# **Tensor Networks**

How physicists can tackle exponentially hard problems

March 4 – 7, 2019 | Patrick Emonts | Max Planck Institute of Quantum Optics



## **Overview**

Introduction

Matrix Product States

**iTEBD** 

References

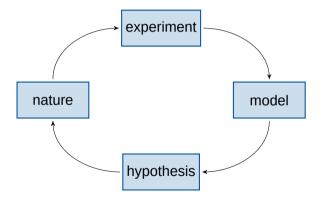


# Section 1

Introduction

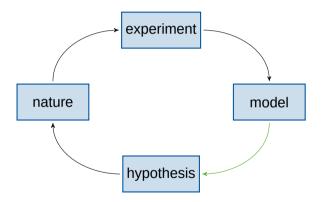


## **Motivation**





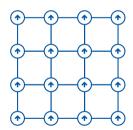
## **Motivation**





## How complex is this problem?

We take a system that can take two states  $\uparrow$  and  $\psi$ 

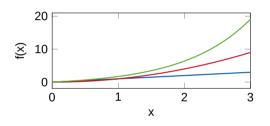


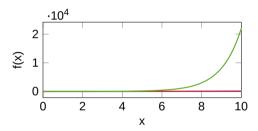
## Number of possibilities

$$Z = 2^N$$



## How bad is exponential scaling?





## Physical example

- 10<sup>23</sup> Number of atoms in 12 g of carbon
- 10<sup>80</sup> Number of atoms in the visible universe



## Quantum Mechanics in 2 slides - Slide 1



Hilbert space  $\mathcal H$  vector space of all possible configurations state  $|\Psi\rangle$  vector in  $\mathcal H$  that describes the state of the system Hamilton operator  $\mathcal H$  Linear operator that describes the energy of the system

#### Note on Notation: Bra and Ket vectors

 $|\Psi\rangle$  is a column vector  $\frac{\Psi}{\Psi}$ 

or  $\begin{vmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \end{vmatrix}$ 

 $\langle \Psi |$  is a row vector

$$\overline{\psi}_0 | \overline{\psi}_1 | \overline{\psi}_2$$



## **Quantum Mechanics in 2 slides – Slide 2**

## Schrödinger equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = H|\Psi(t)\rangle$$

time-independent Schrödinger equation (time-ind. Hamiltonian)

$$H|\Psi\rangle = E|\Psi\rangle$$



## **Quantum Mechanics in 2 slides - Slide 2**

## Schrödinger equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}|\Psi(t)\rangle = H|\Psi(t)\rangle$$

## time-independent Schrödinger equation (time-ind. Hamiltonian)

$$H|\Psi\rangle = E|\Psi\rangle$$

## **Expectation values**

Probability theory 
$$\langle X \rangle = P(X)X$$

Quantum mechanics 
$$\langle E \rangle = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$



# **Expressing spins with matrices**

## **Definitions**

$$|\uparrow\rangle = \begin{pmatrix} 1\\0 \end{pmatrix}$$

$$| \mathbf{\Psi} \rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$S_z = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

## Calculating with spins

$$S_{z}|\uparrow\uparrow\rangle = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
$$= \frac{1}{2} |\uparrow\uparrow\rangle$$



## **Combining multiple spins**

Consider a system consisting of two spins that can two values ( $\checkmark$  and  $^{\land}$ )

## Hilbert space $\mathcal{H}$

$$\mathcal{H} = \operatorname{span} \{ | \mathbf{\psi}_1 \rangle | \mathbf{\psi}_2 \rangle, | \mathbf{\psi}_1 \rangle | \mathbf{\uparrow}_2 \rangle, | \mathbf{\uparrow}_1 \rangle | \mathbf{\psi}_2 \rangle, | \mathbf{\uparrow}_1 \rangle | \mathbf{\uparrow}_2 \rangle \}$$

Spins on different sites are combined by tensor products

$$|\mathbf{\Psi}_1\rangle|\mathbf{\Psi}_2\rangle = \begin{pmatrix} 0\\1 \end{pmatrix} \otimes \begin{pmatrix} 0\\1 \end{pmatrix} = \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix}$$

$$| \bigstar_1 \rangle | \bigstar_2 \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

$$| \mathbf{\Psi}_1 \rangle | \mathbf{\Phi}_2 \rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$| \mathbf{\uparrow}_1 \rangle | \mathbf{\uparrow}_2 \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

