## 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


## Number of possibilities

$$
Z=2^{N}
$$

## How bad is exponential scaling?




Physical example

- $10^{23}$ Number of atoms in 12 g of carbon
- $10^{80}$ 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 $H$ Linear operator that describes the energy of the system

## Note on Notation: Bra and Ket vectors

$|\Psi\rangle$ is a column vector | $\Psi_{0}$ |
| :--- |
| $\Psi_{1}$ |
| $\Psi_{2}$ |

$\langle\psi|$ is a row vector

$$
\begin{array}{|l|l|l|}
\hline \bar{\psi}_{0} & \bar{\psi}_{1} & \bar{\psi}_{2} \\
\hline
\end{array}
$$

## 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

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

## Expressing spins with matrices

Definitions

$$
\begin{aligned}
& |\uparrow\rangle=\binom{1}{0} \\
& |\downarrow\rangle=\binom{0}{1}
\end{aligned}
$$

$$
S_{z}=\frac{1}{2}\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)
$$

Calculating with spins

$$
\begin{aligned}
S_{z}|\uparrow\rangle & =\frac{1}{2}\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)\binom{1}{0} \\
& =\frac{1}{2}|\uparrow\rangle
\end{aligned}
$$

## Combining multiple spins

Consider a system consisting of two spins that can two values ( $\downarrow$ and $\uparrow$ )

## Hilbert space $\mathcal{H}$

$\mathcal{H}=\operatorname{span}\left\{\left|\downarrow_{1}\right\rangle\left|\downarrow_{2}\right\rangle,\left|\downarrow_{1}\right\rangle\left|\uparrow_{2}\right\rangle,\left|\uparrow_{1}\right\rangle\left|\downarrow_{2}\right\rangle,\left|\uparrow_{1}\right\rangle\left|\uparrow_{2}\right\rangle\right\}$
Spins on different sites are combined by tensor products

$$
\begin{aligned}
& \left|\boldsymbol{\Downarrow}_{1}\right\rangle\left|\boldsymbol{\Psi}_{2}\right\rangle=\binom{0}{1} \otimes\binom{0}{1}=\left(\begin{array}{l}
0 \\
0 \\
0 \\
1
\end{array}\right) \\
& \left|\boldsymbol{\Downarrow}_{1}\right\rangle\left|\uparrow_{2}\right\rangle=\binom{0}{1} \otimes\binom{1}{0}=\left(\begin{array}{l}
0 \\
0 \\
1 \\
0
\end{array}\right) \\
& \left|\uparrow_{1}\right\rangle\left|\boldsymbol{\Psi}_{2}\right\rangle=\binom{1}{0} \otimes\binom{0}{1}=\left(\begin{array}{l}
0 \\
1 \\
0 \\
0
\end{array}\right) \\
& \left|\uparrow_{1}\right\rangle\left|\uparrow_{2}\right\rangle=\binom{1}{0} \otimes\binom{1}{0}=\left(\begin{array}{l}
1 \\
0 \\
0 \\
0
\end{array}\right)
\end{aligned}
$$

## Letting spins interact

## Interaction of two spins

$$
H=-J\left(S_{1}^{z} \otimes S_{2}^{Z}\right)
$$

## Matrix representation

$$
\begin{aligned}
H & =-J\left(\frac{1}{2}\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)\right) \otimes\left(\frac{1}{2}\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)\right) \\
& =-\frac{J}{4}\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right) \otimes\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)=-\frac{J}{4}\left(\begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1
\end{array}\right)
\end{aligned}
$$

## Calculating an expectation value

## Preparation of a state

$$
\begin{aligned}
|\Psi\rangle & =\sqrt{0.5}\left|\uparrow_{1}\right\rangle\left|\downarrow_{2}\right\rangle+\sqrt{0.5}\left|\downarrow_{1}\right\rangle\left|\uparrow_{2}\right\rangle \\
& =\sqrt{0.5}\left|\uparrow_{1} \downarrow_{2}\right\rangle+\sqrt{0.5}\left|\downarrow_{1} \uparrow_{2}\right\rangle \\
& =\sqrt{0.5}|\uparrow \downarrow\rangle+\sqrt{0.5}|\downarrow \uparrow\rangle \\
& =\left(\begin{array}{c}
0 \\
\sqrt{0.5} \\
\sqrt{0.5} \\
0
\end{array}\right)
\end{aligned}
$$

