Matrix Product States
for frustrated spin chains, lattices with an extended Hilbert space and constrained models in 1D

Natalia Chepiga

Swiss National Science Foundation
University of Amsterdam, The Netherlands

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Scope

- Basics of DMRG
  - Area law
  - Graphical notations
  - MPO construction
  - Variational optimization (finite- and infinite-size DMRG)
  - Abelian symmetry
- Spin-1 chain with three-site interactions
  - Phase diagram
  - Excitation spectrum and DMRG iterations. Conformal towers
- Comb tensor networks
  - Tree tensor network
- DMRG investigation of a hard-boson model of Rydberg atoms
  - Implementing local constraint into DMRG
  - Floating phase versus chiral transition

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.

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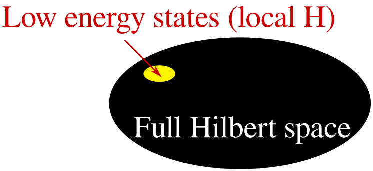
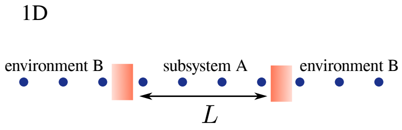
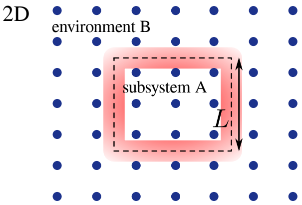
Area law for the entanglement entropy



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: $S_A(L) \propto L$

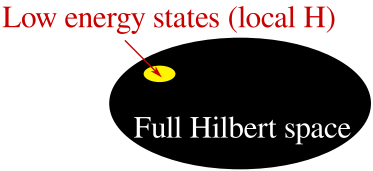
Random state

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

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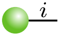
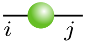
Graphical notations

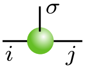
C Number



A_i Vector

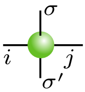


$A_{i,j}$ Matrix



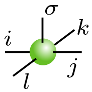
$A^{\sigma}_{i,j}$

rank-3 tensor (MPS)



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

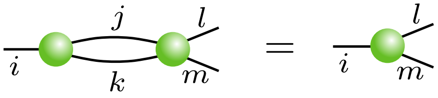
rank-4 tensor (MPO)



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

rank-5 tensor (PEPS)

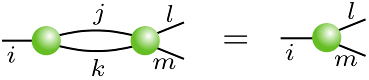
Contraction



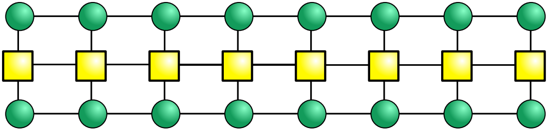
$$\sum_{j,k} A_{i,j,k} \; B_{j,k,l,m} = T_{i,l,m}$$

- Summation over connected bonds
- In practice: reshape tensors into matrices and use optimized matrix multipliers
- 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!



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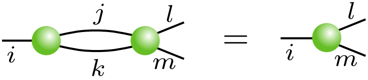

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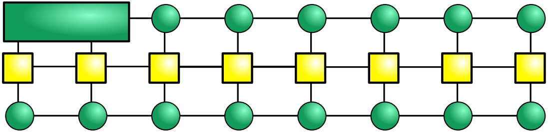

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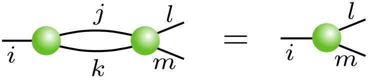

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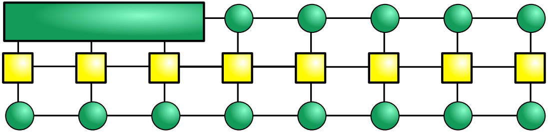

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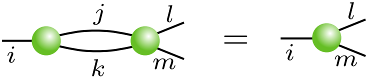

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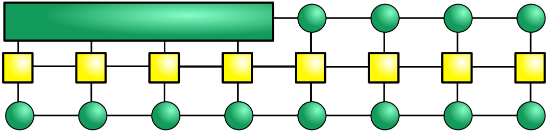

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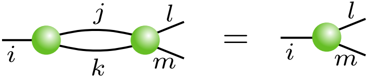

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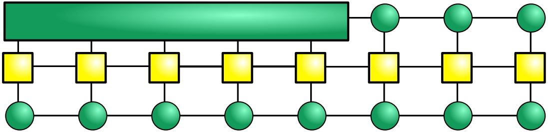
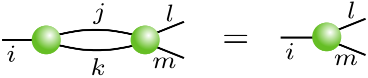


Exponential growth of complexity!

Contraction



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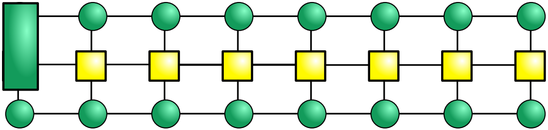

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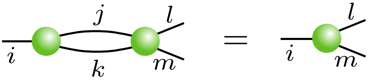

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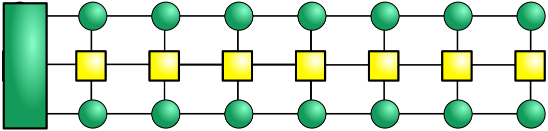

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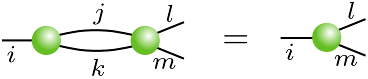

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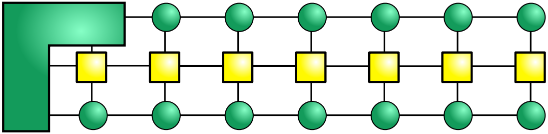

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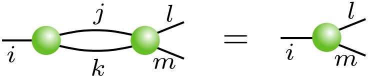

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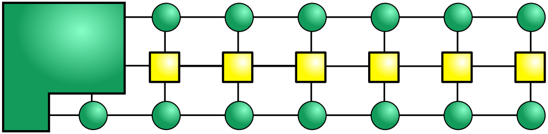

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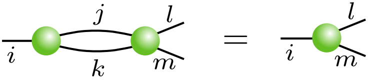

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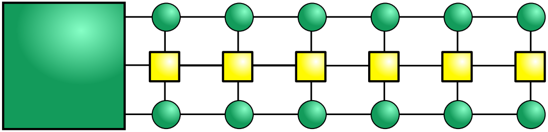

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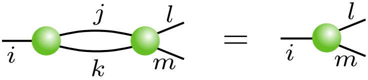

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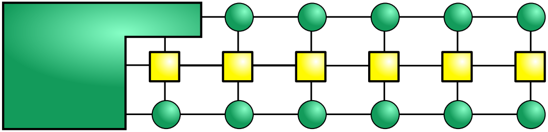

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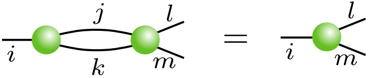

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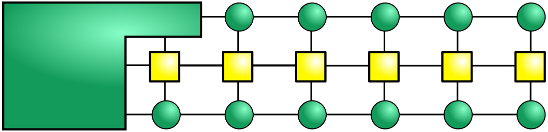

Complexity stays finite!

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:

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  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

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

Bring quantum states into MPS

$|\psi\rangle =$ 

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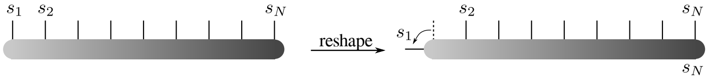
$|\psi\rangle =$ 

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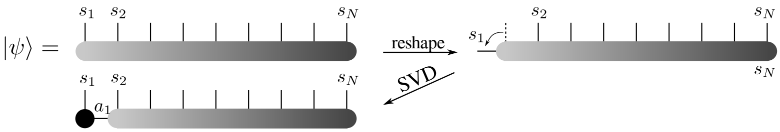

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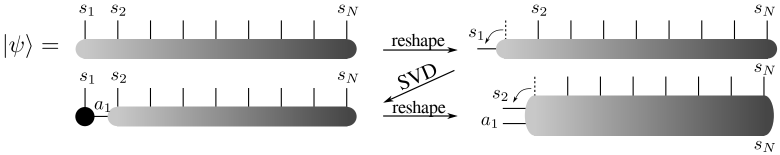

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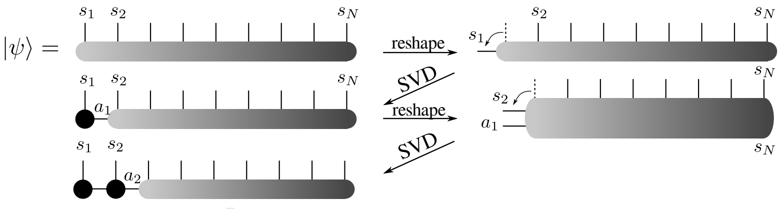

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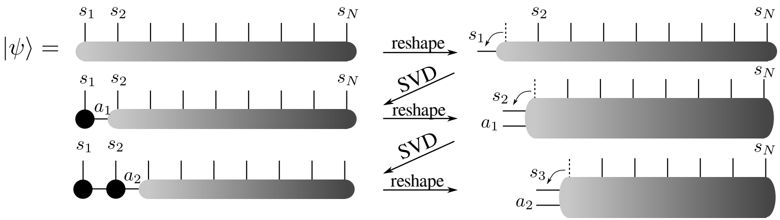

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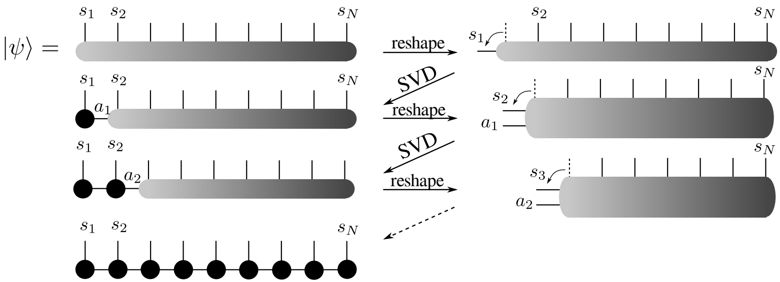