# **Letting spins interact**

## Interaction of two spins

$$H = -J\left(S_1^z \otimes S_2^z\right)$$

## Matrix representation

$$\begin{split} H &= -J \left( \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \otimes \left( \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \\ &= -\frac{J}{4} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = -\frac{J}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \end{pmatrix} \end{split}$$



## Calculating an expectation value

## Preparation of a state

$$\begin{aligned} |\Psi\rangle &= \sqrt{0.5} | \mathbf{\uparrow}_1 \rangle | \mathbf{\downarrow}_2 \rangle + \sqrt{0.5} | \mathbf{\downarrow}_1 \rangle | \mathbf{\uparrow}_2 \rangle \\ &= \sqrt{0.5} | \mathbf{\uparrow}_1 \mathbf{\downarrow}_2 \rangle + \sqrt{0.5} | \mathbf{\downarrow}_1 \mathbf{\uparrow}_2 \rangle \\ &= \sqrt{0.5} | \mathbf{\uparrow} \mathbf{\downarrow} \rangle + \sqrt{0.5} | \mathbf{\downarrow} \mathbf{\uparrow} \rangle \\ &= \begin{pmatrix} 0 \\ \sqrt{0.5} \\ \sqrt{0.5} \\ 0 \end{pmatrix} \end{aligned}$$

## Calculating an expectation value

## Preparation of a state

$$\begin{aligned} |\Psi\rangle &= \sqrt{0.5} | \uparrow \uparrow_1 \rangle | \downarrow \downarrow_2 \rangle + \sqrt{0.5} | \downarrow \uparrow_1 \rangle | \uparrow \uparrow_2 \rangle \\ &= \sqrt{0.5} | \uparrow \uparrow_1 \downarrow \downarrow_2 \rangle + \sqrt{0.5} | \downarrow \uparrow \uparrow_2 \rangle \\ &= \sqrt{0.5} | \uparrow \downarrow \downarrow \rangle + \sqrt{0.5} | \downarrow \uparrow \uparrow \rangle \\ &= \begin{pmatrix} 0 \\ \sqrt{0.5} \\ \sqrt{0.5} \\ 0 \end{pmatrix} \end{aligned}$$

## **Expectation value**

$$\begin{split} \langle H \rangle &= \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle \\ &= \langle \Psi | H | \Psi \rangle \\ &= -\frac{J}{4} ( \circ \sqrt{0.5} \sqrt{0.5} \circ ) \begin{pmatrix} \frac{1}{0} & \frac{0}{-1} & \frac{0}{0} & \frac{0}{0} \\ \frac{0}{0} & \frac{-1}{0} & \frac{0}{1} & 0 \end{pmatrix} \begin{pmatrix} \frac{0}{\sqrt{0.5}} \\ \sqrt{0.5} \\ 0 & 0 & 0 & 1 \end{pmatrix} \\ &= \frac{J}{4} \end{split}$$

# **Summary – Introduction**

## Computation

- Computational complexity of many-body systems scales exponentially with the system size
- We cannot solve those systems exactly and have to use approximate methods

## **Physics**

- Quantum mechanical systems evolve according to the Schrödinger equation
- We are interested in the ground-state  $|\Psi\rangle$  and expectation values  $\langle E\rangle = \frac{\langle \Psi|H|\Psi\rangle}{\langle \Psi|\Psi\rangle}$

## Section 2

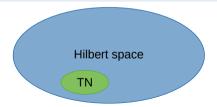
## **Matrix Product States**



#### **Tensor Networks**

## Idea

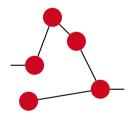
Use an Ansatz with polynomially many parameters although the Hilbert space has exponentially many states



We explore only a small part of the Hilbert space

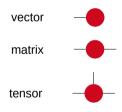


## What is a tensor network?



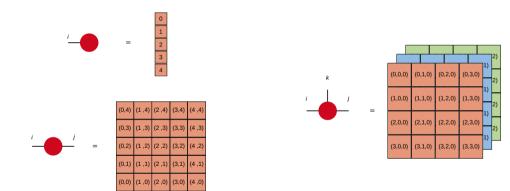


## **Pictorial representation**



- The number of legs determines the number of indices of the object
- A connection ⇔ Contraction of indices