## Calculating an expectation value

Preparation of a state

$$
\begin{aligned}
|\Psi\rangle & =\sqrt{0.5}\left|\uparrow_{1}\right\rangle\left|\downarrow_{2}\right\rangle+\sqrt{0.5}\left|\downarrow_{1}\right\rangle\left|\uparrow_{2}\right\rangle \\
& =\sqrt{0.5}\left|\uparrow_{1} \downarrow_{2}\right\rangle+\sqrt{0.5}\left|\downarrow_{1} \uparrow_{2}\right\rangle \\
& =\sqrt{0.5}|\uparrow \downarrow\rangle+\sqrt{0.5}|\downarrow \uparrow\rangle \\
& =\left(\begin{array}{c}
0 \\
\sqrt{0.5} \\
\sqrt{0.5} \\
0
\end{array}\right)
\end{aligned}
$$

## Expectation value

$$
\begin{aligned}
\langle H\rangle & =\langle\Psi| H|\Psi\rangle /\langle\Psi \mid \Psi\rangle \\
& =\langle\Psi| H|\Psi\rangle \\
& =-\frac{J}{4}\left(\begin{array}{llll}
0 & \sqrt{0.5} & \sqrt{0.5} & 0
\end{array}\right)\left(\begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1
\end{array}\right)\left(\begin{array}{c}
\frac{0}{\sqrt{0.5}} \\
\sqrt{0.5} \\
0
\end{array}\right) \\
& =\frac{J}{4}
\end{aligned}
$$

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


## 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 $\Leftrightarrow$ Contraction of indices


## Pictorial representation as Arrays



## Calculations with pictures

## Matrix-Vector Multiplication

$$
\mathbf{v}_{i}=\sum_{i, j} A_{i j} \mathbf{b}_{j}
$$

$$
{ }^{i} \mathrm{v}=\mathrm{i}^{i} \mathrm{~A}
$$

Matrix-Matrix Multiplication

$$
\begin{aligned}
C_{k l} & =\sum_{i, k, l} A_{k i} B_{i l} \\
k C^{\prime} & =k A B^{\prime}
\end{aligned}
$$

## Calculations with pictures - Quiz



## Calculations with pictures - Quiz

$$
C=A{ }_{j} B
$$

Trace

$$
\begin{aligned}
c & =\sum_{i, j} A_{i j} B_{j i} \\
& =\operatorname{Tr}[A B]
\end{aligned}
$$

## Tensor manipulations - Grouping

## Tensor to Matrix

## Pictorial language

$$
\begin{aligned}
A_{i, j, k} & =A_{i, j k)} \\
& =A_{i, m}
\end{aligned}
$$




## Tensor manipulations - Splitting

Splitting of tensor

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



## Singular Value Decomposition

Singular Value Decomposition


$$
\begin{aligned}
& M=U \cdot S \cdot V^{\dagger} \\
& M \text { arbitrary } m x n \text { matrix } \\
& U \text { unitary } m x m \text { matrix } \\
& S \text { diagonal mxn matrix } \\
& V \text { unitary } n x n \text { matrix }
\end{aligned}
$$

## SVD - Truncation



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

## SVD - Example



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

## A general quantum mechanical state

$$
|\Psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} c_{\sigma_{1}, \sigma_{2} \ldots \sigma_{N}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$

Example: $|\psi\rangle=\sqrt{0.5}|\uparrow\rangle| \rangle+\sqrt{0.5}| \rangle|\uparrow\rangle$

$$
\begin{aligned}
& \mathcal{H}=\operatorname{span}\left\{\left|\boldsymbol{\varpi}_{1}\right\rangle\left|\boldsymbol{\varpi}_{2}\right\rangle,\right. \\
&\left|\boldsymbol{\Psi}_{1}\right\rangle\left|\uparrow_{2}\right\rangle, \\
&\left|\uparrow_{1}\right\rangle\left|\downarrow_{2}\right\rangle, \\
&\left.\left|\uparrow_{1}\right\rangle\left|\uparrow_{2}\right\rangle\right\}
\end{aligned}
$$

$$
\begin{aligned}
& c_{\downarrow_{1}, \downarrow_{2}}=0 \\
& c_{\downarrow_{1}, \uparrow_{2}}=\sqrt{0.5} \\
& c_{\uparrow_{1}, \downarrow_{2}}=\sqrt{0.5} \\
& c_{\uparrow_{1}, \uparrow_{2}}=0
\end{aligned}
$$

