Introduction to Matrix Product States

Natalia Chepiga

Kavli Institute of Nanoscience, TU Delft, The Netherlands

ETN school 2023

Scope

- Area law
- Singular value decomposition
- MPO construction
- Variational optimization (finite- and infinite-size DMRG)
- Entanglement entropy and entanglement spectra
- Boundary conditions
- Excitations
- Abelian symmetries and constraints
- Time evolution
- Outlook

Area law

Why tensor networks work?

Area law

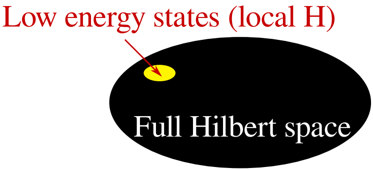
Exponential growth of the Hilbert space $\dim H = d^N$
Exact diagonalization is limited to small clusters.

Area law

Exponential growth of the Hilbert space $\dim H = d^N$

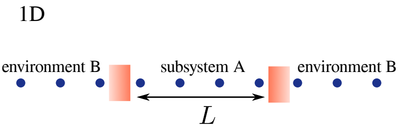
Exact diagonalization is limited to small clusters.

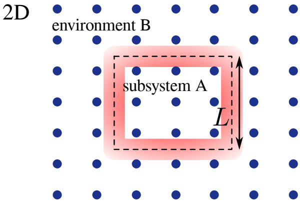
Area law for the entanglement entropy



Ground states of local Hamiltonians are less entangled than a random state in the Hilbert space

Area law





Entanglement entropy: $S_A = -\mathrm{tr}(\rho_A \log \rho_A)$

GS of local Hamiltonians

Area law: $S_A(L) \propto L^{d-1}$

1D: $S_A(L) = \mathrm{const}$
2D: $S_A(L) \propto L$

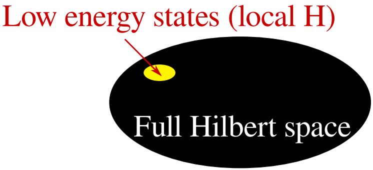
Random state

Volume law: $S_A(L) \propto L^d$

Critical state in 1D

$S_A(L) \propto \log(L)$

Area law



Our goal:
to diagonalize the Hamiltonian directly in the truncated basis

Number of relevant states $D \propto \exp(S)$

GS of local Hamiltonians

Area law: $S_A(L) \propto L^{d-1}$

1D: $S_A(L) = \text{const}$
2D: $S_A(L) \propto L$

Random state

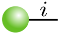
Volume law: $S_A(L) \propto L^d$

Critical state in 1D

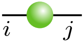
$S_A(L) \propto \log(L)$

Graphical notations

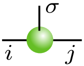
C Number



A_i Vector

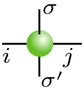


$A_{i,j}$ Matrix



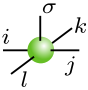
$A^{\sigma}_{i,j}$

rank-3 tensor (MPS)



$A^{\sigma,\sigma'}_{i,j}$

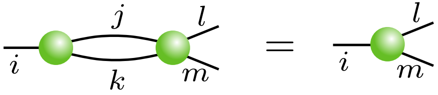
rank-4 tensor (MPO)



$A^{\sigma}_{i,j,k,l}$

rank-5 tensor (PEPS)

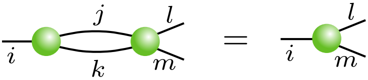
Contraction



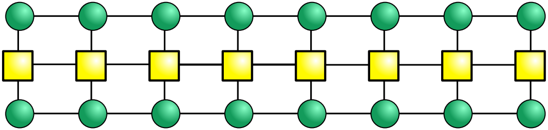
$$\sum_{j,k} A_{i,j,k} \; B_{j,k,l,m} = T_{i,l,m}$$

- Summation over connected bonds
- Rank of the resulting tensor = number of open legs

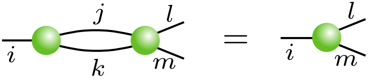
Contraction



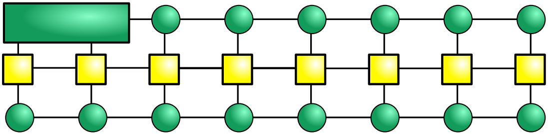
- Complexity $\prod_{i \in \text{ connected legs}} D_i \cdot \prod_{j \in \text{ open legs}} D_j$
- The order of contraction matters!



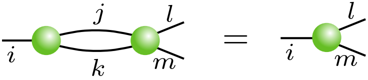
Contraction



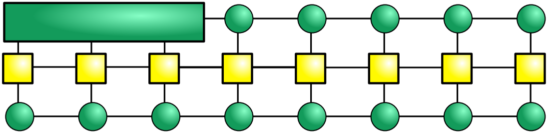
- Complexity $\prod_{i \in \text{ connected legs}} D_i \cdot \prod_{j \in \text{ open legs}} D_j$
- The order of contraction matters!



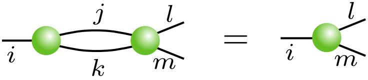
Contraction



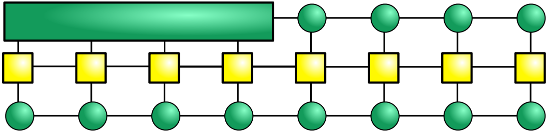
- Complexity $\prod_{i \in \text{ connected legs}} D_i \cdot \prod_{j \in \text{ open legs}} D_j$
- The order of contraction matters!



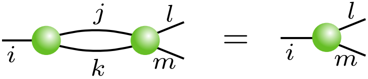
Contraction



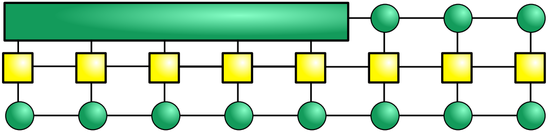
- Complexity $\prod_{i \in \text{ connected legs}} D_i \cdot \prod_{j \in \text{ open legs}} D_j$
- The order of contraction matters!



Contraction

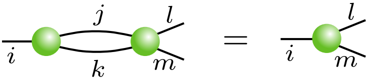


- Complexity $\prod_{i \in \text{ connected legs}} D_i \cdot \prod_{j \in \text{ open legs}} D_j$
- The order of contraction matters!

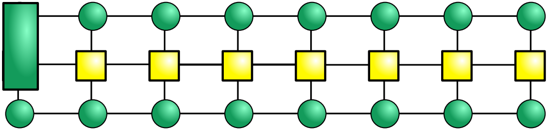


Exponential growth of complexity!

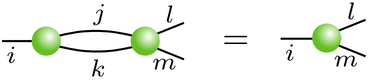
Contraction



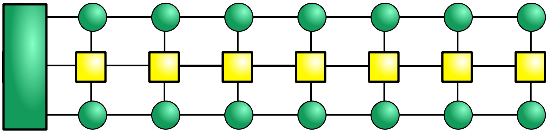
- Complexity $\prod_{i \in \text{ connected legs}} D_i \cdot \prod_{j \in \text{ open legs}} D_j$
- The order of contraction matters!



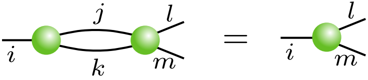
Contraction



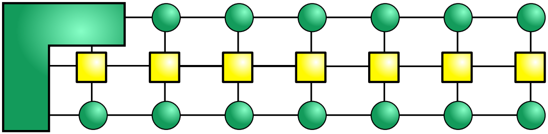
- Complexity $\displaystyle\prod_{i\in \text{ connected legs}} D_i \cdot \prod_{j\in \text{ open legs}} D_j$
- The order of contraction matters!



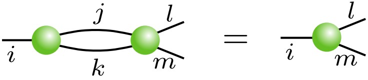
Contraction



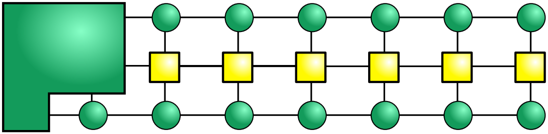
- Complexity $\prod_{i \in \text{ connected legs}} D_i \cdot \prod_{j \in \text{ open legs}} D_j$
- The order of contraction matters!



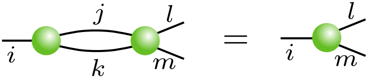
Contraction



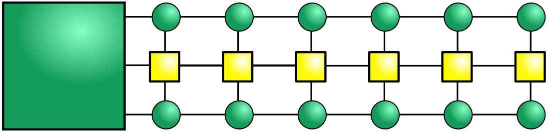
- Complexity $\prod_{i \in \text{ connected legs}} D_i \cdot \prod_{j \in \text{ open legs}} D_j$
- The order of contraction matters!



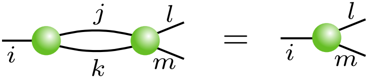
Contraction



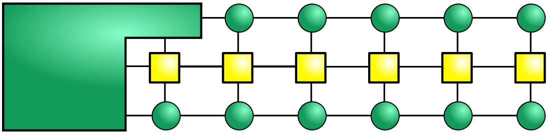
- Complexity $\prod_{i \in \text{ connected legs}} D_i \cdot \prod_{j \in \text{ open legs}} D_j$
- The order of contraction matters!



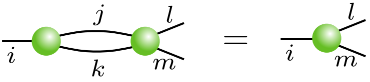
Contraction



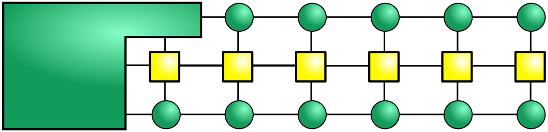
- Complexity $\prod_{i \in \text{ connected legs}} D_i \cdot \prod_{j \in \text{ open legs}} D_j$
- The order of contraction matters!



Contraction



- Complexity $\prod_{i \in \text{ connected legs}} D_i \cdot \prod_{j \in \text{ open legs}} D_j$
- The order of contraction matters!



Complexity stays finite!

SVD

singular values decomposition

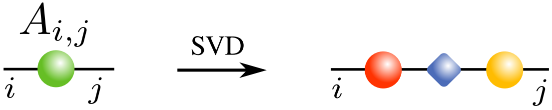
Singular Values Decomposition (SVD)

For any rectangular matrix $M_{i,j}$ exists a decomposition

$$M = U_{i,k} S_{k,k} V^{\dagger}_{k,j}$$

such that:

- $U^{\dagger} U = \mathbb{I}$
- S is a diagonal matrix with non-negative entries
- $V^{\dagger} V = \mathbb{I}$



Schmidt decomposition

- Quantum state:

$$|\psi\rangle = \sum_{i,j} \Psi_{i,j} |i\rangle_A |j\rangle_B,$$

  where $|i\rangle_A$ and $|j\rangle_B$ are orthonormal basis of subsystems A and B.
- Treat $\Psi_{i,j}$ as a matrix and perform SVD
- Schmidt decomposition

$$|\psi\rangle = \sum_{i,j} \sum_{k} U_{i,k} S_{k,k} V^{\dagger}_{k,j} |i\rangle_A |j\rangle_B$$

Schmidt decomposition

- Quantum state:

$$|\psi\rangle = \sum_{i,j} \Psi_{i,j} |i\rangle_A |j\rangle_B,$$

where $|i\rangle_A$ and $|j\rangle_B$ are orthonormal basis of subsystems A and B.

- Treat $\Psi_{i,j}$ as a matrix and perform SVD
- Area law - D relevant states only

$$|\psi\rangle = \sum_{i,j} \sum_{k}^{D} U_{i,k} S_{k,k} V^{\dagger}_{k,j} |i\rangle_A |j\rangle_B$$

Some states have exact MPS representations

Majumdar-Ghosh chain:

$$H = \sum_i J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{J_2}{2} \mathbf{S}_i \cdot \mathbf{S}_{i+2} \tag{1}$$

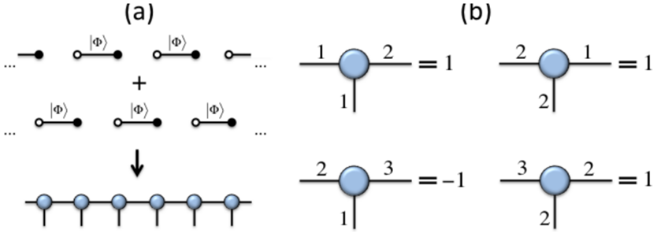
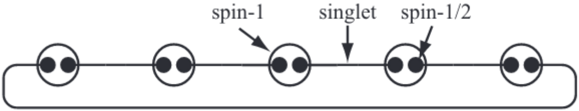


Figure 24: (color online) MPS for the Majumdar-Gosh state: (a) the superposition of two dimerized states of singlets $|\Phi\rangle$ in (a) can be written in terms of an infinite MPS with 1-site unit cell, with non-zero coefficients as in (b).

