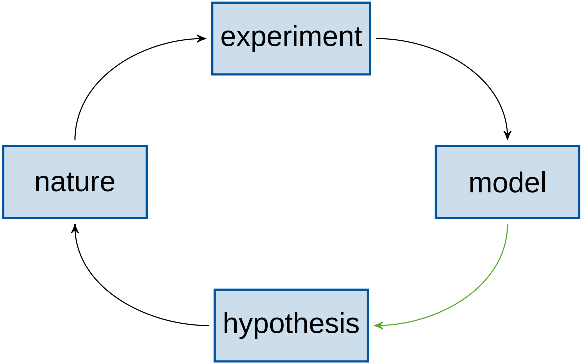
Tensor Networks

How physicists can tackle exponentially hard problems

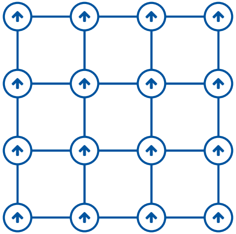
March 5, 2019 | Patrick Emonts | Max Planck Institute of Quantum Optics

Motivation



How complex is this problem?

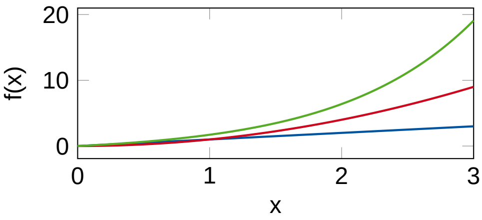
We take a system that can take two states ↑ and ↓

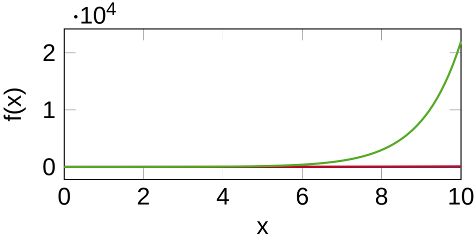


Number of possibilities

$$Z = 2^N$$

How bad is exponential scaling?

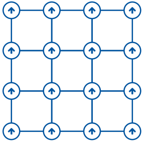




Physical example

- 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 $\begin{bmatrix} \Psi_0 \\ \Psi_1 \\ \Psi_2 \end{bmatrix}$

$\langle\Psi|$ is a row vector

$\begin{bmatrix} \overline{\Psi}_0 & \overline{\Psi}_1 & \overline{\Psi}_2 \end{bmatrix}$

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

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

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

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

Calculating with spins

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

Combining multiple spins

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

Hilbert space $\mathcal{H}$

$$\mathcal{H} = \mathrm{span}\left\{ \left|\downarrow_1\right\rangle \left|\downarrow_2\right\rangle, \left|\downarrow_1\right\rangle \left|\uparrow_2\right\rangle, \left|\uparrow_1\right\rangle \left|\downarrow_2\right\rangle, \left|\uparrow_1\right\rangle \left|\uparrow_2\right\rangle \right\}$$

Spins on different sites are combined by tensor products

$$\left|\downarrow_1\right\rangle \left|\downarrow_2\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \qquad \left|\downarrow_1\right\rangle \left|\uparrow_2\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\left|\uparrow_1\right\rangle \left|\downarrow_2\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} \qquad \left|\uparrow_1\right\rangle \left|\uparrow_2\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Letting spins interact

Interaction of two spins

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

Matrix representation

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

Calculating an expectation value

Preparation of a state

$$
\begin{aligned}
|\Psi\rangle &= \sqrt{0.5}\,|\uparrow_1\rangle\,|\downarrow_2\rangle + \sqrt{0.5}\,|\downarrow_1\rangle\,|\uparrow_2\rangle \\
&= \sqrt{0.5}\,|\uparrow_1\downarrow_2\rangle + \sqrt{0.5}\,|\downarrow_1\uparrow_2\rangle \\
&= \sqrt{0.5}\,|\uparrow\downarrow\rangle + \sqrt{0.5}\,|\downarrow\uparrow\rangle \\
&= \begin{pmatrix} 0 \\ \sqrt{0.5} \\ \sqrt{0.5} \\ 0 \end{pmatrix}
\end{aligned}
$$