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

## A general quantum mechanical state

$$
|\Psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} c_{\sigma_{1}, \sigma_{2} \ldots \sigma_{N}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$

## 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

$$
|\Psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} c_{\sigma_{1}, \sigma_{2} \ldots \sigma_{N}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$

## 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

$$
|\psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} \underbrace{\sum_{a_{n}}}_{c_{a_{1}, \sigma_{2}, \ldots, a_{n}}} A_{a_{1}}^{\sigma_{1}} A_{a_{1}, a_{2}}^{\sigma_{2}} \cdots A_{a_{n-2}, a_{n-1}}^{\sigma_{n-1}} A_{a_{n-1}}^{\sigma_{n}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$

## Tensor Networks - Thinking about Indices

## A Tensor Network State

$$
|\psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} \sum_{a_{1}, \ldots, a_{n-1}} A_{a_{1}}^{\sigma_{1}} A_{1_{1}, a_{2}}^{\sigma_{2}} \cdots A_{a_{n-2}, a_{n-1}}^{\sigma_{n-1}} A_{a_{n-1}}^{\sigma_{n}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$

## Dimensions of object A

$$
\sigma: \text { physical index: }(\uparrow, \downarrow)
$$

$A_{a_{j}, a_{j+1}}^{\sigma}$
a: virtual index

Dimension of physical index

$$
d \quad(\sim 10)
$$

Dimension of virtual index
D (~100)

## Matrix Product States

## A Tensor Network State

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



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


## Matrix Product States - How to get the Tensors?

A general quantum mechanical state

$$
|\Psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} c_{\sigma_{1}, \sigma_{2} \ldots \sigma_{N}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$



Matrix Product state

$$
|\psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} \sum_{a_{1}, \ldots, a_{n-1}} A_{a_{1}}^{\sigma_{1}} A_{a_{1}, a_{2}}^{\sigma_{2}} \cdots A_{a_{n-2}, a_{n-1}}^{\sigma_{n-1}} A_{a_{n-1}}^{\sigma_{n}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$

## Matrix Product States - How to get the Tensors?

A general quantum mechanical state

$$
|\Psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} c_{\sigma_{1}, \sigma_{2} \ldots \sigma_{N}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$



Matrix Product state

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

## Matrix Product States - How to get the Tensors?

A general quantum mechanical state

$$
|\psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} c_{\sigma_{1}, \sigma_{2} \ldots \sigma_{N}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$



Matrix Product state

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

## Matrix Product States - How to get the Tensors?

A general quantum mechanical state

$$
|\psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} c_{\sigma_{1}, \sigma_{2} \ldots \sigma_{N}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$



## Matrix Product state

$$
|\psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} \sum_{a_{1}, \ldots, a_{n-1}} A_{a_{1}}^{\sigma_{1}} A_{1_{1}, a_{2}}^{\sigma_{2}} \cdots A_{a_{n-2}, a_{n-1}}^{\sigma_{n-1}} A_{a_{n-1}}^{\sigma_{n}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$

## Matrix Product States - How to get the Tensors?

A general quantum mechanical state

$$
|\psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} c_{\sigma_{1}, \sigma_{2} \ldots \sigma_{N}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$



## Matrix Product state

$$
|\psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} \sum_{a_{1}, \ldots, a_{n-1}} A_{a_{1}}^{\sigma_{1}} A_{1_{1}, a_{2}}^{\sigma_{2}} \cdots A_{a_{n-2}, a_{n-1}}^{\sigma_{n-1}} A_{a_{n-1}}^{\sigma_{n}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$

## Matrix Product States - How to get the Tensors?

A general quantum mechanical state

$$
|\Psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} c_{\sigma_{1}, \sigma_{2} \ldots \sigma_{N}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$



## Matrix Product state

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

## Matrix Product States - How to get the Tensors?

A general quantum mechanical state

$$
|\Psi\rangle=\sum_{\sigma_{1} \ldots \sigma_{n}} c_{\sigma_{1}, \sigma_{2} \ldots \sigma_{N}}\left|\sigma_{1} \sigma_{2} \ldots \sigma_{n}\right\rangle
$$