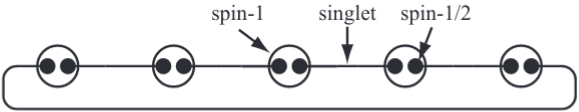
Some states have exact MPS representations

$$\text{AKLT}: \qquad H = \sum_i J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{J_b}{3} \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} \right)^2 \tag{2}$$



Some states have exact MPS representations

$$\text{AKLT}: \qquad H = \sum_i J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{J_b}{3} \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1}\right)^2 \tag{3}$$



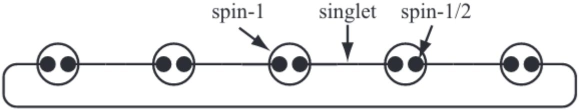
$$\Sigma = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}.$$

$$M^+ = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad M^0 = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \quad M^- = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}.$$

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \mathrm{Tr}(M^{\sigma_1}\Sigma M^{\sigma_2}\Sigma \ldots M^{\sigma_L}\Sigma])|\boldsymbol{\sigma}\rangle,$$

Some states have exact MPS representations

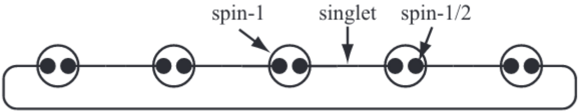
$$\text{AKLT}: \qquad H = \sum_i J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{J_b}{3} \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1}\right)^2 \qquad (4)$$



$$\tilde{A}^+ = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{bmatrix} \quad \tilde{A}^0 = \begin{bmatrix} -\frac{1}{2} & 0 \\ 0 & +\frac{1}{2} \end{bmatrix} \quad \tilde{A}^- = \begin{bmatrix} 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

Some states have exact MPS representations

$$\text{AKLT}: \qquad H = \sum_i J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{J_b}{3} \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} \right)^2 \qquad (5)$$



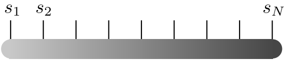
$$\tilde{A}^+ = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{bmatrix} \quad \tilde{A}^0 = \begin{bmatrix} -\frac{1}{2} & 0 \\ 0 & +\frac{1}{2} \end{bmatrix} \quad \tilde{A}^- = \begin{bmatrix} 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

Interestingly, often (always?) exact MPS states corresponds to a disorder point signaling the appearance of incommensurability

Bring quantum states into MPS

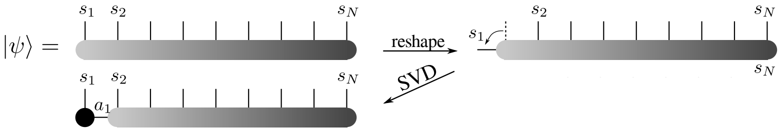
$$
\begin{aligned}
c_{\sigma_1\ldots\sigma_L} &= \Psi_{(\sigma_1\ldots\sigma_{L-1}),\sigma_L} \\
&= \sum_{a_{L-1}} U_{(\sigma_1\ldots\sigma_{L-1}),a_{L-1}} S_{a_{L-1},a_{L-1}} (V^\dagger)_{a_{L-1},\sigma_L} \\
&= \sum_{a_{L-1}} \Psi_{(\sigma_1\ldots\sigma_{L-2}),(\sigma_{L-1}a_{L-1})} B^{\sigma_L}_{a_{L-1}} \\
&= \sum_{a_{L-2},a_{L-1}} U_{(\sigma_1\ldots\sigma_{L-2}),a_{L-2}} S_{a_{L-2},a_{L-2}} (V^\dagger)_{a_{L-2},(\sigma_{L-1}a_{L-1})} B^{\sigma_L}_{a_{L-1}} \\
&= \sum_{a_{L-2},a_{L-1}} \Psi_{(\sigma_1\ldots\sigma_{L-3}),(\sigma_{L-2}a_{L-2})} B^{\sigma_{L-1}}_{a_{L-2},a_{L-1}} B^{\sigma_L}_{a_{L-1}} = \ldots \\
&= \sum_{a_1,\ldots,a_{L-1}} B^{\sigma_1}_{a_1} B^{\sigma_2}_{a_1,a_2} \ldots B^{\sigma_{L-1}}_{a_{L-2},a_{L-1}} B^{\sigma_L}_{a_{L-1}}.
\end{aligned}
$$

Bring quantum states into MPS

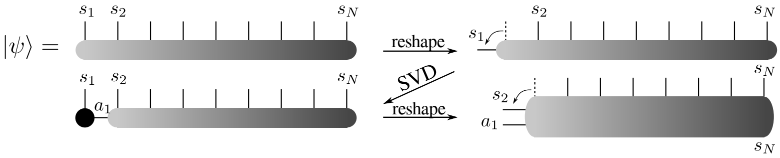
$|\psi\rangle =$ 

Bring quantum states into MPS

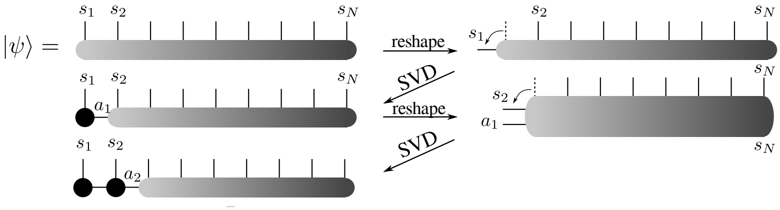
Bring quantum states into MPS



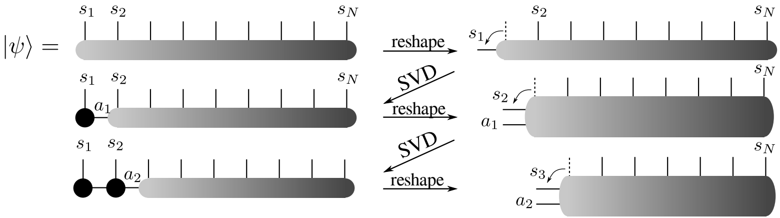
Bring quantum states into MPS



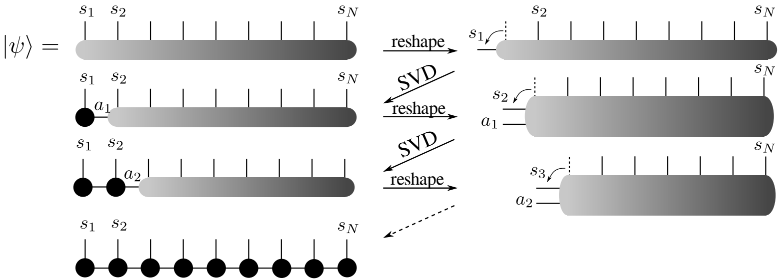
Bring quantum states into MPS



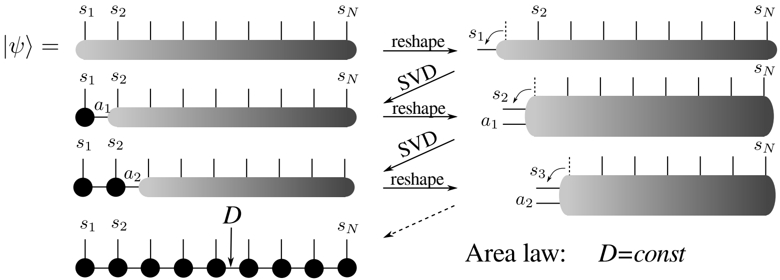
Bring quantum states into MPS



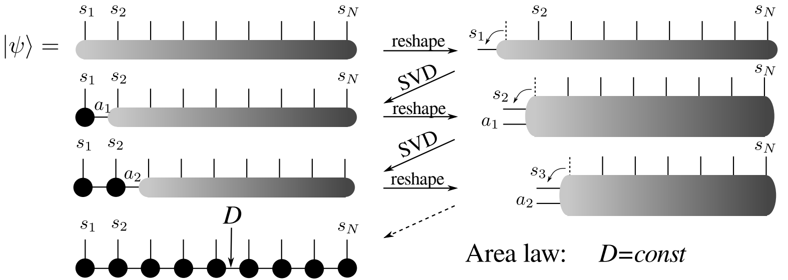
Bring quantum states into MPS



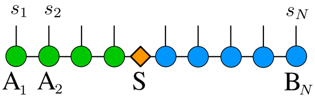
Bring quantum states into MPS



Bring quantum states into MPS



Mixed-canonical form



Normalization:

Normalization

The goal is to find $|\Psi\rangle$ that minimizes the energy:

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

If norm is fixed $\langle\Psi|\Psi\rangle = 1$, it becomes

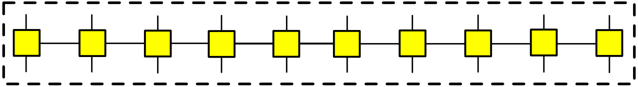
$$E = \langle\Psi|\hat{H}|\Psi\rangle$$

In variational optimization a generalized eigenvalue problem is reduced to a generalized eigvenvalue problem:

$$\hat{H}_{eff}|\psi\rangle = E|\psi\rangle \qquad \text{instead of} \qquad \hat{H}_{eff}|\psi\rangle = E\hat{N}_{eff}|\psi\rangle$$

MPO

Matrix Product Operators



$d^N \times d^N$
Hamiltonian

MPO construction

$$H = \sum_j J(S^x_j S^x_{j+1} + S^y_j S^y_{j+1}) + BS^z_j$$

For a given site j write all possible terms in the Hamiltonian:

$I...I$	BS^z_j	$I...I$
$I...IJS^x_{j-1}$	S^x_j	$I...I$
$I...IJS^y_{j-1}$	S^y_j	$I...I$
$I...I$	JS^x_j	$S^x_{j+1}I...I$
$I...I$	JS^y_j	$S^y_{j+1}I...I$
$I...JS^x_i S^x_{i+1}...I$	I	$I...I$
$I...JS^y_i S^y_{i+1}...I$	I	$I...I$
$I...BS^z_i...I$	I	$I...I$
$I...I$	I	$I...JS^x_i S^x_{i+1}...I$
$I...I$	I	$I...JS^y_i S^y_{i+1}...I$
$I...I$	I	$I...BS^z_i...I$

MPO construction

$$H = \sum_j J(S^x_j S^x_{j+1} + S^y_j S^y_{j+1}) + BS^z_j$$

For a given site j write all possible terms in the Hamiltonian:

$I...I$	BS^z_j	$I...I$
$I...IJS^x_{j-1}$	S^x_j	$I...I$
$I...IJS^y_{j-1}$	S^y_j	$I...I$
$I...I$	JS^x_j	$S^x_{j+1}I...I$
$I...I$	JS^y_j	$S^y_{j+1}I...I$
$I...JS^x_i S^x_{i+1}...I$	I	$I...I$
$I...JS^y_i S^y_{i+1}...I$	I	$I...I$
$I...BS^z_i...I$	I	$I...I$
$I...I$	I	$I...JS^x_i S^x_{i+1}...I$
$I...I$	I	$I...JS^y_i S^y_{i+1}...I$
$I...I$	I	$I...BS^z_i...I$

MPO construction

$$H = \sum_j J(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + BS_j^z$$

For a given site j write all possible terms in the Hamiltonian:

$I...I$	BS_j^z	$I...I$
$I...IJS_{j-1}^x$	S_j^x	$I...I$
$I...IJS_{j-1}^y$	S_j^y	$I...I$
$I...I$	JS_j^x	$S_{j+1}^x I...I$
$I...I$	JS_j^y	$S_{j+1}^y I...I$
I...Full...I	I	$I...I$
$I...I$	I	I...Full...I

- Seven non-zero entries in the MPO

MPO construction

$$H = \sum_j J(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + BS_j^z$$

For a given site j write all possible terms in the Hamiltonian:

$I...I$	BS_j^z	$I...I$
$I...IJS_{j-1}^x$	S_j^x	$I...I$
$I...IJS_{j-1}^y$	S_j^y	$I...I$
$I...I$	JS_j^x	$S_{j+1}^x I...I$
$I...I$	JS_j^y	$S_{j+1}^y I...I$
I...Full...I	I	$I...I$
$I...I$	I	I...Full...I

- Seven non-zero entries in the MPO
- Look at the left and right basis in which the MPO is going to be written

MPO construction

- For a given site j write all possible terms in the Hamiltonian:
- Seven non-trivial entries in the MPO
- Look at the left and right basis in which the MPO is going to be written

I...Full...I				
$I...IJS^x_{j-1}$				
$I...IJS^y_{j-1}$				
$I...I$				
	$I...I$	$S^x_{j+1}I...I$	$S^y_{j+1}I...I$	I...Full...I

MPO construction

- For a given site j write all possible terms in the Hamiltonian:
- Five non-trivial entries in the MPO
- Look at the left and right basis in which the MPO is going to be written
- Fill-in the matrix:

$I\ldots\text{Full}\ldots I$	I	0	0	0
$I\ldots IJS^x_{j-1}$	S^x_j	0	0	0
$I\ldots IJS^y_{j-1}$	S^y_j	0	0	0
$I\ldots I$	BS^z_j	JS^x_j	JS^y_j	I
	$I\ldots I$	$S^x_{j+1}I\ldots I$	$S^y_{j+1}I\ldots I$	$I\ldots\text{Full}\ldots I$

MPO answers:

$$H = \sum_j J(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + BS_j^z$$

$$H_j = \begin{pmatrix} I & . & . & . \\ S_j^x & . & . & . \\ S_j^y & . & . & . \\ BS_j^z & JS_j^x & JS_j^y & I \end{pmatrix}$$

MPO answers:

$$H = \sum_j J(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + BS_j^z$$

Bulk MPO:

$$H_j = \begin{pmatrix} I & . & . & . \\ S_j^x & . & . & . \\ S_j^y & . & . & . \\ BS_j^z & JS_j^x & JS_j^y & I \end{pmatrix}$$

First and last sites:

$$H_1 = \begin{pmatrix} BS_j^z & JS_j^x & JS_j^y & I \end{pmatrix} \qquad H_j = \begin{pmatrix} I \\ S_j^x \\ S_j^y \\ BS_j^z \end{pmatrix}$$

