
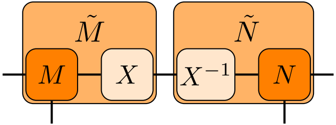


$$|j_1, \ldots, j_N\rangle$$

free parameters $\mathcal{O}(d^N) \to \mathcal{O}(N\chi^2)$

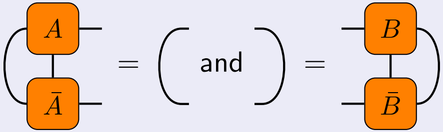


gauge freedom on contracted legs:

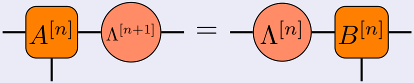


Canonical Form

ONB of Schmidt states



in canonical form with

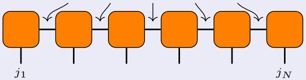


Matrix Product States (MPS)

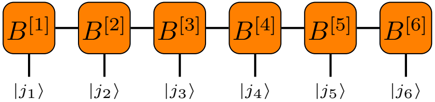
Definition (MPS)

Variational Ansatz

max. bond dimension $\chi \approx 1000$

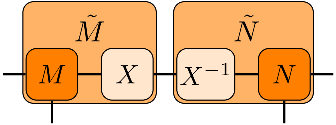
$|\psi\rangle = \sum_{j_1 \ldots j_N}$  $|j_1, \ldots, j_N\rangle$

free parameters $\mathcal{O}(d^N) \to \mathcal{O}(N\chi^2)$



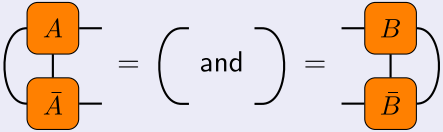
$\to$ in *right* canonical form

gauge freedom on contracted legs:

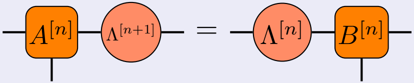


Canonical Form

ONB of Schmidt states



in canonical form with



Matrix Product States (MPS)

Definition (MPS)

Variational Ansatz

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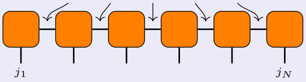
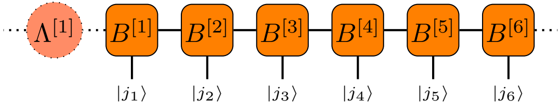
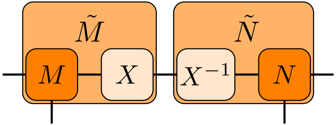
$|\psi\rangle = \sum_{j_1 \dots j_N}$  $|j_1, \dots, j_N\rangle$

free parameters $\mathcal{O}(d^N) \to \mathcal{O}(N\chi^2)$



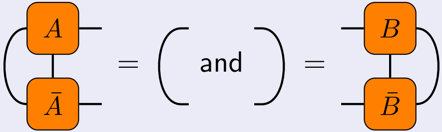
$\to$ in *right* canonical form

gauge freedom on contracted legs:

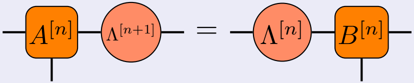


Canonical Form

ONB of Schmidt states



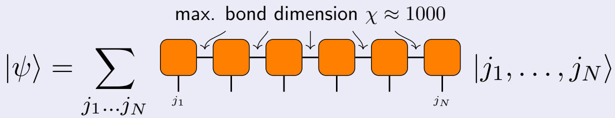
in canonical form with



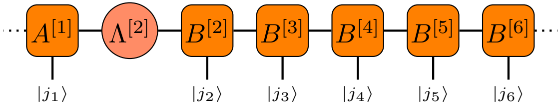
Matrix Product States (MPS)

Definition (MPS)

Variational Ansatz

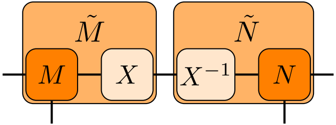


free parameters $\mathcal{O}(d^N) \to \mathcal{O}(N\chi^2)$



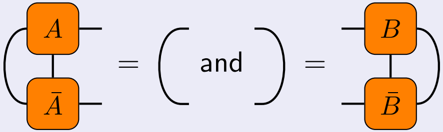
$\to$ in *mixed* canonical form

gauge freedom on contracted legs:

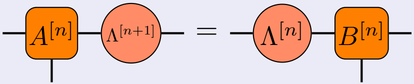


Canonical Form

ONB of Schmidt states



in canonical form with



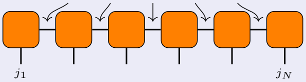
Matrix Product States (MPS)

Definition (MPS)

Variational Ansatz

max. bond dimension $\chi \approx 1000$

$$|\psi\rangle = \sum_{j_1 \dots j_N}$$



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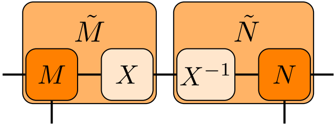
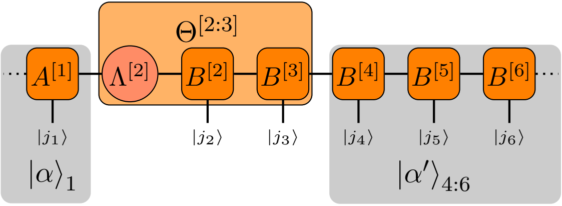
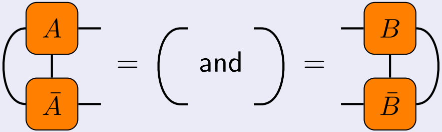




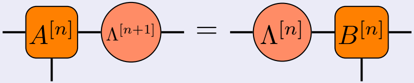
$\to$ in *mixed* canonical form

Canonical Form

ONB of Schmidt states



in canonical form with



Matrix Product States (MPS)

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Variational Ansatz

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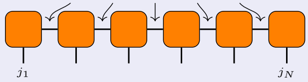
$|\psi\rangle = \sum_{j_1 \dots j_N}$  $|j_1, \dots, j_N\rangle$

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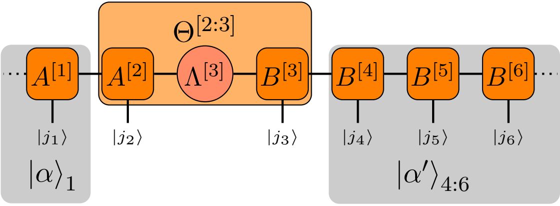
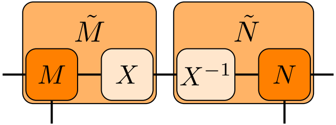


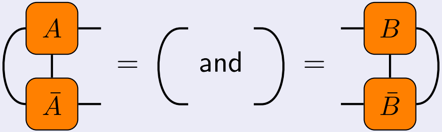
$\to$ in *mixed* canonical form

gauge freedom on contracted legs:



Canonical Form

ONB of Schmidt states



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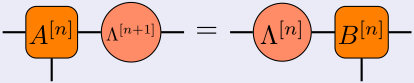

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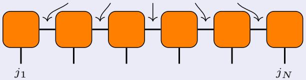
$|\psi\rangle = \sum_{j_1 \ldots j_N}$  $|j_1, \ldots, j_N\rangle$

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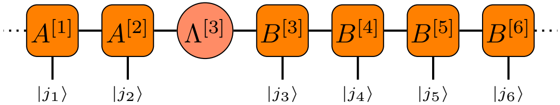

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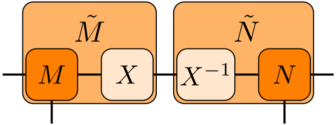
gauge freedom on contracted legs:



Canonical Form

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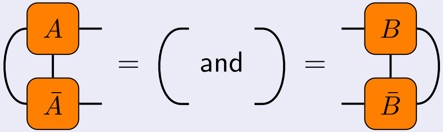

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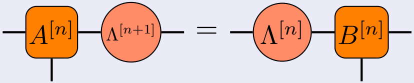

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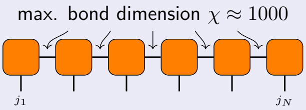
$|\psi\rangle = \sum_{j_1 \dots j_N}$  $|j_1, \dots, j_N\rangle$