## **Pictorial representation as Arrays**



## **Calculations with pictures**

## Matrix-Vector Multiplication

$$\mathbf{v}_i = \sum_{i,j} A_{ij} \mathbf{b}_j$$

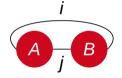
$$\frac{i}{\mathbf{v}} = \frac{i}{\mathbf{A}} \frac{j}{b}$$

## Matrix-Matrix Multiplication

$$C_{kl} = \sum_{i,k,l} A_{ki} B_{il}$$

$$\frac{k}{C} = \frac{k}{A} \frac{i}{B} \frac{I}{B}$$

# **Calculations with pictures – Quiz**





## **Calculations with pictures – Quiz**

$$C = A_{j}B$$

## Trace

$$c = \sum_{i,j} A_{ij} B_j$$
$$= Tr[AB]$$

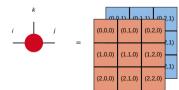


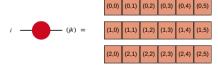
## **Tensor manipulations – Grouping**

## **Tensor to Matrix**

$$A_{i,j,k} = A_{i,(jk)}$$
$$= A_{i,m}$$

# Pictorial language

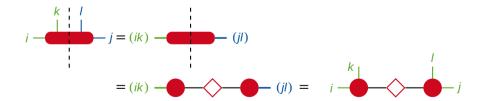




# **Tensor manipulations – Splitting**

## Splitting of tensor

$$A = U \cdot S \cdot V^{\dagger}$$



## **Singular Value Decomposition**



# Singular Value Decomposition

$$M = U \cdot S \cdot V^{\dagger}$$

- ↑ arbitrary mxn matrix
- *U* unitary *mxm* matrix
- S diagonal mxn matrix
- V unitary nxn matrix



## **SVD** - Truncation





The shape of M does not change since we are only manipulating an index which we contract.

# **SVD - Example**





Truncated Image (20 SV)



#### Back to formulas: What is a Tensor Network?

## A general quantum mechanical state

$$|\Psi\rangle = \sum_{\sigma_1...\sigma_n} c_{\sigma_1,\sigma_2...\sigma_N} |\sigma_1\sigma_2...\sigma_n\rangle$$

# Example: $|\Psi\rangle = \sqrt{0.5} |\uparrow\rangle |\downarrow\rangle + \sqrt{0.5} |\downarrow\rangle |\uparrow\rangle$

$$\mathcal{H} = \operatorname{span}\{|\mathbf{\psi}_{1}\rangle|\mathbf{\psi}_{2}\rangle, \\ |\mathbf{\psi}_{1}\rangle|\mathbf{\uparrow}_{2}\rangle, \\ |\mathbf{\uparrow}_{1}\rangle|\mathbf{\psi}_{2}\rangle, \\ |\mathbf{\uparrow}_{1}\rangle|\mathbf{\uparrow}_{2}\rangle\}$$

$$c_{\mathbf{\psi}_1,\mathbf{\psi}_2} = 0$$

$$c_{\mathbf{\psi}_1,\mathbf{\psi}_2} = \sqrt{0.5}$$

$$c_{\mathbf{\psi}_1,\mathbf{\psi}_2} = \sqrt{0.5}$$

$$\sqrt{\mathbf{p}_1,\mathbf{p}_2} = \sqrt{0.5}$$

$$\mathbf{A}_{1}, \mathbf{\Psi}_{2} = \sqrt{0.5}$$

$$c_{\uparrow_1,\uparrow_2} = 0$$



#### Back to formulas: What is a Tensor Network?

## A general quantum mechanical state

$$|\Psi\rangle = \sum_{\sigma_1...\sigma_n} c_{\sigma_1,\sigma_2...\sigma_N} |\sigma_1 \sigma_2 ... \sigma_n\rangle$$

#### Problem

The coefficients depend on the configuration of all spins. Thus, there are exponentially many coefficients.



#### Back to formulas: What is a Tensor Network?

## A general quantum mechanical state

$$|\Psi\rangle = \sum_{\sigma_1...\sigma_n} c_{\sigma_1,\sigma_2...\sigma_N} |\sigma_1\sigma_2...\sigma_n\rangle$$

#### **Problem**

The coefficients depend on the configuration of all spins. Thus, there are exponentially many coefficients.