Expectation value

$$
\begin{aligned}
\langle H\rangle &= \langle\Psi|\,H\,|\Psi\rangle \,/\, \langle\Psi|\Psi\rangle \\
&= \langle\Psi|\,H\,|\Psi\rangle \\
&= \frac{J}{4}\begin{pmatrix} 0 & \sqrt{0.5} & \sqrt{0.5} & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} 0 \\ \sqrt{0.5} \\ \sqrt{0.5} \\ 0 \end{pmatrix} \\
&= -\frac{J}{4}
\end{aligned}
$$

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

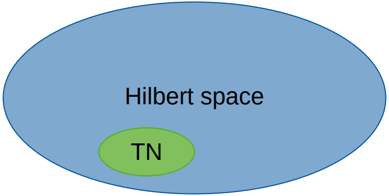
Physics

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

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?

A general quantum mechanical state

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

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

$$\begin{aligned}\mathcal{H} = \mathrm{span}\{&|\downarrow_1\rangle\,|\downarrow_2\rangle\,,\\ &|\downarrow_1\rangle\,|\uparrow_2\rangle\,,\\ &|\uparrow_1\rangle\,|\downarrow_2\rangle\,,\\ &|\uparrow_1\rangle\,|\uparrow_2\rangle\}\end{aligned}$$

$$c_{\downarrow_1,\downarrow_2} = 0$$

$$c_{\downarrow_1,\uparrow_2} = \sqrt{0.5}$$

$$c_{\uparrow_1,\downarrow_2} = \sqrt{0.5}$$

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

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

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

Tensor Networks – Thinking about Indices

A Tensor Network State

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

Dimensions of object *A*

σ: *physical index*: ($\uparrow$, $\downarrow$)

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

a: *virtual index*

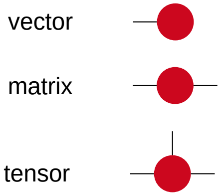
Dimension of physical index

$d \quad (\sim 10)$

Dimension of virtual index

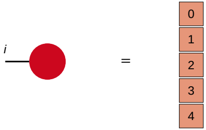
$D \quad (\sim 100)$

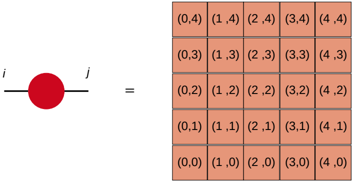
Pictorial representation

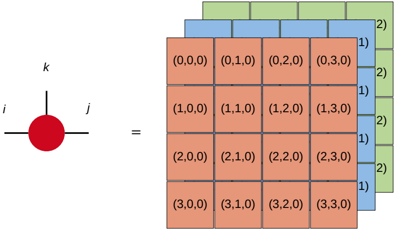


- The number of legs determines the number of indices of the object
- A connection $\Leftrightarrow$ Contraction of indices

Pictorial representation as Arrays



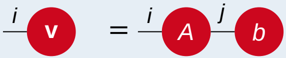




Calculations with pictures

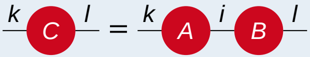
Matrix-Vector Multiplication

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

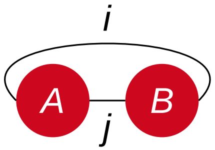


Matrix-Matrix Multiplication

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



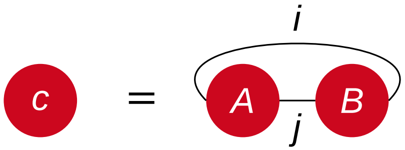
Calculations with pictures – Quiz



Trace

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

Calculations with pictures – Quiz



Trace

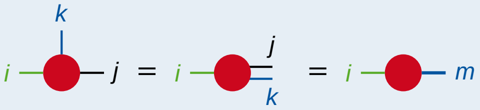
$$c = \sum_{i,j} A_{ij} B_{ji}$$
$$= \mathrm{Tr}[AB]$$