## Matrix Product state

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

## Matrix Product States - Bra, Ket and Norms



## Matrix Product States - Why contraction order matters!

Different contraction orders yield different contraction complexities


## Matrix Product States - Why contraction order matters!



Number of operations

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


## Matrix Product States - Why contraction order matters!



Number of operations

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


## Matrix Product States - Why contraction order matters!



Number of operations

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


## Matrix Product States - Why contraction order matters!



Number of operations

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


## Matrix Product States - Why contraction order matters!



Number of operations

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


## Matrix Product States - Why contraction order matters!



Number of operations

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


## Matrix Product States - Why contraction order matters!



## Number of operations

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


## Matrix Product States - Why contraction order matters!



## Number of operations

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


## Matrix Product States - Why contraction order matters!



## Number of operations

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


## Matrix Product States - Why contraction order matters!

## Number of operations

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


## ! Don't try this at home !

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

## Matrix Product States - Why contraction order matters!



Number of operations

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


## Matrix Product States - Why contraction order matters!



Number of operations

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


## Matrix Product States - Why contraction order matters!



Number of operations

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


## Matrix Product States - Why contraction order matters!



Number of operations

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


## Matrix Product States - Why contraction order matters!



Number of operations

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


## Matrix Product States - Why contraction order matters!



Number of operations

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


## Matrix Product States - Why contraction order matters!



## Number of operations

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


## Matrix Product States - Why contraction order matters!



Number of operations

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


## Matrix Product States - Why contraction order matters!

## Number of operations

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


## Matrix Product States - Why contraction order matters!

## Number of operations

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


## 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

$$
\begin{aligned}
\langle O\rangle & =\frac{\langle\Psi| O|\Psi\rangle}{\langle\Psi \mid \Psi\rangle} \\
\left\langle O_{i}\right\rangle & =\frac{\langle\Psi| O_{i}|\Psi\rangle}{\langle\psi \mid \Psi\rangle}
\end{aligned}
$$

## Example - DMRG calculation

## Spin 1 Heisenberg chain

$$
H=\sum_{i} S_{i}^{x} S_{i+1}^{X}+S_{i}^{y} S_{i+1}^{y}+S_{i}^{z} S_{i+1}^{z}
$$



## 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.

## Classical mechanics



## Quantum mechanics

Find $\left|\Psi_{\text {min }}\right\rangle$ such that
$E_{\text {min }}=\frac{\left\langle\Psi_{\text {min }}\right| H\left|\Psi_{\text {min }}\right\rangle}{\left\langle\Psi_{\text {min }} \mid \Psi_{\text {min }}\right\rangle}$
is minimal.

## Reminder - Tensor network notation

## A Tensor Network State

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



$$
|\psi\rangle=\xi
$$

$\langle\Psi|=$


## Reminder - Calculation of energies

## Expectation value

$$
\langle E\rangle=\frac{\langle\varphi|| ||\psi\rangle}{\langle\psi \mid \psi\rangle}
$$

Calculation of an observable


## 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

$$
\begin{aligned}
\left|\Psi_{0}\right\rangle & =\lim _{\delta \rightarrow \infty} \frac{\exp (-H \delta)|\Psi\rangle}{\| \exp (-H \delta)|\Psi\rangle \|} \\
& =\lim _{\delta \rightarrow \infty} \frac{U(\delta)|\Psi\rangle}{\| U(\delta)|\Psi\rangle \|}
\end{aligned}
$$

## Trotterization of an operator

Evolution operator

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

## Ising Model

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

(〇) (O)
0 O

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

## Trotterization of an operator

## Evolution operator

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

## Ising Model

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

(〇) (〇)

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

## Trotterization of an operator

## Evolution operator

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

## Trotterization of an operator

$$
\begin{aligned}
U(\delta) & =e^{-\delta H} \\
& =e^{-\delta H_{\text {even }}} e^{-\delta H_{\text {odd }}} e^{-\delta^{2}\left[H_{\text {even }}, H_{\text {odd }}\right]} \\
& \approx e^{-\delta H_{\text {even }}} e^{-\delta H_{\text {odd }}}
\end{aligned}
$$

## Pictorial representation



## Making life easy: infinite systems

## General MPS



Translationally invariant MPS


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

We started with

and got


## The iTEBD algorithm

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.

## The iTEBD algorithm

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.

## The iTEBD algorithm

- Apply the operator $U$ to sites $A$ and $B$


## The iTEBD algorithm



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



## The iTEBD algorithm



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


## The iTEBD algorithm



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


## The iTEBD algorithm



- 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 $\Gamma_{B}$


## The iTEBD algorithm



- 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

Application to even sites


Application to odd sites


## Results for an Ising spin system

## Ising Model

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



Parameters

- $D=1$
- $\delta=0.001$


## Outlook



MERA


## 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)