Exponentially decaying interactions

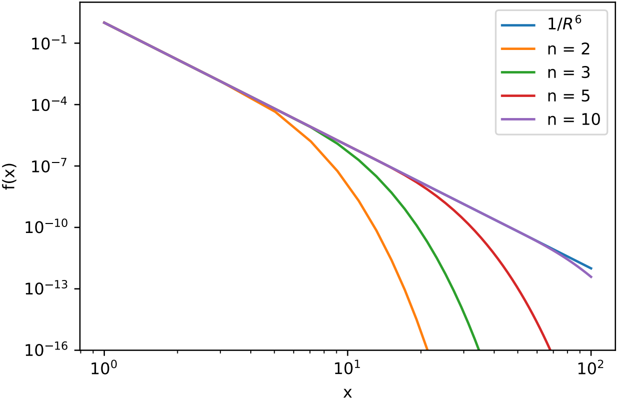
- Long-range interactions are in general difficult
- ... but there is one exception - exponentially decaying potential

$$H = \sum_j J(r) S^z_j S^z_{j+1} \qquad \text{with} \qquad J(r) = Je^{-r/\xi} = J\lambda^r$$

$$H_j = \begin{pmatrix} I & . & . \\ S^z & \lambda S^z_j & . \\ . & J\lambda S^z_j & I \end{pmatrix}$$

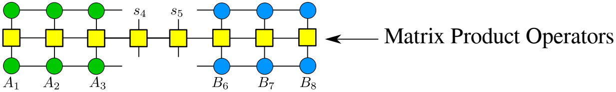
Exponentially decaying interactions

- Long-range interactions are in general difficult
- ... but there is one exception - exponentially decaying potential
- Approximate long-range interactions with exponentials

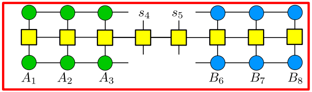


DMRG / variational MPS

DMRG sweep



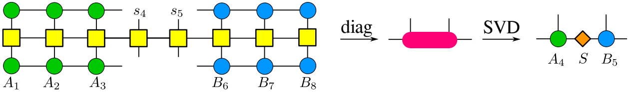
DMRG sweep



Group the legs and treat this rank-8 tensor as a matrix

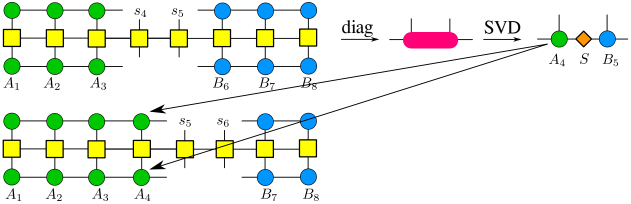
DMRG sweep

Left-to-right:



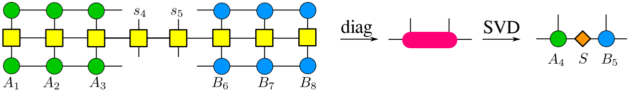
DMRG sweep

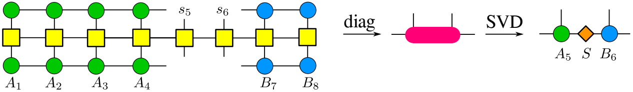
Left-to-right:



DMRG sweep

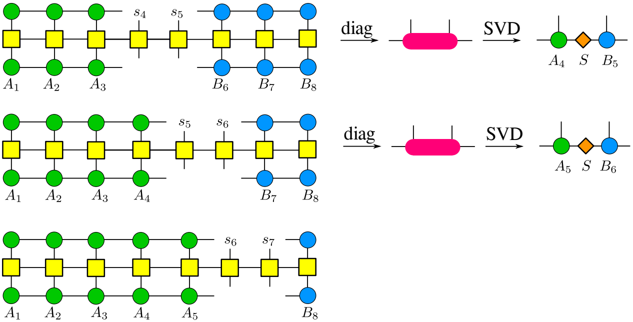
Left-to-right:





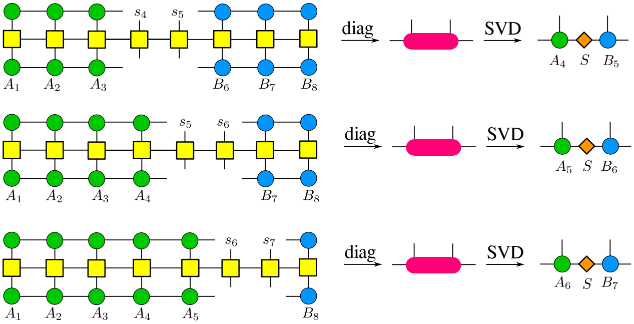
DMRG sweep

Left-to-right:



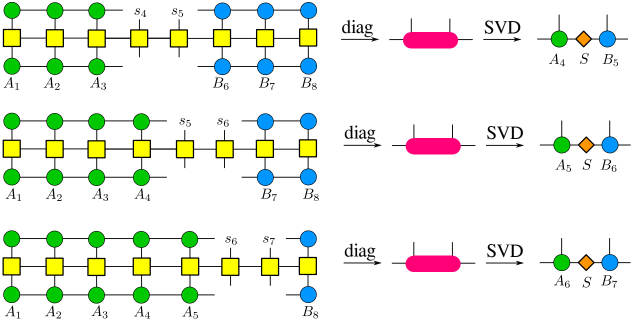
DMRG sweep

Left-to-right:

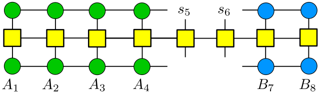


DMRG sweep

Left-to-right:

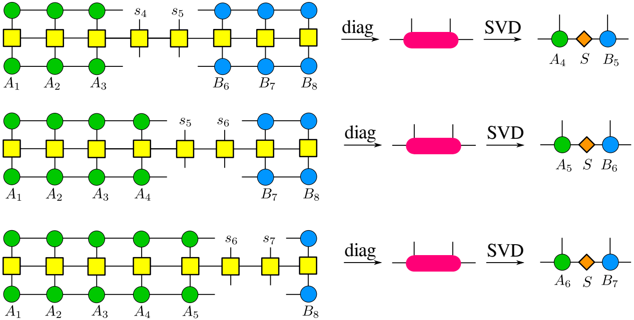


Right-to-left:

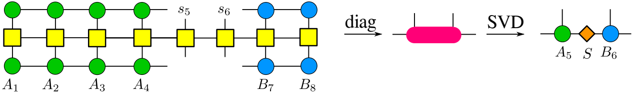


DMRG sweep

Left-to-right:



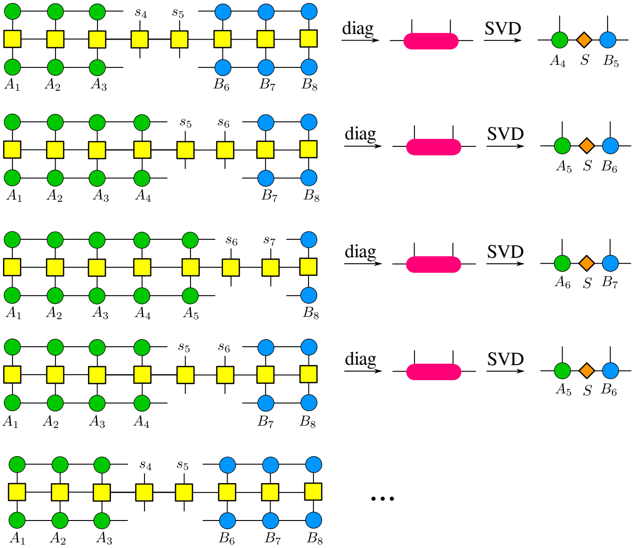
Right-to-left:



DMRG sweep

Left-to-right:

Right-to-left:



Convergence criteria

Convergence criteria

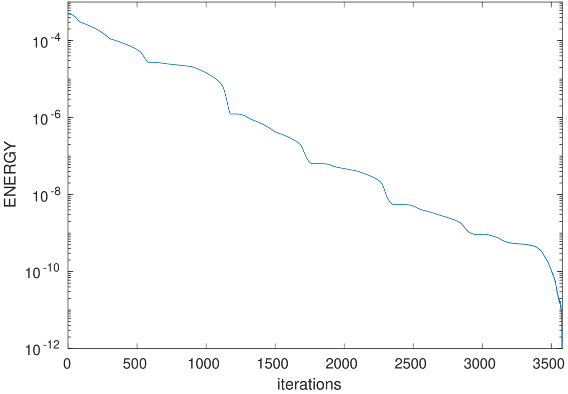
- Energy
- Entanglement
- Observable of interest:
  - Local magnetization/density
  - Dimerization / local oscillations
  - Distant correlations $\langle O_i O_j \rangle$
  - Extreme values (disorder)
  - ...

Convergence criteria

- Local magnetization/density
- Dimerization / local oscillations
- Extreme values (disorder)
- Energy
- Distant correlations $\langle O_i O_j \rangle$
- Entanglement

Convergence criteria

Typical energy convergence:



DMRG is variational!

Convergence criteria

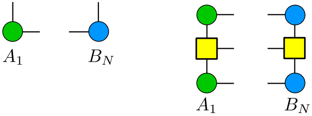
- Local magnetization/density
- Dimerization / local oscillations
- Extreme values (disorder)
- Energy
- Distant correlations $\langle O_i O_j \rangle$
- Entanglement

DMRG has to converge with respect to BOTH
the bond dimension D and the number of iterations!

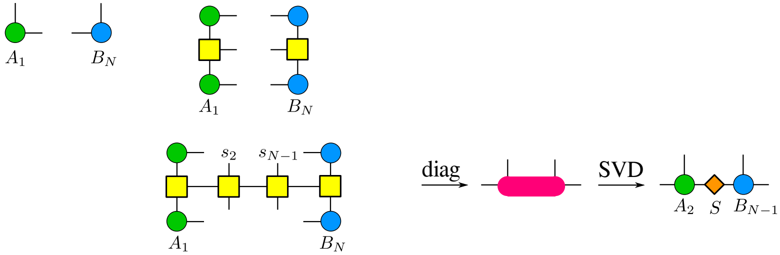
Initial guess

- Product state
- Random state
- Infinite-size DMRG

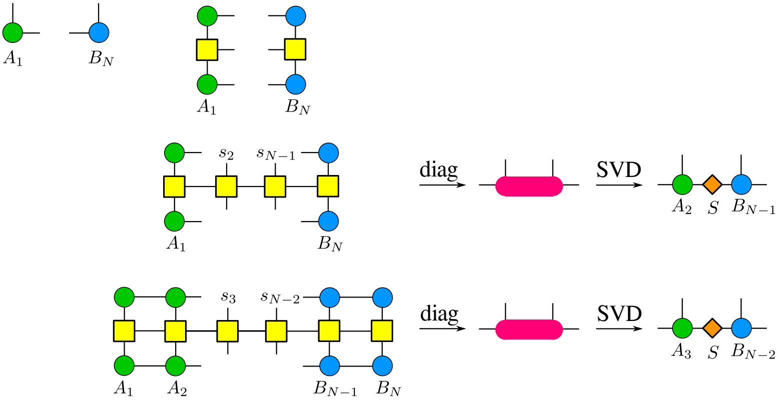
Infinite-size DMRG



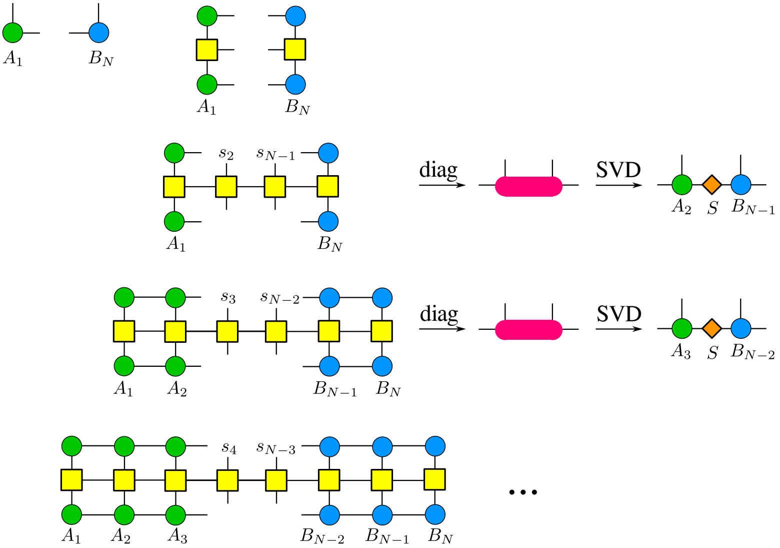
Infinite-size DMRG



Infinite-size DMRG

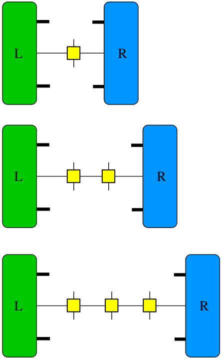


Infinite-size DMRG



One-, two- and multi-site DMRG

?-site DMRG



- Traditionally DMRG is a two-site algorithm.
- Single-site is cheaper by a factor d^2
- Naively the bond dimension in one-site DMRG is fixed
- Now there are now efficient ways to increase it:
  - Hubig et al (PRB 2015)
  - von Delft et al (PRL 2022)
- Multi-site provide stability but they are expensive, though there are tricks like DMRG^2