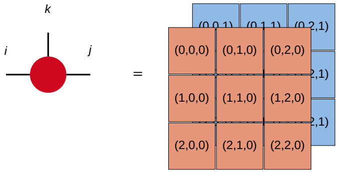
Tensor manipulations – Grouping

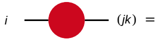
Tensor to Matrix

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

Pictorial language





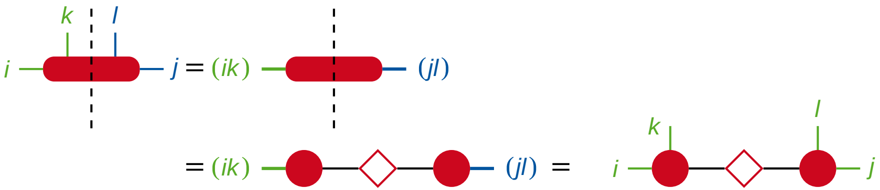


(0,0)	(0,1)	(0,2)	(0,3)	(0,4)	(0,5)	(0,6)
(1,0)	(1,1)	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)
(2,0)	(2,1)	(2,2)	(2,3)	(2,4)	(2,5)	(2,6)

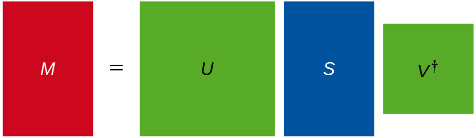
Tensor manipulations – Splitting

Splitting of tensor

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



Singular Value Decomposition

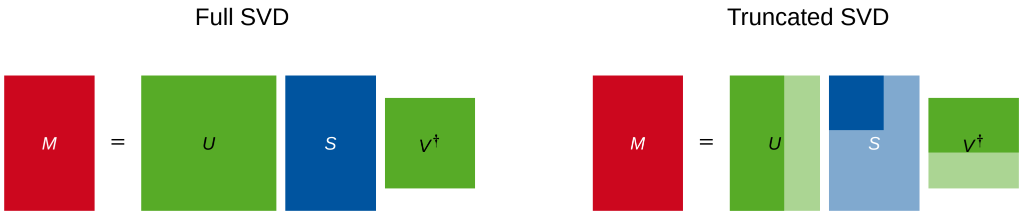


Singular Value Decomposition

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

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

SVD – Truncation



Note

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

SVD – Example

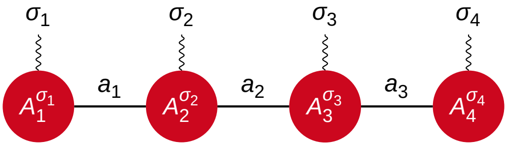
Original Image

Truncated Image (20 SV)

Matrix Product States

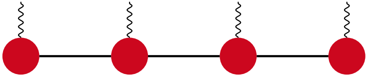
A Tensor Network State

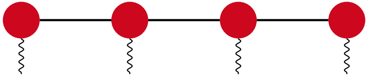
$$|\Psi\rangle = \sum_{\sigma_1 \ldots \sigma_n} \sum_{a_1,\ldots,a_{n-1}} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \cdots A^{\sigma_{n-1}}_{a_{n-2},a_{n-1}} A^{\sigma_n}_{a_{n-1}} \left|\sigma_1 \sigma_2 \ldots \sigma_n\right\rangle$$

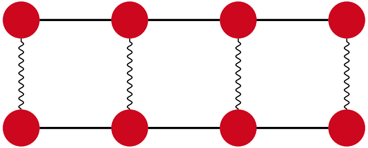


- Dimension: 1D
- Typical quantities
  - correlations
  - expectation values of observables

Matrix Product States – Bra, Ket and Norms

$|\Psi\rangle =$ 

$\langle\Psi| =$ 

$\langle\Psi|\Psi\rangle =$ 

Matrix Product States – How to get the Tensors?

A general quantum mechanical state

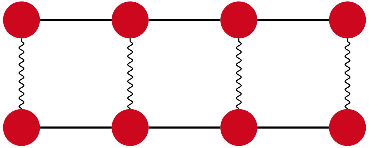
$$|\Psi\rangle = \sum_{\sigma_1 \ldots \sigma_n} c_{\sigma_1,\sigma_2 \ldots \sigma_N} |\sigma_1 \sigma_2 \ldots \sigma_n\rangle$$

Matrix Product state

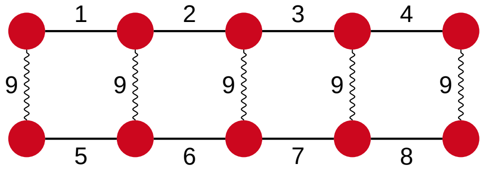
$$|\Psi\rangle = \sum_{\sigma_1 \ldots \sigma_n} \sum_{a_1,\ldots,a_{n-1}} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \cdots A^{\sigma_{n-1}}_{a_{n-2},a_{n-1}} A^{\sigma_n}_{a_{n-1}} |\sigma_1 \sigma_2 \ldots \sigma_n\rangle$$

Matrix Product States – Why contraction order matters!