## A fancy way to write a quantum mechanical state

$$|\Psi\rangle = \sum_{\sigma_1 \dots \sigma_n} \underbrace{\sum_{a_1,\dots,a_{n-1}} A_{a_1}^{\sigma_1} A_{a_1,a_2}^{\sigma_2} \cdots A_{a_{n-2},a_{n-1}}^{\sigma_{n-1}} A_{a_{n-1}}^{\sigma_n}}_{c_{\sigma_1,\sigma_2\dots\sigma_N}} |\sigma_1 \sigma_2 \dots \sigma_n\rangle$$



# **Tensor Networks – Thinking about Indices**

#### A Tensor Network State

$$|\Psi\rangle=\sum_{\sigma_1\dots\sigma_n}\sum_{a_1,\dots,a_{n-1}}A_{a_1}^{\sigma_1}A_{a_1,a_2}^{\sigma_2}\cdots A_{a_{n-2},a_{n-1}}^{\sigma_{n-1}}A_{a_{n-1}}^{\sigma_n}\left|\sigma_1\sigma_2\dots\sigma_n\right\rangle$$

## Dimensions of object A

 $\sigma$ : physical index: ( $\uparrow$ ,  $\psi$ )

$$A_{a_j,a_{j+1}}^{\sigma}$$

a: virtual index

Dimension of physical index  $d (\sim 10)$ 

Dimension of virtual index

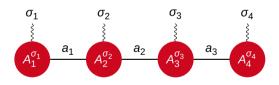
 $D (\sim 100)$ 



#### **Matrix Product States**

## A Tensor Network State

$$|\Psi\rangle = \sum_{\sigma_1 \dots \sigma_n} \sum_{a_1, \dots, a_{n-1}} A_{a_1}^{\sigma_1} A_{a_1, a_2}^{\sigma_2} \cdots A_{a_{n-2}, a_{n-1}}^{\sigma_{n-1}} A_{a_{n-1}}^{\sigma_n} \left| \sigma_1 \sigma_2 \dots \sigma_n \right\rangle$$



- Dimension: 1D
- Typical quantities
  - correlations
  - expectation values of observables



## **Matrix Product States – How to get the Tensors?**

## A general quantum mechanical state

$$|\Psi\rangle = \sum_{\sigma_1...\sigma_n} c_{\sigma_1,\sigma_2...\sigma_N} |\sigma_1 \sigma_2 ... \sigma_n\rangle$$

$$c_{\sigma_1,\sigma_2,...,\sigma_N} =$$

#### Matrix Product state

$$|\Psi\rangle = \sum_{\sigma_1 \dots \sigma_n} \sum_{a_1, \dots, a_{n-1}} A_{a_1}^{\sigma_1} A_{a_1, a_2}^{\sigma_2} \cdots A_{a_{n-2}, a_{n-1}}^{\sigma_{n-1}} A_{a_{n-1}}^{\sigma_n} \left| \sigma_1 \sigma_2 \dots \sigma_n \right\rangle$$



## **Matrix Product States – How to get the Tensors?**

#### A general quantum mechanical state

$$|\Psi\rangle = \sum_{\sigma_1...\sigma_n} c_{\sigma_1,\sigma_2...\sigma_N} |\sigma_1 \sigma_2 ... \sigma_n\rangle$$



#### Matrix Product state

$$|\Psi\rangle=\sum_{\sigma_1\dots\sigma_n}\sum_{a_1,\dots,a_{n-1}}A_{a_1}^{\sigma_1}A_{a_1,a_2}^{\sigma_2}\cdots A_{a_{n-2},a_{n-1}}^{\sigma_{n-1}}A_{a_{n-1}}^{\sigma_n}\left|\sigma_1\sigma_2\dots\sigma_n\right\rangle$$



#### A general quantum mechanical state

$$|\Psi\rangle = \sum_{\sigma_1...\sigma_n} c_{\sigma_1,\sigma_2...\sigma_N} |\sigma_1\sigma_2...\sigma_n\rangle$$

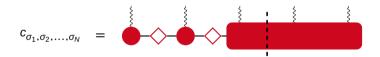
$$c_{\sigma_1,\sigma_2,...,\sigma_N} =$$

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#### A general quantum mechanical state

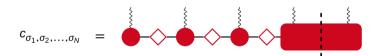
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$$|\Psi\rangle=\sum_{\sigma_1\dots\sigma_n}\sum_{a_1,\dots,a_{n-1}}A_{a_1}^{\sigma_1}A_{a_1,a_2}^{\sigma_2}\cdots A_{a_{n-2},a_{n-1}}^{\sigma_{n-1}}A_{a_{n-1}}^{\sigma_n}\left|\sigma_1\sigma_2\dots\sigma_n\right\rangle$$