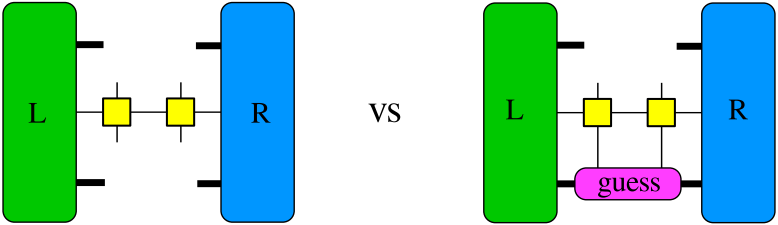
Lanczos algorithm

Iterative eigensolver

Lanczos algorithm

1. Let $v_1 \in \mathbb{C}^n$ be an arbitrary vector with Euclidean norm 1.
2. Abbreviated initial iteration step:
    1. Let $w_1' = Av_1$.
    2. Let $\alpha_1 = w_1'^* v_1$.
    3. Let $w_1 = w_1' - \alpha_1 v_1$.
3. For $j = 2, \ldots, m$ do:
    1. Let $\beta_j = \|w_{j-1}\|$ (also Euclidean norm).
    2. If $\beta_j \neq 0$, then let $v_j = w_{j-1}/\beta_j$,
       else pick as v_j an arbitrary vector with Euclidean norm 1 that is orthogonal to all of $v_1, \ldots, v_{j-1}$.
    3. Let $w_j' = Av_j$.
    4. Let $\alpha_j = w_j'^* v_j$.
    5. Let $w_j = w_j' - \alpha_j v_j - \beta_j v_{j-1}$.
4. Let V be the matrix with columns $v_1, \ldots, v_m$. Let $T = \begin{pmatrix} \alpha_1 & \beta_2 & & & & 0 \\ \beta_2 & \alpha_2 & \beta_3 & & & \\ & \beta_3 & \alpha_3 & \ddots & & \\ & & \ddots & \ddots & \beta_{m-1} & \\ & & & \beta_{m-1} & \alpha_{m-1} & \beta_m \\ 0 & & & & \beta_m & \alpha_m \end{pmatrix}$.

Lanczos in MPS



- H_{eff} is too expensive
- In Lanczos: $H_{\text{eff}} \cdot v_{\text{guess}}$ - much cheaper! (see tutorials)

Control parameters

Control parameters

- Bond dimension
- Truncation weight
- Number of sweeps
- Number of Lanczos iterations

Control parameters

- Bond dimension
- Truncation weight
- Number of sweeps
- Number of Lanczos iterations

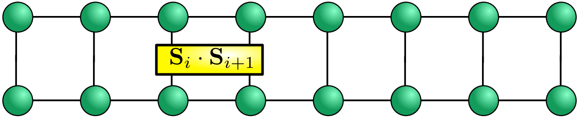
Two main DMRG practices:

- A few Lanczos iterations (≈ 5) + Many sweeps (≈ 100); D increases after the convergence is reached
- D increases every sweep, many Lanczos iterations (≈ 100), a few sweeps (≈ 5).

Observables

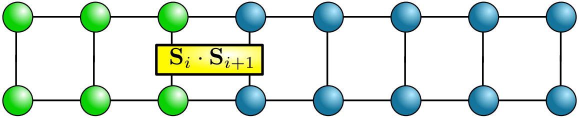
Observables

Nearest-neighbor correlations $\langle\Psi|\mathbf{S}_i \cdot \mathbf{S}_{i+1}|\Psi\rangle$



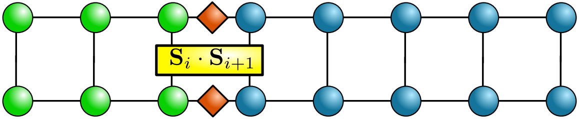
Observables

Nearest-neighbor correlations $\langle\Psi|\mathbf{S}_i \cdot \mathbf{S}_{i+1}|\Psi\rangle$



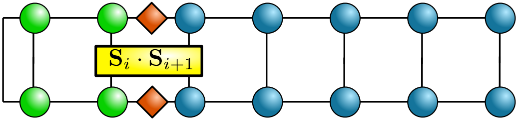
Observables

Nearest-neighbor correlations $\langle \Psi | \mathbf{S}_i \cdot \mathbf{S}_{i+1} | \Psi \rangle$



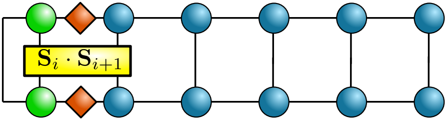
Observables

Nearest-neighbor correlations $\langle\Psi|\mathbf{S}_i \cdot \mathbf{S}_{i+1}|\Psi\rangle$



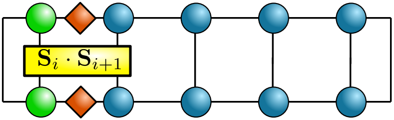
Observables

Nearest-neighbor correlations $\langle\Psi|\mathbf{S}_i \cdot \mathbf{S}_{i+1}|\Psi\rangle$



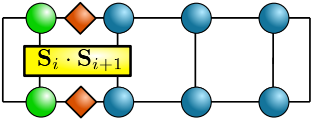
Observables

Nearest-neighbor correlations $\langle\Psi|\mathbf{S}_i \cdot \mathbf{S}_{i+1}|\Psi\rangle$



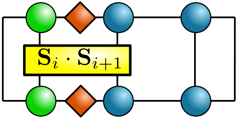
Observables

Nearest-neighbor correlations $\langle \Psi | \mathbf{S}_i \cdot \mathbf{S}_{i+1} | \Psi \rangle$



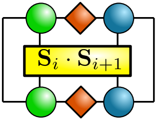
Observables

Nearest-neighbor correlations $\langle\Psi|\mathbf{S}_i \cdot \mathbf{S}_{i+1}|\Psi\rangle$



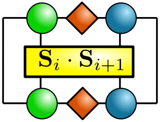
Observables

Nearest-neighbor correlations $\langle\Psi|\mathbf{S}_i \cdot \mathbf{S}_{i+1}|\Psi\rangle$

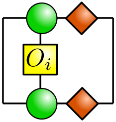


Observables

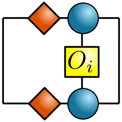
Nearest-neighbor correlations $\langle\Psi|\mathbf{S}_i\cdot\mathbf{S}_{i+1}|\Psi\rangle$



On-site measures $\langle\Psi|O_i|\Psi\rangle$

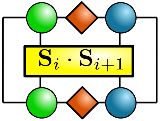


or

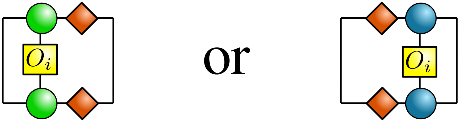


Observables

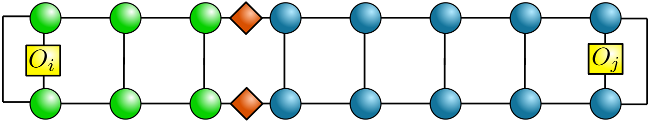
Nearest-neighbor correlations $\langle\Psi|\mathbf{S}_i\cdot\mathbf{S}_{i+1}|\Psi\rangle$



On-site measures $\langle\Psi|O_i|\Psi\rangle$

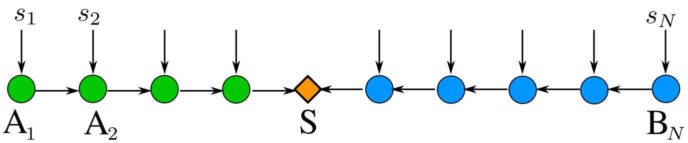


Long range correlations $\langle\Psi|O_i\cdot O_j|\Psi\rangle$



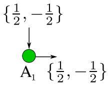
Abelian symmetries

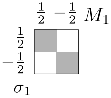
Abelian symmetry



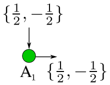
- Assign quantum numbers - labels to physical bonds of MPS
- Using fusion rules of the symmetry, find quantum numbers on auxiliary legs
- When local basis is sorted according to the quantum number of states, the MPS takes a block-diagonal form

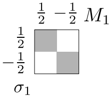
Abelian symmetry. Examples

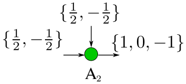


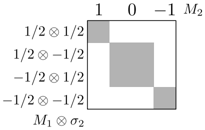


Abelian symmetry. Examples

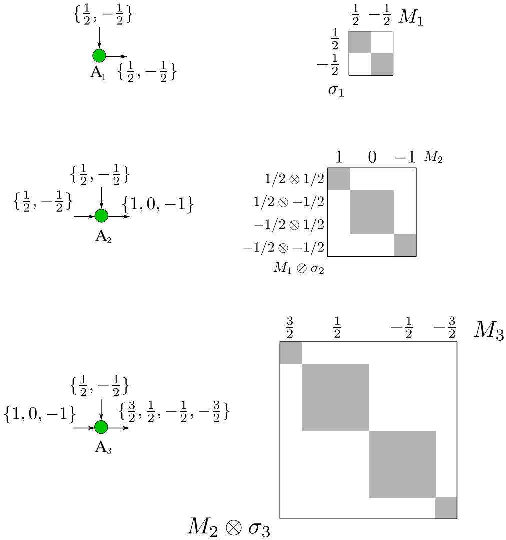




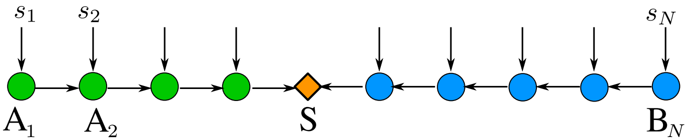




Abelian symmetry. Examples



Abelian symmetry



- Assign quantum numbers - labels to physical bonds of MPS
- Using fusion rules of the symmetry, find quantum numbers on auxiliary legs
- When local basis is sorted according to the quantum number of states, the MPS takes a block-diagonal form
- Select the right symmetry sector by matching the right combination of quantum numbers

Not implemented symmetries

Keep your guess in the right sector

Constraints

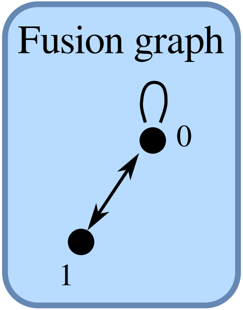
Nearest-neighbor blockade: $n_i n_{i+1} = 0$

Fusion graph for $r = 1$ Rydberg blockade

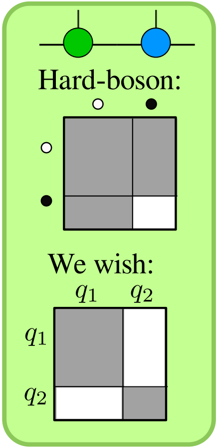
...○ + ● = ...○●

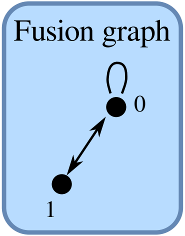
...● + ○ = ...●○

...○ + ○ = ...○○

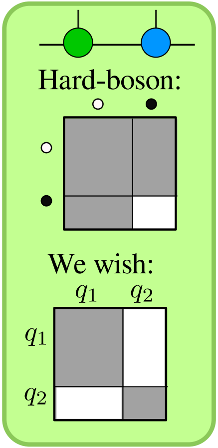


Encoding the $r = 1$ Rydberg blockade

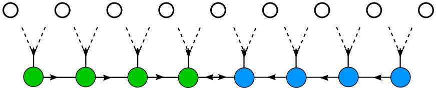




Encoding the $r = 1$ Rydberg blockade



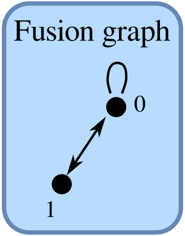
$|l_1\rangle = |\circ\rangle$ $|l_2\rangle = |\bullet\rangle$



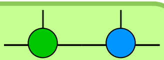
New local Hilbert space:

$|h_1\rangle = |\circ\,\circ\rangle$ $|h_2\rangle = |\circ\,\bullet\rangle$ $|h_3\rangle = |\bullet\,\circ\rangle$

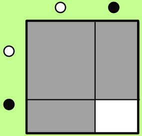
Span local degrees of freedom over two sites



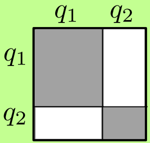
Encoding the $r = 1$ Rydberg blockade



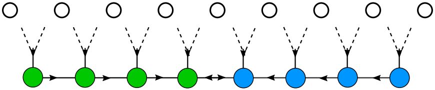
Hard-boson:



We wish:



$|l_1\rangle = |\circ\rangle$ $|l_2\rangle = |\bullet\rangle$



New local Hilbert space:

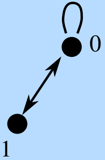
$|h_1\rangle = |\circ\circ\rangle$ $|h_2\rangle = |\circ\bullet\rangle$ $|h_3\rangle = |\bullet\circ\rangle$

Span local degrees of freedom over two sites

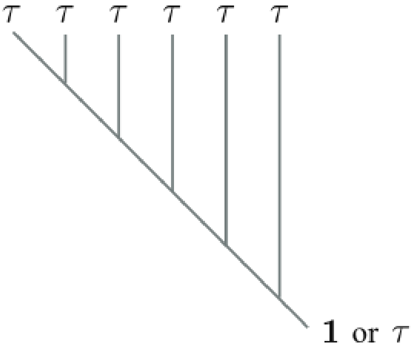
For each neighbors there is a common boson site:

use its states as **quantum labels!**

Fusion graph



Fusion graph for Fibonacci anyons



$$I \times \tau = \tau$$

$$\tau \times \tau = I + \tau$$

Trebst et al., Prog. Theor. Phys. Supp. 176, 384 (2008)

