Matrix Product States, Operators, and the Thermodynamic Limit of DMRG

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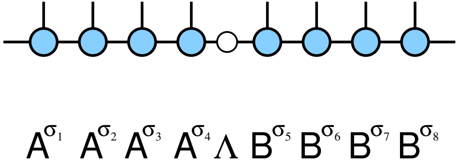
Outline

1. MPS Introduction
2. Infinite size DMRG
3. Scaling relations in the thermodynamic limit
4. Expectation values of iMPO's
5. Conclusions

MPS representations

DMRG produces a matrix product state wavefunction.

$$|\Psi\rangle = \mathrm{Tr} \sum_{s_1, s_2, \ldots} A^{s_1} A^{s_2} A^{s_3} A^{s_4} \cdots |s_1\rangle |s_2\rangle |s_3\rangle |s_4\rangle \cdots$$

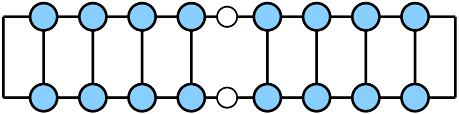


Λ is the wavefunction in the *Schmidt basis*
$|\Psi\rangle = \sum_i \Lambda_{ii} |i\rangle_L |i\rangle_R$

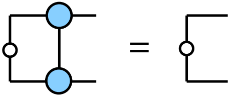
Key advantage of the MPS representation:
Manipulations of the wavefunction are easy - both conceptually and numerically

MPS operations - normalization

Simple example: how do we calculate the norm?

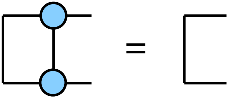


Sequential contractions:

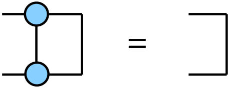


$$\tilde{E}_n = \sum_s A^{s\dagger} \, \tilde{E}_{n-1} \, A^s$$

This process is greatly simplified if we require that the MPS is *orthonormalized*

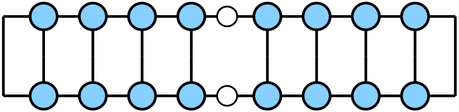


$$\sum_s A^{s\dagger} A^s = I$$



$$\sum_s B^s B^{s\dagger} = I$$

Sequential contraction for the norm



Remaining tensor:

$$|\Psi\rangle = \sum_i \Lambda_{ii} |i\rangle_L |i\rangle_R$$

$$\mathrm{Tr}\, \Lambda^\dagger \Lambda = \langle\Psi|\Psi\rangle = 1$$

This works because we know how to contract tensors at the boundary

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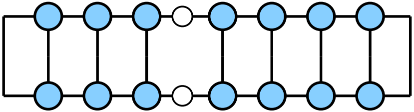

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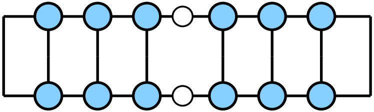

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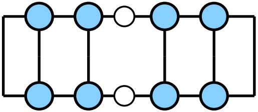

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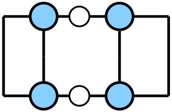

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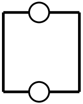

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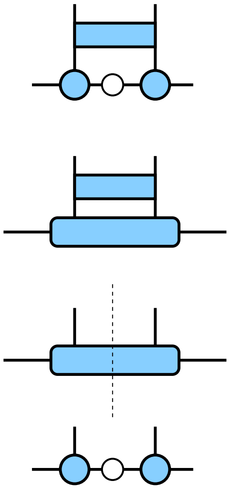
Bond Evolution



Apply operator $U_{s_1 s_2}^{s_1' s_2'}$ to two sites:

$A'^{s_1'} \; \Lambda' \; B'^{s_2'} = U_{s_1 s_2}^{s_1' s_2'} \, A^{s_1} \; \Lambda \; B^{s_2}$

Merge tensors:

$X^{s_1 s_2} = A^{s_1} \; \Lambda \; B^{s_2}$

Apply evolution operator:

$X' s_1' s_2' = U_{s_1 s_2}^{s_1' s_2'} \, X^{s_1 s_2}$

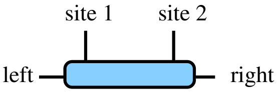
Singular value decomposition:

$X' s_1' s_2' = A'^{s_1'} \; \Lambda' \; B'^{s_2'}$

This is the basis of TEBD

DMRG: Local minimization of the Hamiltonian with an eigensolver

- We need a representation of the Hamiltonian operator in the Hilbert space of the tensors at the center of the lattice



Partition the Hamiltonian operator:

$$
\begin{array}{rcl cccc}
 & & & \text{left} & \text{site 1} & \text{site 2} & \text{right} \\
H & = & & \tilde{H} & I & I & \tilde{I} \\
 & & + & \tilde{I} & H & I & \tilde{I} \\
 & & + & \tilde{I} & I & H & \tilde{I} \\
 & & + & \tilde{I} & I & I & \tilde{H} \\
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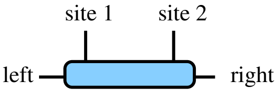

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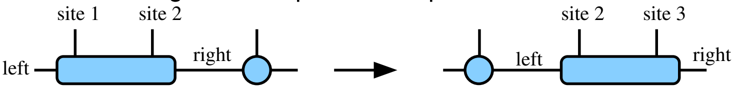
The second ingredient: update the operators in the course of a DMRG sweep