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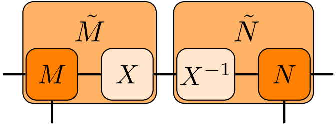
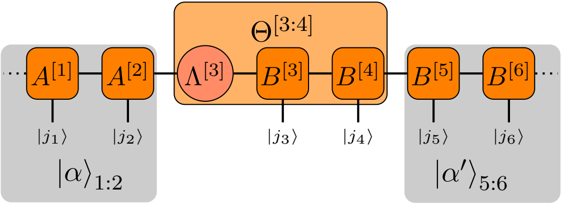
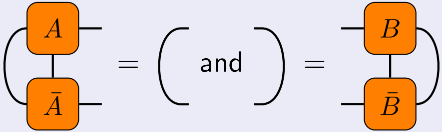




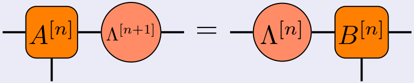
$\to$ in *mixed* canonical form

Canonical Form

ONB of Schmidt states



in canonical form with



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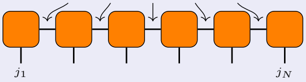

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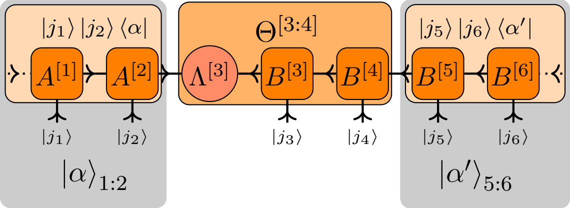

$\to$ in *mixed* canonical form

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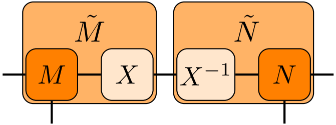
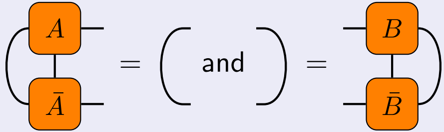
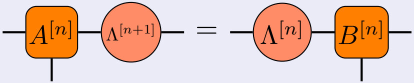


Canonical Form

ONB of Schmidt states

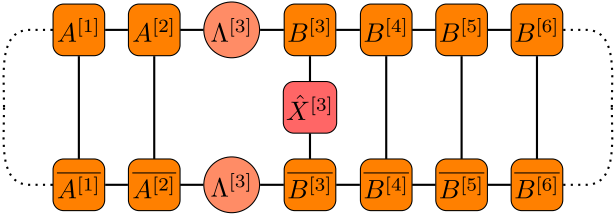


in canonical form with



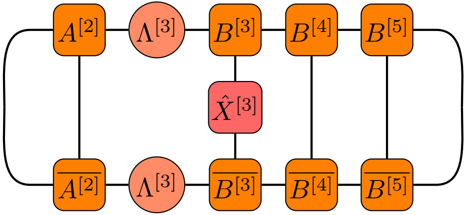
MPS Expectation values

$$\langle\psi|\hat{X}_3|\psi\rangle =$$



$\Rightarrow$ always contract *locally*, never top to bottom!

MPS Expectation values

$\langle\psi|\hat{X}_3|\psi\rangle =$ 

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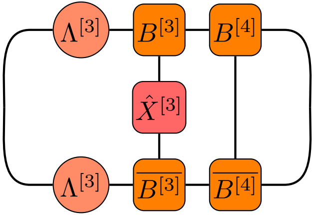

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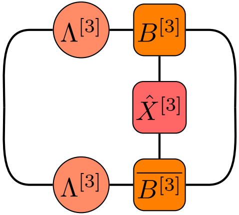
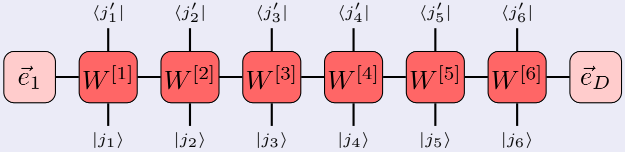


$\Rightarrow$ always contract *locally*, never top to bottom!