Fusion graph for Fibonacci anyons

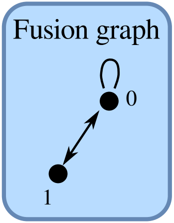
$$I \times \tau = \tau$$

$$\tau \times \tau = I + \tau$$

...○ + ● = ...○●

...● + ○ = ...●○

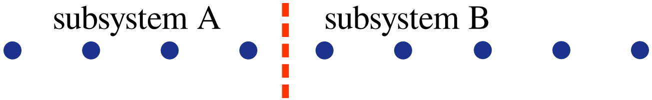
...○ + ○ = ...○○



Entanglement

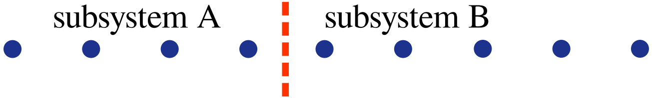
Entanglement entropy

$$S_{A|B} = -\mathrm{Tr}\rho_A \log \rho_A = -\sum_{a=1}^{D} s_a^2 \log s_a^2 \tag{6}$$

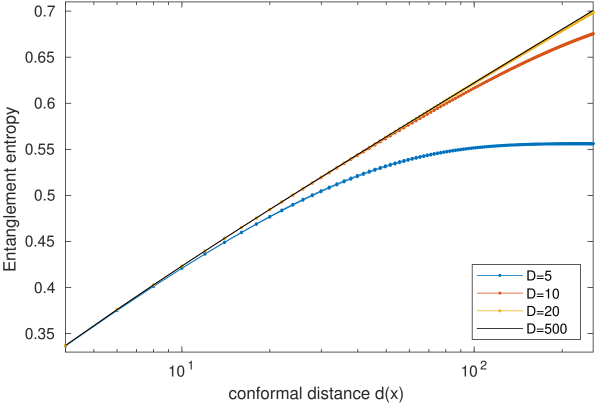


- DMRG is a low entangled approximation of a quantum state

Entanglement entropy

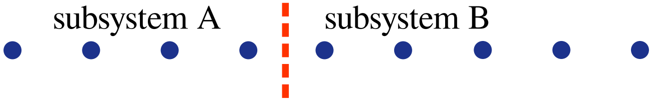


- DMRG is a low entangled approximation of a quantum state



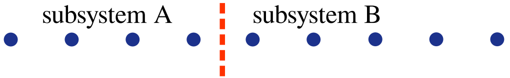
Entanglement entropy

$$S_{A|B} = -\mathrm{Tr}\rho_A \log \rho_A = -\sum_{a=1}^{D} s_a^2 \log s_a^2 \qquad (7)$$

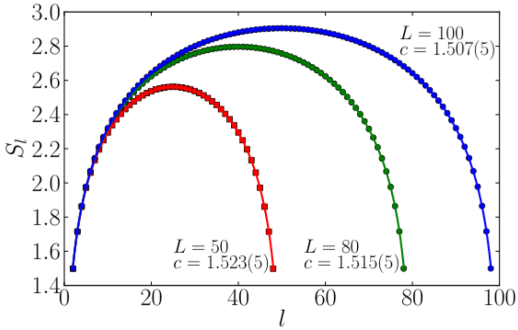


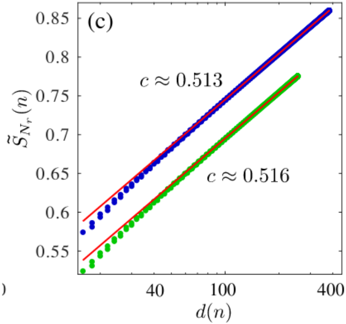
- DMRG is a low entangled approximation of a quantum state
- But the entanglement can itself be an observable

Central charge



Calabrese-Cardy formula: $S_{\text{PBC}} = \frac{c}{3} \log\left(\frac{L}{\pi a} \sin \frac{\pi l}{L}\right) + c_1'$

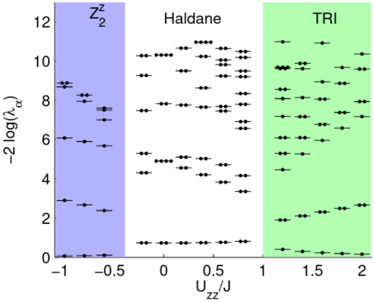




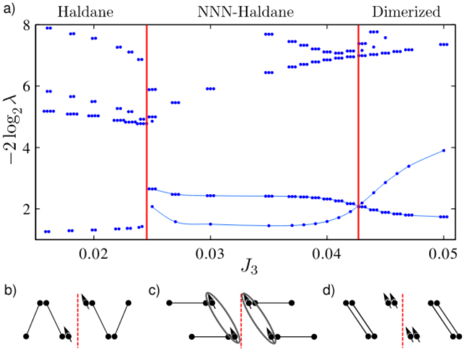
Michaud et al.Phys. Rev. Lett. 108, 127202 (2012)

Entanglement spectra

$$\epsilon_a = -\log_2 s_a^2$$



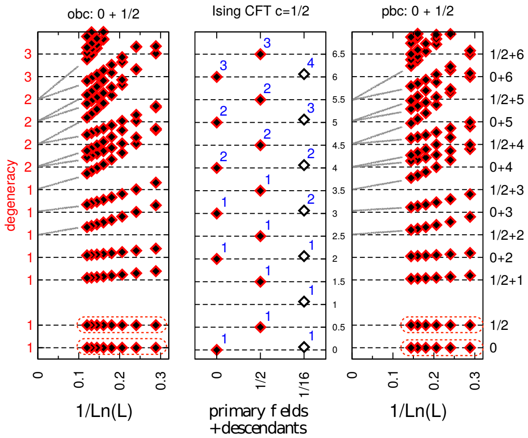
Pollmann et al., Phys. Rev. B 81, 064439 (2010)



- Identify topologically non-trivial phases
- Locate quantum phase transitions

Conformal towers from entanglement spectrum

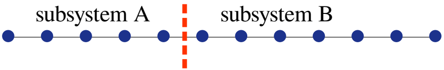
Transverse field Ising model

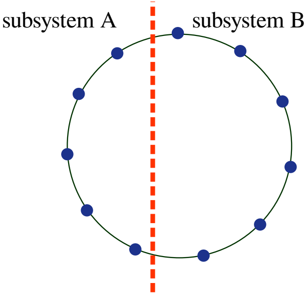


A.Läuchli, arxiv:1303.0741

Boundary conditions

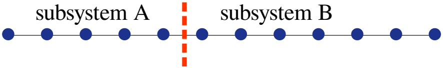
Periodic vs open boundary conditions

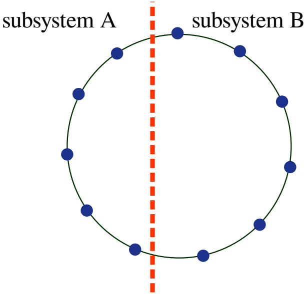




For periodic chains the entanglement is usually higher than for open ones

Periodic vs open boundary conditions





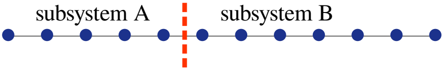
For periodic chains the entanglement is usually higher than for open ones

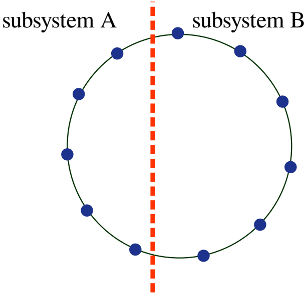
Calabrese-Cardy formulas for critical systems:

$$S_{\mathrm{PBC}} = \frac{c}{3} \log \left(\frac{L}{\pi a} \sin \frac{\pi l}{L} \right) + c_1', \tag{8}$$

$$S_{\mathrm{OBC}} = \frac{c}{6} \log \left(\frac{2L}{\pi a} \sin \frac{\pi l}{L} \right) + c_1'/2 + \log \tilde{g}. \tag{9}$$

Periodic vs open boundary conditions





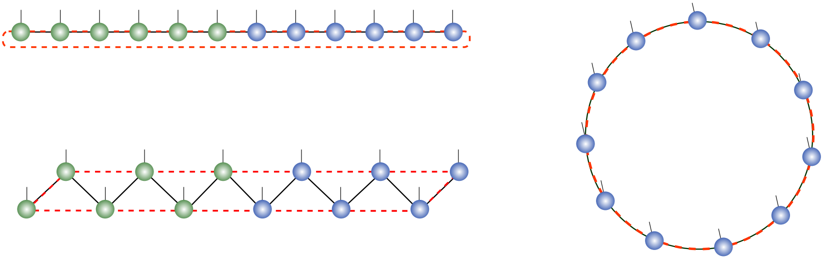
For periodic chains the entanglement is usually higher than for open ones

Calabrese-Cardy formulas for critical systems.

$$S_{\mathrm{PBC}} = \frac{c}{3} \log\left(\frac{L}{\pi a} \sin\frac{\pi l}{L}\right) + c_1', \tag{10}$$

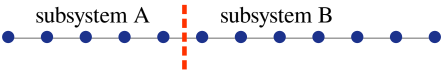
$$S_{\mathrm{OBC}} = \frac{c}{6} \log\left(\frac{2L}{\pi a} \sin\frac{\pi l}{L}\right) + c_1'/2 + \log\tilde{g}. \tag{11}$$

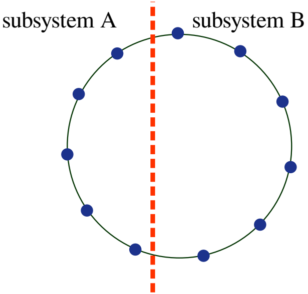
PBC with MPS



red = lattice; black = tensor network

Periodic vs open boundary conditions





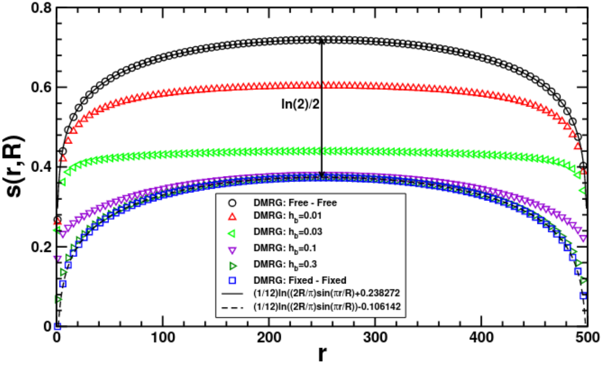
For periodic chains the entanglement is usually higher than for open ones

Calabrese-Cardy formulas for critical systems. Note: the boundary term $\tilde{g}$

$$S_{\mathrm{PBC}} = \frac{c}{3} \log\left(\frac{L}{\pi a} \sin\frac{\pi l}{L}\right) + c_1', \qquad (12)$$

$$S_{\mathrm{OBC}} = \frac{c}{6} \log\left(\frac{2L}{\pi a} \sin\frac{\pi l}{L}\right) + c_1'/2 + \log\tilde{g} \qquad (13)$$

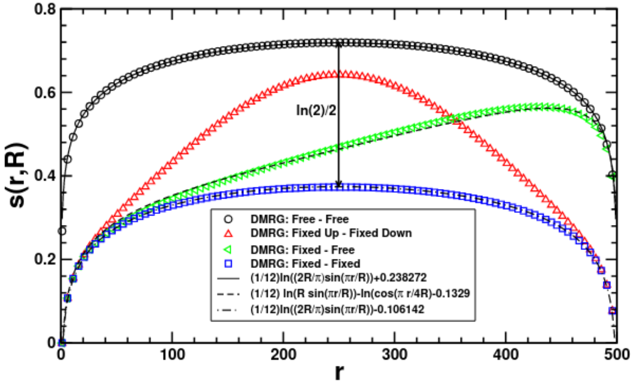
Fixed BC = Lower entanglement



Affleck, Laflorencie, Sorensen, J. Phys. A: Math. Theor. 42 504009 (2009)

Sometimes boundary conditions are unintentionally "fixed" by the model (e.g. Heisenberg chain)

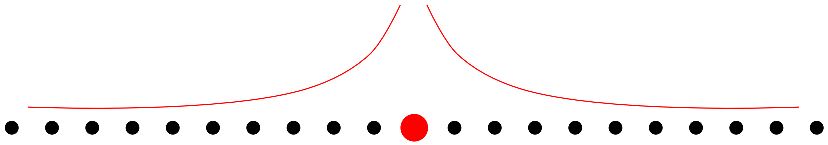
Non-symmetric BC = different scaling!