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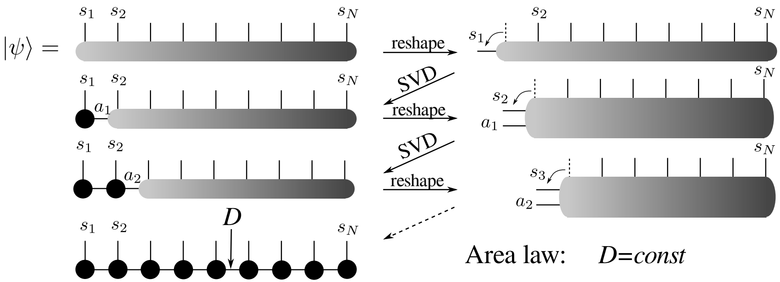
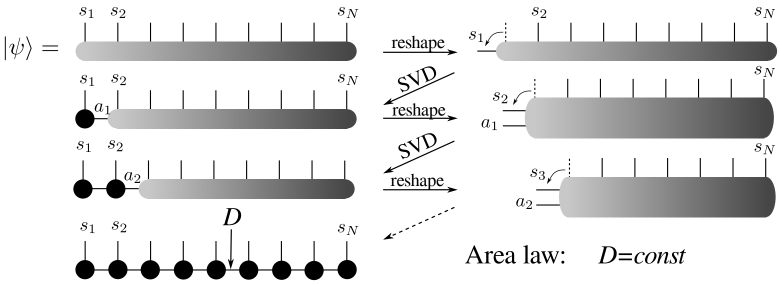


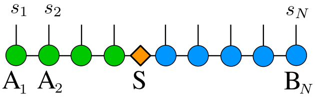
Area law: D=*const*

Bring quantum states into MPS



Area law: *D=const*

Mixed-canonical form



Normalization:

Normalization

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

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

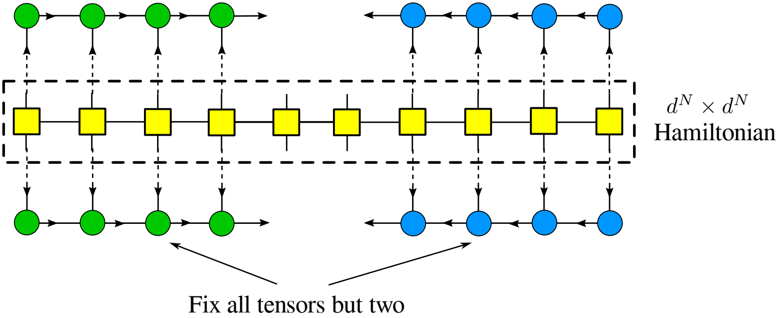
If norm is fixed $\langle\Psi|\Psi\rangle = 1$, it becomes

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

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

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

Variational optimization of the MPS



MPO

Full Hamiltonian as a product of local tensors

MPO construction

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

Transverse field Ising model: $H = \sum J S_i^x S_{i+1}^x + \sum h S_i^z$

$$
\begin{array}{l|c|r}
I...I & hS_j^z & I...I \\
I...IJS_{j-1}^x & S_j^x & I...I \\
I...I & JS_j^x & S_{j+1}^x I...I \\
I...JS_i^x S_{i+1}^x...I & I & I...I \\
I...hS_i^z...I & I & I...I \\
I...I & I & I...JS_i^x S_{i+1}^x...I \\
I...I & I & I...hS_i^z...I
\end{array}
$$

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I...IJS_{j-1}^x & S_j^x & I...I \\
I...I & JS_j^x & S_{j+1}^x I...I \\
I...JS_i^x S_{i+1}^x...I & I & I...I \\
I...hS_i^z...I & I & I...I \\
I...I & I & I...JS_i^x S_{i+1}^x...I \\
I...I & I & I...hS_i^z...I
\end{array}
$$

MPO construction

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$$
\begin{array}{l|c|r}
I ... I & hS_j^z & I ... I \\
I ... I J S_{j-1}^x & S_j^x & I ... I \\
I ... I & J S_j^x & S_{j+1}^x I ... I \\
I ... \text{Full} ... I & I & I ... I \\
I ... I & I & I ... \text{Full} ... I
\end{array}
$$

- Five non-trivial entries in the MPO

MPO construction

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

  Transverse field Ising model: $H = \sum J S_i^x S_{i+1}^x + \sum h S_i^z$

$$\begin{array}{l|c|r} I \ldots I & h S_j^z & I \ldots I \\ I \ldots I J S_{j-1}^x & S_j^x & I \ldots I \\ I \ldots I & J S_j^x & S_{j+1}^x I \ldots I \\ I \ldots \text{Full} \ldots I & I & I \ldots I \\ I \ldots I & I & I \ldots \text{Full} \ldots I \end{array}$$

- Five non-trivial 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:
- Five non-trivial entries in the MPO
- Look at the left and right basis in which the MPO is going to be written

$$
\begin{array}{l|lll}
I \ldots \mathrm{Full} \ldots I & & & \\
I \ldots I J S^x_{j-1} & & & \\
I \ldots I & & & \\
\hline
 & I \ldots I & S^x_{j+1} I \ldots I & I \ldots \mathrm{Full} \ldots I
\end{array}
$$

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:

$$
\begin{array}{l|ccc}
I...\text{Full}...I & I & 0 & 0 \\
I...IJS^x_{j-1} & S^x_j & 0 & 0 \\
I...I & hS^z_j & JS^x_j & I \\
\hline
 & I...I & S^x_{j+1}I...I & I...\text{Full}...I
\end{array}
$$

MPO exercise:

- Heisenberg nearest-neighbor:

$$H = J \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$
$$= J \sum_j \frac{1}{2} \left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+ \right) + S_j^z S_{j+1}^z \quad (1)$$

- $J_1 - J_2$ model:

$$H_{J_1-J_2} = J_1 \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1} + J_2 \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+2} \quad (2)$$

- Three-site interaction:

$$H = H_{J_1-J_2} + J_3 \sum_j \left[(\mathbf{S}_j \cdot \mathbf{S}_{j+1})(\mathbf{S}_{j+1} \cdot \mathbf{S}_{j+2}) + \text{h.c.} \right] \quad (3)$$

MPO answers:

- Heisenberg nearest-neighbor:

$$H = J \sum_j \frac{1}{2}\left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right) + S_j^z S_{j+1}^z \tag{4}$$

$$H_j = \begin{pmatrix} I & . & . & . & \\ S_j^- & . & . & . & \\ S_j^+ & . & . & . & \\ S_j^z & . & . & . & \\ . & \frac{J}{2}S_j^+ & \frac{J}{2}S_j^- & JS_j^z & I \end{pmatrix}$$

MPO answers:

- $J_1 - J_2$ model:

$$H_{J_1-J_2} = J_1 \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1} + J_2 \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+2} \tag{5}$$

$$H_j = \begin{pmatrix} I & . & . & . & . & . & . & \\ S_j^- & . & . & . & . & . & . & \\ S_j^+ & . & . & . & . & . & . & \\ S_j^z & . & . & . & . & . & . & \\ . & I & . & . & . & . & . & \\ . & . & I & . & . & . & . & \\ . & . & . & I & . & . & . & \\ . & \frac{J_1}{2}S_j^+ & \frac{J_1}{2}S_j^- & J_1 S_j^z & \frac{J_2}{2}S_j^+ & \frac{J_2}{2}S_j^- & J_2 S_j^z & I \end{pmatrix}$$

MPO answers:

- Three-site interaction:

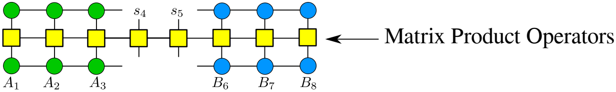
$$H = H_{J_1 - J_2} + J_3 \sum_j [(\mathbf{S}_j \cdot \mathbf{S}_{j+1})(\mathbf{S}_{j+1} \cdot \mathbf{S}_{j+2}) + \text{h.c.}] \qquad (6)$$

$$H_i = \begin{pmatrix} I & . & . & . & . & . & . & \\ S_i^- & . & . & . & . & . & . & \\ S_i^+ & . & . & . & . & . & . & \\ S_i^z & . & . & . & . & . & . & \\ . & \frac{J_2}{2} I + J_3 Q^{+-} & J_3 Q^{--} & J_3 Q^{-z} & . & . & . & \\ . & J_3 Q^{++} & \frac{J_2}{2} I + J_3 Q^{+-} & J_3 Q^{+z} & . & . & . & \\ . & J_3 Q^{+z} & J_3 Q^{-z} & J_2 I + J_3 Q^{zz} & . & . & . & \\ . & \frac{J_1}{2} S_i^+ & \frac{J_1}{2} S_i^- & J_1 S_i^z & S_i^+ & S_i^- & S_i^z & I \end{pmatrix},$$

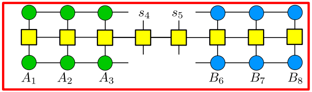
where $Q_i^{\alpha\beta} = S_i^\alpha S_i^\beta + S_i^\beta S_i^\alpha$ with $S^\alpha = \{\frac{S^+}{\sqrt{2}}, \frac{S^-}{\sqrt{2}}, S^z\}$

DMRG / variational MPS

DMRG sweep



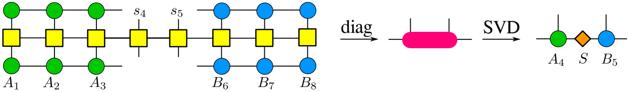
DMRG sweep



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

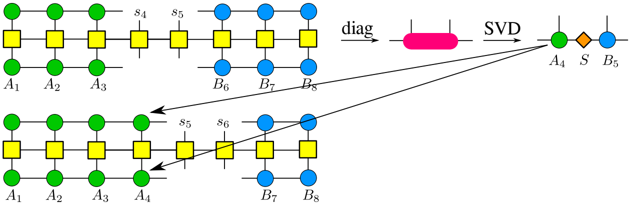
DMRG sweep

Left-to-right:



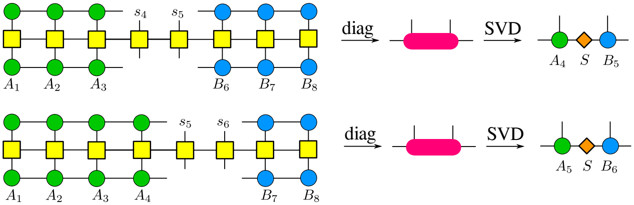
DMRG sweep

Left-to-right:



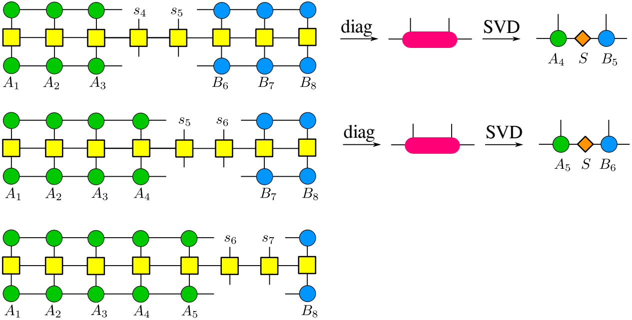
DMRG sweep

Left-to-right:



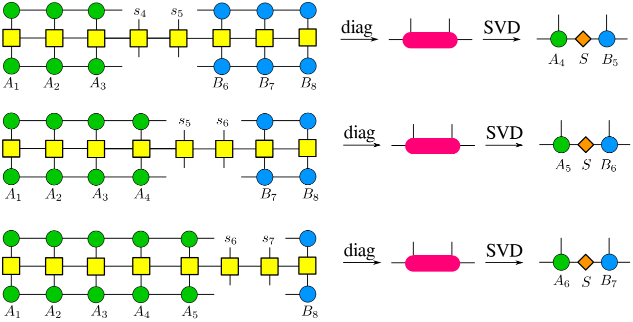
DMRG sweep

Left-to-right:



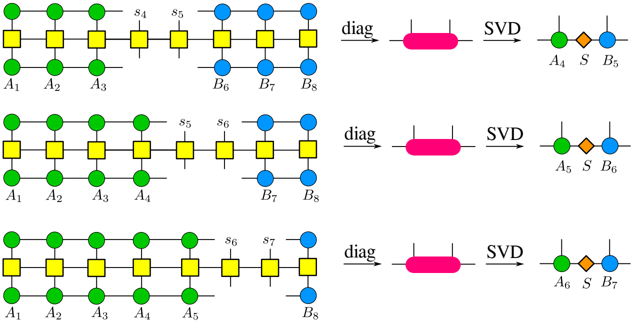
DMRG sweep

Left-to-right:

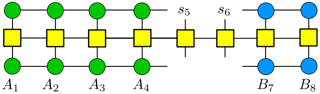


DMRG sweep

Left-to-right:

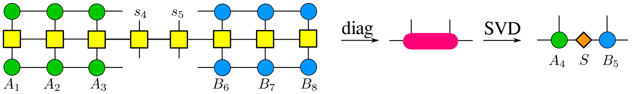


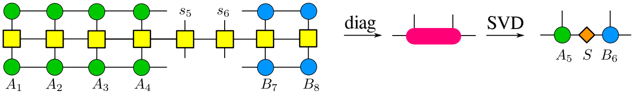
Right-to-left:

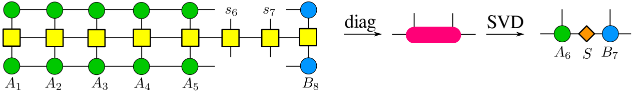


DMRG sweep

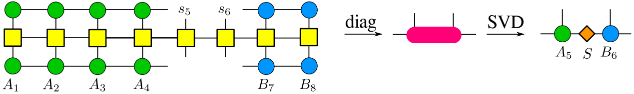
Left-to-right:





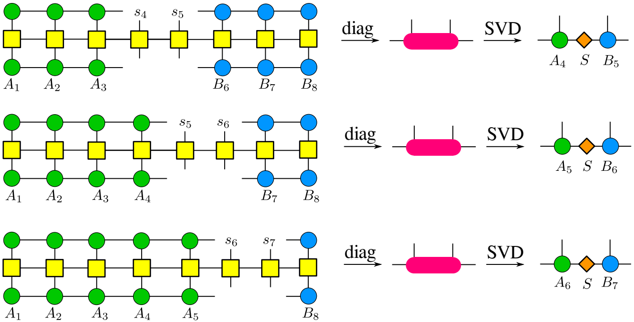


Right-to-left:

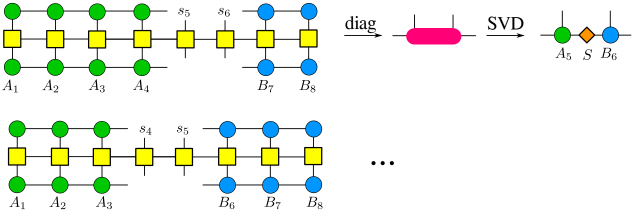


DMRG sweep

Left-to-right:



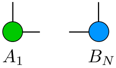
Right-to-left:

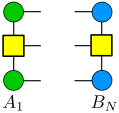


Initial guess

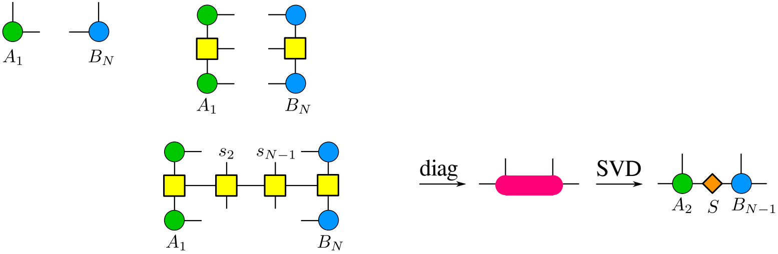
- Product state
- Random state
- Infinite-size DMRG

Infinite-size DMRG

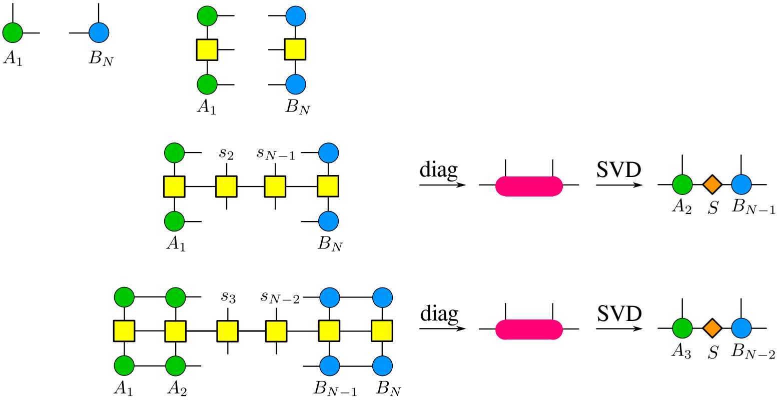




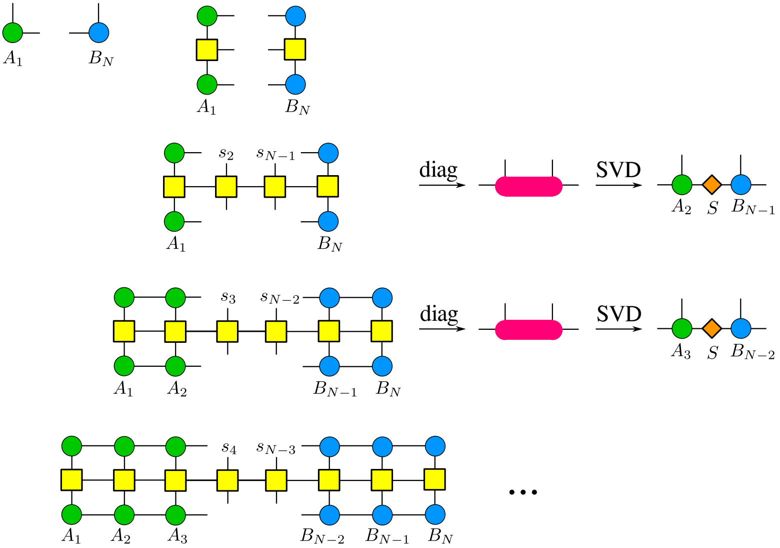
Infinite-size DMRG



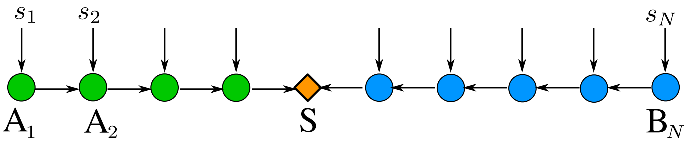
Infinite-size DMRG



Infinite-size DMRG

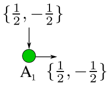


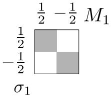
Abelian symmetry



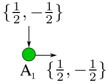
- Assign quantum numbers - labels to physical bonds of MPS
- Using fusion rules of the symmetry, find quantum numbers on auxiliary legs
- When local basis is sorted according to the quantum number of states, the MPS takes a block-diagonal form

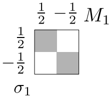
Abelian symmetry. Examples

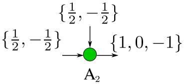


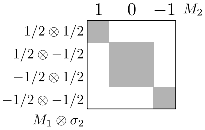


Abelian symmetry. Examples

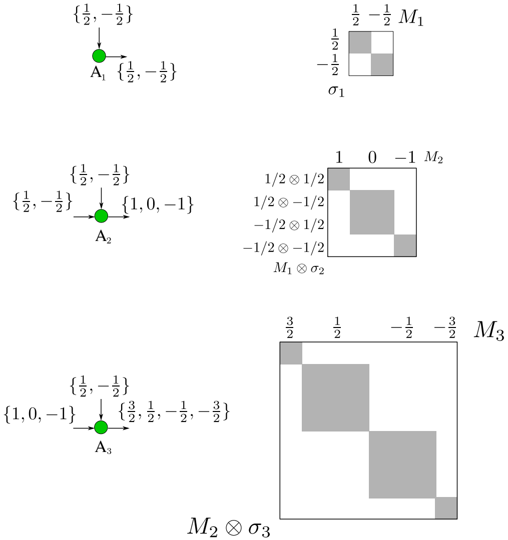








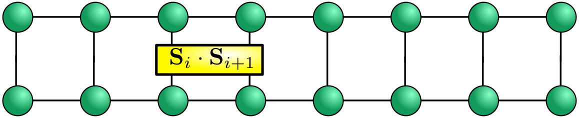
Abelian symmetry. Examples



Observables

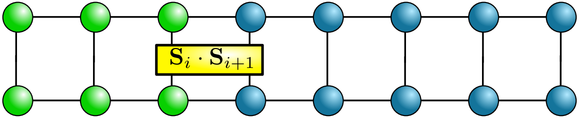
Observables

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



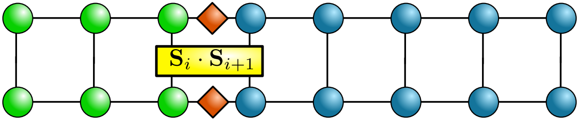
Observables

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



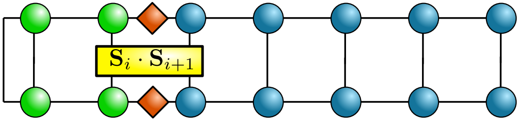
Observables

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



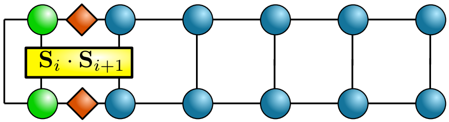
Observables

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



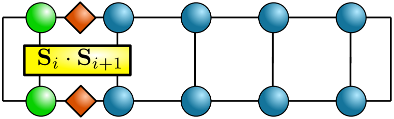
Observables

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



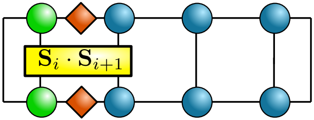
Observables

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



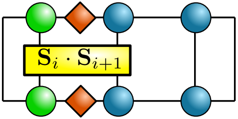
Observables

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



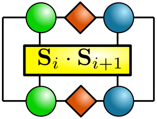
Observables

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



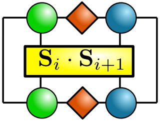
Observables

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

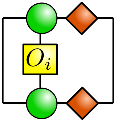


Observables

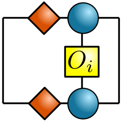
Nearest-neighbor correlations $\langle \Psi | \mathbf{S}_i \cdot \mathbf{S}_{i+1} | \Psi \rangle$