Different contraction orders yield different contraction complexities

$\langle \Psi | \Psi \rangle =$ 

Matrix Product States – Why contraction order matters!



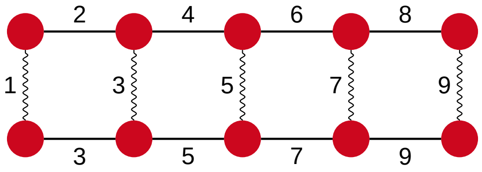
Number of operations

1. $\mathcal{O}(D^2d^2)$
2. $\mathcal{O}(D^2d^3)$
3. $\mathcal{O}(D^2d^4)$
4. $\mathcal{O}(Dd^5)$
5. $\mathcal{O}(D^2d^2)$
6. $\mathcal{O}(D^2d^3)$
7. $\mathcal{O}(D^2d^4)$
8. $\mathcal{O}(Dd^5)$
9. $\mathcal{O}(d^6)$

! 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

1. $\mathcal{O}(D^2 d)$
2. $\mathcal{O}(D^3 d)$
3. $\mathcal{O}(D^3 d)$
4. $\mathcal{O}(D^3 d)$
5. $\mathcal{O}(D^3 d)$
6. $\mathcal{O}(D^3 d)$
7. $\mathcal{O}(D^3 d)$
8. $\mathcal{O}(D^2 d)$
9. $\mathcal{O}(Dd)$

Complexity

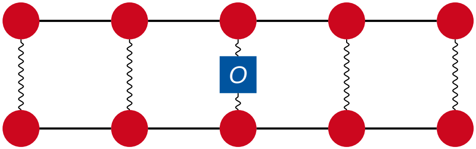
The number of matrix elements does not dependent on the number of sites N at all and the procedure scales linear in time with N.

Matrix Product States – Calculation of an expectation value

Expectation values

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

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

$\langle \Psi | O | \Psi \rangle =$ 

Summary – MPS

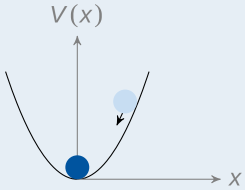
- MPS is an Ansatz to describe many-body states with polynomially many parameters
- The pictorial description simplifies the formulation of calculations and algorithms
- We have to be careful about the order of contractions

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 $|\Psi_{\text{min}}\rangle$ such that

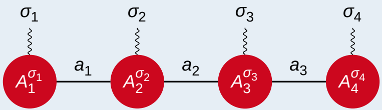
$$E_{\text{min}} = \frac{\langle \Psi_{\text{min}} | H | \Psi_{\text{min}} \rangle}{\langle \Psi_{\text{min}} | \Psi_{\text{min}} \rangle}$$

is minimal.

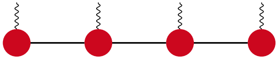
Tensor network notation

A Tensor Network State

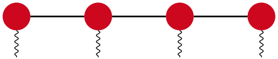
$$|\Psi\rangle = \sum_{\sigma_1 \ldots \sigma_n} \sum_{a_1,\ldots,a_{n-1}} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1,a_2} \cdots A^{\sigma_{n-1}}_{a_{n-2},a_{n-1}} A^{\sigma_n}_{a_{n-1}} |\sigma_1 \sigma_2 \ldots \sigma_n\rangle$$