Affleck, Laflorencie, Sorensen, J. Phys. A: Math. Theor. 42 504009 (2009)

Friedel oscillations

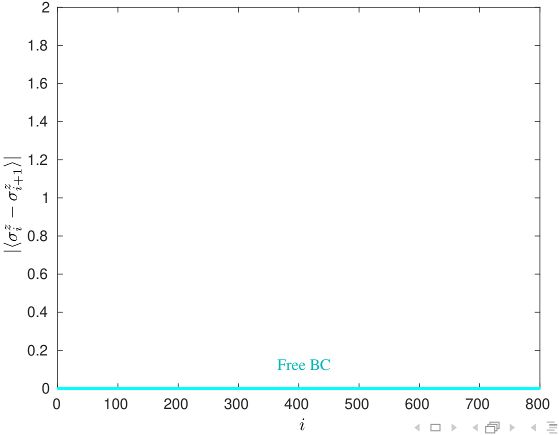
- Response of the system to an impurity
- In the gapped phase it decays exponentially
- At the critical point - with the corresponding critical exponent
- Open boundary conditions = impurity
- Prediction by boundary-CFT



Broken symmetry

Transverse field Ising model:

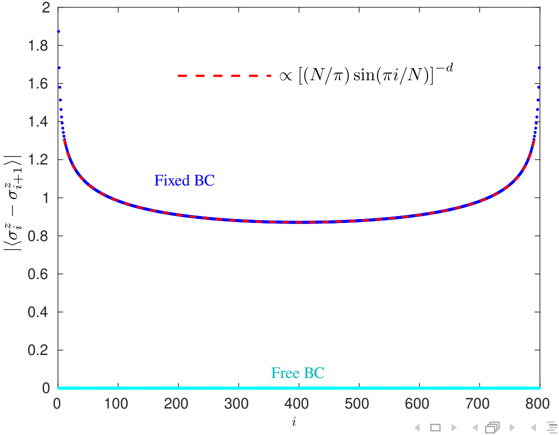
$$H = \sum_i \sigma_i^z \sigma_{i+1}^z + h\sigma_i^x$$



Fixed BC = Friedel oscillations

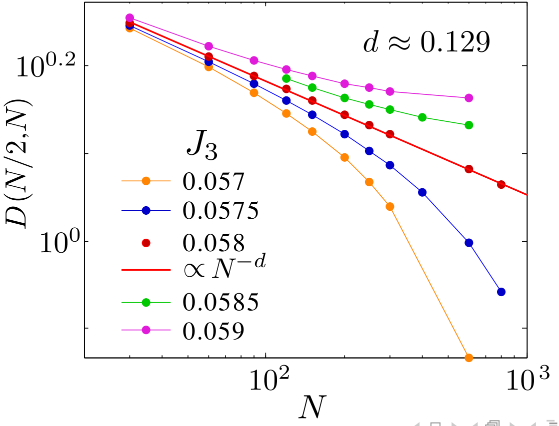
Transverse field Ising model:

$$H = \sum_i \sigma_i^z \sigma_{i+1}^z + h\sigma_i^x$$



Locate phase transitions

$$H = \sum_i \sigma_i^z \sigma_{i+1}^z + h\sigma_i^x$$



By-path in computing correlations

Distant correlations

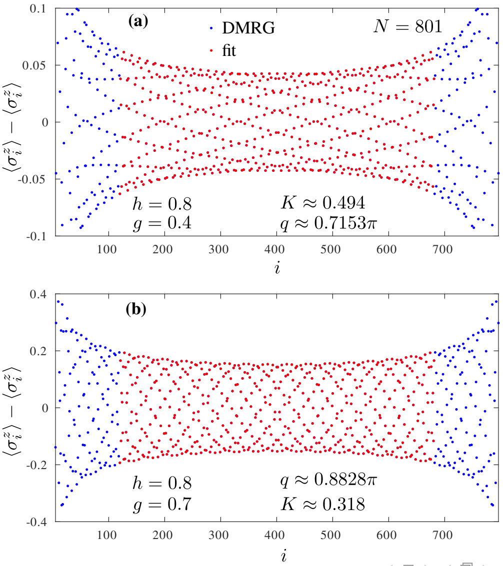
$$\langle O_i O_{i+r} \rangle - \langle O_i \rangle \langle O_{i+r} \rangle \propto r^{\eta}$$

$$\Downarrow$$

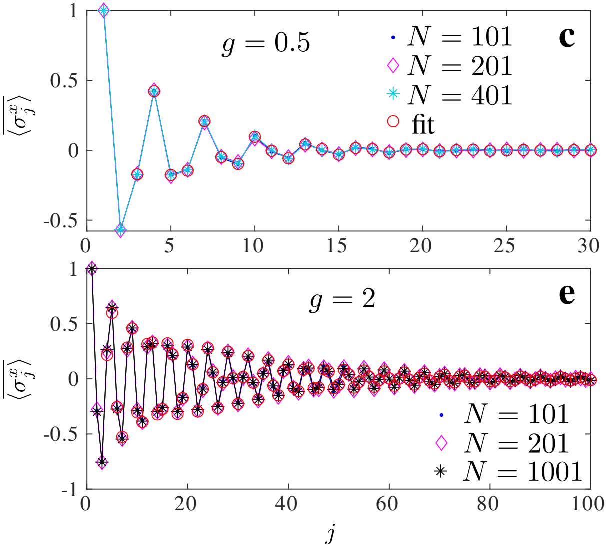
Friedel oscillations

$$\langle O_r \rangle \propto r^{\eta/2}$$

Extract Luttinger liquid exponents



Way more accurate in case of disorder and noise



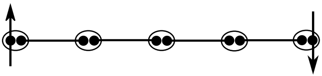
Excitation spectrum

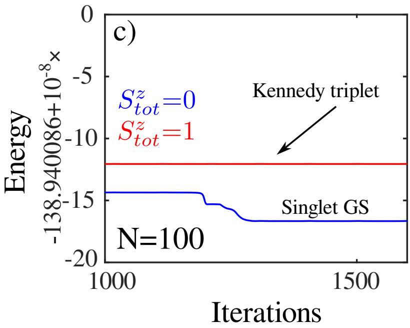
Excitation spectrum with DMRG/MPS

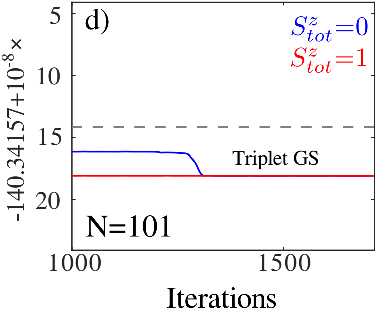
1. The excited state is the 'ground-state' of the different symmetry sector

Example: Kennedy triplet in Haldane chain

$$H = J \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$







Excitation spectrum with DMRG/MPS

1. The excited state is the 'ground-state' of the different symmetry sector
2. Conventional DMRG: Mixed states
   - The ground-state is spoiled
   - Heavy memory usage

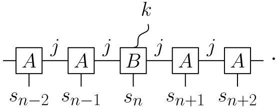
Excitation spectrum with DMRG/MPS

1. The excited state is the 'ground-state' of the different symmetry sector
2. Conventional DMRG: Mixed states
   - No longer variational
   - Heavy memory usage
3. MPS: Construct the lowest-energy state orthogonal to the previously constructed ones
   - Time consuming
   - Accumulation of the error

Excitation spectrum with DMRG/MPS

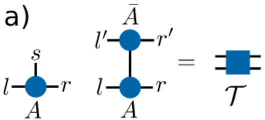
1. The excited state is the 'ground-state' of the different symmetry sector
2. Conventional DMRG: Mixed states
   - No longer variational
   - Heavy memory usage
3. MPS: Construct the lowest-energy state orthogonal to the previously constructed ones
   - Time consuming
   - Accumulation of the error
4. Elementary excitations + plane-wave superposition
   - Translation invariant MPS
   - Not suitable for OBC

$$|\Phi_p^k(B)\rangle = \sum_n e^{ipn}$$

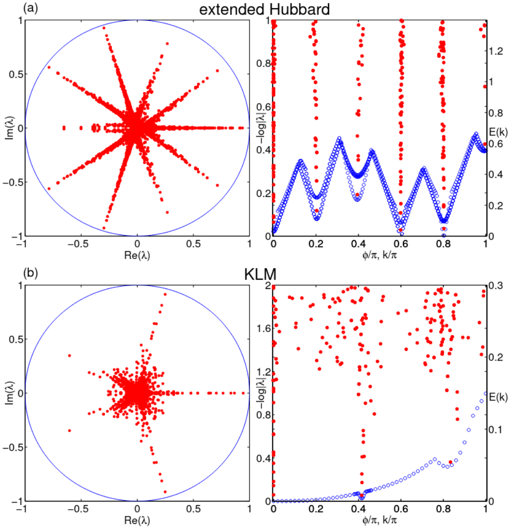


Vanderstraeten, Wybo, NC, Verstraete, Mila, PRB (2020)

Transfer matrix



Zauner et al, New J. Phys. 17 (2015) 053002



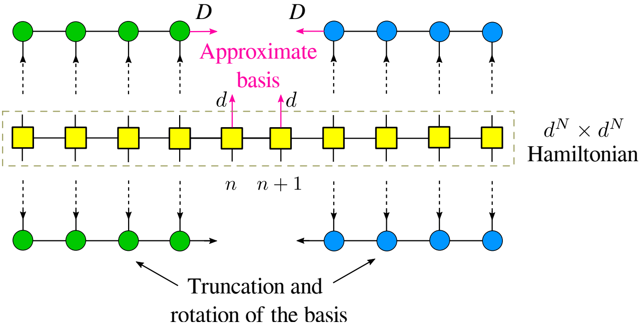
Excitation spectrum with DMRG/MPS

1. The excited state is the 'GS' of the different symmetry sector
2. Conventional DMRG: Mixed states
   - No longer variational & Heavy memory usage
3. MPS: Construct the lowest-energy state orthogonal to the previously constructed ones
   - Time consuming & Accumulation of the error
4. MPS: Domain wall/ special tensor/ transfer matrix
   - Translation invariant MPS

There is a cheaper option:

Sometimes it is sufficient to target multiple eigenstates of the effective Hamiltonian and keep track of the energies as a function of iterations [NC, Mila, Phys.Rev.B **96**, 054425 (2017)]

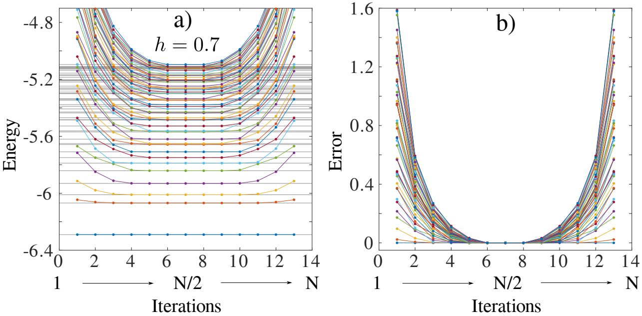
Effective Hamiltonian



- The Hamiltonian is written in a truncated and rotated basis.
- This basis is selected for the ground state.
- Could this basis be suitable for other low-energy states?

Trivial case - non-truncated MPS

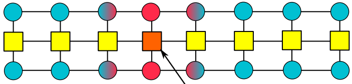
When no truncation is imposed and all basis states are kept in MPS, the DMRG is equivalent to exact diagonalization and one can access the entire spectrum!



When does it work?

Local impurities

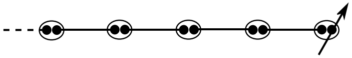
- Localized excitations
- MPS is the same except for a few sites



When does it work?

Edge states

- Edge spins are entangled through the entire network
- All edge states are in the basis



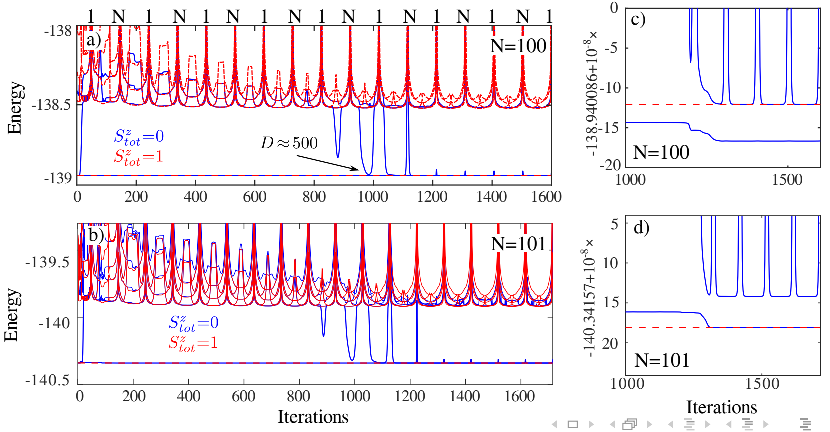
$$\left(\frac{B}{2}\otimes\uparrow\right)\oplus\left(\frac{B}{2}\otimes\downarrow\right)$$

Local impurities

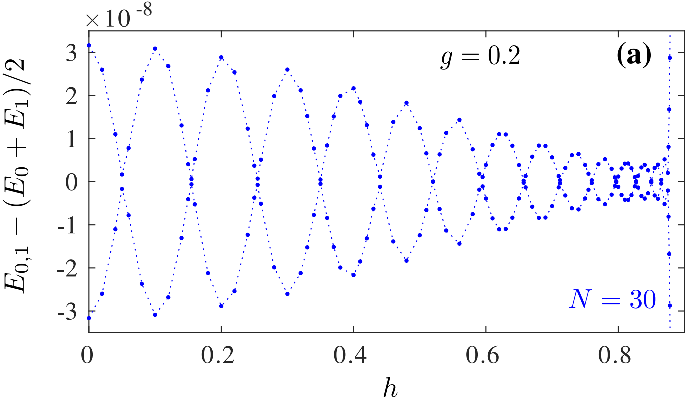
- Localized excitations
- MPS is the same except for a few sites

Edge states in the Haldane chain

$$H = J \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$



Exact zero modes in Majorana chain



When correlations are incommensurate the effective coupling between edge states can be continuously tuned $J_{\text{eff}} \propto \cos(q \cdot L)$

Zero modes appear and we can capture them with nearly machine precision!