#### A general quantum mechanical state

$$|\Psi\rangle = \sum_{\sigma_1...\sigma_n} c_{\sigma_1,\sigma_2...\sigma_N} |\sigma_1 \sigma_2 ... \sigma_n\rangle$$



$$|\Psi\rangle=\sum_{\sigma_1\dots\sigma_n}\sum_{a_1,\dots,a_{n-1}}A_{a_1}^{\sigma_1}A_{a_1,a_2}^{\sigma_2}\cdots A_{a_{n-2},a_{n-1}}^{\sigma_{n-1}}A_{a_{n-1}}^{\sigma_n}\left|\sigma_1\sigma_2\dots\sigma_n\right\rangle$$



#### A general quantum mechanical state

$$|\Psi\rangle = \sum_{\sigma_1...\sigma_n} c_{\sigma_1,\sigma_2...\sigma_N} |\sigma_1 \sigma_2 ... \sigma_n\rangle$$

$$c_{\sigma_1,\sigma_2,...,\sigma_N} =$$

$$|\Psi\rangle = \sum_{\sigma_1...\sigma_n} \sum_{a_1,...,a_{n-1}} A_{a_1}^{\sigma_1} A_{a_1,a_2}^{\sigma_2} \cdots A_{a_{n-2},a_{n-1}}^{\sigma_{n-1}} A_{a_{n-1}}^{\sigma_n} |\sigma_1 \sigma_2 \dots \sigma_n\rangle$$



#### A general quantum mechanical state

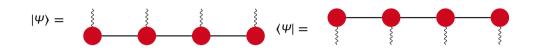
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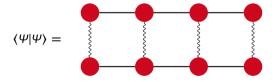


$$|\Psi\rangle=\sum_{\sigma_1\dots\sigma_n}\sum_{a_1,\dots,a_{n-1}}A_{a_1}^{\sigma_1}A_{a_1,a_2}^{\sigma_2}\cdots A_{a_{n-2},a_{n-1}}^{\sigma_{n-1}}A_{a_{n-1}}^{\sigma_n}\left|\sigma_1\sigma_2\dots\sigma_n\right\rangle$$

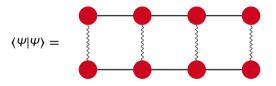


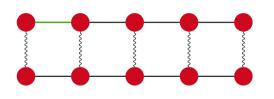
#### Matrix Product States - Bra, Ket and Norms





Different contraction orders yield different contraction complexities

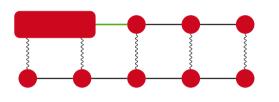




#### Number of operations

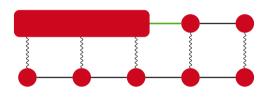
•  $\mathcal{O}(D^2d^2)$ 





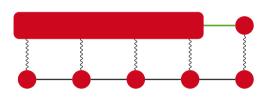
- \$\mathcal{O}(D^2d^2)\$
   \$\mathcal{O}(D^2d^3)\$





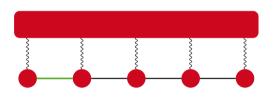
- $\mathcal{O}(D^2d^2)$
- $\mathcal{O}(D^2d^3)$
- $\mathcal{O}(D^2d^4)$





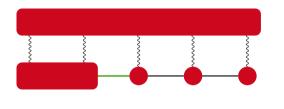
- $\mathcal{O}(D^2d^2)$
- $\mathcal{O}(D^2d^3)$
- $\mathcal{O}(D^2d^4)$
- $\mathcal{O}(Dd^5)$





- $\mathcal{O}(D^2d^2)$
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- $\mathcal{O}(D^2d^4)$
- $\mathcal{O}(Dd^5)$
- $\mathcal{O}(D^2d^2)$



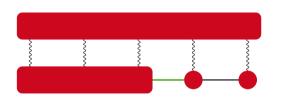


#### Number of operations

- $\mathcal{O}(D^2d^2)$
- $O(D^2d^3)$
- $\mathcal{O}(D^2d^4)$
- $\mathcal{O}(Dd^5)$
- $\mathcal{O}(D^2d^2)$



•  $\mathcal{O}(D^2d^3)$ 



#### Number of operations

- $\mathcal{O}(D^2d^2)$
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- $\mathcal{O}(D^2d^4)$
- $\mathcal{O}(Dd^5)$
- $\mathcal{O}(D^2d^2)$