Matrix Product Operator (MPO)

Definition (MPO)

write Hamiltonian $\hat{H}$ as



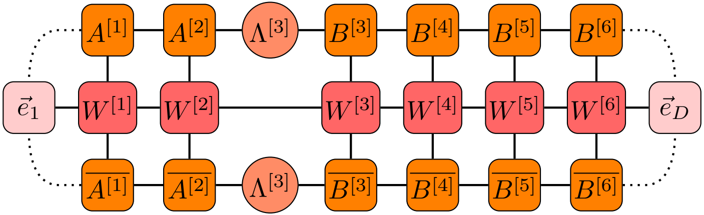
Example (Transverse Field Ising)

$$\hat{H} = -J \sum_i \hat{Z}_i \hat{Z}_{i+1} - g \sum_i \hat{X}_i$$

$$W^{[n]}_{\alpha,\alpha'} = \begin{pmatrix} \mathbb{1} & \hat{Z}_n & -g\hat{X}_n \\ & & J\hat{Z}_n \\ & & \mathbb{1} \end{pmatrix}$$

bond dimension D depends on $\hat{H}$

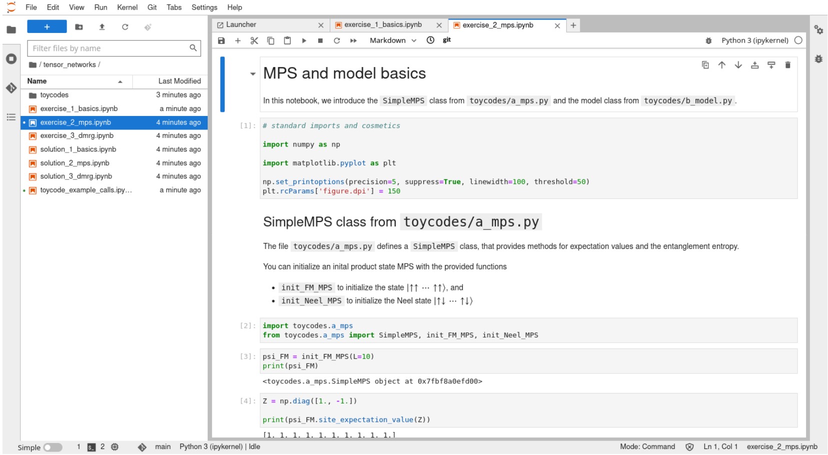
$E = \langle\psi|\hat{H}|\psi\rangle =$



Exercise 2: MPS and Model

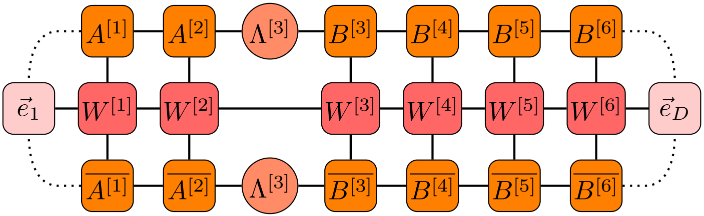
`https://quanthub.pks.mpg.de`, Login and Passwort same as for WiFi