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

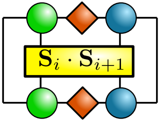


or

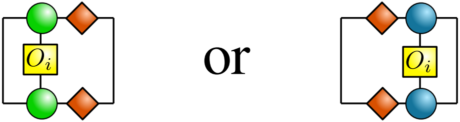


Observables

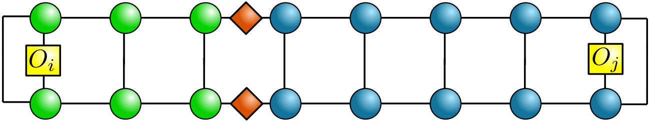
Nearest-neighbor correlations $\langle\Psi|\mathbf{S}_i \cdot \mathbf{S}_{i+1}|\Psi\rangle$



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



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



Dimerization transition in frustrated spin-1 chain

in collaboration with

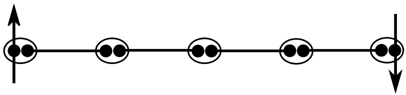
Frederic Mila (EPFL) and Ian Affleck (UBC)

Spin chains

Heisenberg Hamiltonian:

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

- Spin-1/2 chain is critical
- Spin-1 chain:
  - finite bulk gap
  - topologically non-trivial ground state
  - spin-1/2 edge states

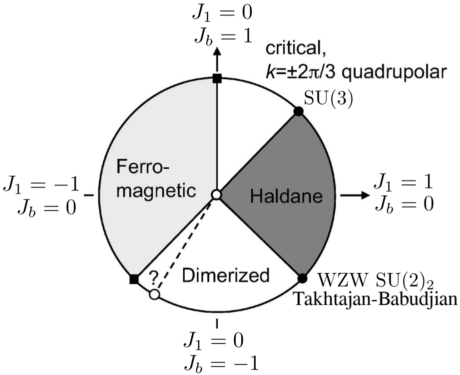


- Haldane, Phys. Lett. A **93**, 464 '83
- Affleck, Kennedy, Lieb, Tasaki, PRL **59**, 799 '87
- Kennedy J. Phys: Cond. Mat **2**, 5737 '90

Introduction

Add biquadratic interaction:

$$H = \sum_i J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_b (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$$



Critical spin-1 chains:

- WZW SU(2)$_2$
- SU(3)

- Affleck, Nucl.Phys.B **265**, 409 '86
- Fáth, Sólyom, PRB **44**,11836 '91
- Schollwöck, Jolicœur, Garel, PRB **53**, 3304 '96
- Läuchli, Schmid, Trebst, PRB **74**, 144426 '06

The model

Hamiltonian:

$$H = \sum_i (J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_{i-1} \cdot \mathbf{S}_{i+1}) + \sum_i J_3 \left[(\mathbf{S}_{i-1} \cdot \mathbf{S}_i)(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \mathrm{H.c.} \right]$$

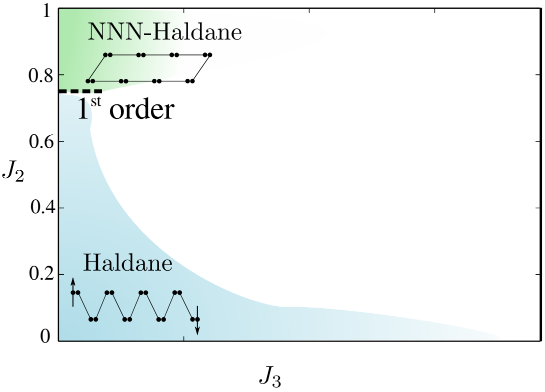
Three-site term:

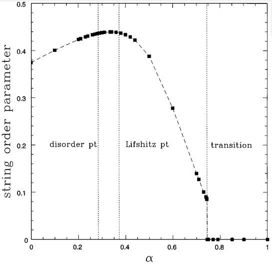
- Appears in next-to-leading order in the strong coupling expansion of the two-band Hubbard model
- Induces spontaneous dimerization
- Reduces to next-nearest-neighbor interaction for spin-1/2

Motivation

$$H = \sum_i (J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_{i-1} \cdot \mathbf{S}_{i+1})$$

$$+ \sum_i J_3 \left[(\mathbf{S}_{i-1} \cdot \mathbf{S}_i)(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \mathrm{H.c.} \right]$$





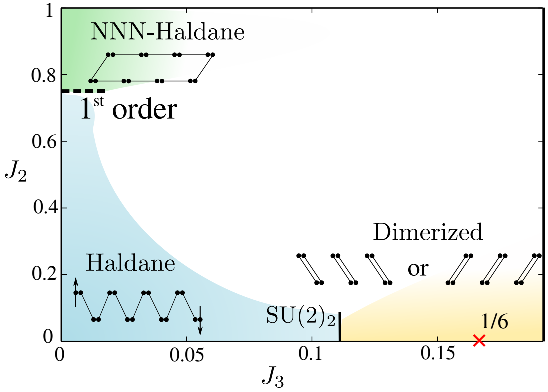
1^{st} order transition between two topologically different phases

- Kolezhuk, Roth, Scholwöck, PRL **77**, 5142 '96
- Kolezhuk, Scholwöck, PRB **65**, 100401 '01

Motivation

$$H = \sum_i (J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_{i-1} \cdot \mathbf{S}_{i+1})$$

$$+ \sum_i J_3 \left[(\mathbf{S}_{i-1} \cdot \mathbf{S}_i)(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \mathrm{H.c.} \right]$$



Generalization of the Majumdar-Ghosh model: fully dimerized state is an exact ground state at $J_3/J_1 = 1/6$

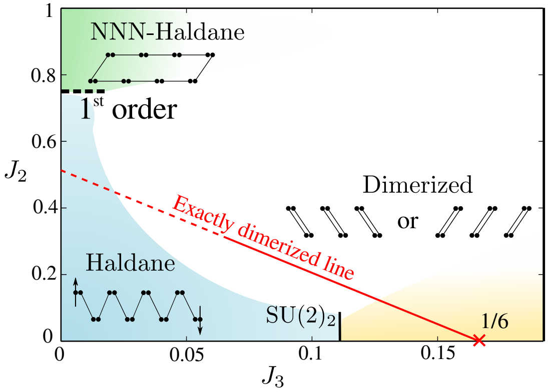
Continuous WZW $SU(2)_{k=2}$ transition at $J_3/J_1 = 0.111$

- Michaud, Vernay, Manmana, Mila, PRL **108**, 127202 '12

Motivation

$$H = \sum_i (J_1 \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_2 \mathbf{S}_{i-1} \cdot \mathbf{S}_{i+1})$$

$$+ \sum_i J_3 \left[(\mathbf{S}_{i-1} \cdot \mathbf{S}_i)(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \mathrm{H.c.} \right]$$

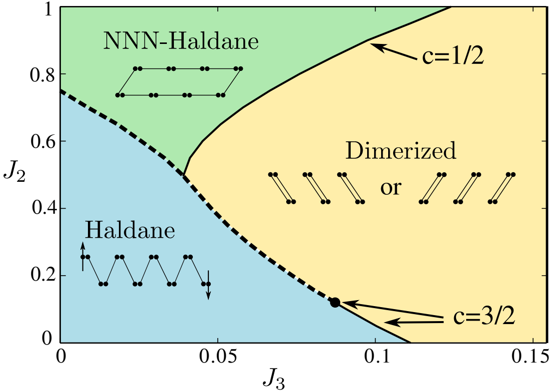


There is a line in $J_2 - J_3$ parameter space, at which the fully dimerized state is exact eigenstate

First order phase transition has to appear between the Haldane and dimerized phases

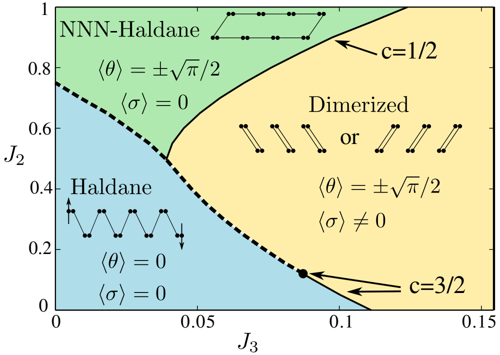
- Michaud, Vernay, Manmana, Mila, PRL **108**, 127202 '12
- Wang, Furuya, Nakamura, Komakura, PRB **88**, 224419'13

Phase diagram



- The transition between the Haldane and dimerized phases is **continuous WZW SU(2)$_2$** below and including at the end point
- The transition between the NNN-Haldane phase and the dimerized phase is in the **Ising universality class**
- Topological transition between the Haldane and NNN-Haldane phases is **always first order**

Phase diagram. Field theory



Effective Hamiltonian:

$$\mathcal{H} = \mathcal{H}_{\mathrm{WZW}} + \lambda_1(\mathrm{tr}g)^2 + \lambda_2 \vec{J}_R \cdot \vec{J}_L$$

- $\lambda_2 < 0$ Continuous $SU(2)_2$
- $\lambda_2 = 0$ End point
- $\lambda_2 > 0$ First order

Free boson and Ising fields:

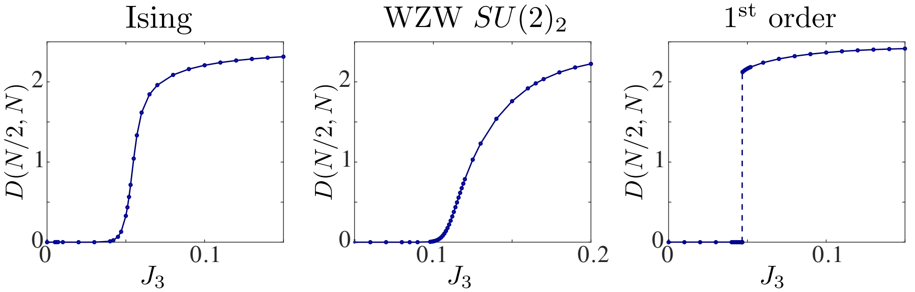
$$\mathrm{tr}g \propto \sigma \sin\sqrt{\pi}\theta$$
$$(\mathrm{tr}g)^2 \propto \epsilon - C_1 \cos\sqrt{4\pi}\theta$$
$$\vec{J}_L \cdot \vec{J}_R \propto \epsilon \cos\sqrt{4\pi}\theta + C_2 \partial_x\phi_L \partial_x\phi_R$$

Second order transition between the Haldane and dimerized phases occurs **simultaneously in Ising and boson sectors**. Far from the WZW critical end point the Ising and boson critical lines could split

Dimerization

Local dimerization:

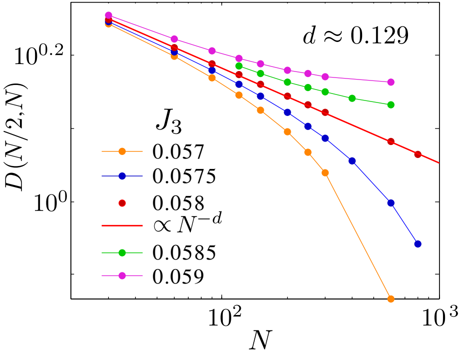
$$D(j, N) = |\langle \mathbf{S}_j \cdot \mathbf{S}_{j+1} \rangle - \langle \mathbf{S}_{j-1} \cdot \mathbf{S}_j \rangle|$$



Ising transition. Dimerization

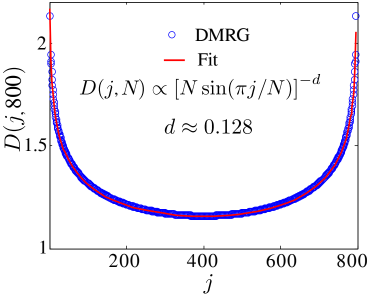
- Local dimerization: $D(j,N) = |\langle \mathbf{S}_j \cdot \mathbf{S}_{j+1} \rangle - \langle \mathbf{S}_{j-1} \cdot \mathbf{S}_j \rangle|$

- Finite-size scaling of the middle-chain dimerization in log-log scale
- The **separatrix** is associated with the phase transition
- The **slope** corresponds to the critical exponent
- Critical exponent in Ising chain: $\mathbf{d = 1/8}$



Ising transition. Dimerization

- Local dimerization: $D(j,N) = |\langle \mathbf{S}_j \cdot \mathbf{S}_{j+1}\rangle - \langle \mathbf{S}_{j-1} \cdot \mathbf{S}_j\rangle|$
- Open boundary favors dimerization
- In the transverse-field Ising chain it is equivalent to the applied **boundary magnetic field**
- At the critical point the magnetization decays away from the edges as $\sigma(x) \propto [N \sin(\pi j/N)]^{-1/8}$



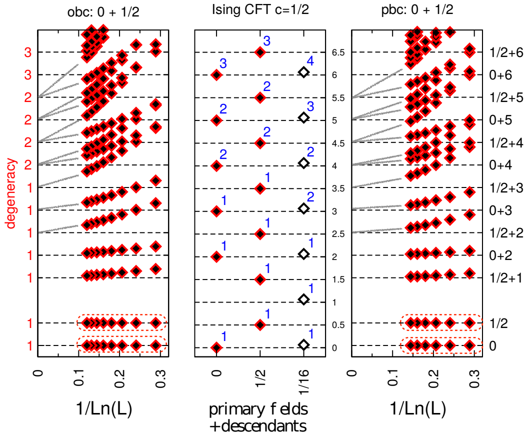
- In spin-1 chain the dimerization decays away from the boundaries in the same way and with the same **critical exponent**

Conformal towers = fingerprints of a critical theory

- Ising critical theory is minimal model of CFT
- It is described by a finite number of primary fields
- Combining boundary CFT with DMRG we can probe all of them numerically!

Conformal towers from entanglement spectrum

Transverse field Ising model:



A.Läuchli, arxiv:1303.0441

Energy excitation spectrum with DMRG

Excitation spectrum with DMRG/MPS

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

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 spoilt
   - Heavy memory usage

Excitation spectrum with DMRG/MPS

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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

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4. MPS: Domain wall or special tensor (see Laurens' talk)
   - Translation invariant MPS

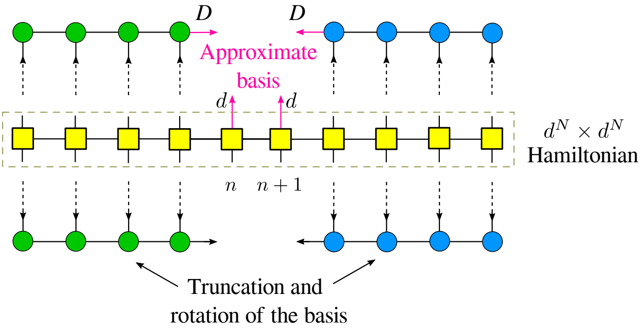
Excitation spectrum with DMRG/MPS

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 or special tensor (see Laurens' talk)
   - 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)]

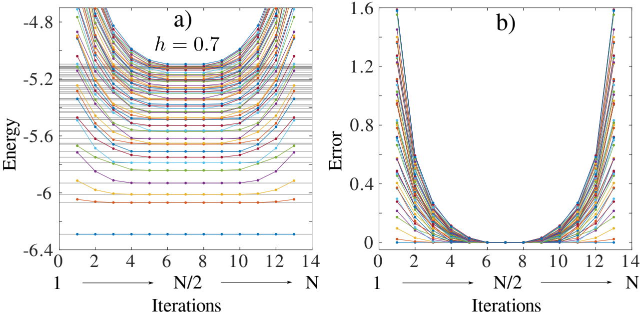
Effective Hamiltonian



- 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

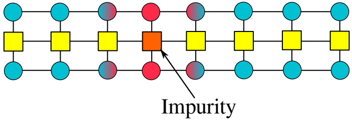
When no truncation is imposed and all basis states are kept in MPS, the DMRG is equivalent to exact diagonalization and one can access the entire spectrum!



When does it work?

Local impurities

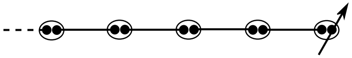
- Localized excitations
- MPS is the same except for a few sites



When does it work?

Edge states

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

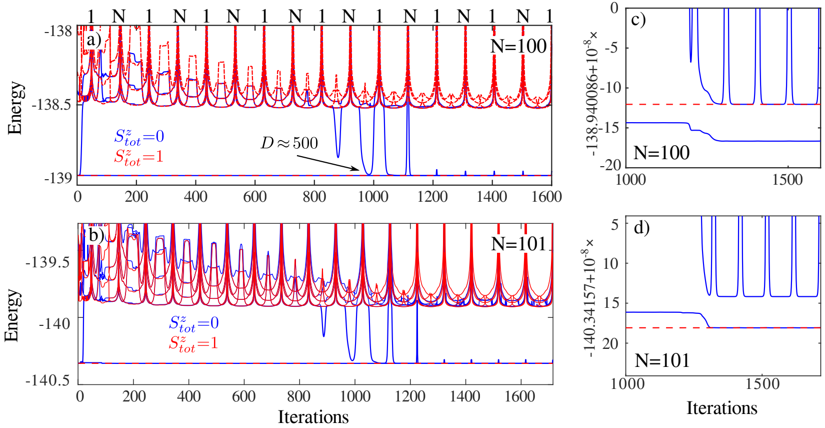


$$\left(\frac{B}{2} \otimes \uparrow\right) \oplus \left(\frac{B}{2} \otimes \downarrow\right)$$

Local impurities

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

Edge states in the Haldane chain



When does it work?

Critical systems

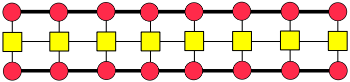
- Divergent correlation length
- Slow decay of Schmidt values
- Special structure of spectrum

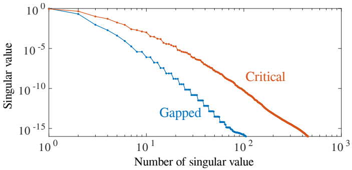
Edge states

- 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



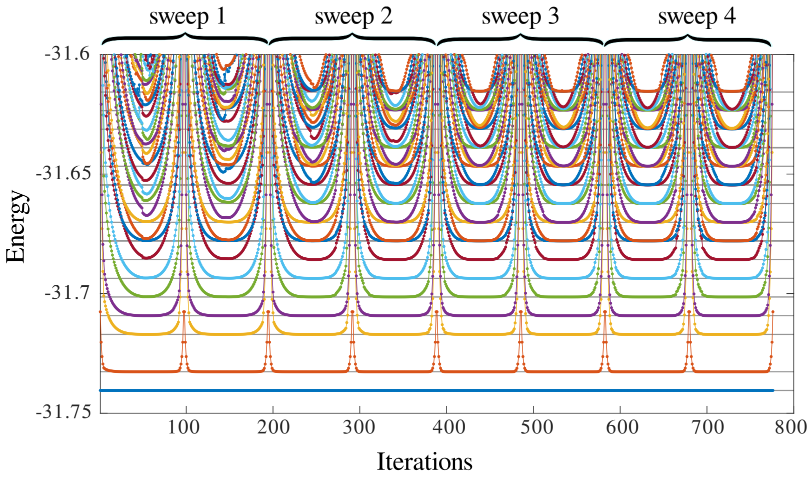


Transverse field Ising model

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

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

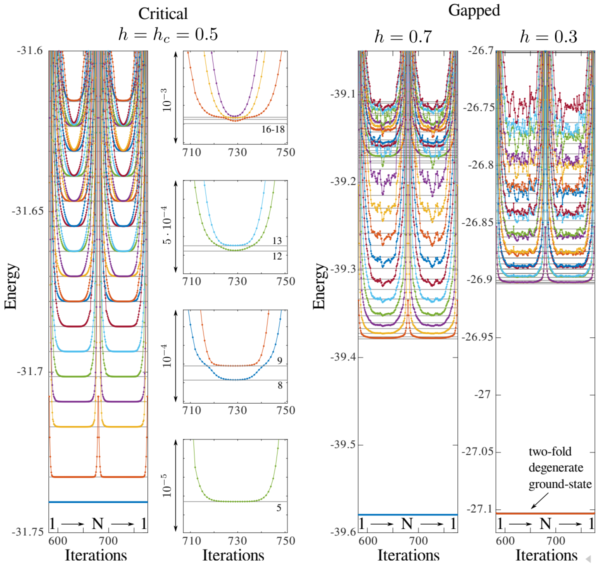
Transverse field Ising model. Excitation spectrum