$|\Psi\rangle =$



$\langle\Psi| =$



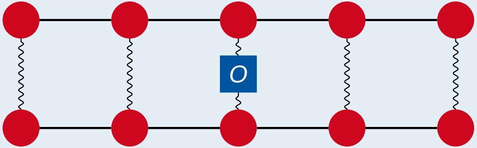
Calculation of energies

Expectation value

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

Calculation of an observable

$$\langle \Psi | O | \Psi \rangle =$$



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

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

Trotterization of an operator

Evolution operator

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

Ising Model

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

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

$$H = H_{\text{even}} + H_{\text{odd}}$$

Trotterization of an operator

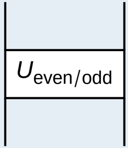
Evolution operator

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

Trotterization of an operator

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

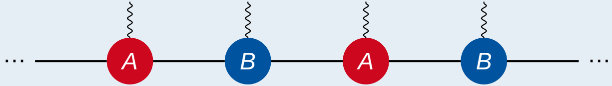
Pictorial representation



Making life easy: infinite systems

General MPS

Translationally invariant MPS



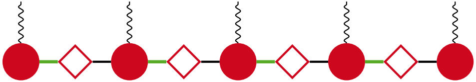
Back to the start: An MPS with diagonal matrices

We started with

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

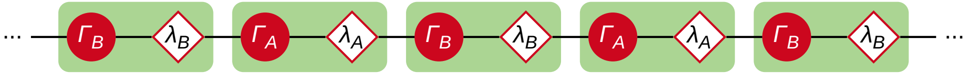
and got

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



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

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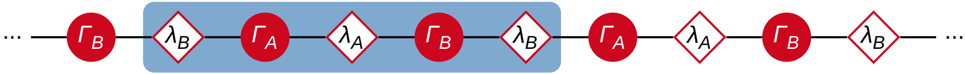

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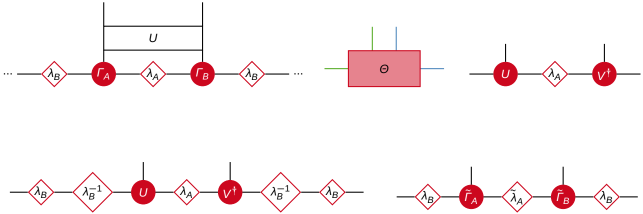
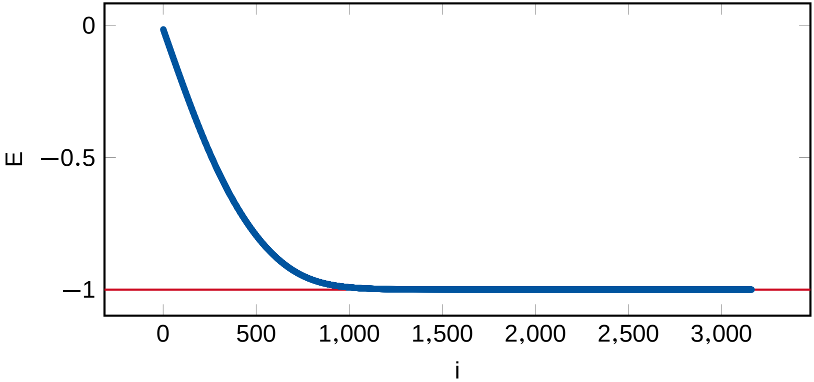
The iTEBD algorithm



1. Apply the operator U to sites A and B
2. Contract all indices and group indices (blue and green)
3. Compute SVD of the tensor
4. Reintroduce λ_B
5. Update Γ_A and Γ_B
6. Repeat the procedure with the sites B and A

Results for an Ising spin system

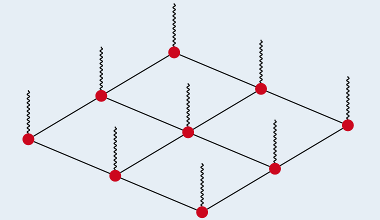


Parameters

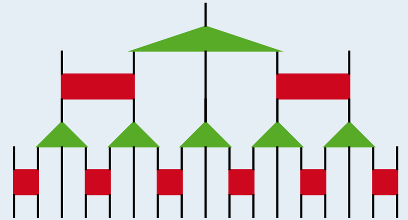
- $D = 10$
- $\delta = 0.001$

Outlook

PEPS



MERA



Tensor Networks

How physicists can tackle exponentially hard problems

March 5, 2019 | Patrick Emonts | Max Planck Institute of Quantum Optics

MPQ

References I

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