When does it work?

Critical systems

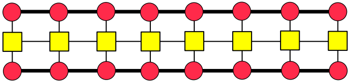
- Divergent correlation length
- Slow decay of Schmidt values
- Special structure of spectrum

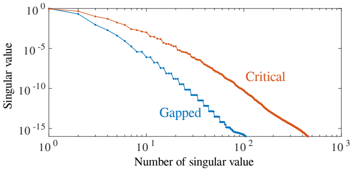
Edge states

- Edge spins are entangled through the entire network
- All edge states are in the basis

Local impurities

- Localized excitations
- MPS is the same except for a few sites



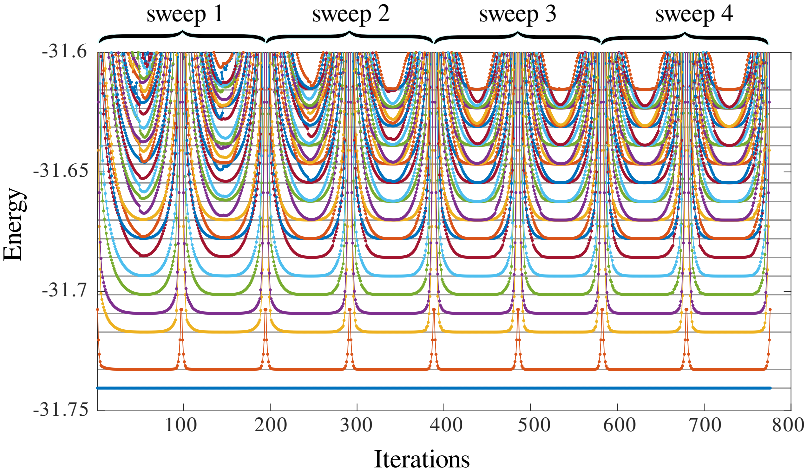


Transverse field Ising model

$$H = \sum_i J S_i^x S_{i+1}^x + h S_i^z$$

- Critical at $h = J/2$
- Solved by Jordan-Wigner transformation
- Corresponds to the minimal model (4,3) in CFT

Transverse field Ising model. Excitation spectrum

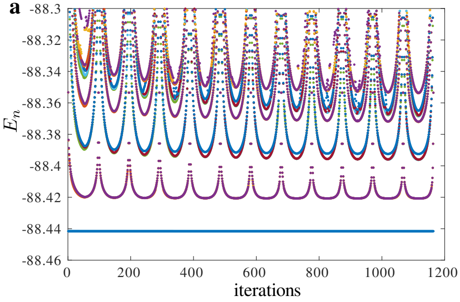


- 30 states within a single run!
- Flat modes signal convergence

NC, F. Mila, Phys. Rev. B 96, 054425'17

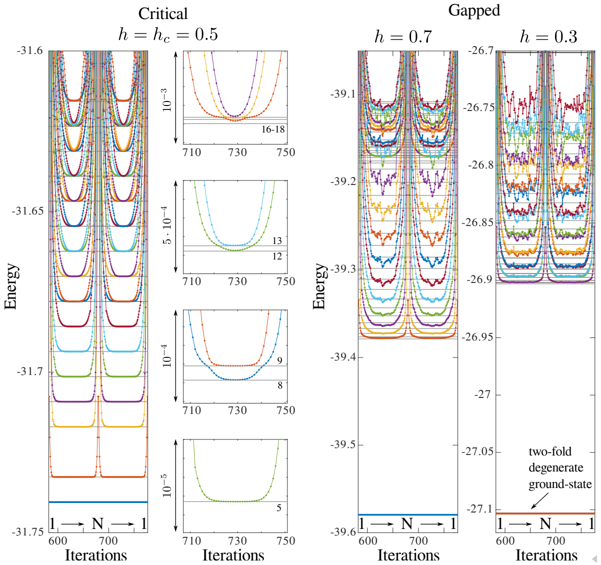
The convergence is sometimes tricky

4-state Potts with free BC:



NC, SciPost Phys. Core 5, 031 (2022)

Transverse field Ising model. Excitation spectrum



- Remarkable accuracy for critical system
- Wrong spectrum for gapped system
- promising results for multi-site DMRG Banuls et al, in prep

NC, F. Mila, Phys. Rev. B 96, 054425'17

Conformally invariant boundary conditions

Ising critical theory:

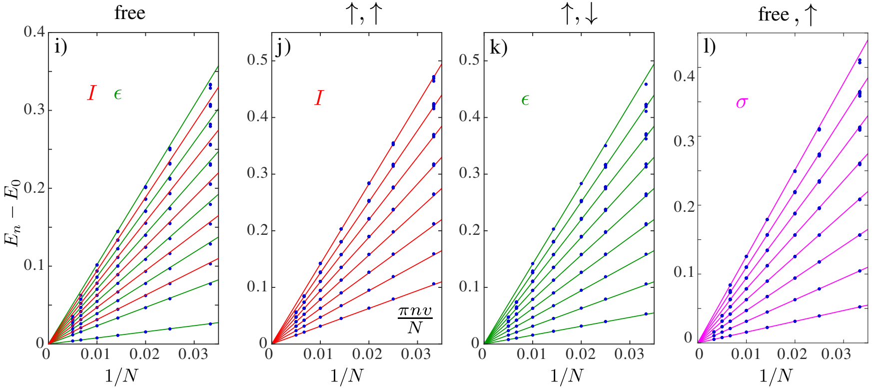
- Free
- Fixed= $\{\uparrow, \downarrow\}$

Two boundaries - 4 combinations:

- Free-Free $\mathbb{I} + \varepsilon$
- $\uparrow, \uparrow$ $\mathbb{I}$ $\chi_I(q) = q^{-1/48}\left(1 + q^2 + q^3 + 2q^4 + 2q^5 + 3q^6 + 3q^7 + \ldots\right)$
- $\uparrow, \downarrow$ ε $\chi_\epsilon(q) = q^{1/2-1/48}\left(1 + q + q^2 + q^3 + 2q^4 + 2q^5 + 3q^6 + 4q^7 + \ldots\right)$
- Free,$\uparrow$ σ $\chi_\sigma = q^{1/16-1/48}\left(1 + q + q^2 + 2q^3 + 2q^4 + 3q^5 + 4q^6 + 5q^7 + \ldots\right)$

BCFT prediction: Cardy, Nuc. Phys. B, **324** 581-596, 1989

Finite-size scaling of the excitation energy



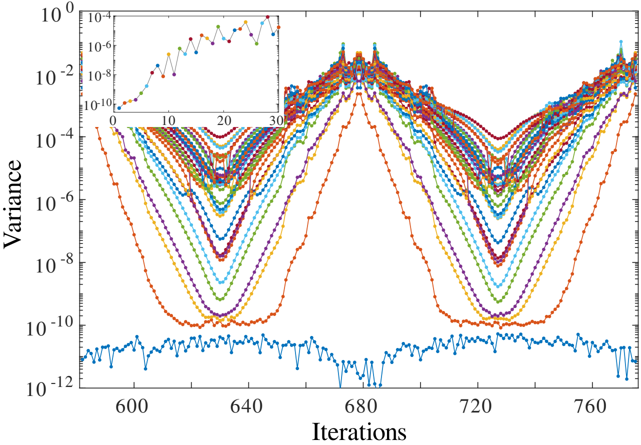
$$\chi_I(q) = q^{-1/48}\left(1 + q^2 + q^3 + 2q^4 + 2q^5 + 3q^6 + 3q^7 + 5q^8\right)$$

$$\chi_\epsilon(q) = q^{1/2-1/48}\left(1 + q + q^2 + q^3 + 2q^4 + 2q^5 + 3q^6 + 4q^7 + 5q^8\right)$$

$$\chi_\sigma = q^{1/16-1/48}\left(1 + q + q^2 + 2q^3 + 2q^4 + 3q^5 + 4q^6 + 5q^7 + 6q^8 + \dots\right)$$

- BCFT prediction: Cardy, Nuc. Phys. B, **324** 581-596'89
- DMRG results: NC, Mila, Phys. Rev. B **96**, 054425'17

States are also good!



NC, Mila, Phys. Rev. B **96**, 054425'17

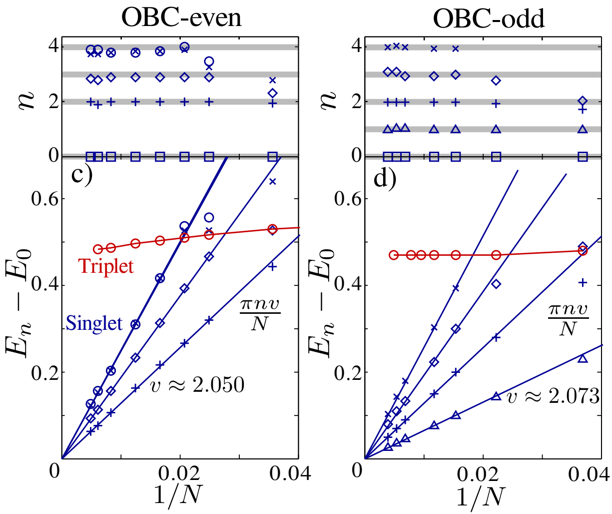
Not only for the simplest models:

Ising transition in spin-1 chain

$$H_{J_1 J_2 J_3} = J_1 \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1} + J_2 \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+2} + J_3 \sum_j \left[(\mathbf{S}_j \cdot \mathbf{S}_{j+1})(\mathbf{S}_{j+1} \cdot \mathbf{S}_{j+2}) + \text{h.c.} \right]$$

NC, Affleck, Mila, Phys. Rev. B **93** 241108, 2016

Ising conformal towers in spin-1 chain



- Singlet-triplet gap is **open**
- Critical scaling of the gap in the singlet sector
- N **even**
  I conformal tower
- N **odd**
  ϵ conformal tower

NC, Affleck, Mila, PRB **93**, 241108'16

There is a reason why it works for CFT

Extracting the Speed of Light from Matrix Product States

arXiv:2303.00663v1 [cond-mat.str-el] 1 Mar 2023

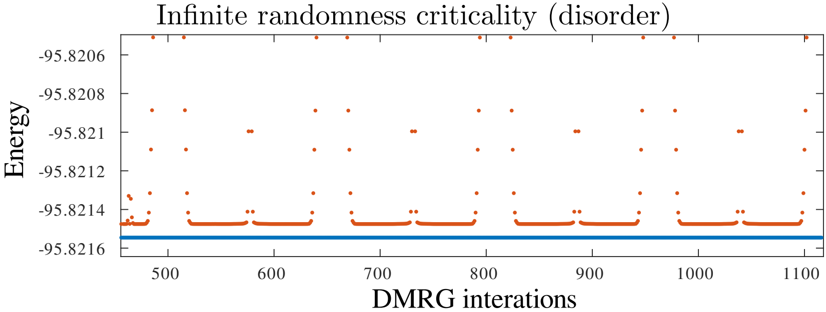
Alexander A. Eberharter,[1] Laurens Vanderstraeten,[2] Frank Verstraete,[2] and Andreas M. Läuchli[3,4]

[1]Institut für Theoretische Physik, Universität Innsbruck, A-6020 Innsbruck, Austria
[2]Department of Physics and Astronomy, University of Ghent, Belgium
[3]Laboratory for Theoretical and Computational Physics, Paul Scherrer Institute, 5232 Villigen, Switzerland
[4]Institute of Physics, École Polytechnique Fédérale de Lausanne (EPFL), 1015 Lausanne, Switzerland

(Dated: March 2, 2023)

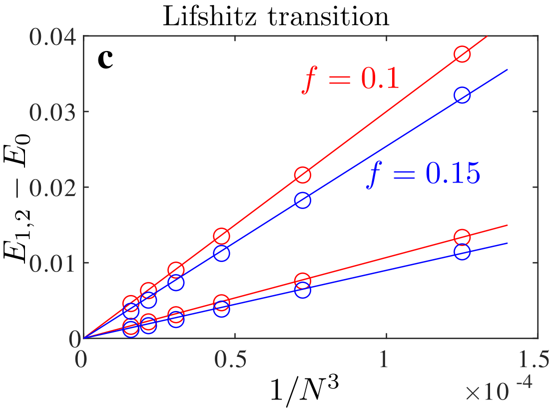
We provide evidence that the spectrum of the local effective Hamiltonian and the transfer operator in inf nite-system matrix product state simulations are identical up to a global rescaling factor, i.e. the speed of light of the system, when the underlying system is described by a 1+1 dimensional CFT. We provide arguments for this correspondence based on a path integral point of view. This observation turns out to yield very precise estimates for the speed of light in practice, conf rming exact results to high precision where available, but also allowing us to f nally determine the speed of light of the non-integrable, critical SU(2) Heisenberg chains with half-

But it also works for non-CFT



accuracy about 10^{-8}

But it also works for non-CFT



Dynamical critical exponent $z = 3$.