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

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

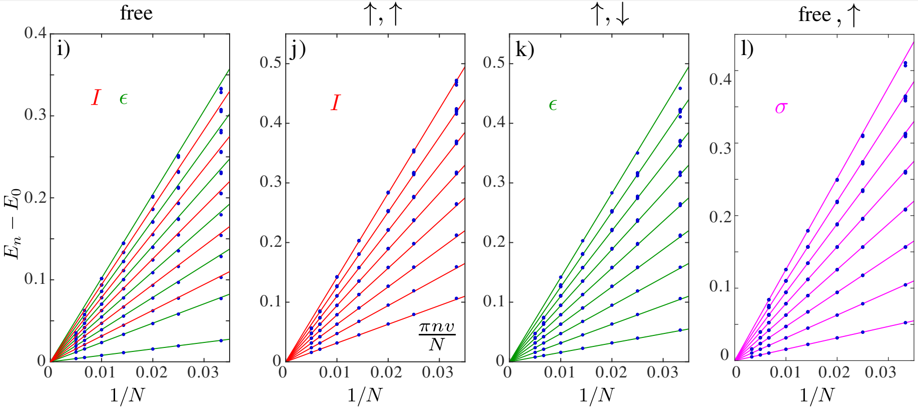
Transverse field Ising model. Excitation spectrum



- Remarkable accuracy for critical system
- Wrong spectrum for gapped system

[NC, F. Mila, Phys. Rev. B 96, 054425’17]

Finite-size scaling of the excitation energy

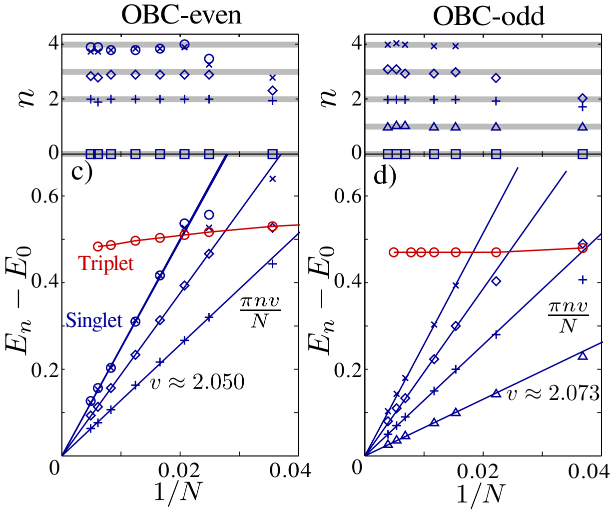


$$\chi_I(q) = q^{-1/48}\left(1 + q^2 + q^3 + 2q^4 + 2q^5 + 3q^6 + 3q^7 + 5q^8\right)$$
$$\chi_\epsilon(q) = q^{1/2-1/48}\left(1 + q + q^2 + q^3 + 2q^4 + 2q^5 + 3q^6 + 4q^7 + 5q^8\right)$$

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

Ising transition in spin-1 chain

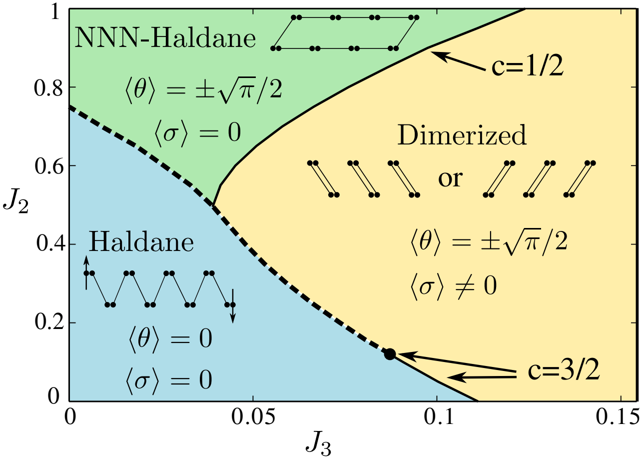
Ising conformal towers in spin-1 chain



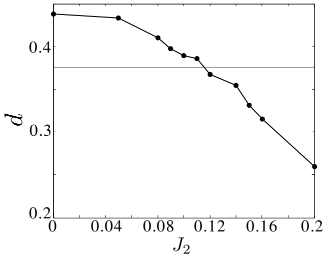
- Singlet-triplet gap is **open**
- Critical scaling of the gap in the singlet sector
- N **even**
  I conformal tower
- N **odd**
  ϵ conformal tower

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

WZW $SU(2)_2$ end point

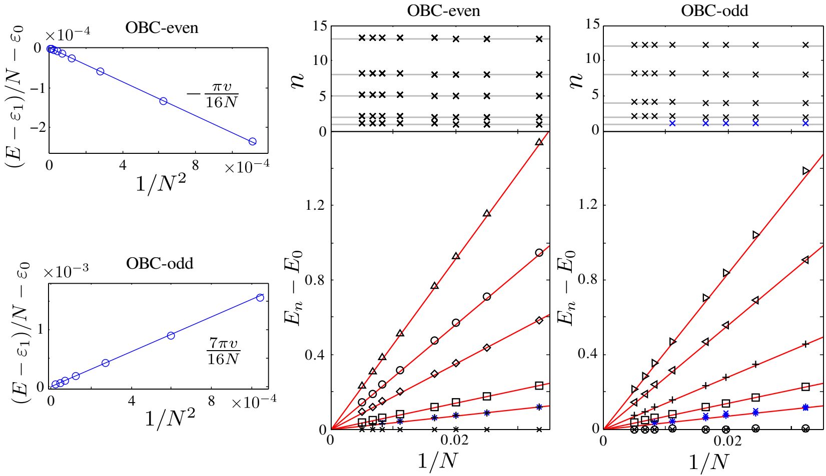


WZW $SU(2)_2$ end point



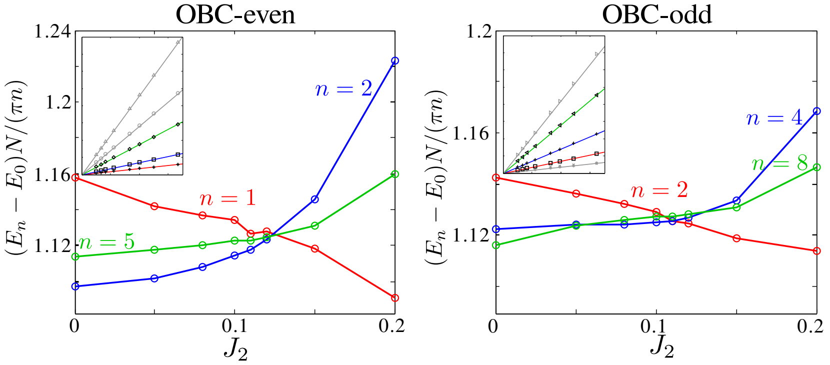
- Associate the critical point with the separatrix in the log-log plot of the finite-size scaling of the dimerization
- The slope gives an **apparent** critical exponent. It is different from the WZW $SU(2)_2$ due to logarithmic corrections
- At the end point the logarithmic corrections vanish and the critical exponent is $\mathbf{d = 3/8}$

WZW $SU(2)_2$ end point



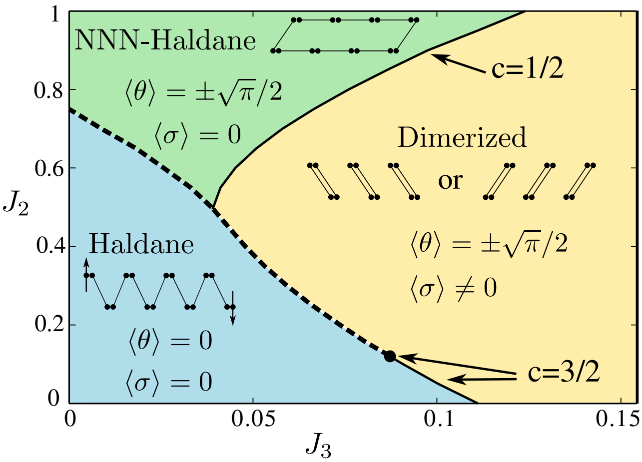
NC, Affleck, Mila, PRB **93**, 241108'16

WZW $SU(2)_2$ end point

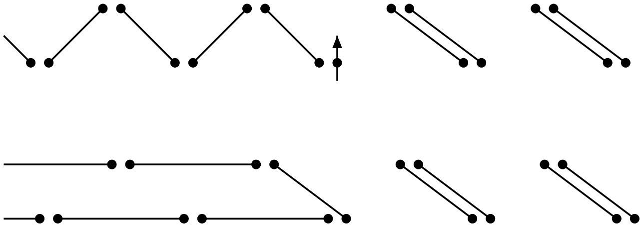


- The 'velocities' extracted from the gap between the ground state and a few lowest excited states cross at the end point
- Away from this point the lines are divergent and the conformal towers are destroyed

Ising vs WZW SU(2)$_2$

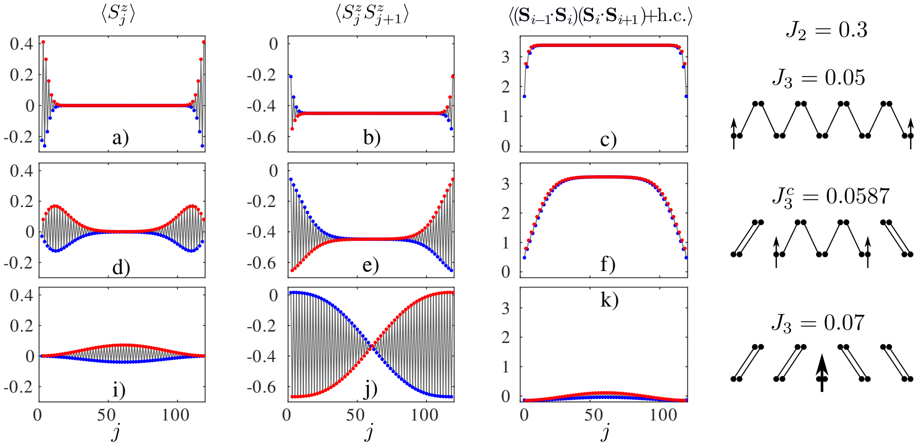


Ising vs WZW $SU(2)_2$



- The domain wall between the Haldane and dimerized phase carries spin-1/2 and corresponds to the **magnetic** WZW $SU(2)_2$ transition
- The domain wall between the NNN-Haldane phased and the dimerized phase does not carry any spin and therefore the singlet-triplet gap remains open