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- $\mathcal{O}(D^2d^2)$
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- $\mathcal{O}(Dd^5)$





- $\mathcal{O}(D^2d^2)$
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- $\mathcal{O}(D^2d^3)$
- $\mathcal{O}(D^2d^4)$
- $\mathcal{O}(Dd^5)$
- $\mathcal{O}(d^6)$

#### Number of operations

- $\mathcal{O}(D^2d^2)$
- $\mathcal{O}(D^2d^3)$

\$\mathcal{O}(D^2d^3)\$
 \$\mathcal{O}(D^2d^4)\$

•  $\mathcal{O}(D^2d^4)$ 

 $\circ$   $\mathcal{O}(Dd^5)$ 

•  $\mathcal{O}(Dd^5)$ 

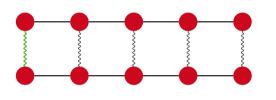
• O(Da<sup>o</sup>)

•  $\mathcal{O}(D^2d^2)$ 

•  $\mathcal{O}(d^6)$ 

# Don't try this at home

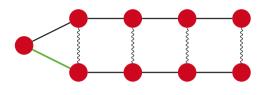
The number of matrix elements needed scales exponentially with the number of sites N.



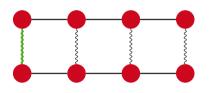
## Number of operations

•  $\mathcal{O}(D^2d)$ 



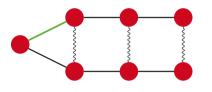


- $\mathcal{O}(D^2d)$
- $\mathcal{O}(D^3d)$



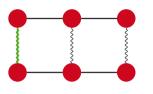
- $\mathcal{O}(D^2d)$
- $\mathcal{O}(D^3d)$
- $\mathcal{O}(D^3d)$



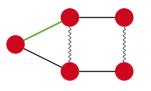


- $\mathcal{O}(D^2d)$
- $\mathcal{O}(D^3d)$
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- $\mathcal{O}(D^2d)$
- $\mathcal{O}(D^3d)$
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- $\mathcal{O}(D^3d)$
- $\mathcal{O}(D^3d)$



#### Number of operations

•  $\mathcal{O}(D^3d)$ 

- $\mathcal{O}(D^2d)$
- $\mathcal{O}(D^3d)$
- $\mathcal{O}(D^3d)$
- $\mathcal{O}(D^3d)$
- $\mathcal{O}(D^3d)$



#### Number of operations

O(D<sup>3</sup>d)
 O(D<sup>3</sup>d)

- $\mathcal{O}(D^2d)$
- $\mathcal{O}(D^3d)$
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- $\mathcal{O}(D^2d)$
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  - $\mathcal{O}(D^2d)$





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- $\mathcal{O}(D^3d)$

- $\mathcal{O}(D^3d)$
- $\mathcal{O}(D^3d)$
- $\mathcal{O}(D^2d)$
- O(Dd)



#### Number of operations

- $\mathcal{O}(D^2d)$
- $\mathcal{O}(D^3d)$
- $\mathcal{O}(D^3d)$
- $\mathcal{O}(D^3d)$
- $\mathcal{O}(D^3d)$

- $\mathcal{O}(D^3d)$
- $\mathcal{O}(D^3d)$
- $\mathcal{O}(D^2d)$
- O(Dd)

## Complexity

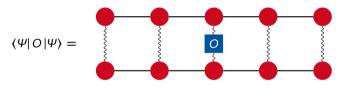
The number of matrix elements does not dependent on the number of sites N at all and the procedure scales linear in time with N.

## Matrix Product States - Calculation of an expectation value

#### **Expectation values**

$$\langle O \rangle = \frac{\langle \Psi | O | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

$$\langle O_i \rangle = \frac{\langle \Psi | O_i | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$



## **Example - DMRG calculation**

#### Spin 1 Heisenberg chain $H = \sum_{i} S_{i}^{x} S_{i+1}^{x} + S_{i}^{y} S_{i+1}^{y} + S_{i}^{z} S_{i+1}^{z}$ 150 Runtime [s] 100 50 SYTEN 0 100 200 300 400 500 600 700 800 900 1,000 System Size L Data provided by Claudius Hubig, MPQ

### **Summary - MPS**

- MPS is an Ansatz to describe many-body states with polynomially many parameters
- The pictorial description simplifies the formulation of calculations and algorithms
- We have to be careful about the order of contractions



Section 3

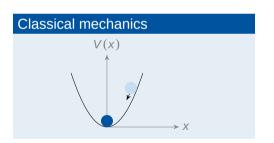
**iTEBD** 



# Minimization of energy

#### Goal

Find the groundstate of a Hamiltonian H, i.e. find the state with the smallest energy eigenvalue.