also `https://github.com/mgbukov/quant22_notebooks`

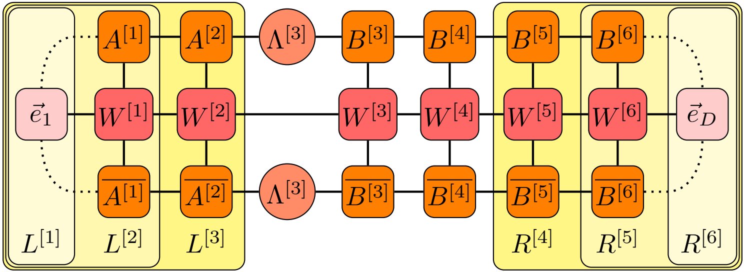


Density matrix renormalization group (DMRG) algorithm

$$E = \langle\psi|\hat{H}|\psi\rangle =$$

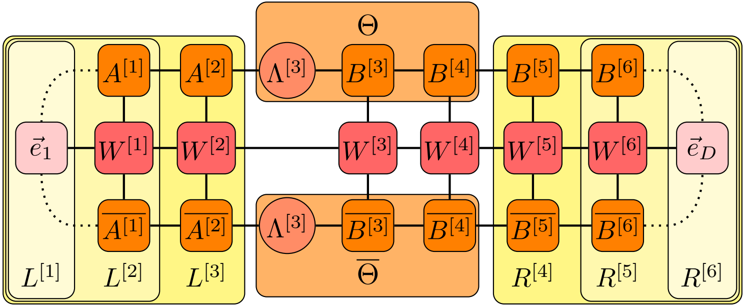


Density matrix renormalization group (DMRG) algorithm

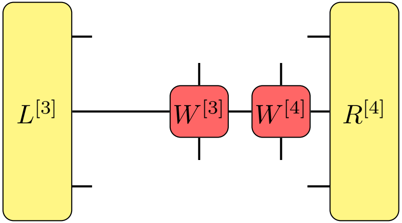
$E = \langle\psi|\hat{H}|\psi\rangle =$ 

Density matrix renormalization group (DMRG) algorithm

$E = \langle\Theta|\hat{H}_{\text{eff}}|\Theta\rangle =$

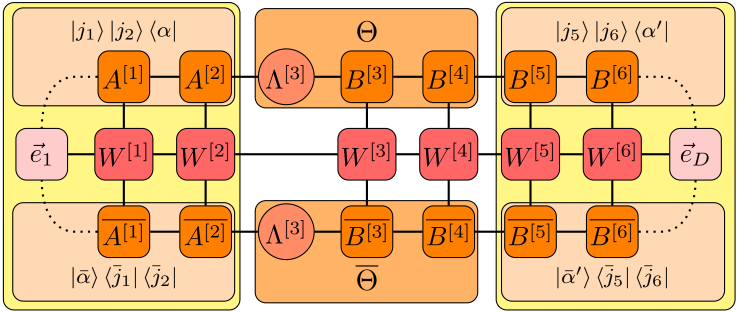


$\hat{H}_{\text{eff}} =$



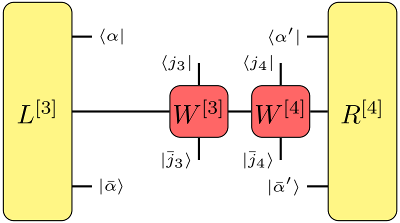
Density matrix renormalization group (DMRG) algorithm

$E = \langle \Theta | \hat{H}_{\text{eff}} | \Theta \rangle =$

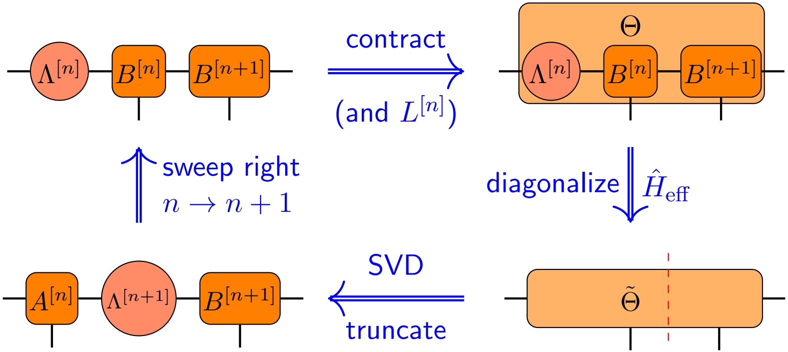


$\Rightarrow$ diagonalize $\hat{H}_{\text{eff}}$
with Lanczos
to update $\Theta \to \tilde{\Theta}$