Solitons at the transition between the Haldane and dimerized phases



NC, Affleck, Mila, PRB **94**, 205112'16

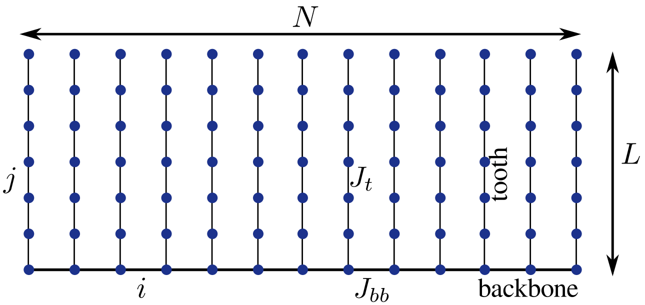
Outlook-1

- In spin-1 chains the transition to spontaneously dimerized phase can be either continuous in the **WZW SU(2)$_2$** or in the **Ising** universality class, or **first order**
- The choice between the Ising and WZW SU(2)$_2$ transition depends on the nature of the **domain walls** between the corresponding phases
- Continuous WZW SU(2)$_2$ critical line turn into a first order phase transition at the end point due to the presence of marginal operator
- Universality class can be deduced from the finite-size scaling of the energy spectrum

Comb tensor networks

in collaboration with S.R.White 

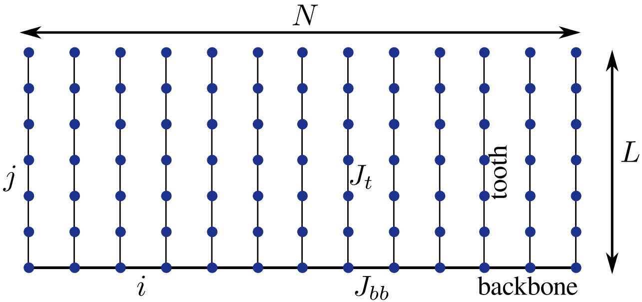
Comb geometry



- Spin chains (teeth) coupled through one edge
- Highly decorated spin chain (backbone)

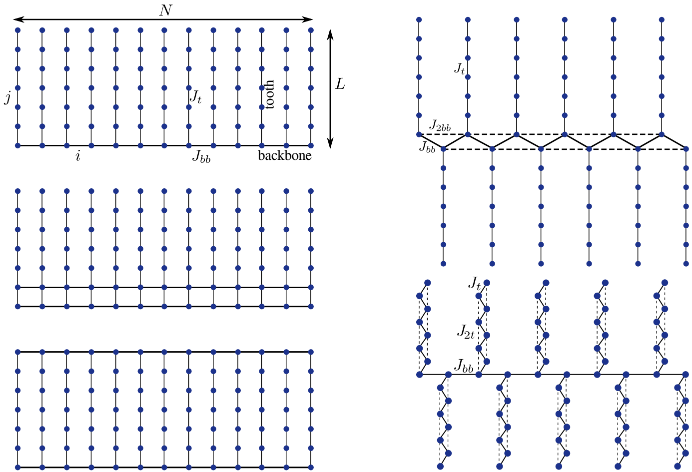
One dimensional... in which direction?

Comb geometry

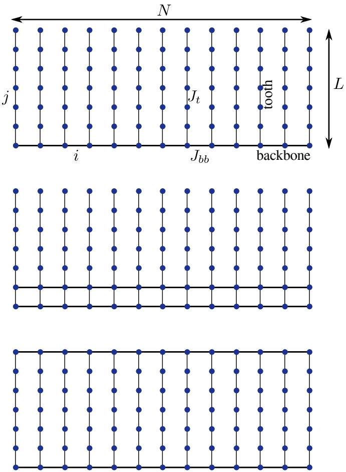


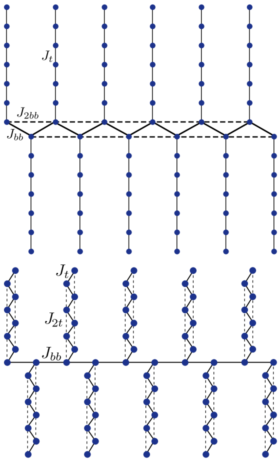
- **Y-DMRG:** Guo, White, Phys. Rev. B **74**, 060401 (2006)
- **Fork tensor networks:**
  Holzner, Weichselbaum, von Delft, Phys. Rev. B **81**, 125126 (2010);
  Bauernfeind, Zingl, Triebl, Aichhorn, Evertz, Phys. Rev. X **7**, 031013 (2017)

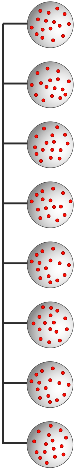
Comb geometry



Comb geometry

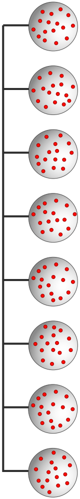




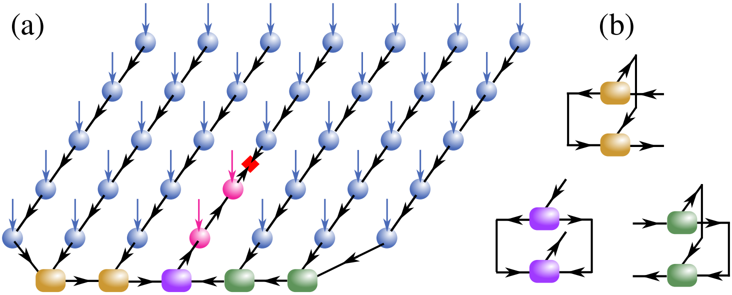


Generic comb

- **The goal is to split two channels of entanglement: along the backbone and within the tooth**
- Finite-size clusters form local degrees of freedom
- Ad-lib complicated interactions within the clusters (DMRG-limited)
- The wave-function is expected to obey the area law



A comb network. Mixed-canonical form

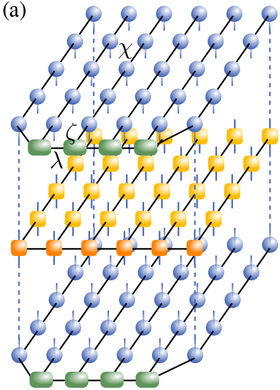


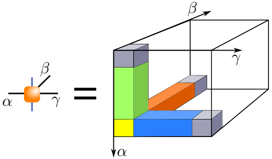
Auxiliary backbone tensors:

- Each tensor is at most of rank 3
- Split degrees of freedom on a backbone

NC, White, Phys. Rev. B **99**, 235426 (2019)

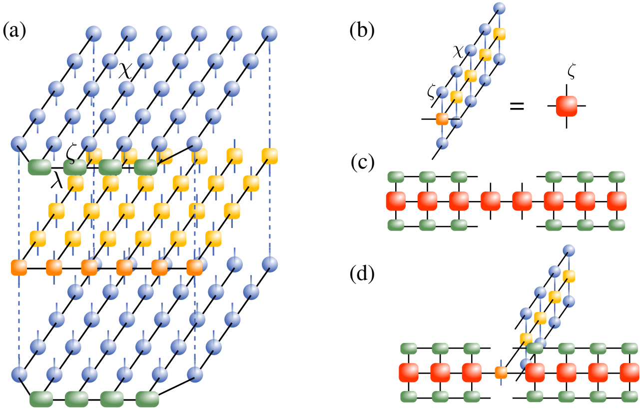
Variational optimization





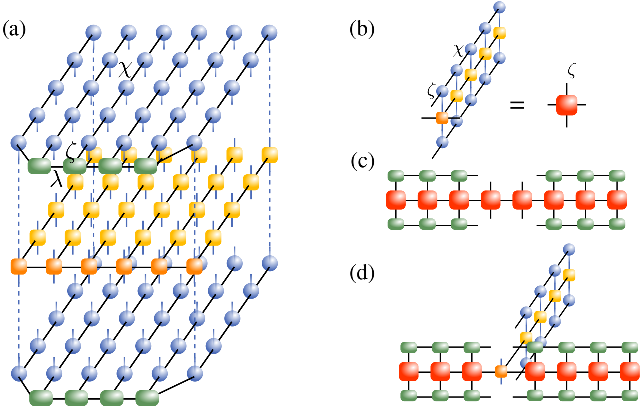
- Hamiltonian in terms of local tensors - PEPO

Variational optimization



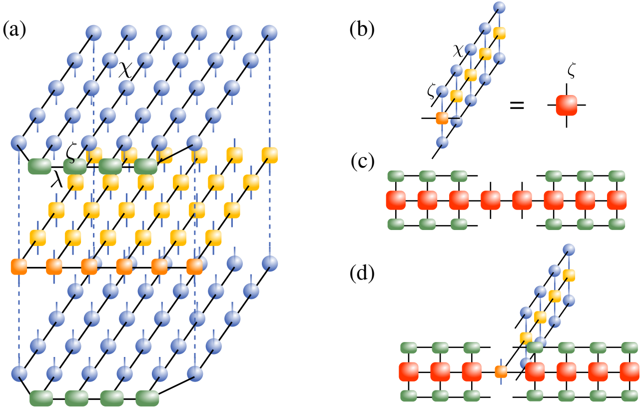
- Hamiltonian in terms of local tensors - PEPO
- Optimization within the tooth = DMRG

Variational optimization



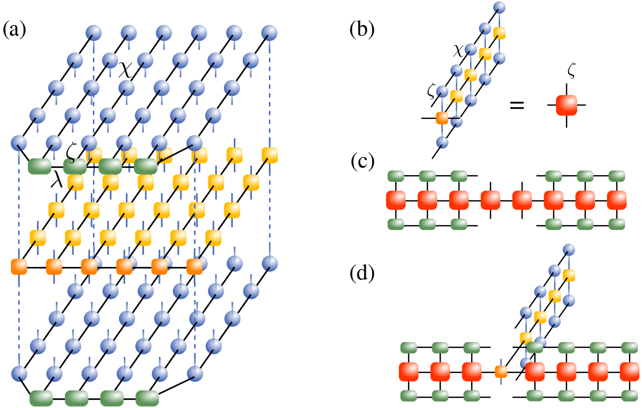
- Hamiltonian in terms of local tensors - PEPO
- Optimization within the tooth = DMRG
- Fully contracted tooth can be viewed as an MPO with fat physical bonds