### Quantum mechanics

Find  $|\Psi_{\rm min}\rangle$  such that

$$E_{\min} = \frac{\left\langle \Psi_{\min} \middle| H \middle| \Psi_{\min} \right\rangle}{\left\langle \Psi_{\min} \middle| \Psi_{\min} \right\rangle}$$

is minimal.



#### Reminder – Tensor network notation

#### A Tensor Network State

$$|\Psi\rangle = \sum_{\sigma_{1}...\sigma_{n}} \sum_{a_{1},...,a_{n-1}} A_{a_{1}}^{\sigma_{1}} A_{a_{1},a_{2}}^{\sigma_{2}} \cdots A_{a_{n-2},a_{n-1}}^{\sigma_{n-1}} A_{a_{n-1}}^{\sigma_{n}} |\sigma_{1}\sigma_{2}...\sigma_{n}\rangle$$







#### **Reminder – Calculation of energies**

#### **Expectation value**

$$\langle E \rangle = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

#### Calculation of an observable

$$\langle \Psi | O | \Psi \rangle = \frac{1}{2}$$



# **Energy minimization via imaginary time evolution**

#### Motivation

The ground state is the state with the smallest energy. All other states are suppressed more quickly by an exponential.

#### Time evolution in imaginary time

$$\begin{split} |\Psi_0\rangle &= \lim_{\delta \to \infty} \frac{\exp(-H\delta) \, |\Psi\rangle}{\|\exp(-H\delta) \, |\Psi\rangle\|} \\ &= \lim_{\delta \to \infty} \frac{U(\delta) \, |\Psi\rangle}{\|U(\delta) \, |\Psi\rangle\|} \end{split}$$



## **Trotterization of an operator**

#### **Evolution operator**

$$U(\delta)=e^{-\delta H}$$

### Ising Model

$$H = \sum_{i} S_{i}^{z} S_{i+1}^{z} = \sum_{i} h_{i,i+1}$$



$$H_{\text{even}} = \sum_{i \text{ even}} h_{i,i+1}$$

$$H_{\text{odd}} = \sum_{i \text{ odd}} h_{i,i+1}$$

### **Trotterization of an operator**

### **Evolution operator**

$$U(\delta) = e^{-\delta H}$$

# Ising Model

$$H = \sum_{i} S_{i}^{z} S_{i+1}^{z} = \sum_{i} h_{i,i+1}$$



$$H_{\text{even}} = \sum_{i \text{ even}} h_{i,i+1}$$
  $H_{\text{odd}} = \sum_{i \text{ odd}} h_{i,i+1}$   $H = H_{\text{even}} + H_{\text{odd}}$ 

# **Trotterization of an operator**

### **Evolution operator**

$$U(\delta) = e^{-\delta H}$$

### Trotterization of an operator

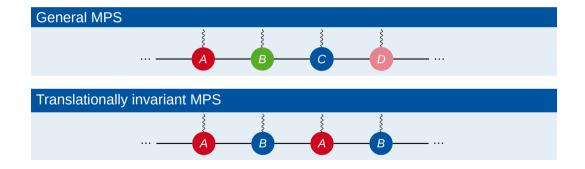
$$U(\delta) = e^{-\delta H}$$

$$= e^{-\delta H_{\text{even}}} e^{-\delta H_{\text{odd}}} e^{-\delta^2 [H_{\text{even}}, H_{\text{odd}}]}$$

$$\approx e^{-\delta H_{\text{even}}} e^{-\delta H_{\text{odd}}}$$

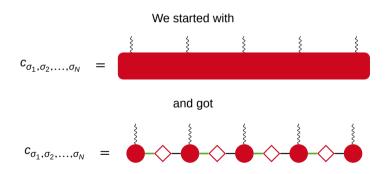
# Pictorial representation Ueven/odd

### Making life easy: infinite systems





### Back to the start: An MPS with diagonal matrices





We start with an infinite system that consists of two sites A and B



### Disclaimer

This algorithm is proven to be numerically unstable. You should NOT use it in research, it is shown here due to its simplicity.