Time evolution

Time evolution: real and imaginary

The goal is to compute action operators:

$$e^{-iHt} \quad \text{and} \quad e^{-\beta H}$$

First-order Trotter decomposition

$$\mathrm{e}^{-\mathrm{i}\hat{H}\tau} = \mathrm{e}^{-\mathrm{i}\hat{h}_1\tau}\mathrm{e}^{-\mathrm{i}\hat{h}_2\tau}\mathrm{e}^{-\mathrm{i}\hat{h}_3\tau}\ldots\mathrm{e}^{-\mathrm{i}\hat{h}_{L-3}\tau}\mathrm{e}^{-\mathrm{i}\hat{h}_{L-2}\tau}\mathrm{e}^{-\mathrm{i}\hat{h}_{L-1}\tau} + O(\tau^2),$$

Second-order Trotter decomposition - better accuracy at no cost

$$\mathrm{e}^{-\mathrm{i}\hat{H}\tau} = \mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{odd}}\tau/2}\mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{even}}\tau}\mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{odd}}\tau/2} + O(\tau^3),$$

Time evolution: real and imaginary

The goal is to compute action operators:

$$e^{-iHt} \quad \text{and} \quad e^{-\beta H}$$

First-order Trotter decomposition

$$\mathrm{e}^{-\mathrm{i}\hat{H}\tau} = \mathrm{e}^{-\mathrm{i}\hat{h}_1\tau}\mathrm{e}^{-\mathrm{i}\hat{h}_2\tau}\mathrm{e}^{-\mathrm{i}\hat{h}_3\tau}\dots\mathrm{e}^{-\mathrm{i}\hat{h}_{L-3}\tau}\mathrm{e}^{-\mathrm{i}\hat{h}_{L-2}\tau}\mathrm{e}^{-\mathrm{i}\hat{h}_{L-1}\tau} + O(\tau^2),$$

Second-order Trotter decomposition - better accuracy at no cost

$$\mathrm{e}^{-\mathrm{i}\hat{H}\tau} = \mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{odd}}\tau/2}\mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{even}}\tau}\mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{odd}}\tau/2} + O(\tau^3),$$

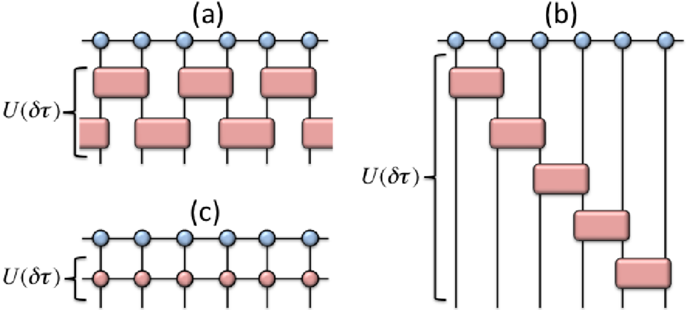
For very long i-times quantum state approaches the ground-state:

$$|E_0\rangle = \lim_{\tau\to\infty} \frac{e^{-\tau H}|\Psi(0)\rangle}{\sqrt{|\langle\Psi(\tau)|\Psi(\tau)\rangle|}} \qquad |\Psi(\tau)\rangle = e^{-\tau H}|\Psi(0)\rangle$$

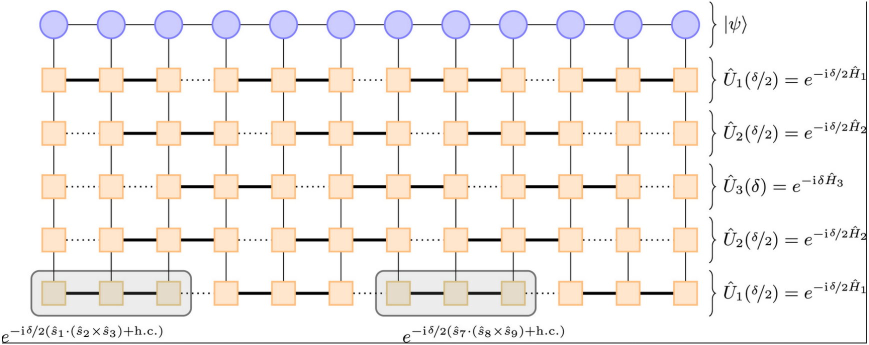
Time evolution: various ways to apply

Second-order Trotter decomposition - better accuracy at no cost

$$e^{-i\hat{H}\tau} = e^{-i\hat{H}_{\text{odd}}\tau/2} e^{-i\hat{H}_{\text{even}}\tau} e^{-i\hat{H}_{\text{odd}}\tau/2} + O(\tau^3),$$



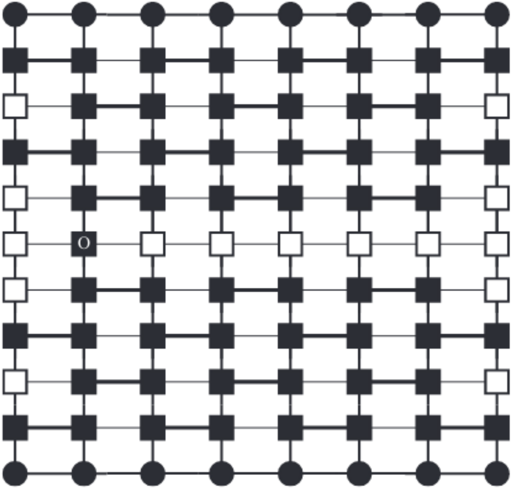
Time evolution: longer-range terms



One can also use swap-gates, but keep an eye on a complexity!

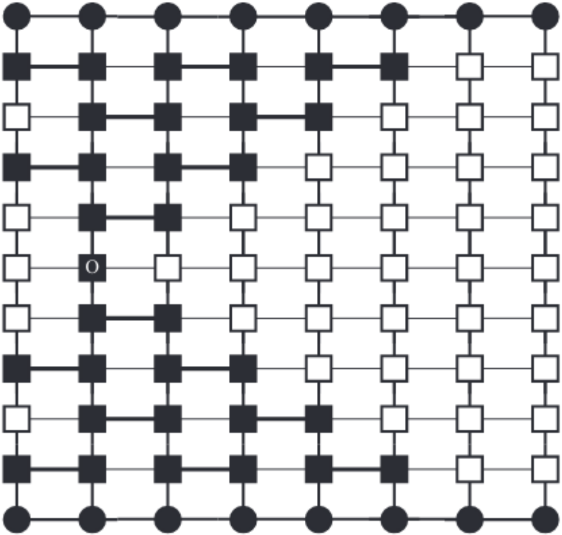
For truly long-range order - TDVP

Extracting observables



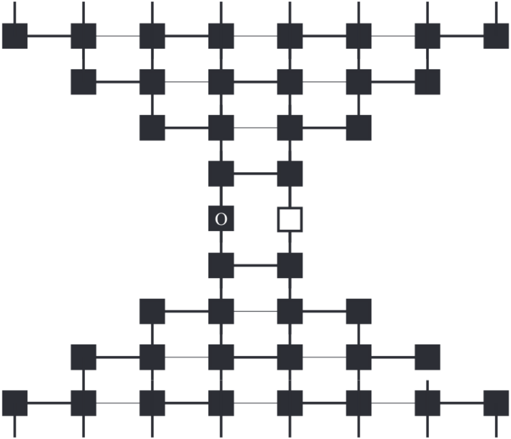
Schollwoeck, Annals of Physics 326, 96 (2011)

Extracting observables



Schollwoeck, Annals of Physics 326, 96 (2011)

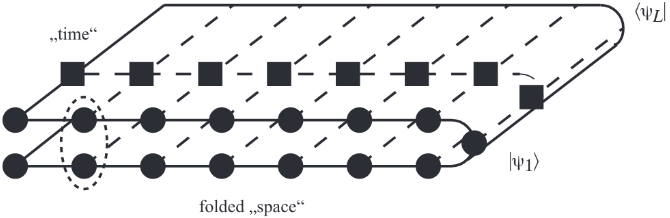
Light cone



Schollwoeck, Annals of Physics 326, 96 (2011)

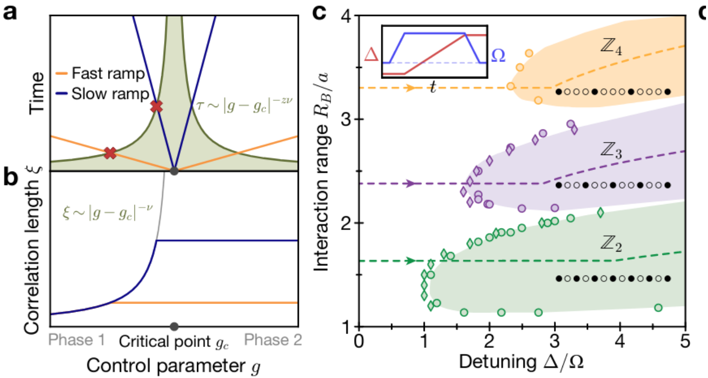
Folding

folding of forward and backward timesteps leads to some cancellations in entanglement



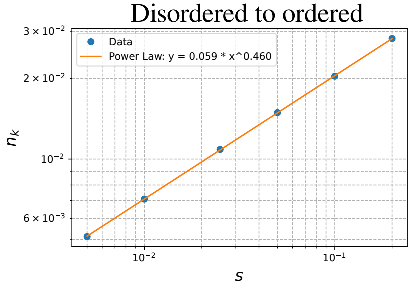
Schollwoeck, Annals of Physics 326, 96 (2011)

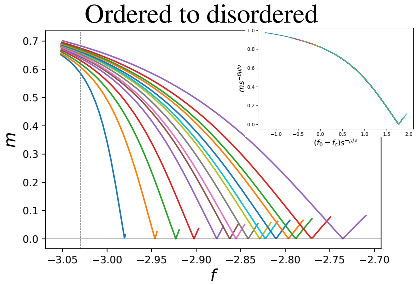
Motivation: Rydberg experiments



Probe quantum phase transitions with Kibble-Zurek mechanism:
The faster you sweep the more domain walls you end up with

Kibble-Zurek and Finite-time scaling

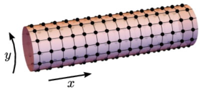


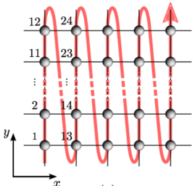


Kibble-Zurek mechanism:
The faster you sweep the more domain walls you end up with

Finite-time scaling:
The slower you sweep the latter the order parameter will vanish

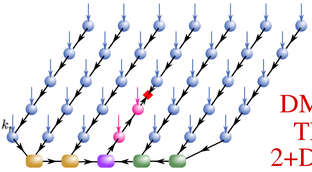
2D-DMRG



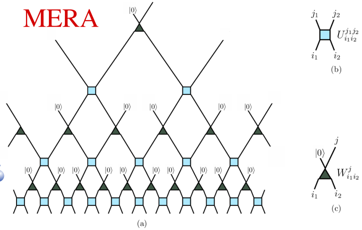


(a)

Y-DMRG
Comb / Fork DMRG
Tree tensor networks

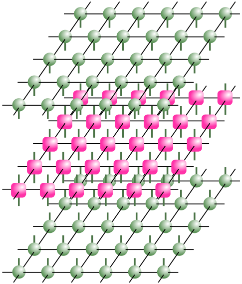


MERA

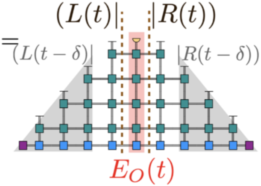


DMRG-X
TDVP
2+D iPEPS

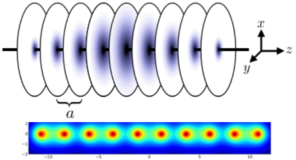
2D iPEPS

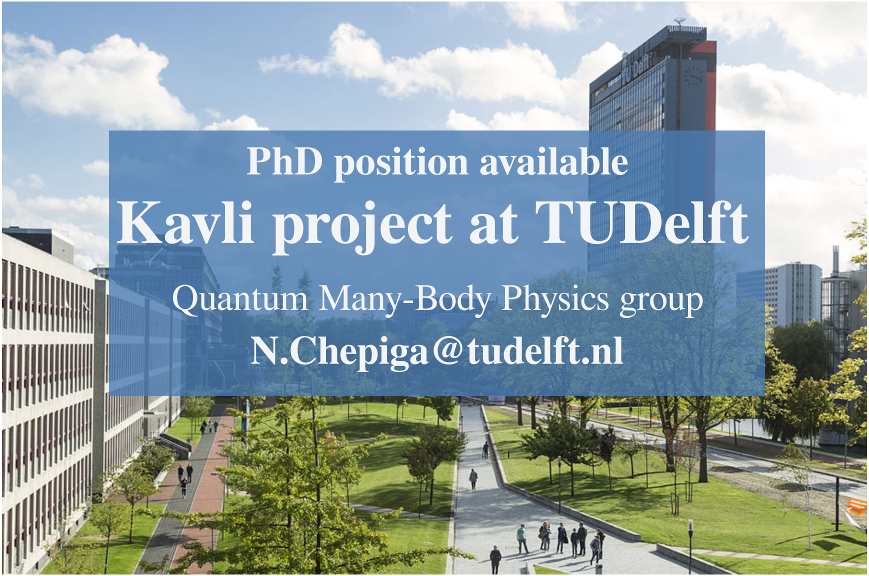


Light-cone TN



Sliced DMRG
Gausslets




PhD position available
Kavli project at TUDelft
Quantum Many-Body Physics group
N.Chepiga@tudelft.nl