Variational optimization



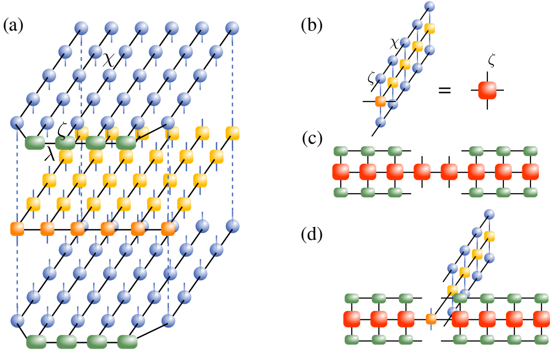
- Optimization within the tooth = DMRG
- Fully contracted tooth can be viewed as an MPO with fat physical bonds
- Optimization of two backbone tensors = DMRG

Variational optimization



- Optimization within the tooth = DMRG
- Optimization of two backbone tensors = DMRG
- Connect update $\neq$ DMRG and involves three environments

Complexity

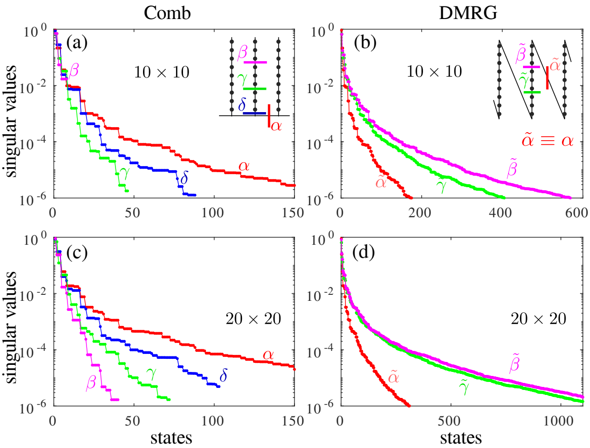


Complexity ($\chi \approx \zeta \approx \lambda \approx D$)

- Backbone update: D^5
- Connect update: D^4
- Tooth update: D^3

For AKLT-like states (finite ξ, ζ) the complexity is λ^3

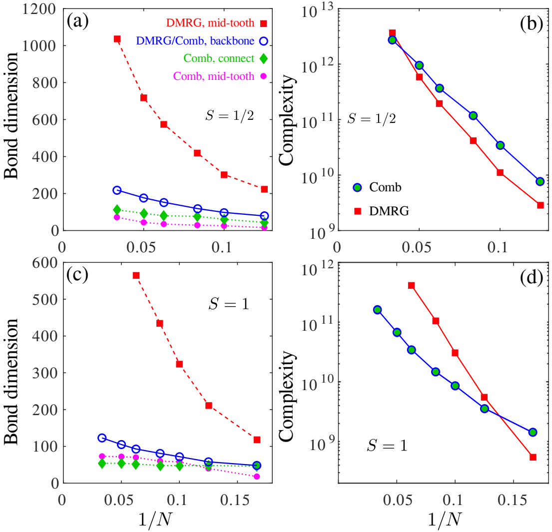
DMRG versus comb. Schmidt values



- Heisenberg spin-1/2
- Backbone cut is the same for the comb and for the DMRG
- DMRG: the largest bond dimension is inside the tooth
- Comb: the bond dimension decreases upon approaching the tip of the tooth

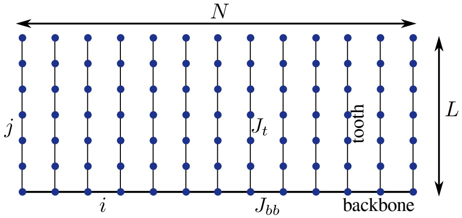
NC, White, Phys. Rev. B **99**, 235426 (2019)

DMRG versus comb. Complexity



Spin-1 Heisenberg comb

$$H = J_{bb} \sum_{i=1}^{N-1} \mathbf{S}_{i,1} \cdot \mathbf{S}_{i+1,1} + J_t \sum_{i=1}^{N} \sum_{j=1}^{L-1} \mathbf{S}_{i,j} \cdot \mathbf{S}_{i,j+1},$$



Spin-1 Heisenberg comb

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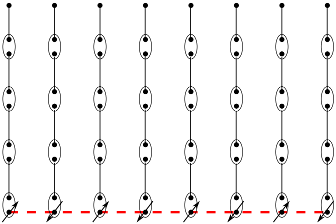
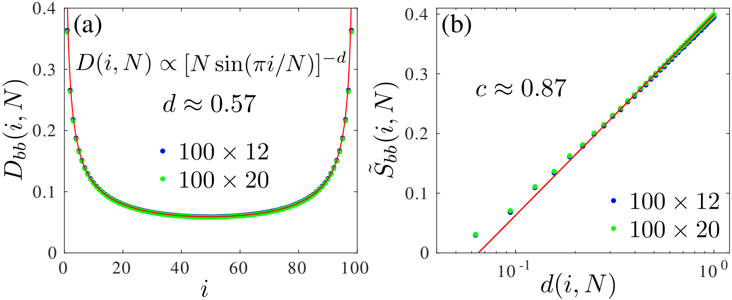
(a)

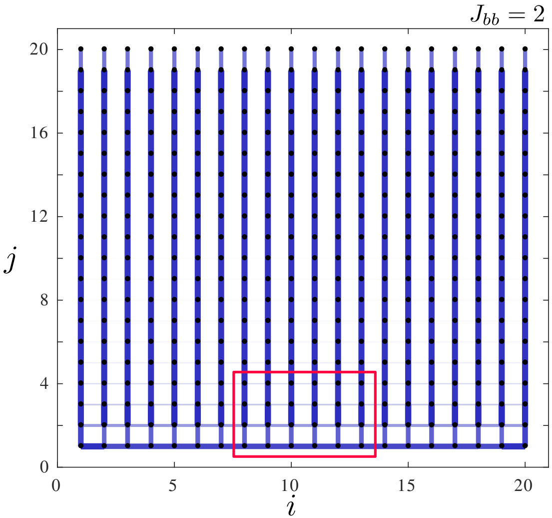


Emergent spin-1/2 chain

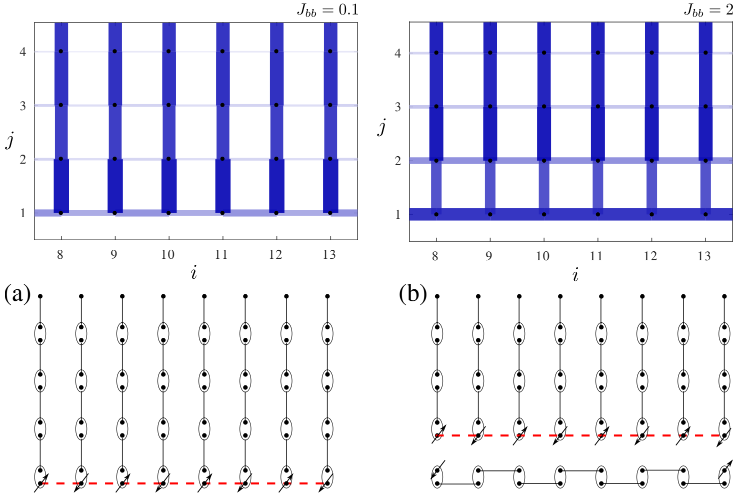


CFT prediction for WZW $SU(2)_1$: $d = 1/2$ and $c = 1$

Spin-1 comb. Correlations

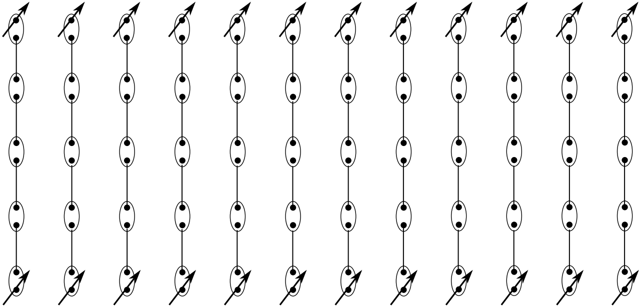


Spin-1 comb



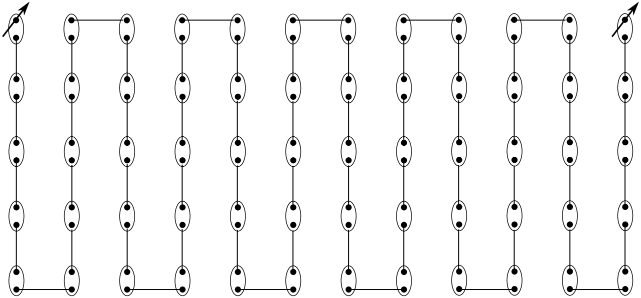
Higher-order edge states

- Tooth with odd number of sites
- Edge states of each tooth couple to a triplet



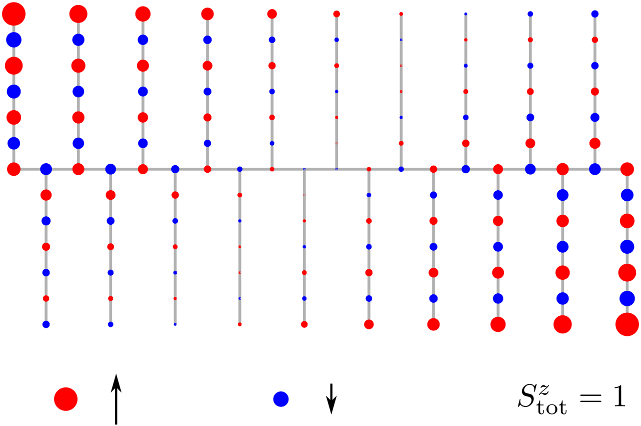
Higher-order edge states

- Tooth with odd number of sites
- Edge states of each tooth couple to a triplet
- Effective spin-1 chain - Haldane state → **Edge states**



Higher-order edge states

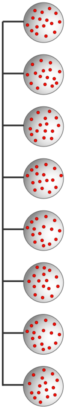
$J_{bb} = J_t$



$S^z_{\mathrm{tot}} = 1$

NC, White, Phys. Rev. B **99**, 235426 (2019)

Outlook-2



- Comb lattice - quasi-one-dimensional system
- Exotic critical behavior induced by the backbone interaction
-
-
- Flexible and powerful algorithm
  ...and many geometries to play with