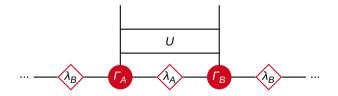
We start with an infinite system that consists of two sites A and B



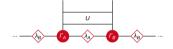
### Disclaimer

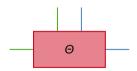
This algorithm is proven to be numerically unstable. You should NOT use it in research, it is shown here due to its simplicity.

 Apply the operator U to sites A and B



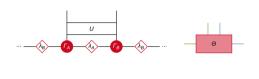






- Apply the operator U to sites A and B
- Contract all indices and group indices (blue and green)

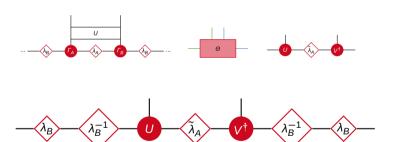




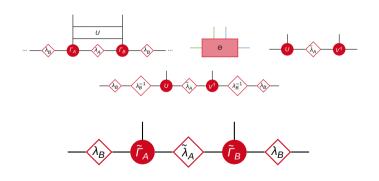


- Apply the operator U to sites A and B
- Contract all indices and group indices (blue and green)
- Compute SVD of the tensor



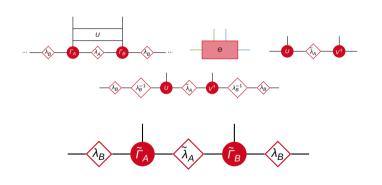


- Apply the operator U to sites A and B
- Contract all indices and group indices (blue and green)
- Compute SVD of the tensor
- Reintroduce  $\lambda_B$



- Apply the operator *U* to sites A and B
- Contract all indices and group indices (blue and green)
- Compute SVD of the tensor
- Reintroduce  $\lambda_B$
- Update  $\Gamma_A$  and  $\Gamma_B$

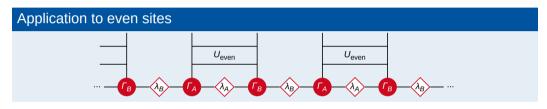


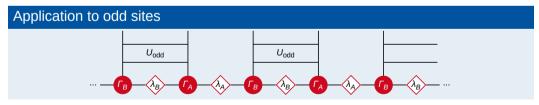


- Apply the operator *U* to sites A and B
- Contract all indices and group indices (blue and green)
- Compute SVD of the tensor
- Reintroduce  $\lambda_B$
- Update  $\Gamma_A$  and  $\Gamma_B$
- Repeat the procedure with the sites B and A



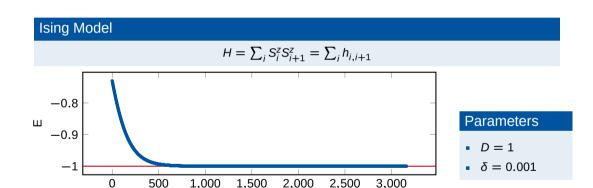
### Application on odd an even sites



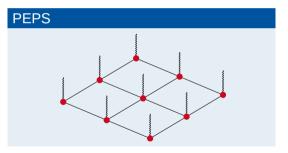


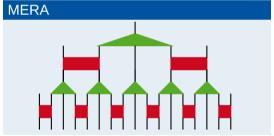


# Results for an Ising spin system



### **Outlook**





# **Tensor Networks**

How physicists can tackle exponentially hard problems

March 4 – 7, 2019 | Patrick Emonts | Max Planck Institute of Quantum Optics



# Section 4

References



### References I

- Bascis Jacob C. Bridgeman and Christopher T. Chubb. "Hand-waving and Interpretive Dance: An Introductory Course on Tensor Networks". In: *Journal of Physics A: Mathematical and Theoretical* 50.22 (June 2, 2017), p. 223001
  - Román Orús. "A practical introduction to tensor networks: Matrix product states and projected entangled pair states". In: Annals of Physics 349 (Oct. 2014), pp. 117–158
  - Ulrich Schollwöck. "The density-matrix renormalization group in the age of matrix product states". In: Annals of Physics 326.1 (Jan. 2011), pp. 96–192
- iTEBD G. Vidal. "Classical Simulation of Infinite-Size Quantum Lattice Systems in One Spatial Dimension". In: Physical Review Letters 98.7 (Feb. 12, 2007)