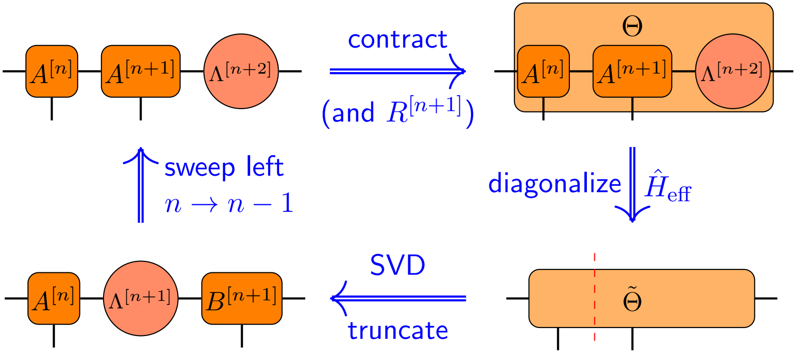
$\hat{H}_{\text{eff}} =$



DMRG update loop



DMRG update loop



Exercise 3: DMRG

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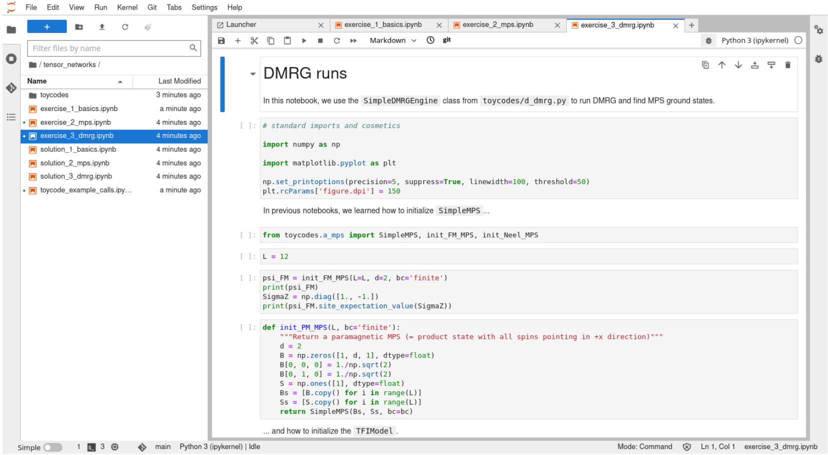
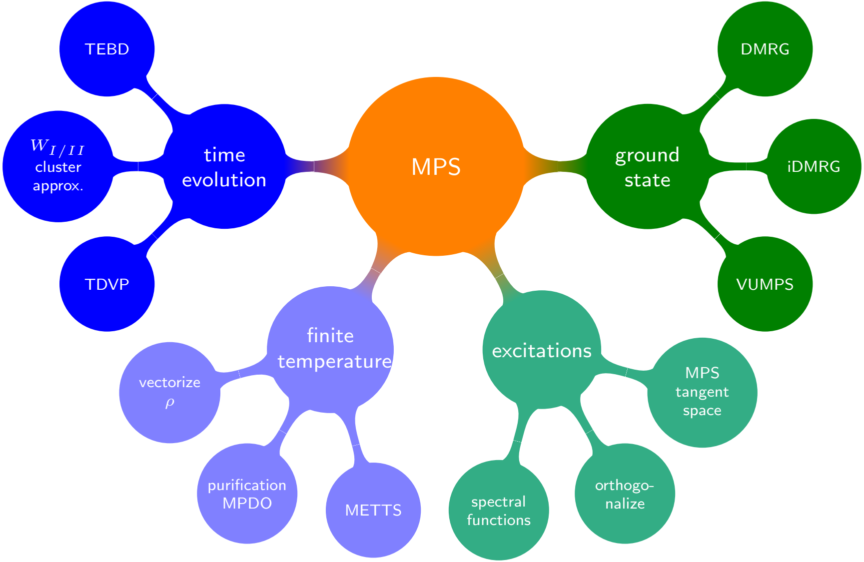


Outlook: other MPS-based algorithms



(Some) References

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- Yearly schools: European tensor network `quantumtensor.eu`

Appendix

More MPO examples

Translation invariant MPO

$$\hat{H} = \sum_{i<k} C_i \left(\prod_{j=i+1}^{k-1} A_j \right) B_k + \sum_i D_i$$

$$W^{[n]}_{\alpha,\alpha'} = \left(\begin{array}{c|c|c} \mathbb{1} & C & D \\ \hline & \mathsf{A} & B \\ \hline & & \mathbb{1} \end{array}\right)$$