New block operator $\tilde{Y} \otimes Z \to \tilde{X}$

$$\sum_{s' s} \langle s' | Z | s \rangle A^{s'\dagger} \tilde{Y} A^{s} = \tilde{X}$$

But our new block operators may be sums of these terms.
Example: $\tilde{H} \leftarrow \tilde{H} \otimes I + \tilde{I} \otimes H + \tilde{b}^{\dagger} \otimes b \ldots$

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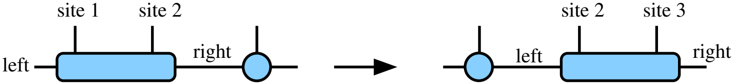

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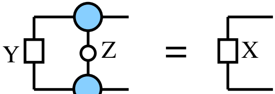

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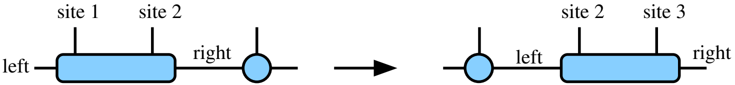

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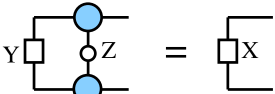

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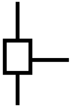
Constructing the block operators

How to we represent the block update in a generic way?

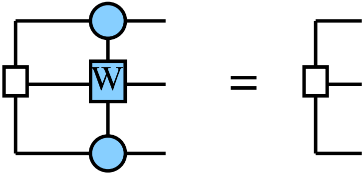
Denote the block operators by a set, labeled by index α



α

$$\tilde{E}^{\alpha},\ \alpha = 1, 2, \ldots, M$$

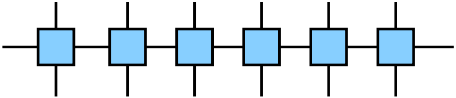
Generalize the local operator into a 4-index *matrix product operator* $W^{s's}_{\alpha'\alpha}$



$$\tilde{E}'^{\alpha'} = \sum_{s' s \alpha} W^{s's}_{\alpha'\alpha} A^{s'\dagger} \tilde{E}^{\alpha} A^{s}$$

Dimension M of the MPO is equal to the number of block operators - typically small

$$X = \mathrm{Tr} \sum_{s_1, s_2, \ldots} W^{s_1' s_1} A^{s_2' s_2} A^{s_3' s_3} A^{s_4' s_4} \cdots |s_1'\rangle\langle s_1| \, |s_2'\rangle\langle s_2| \, |s_3'\rangle\langle s_3| \, |s_4'\rangle\langle s_4| \cdots$$



The principal advantage of the MPO representation is that it allows arithmetic operations on the operators

$$X = Y + Z \to W_X = W_Y \oplus W_Z$$

Dimension increases: $M_X = M_Y + M_Z$

$$X = YZ \to W_X = W_Y \otimes W_Z$$

Dimension increases: $M_X = M_Y M_Z$

For finite, open systems, the boundary components are 1-dimensional.

'Orthogonalization' of the MPO keeps the dimension under control.

Operator arithmetic

IPM J. Stat. Mech. P10014 (2007)

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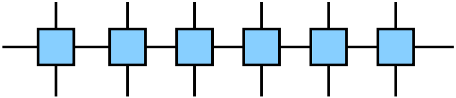

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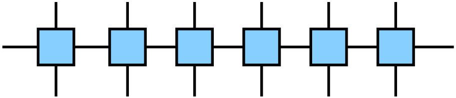

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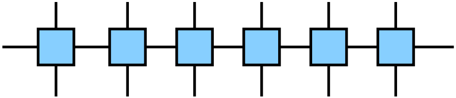

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- Orthonormalizing an MPO in the same way as an MPS is a bad idea
  - Norm of an MPO is the Frobenius norm $\sim \dim(\mathcal{H})$
  - Difference in norms of two operators also scales as $\sim \dim(\mathcal{H})$
  - As soon as this difference exceeds 10^{16}, all precision in the orthogonalization transform is lost
- Instead, collapse only those rows/columns that are *parallel*, ie. identical, up to a constant

Some examples:

Sum of local terms $H = \sum_i X_i$

$$W_H = \begin{pmatrix} I & 0 \\ X & I \end{pmatrix}$$

Boundary vectors $\begin{pmatrix} 0 & I \end{pmatrix}$ and $\begin{pmatrix} I \\ 0 \end{pmatrix}$

Sum of nearest-neighbor terms $H = \sum_i X_i Y_{i+1}$

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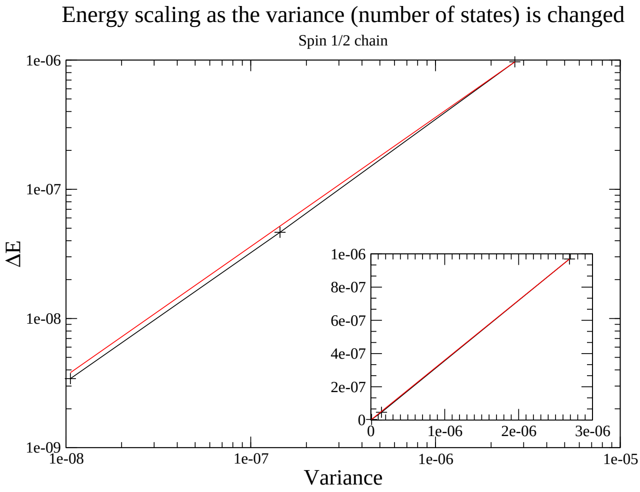
Calculating observables of ‘complicated’ operators is often easy

Error estimates:

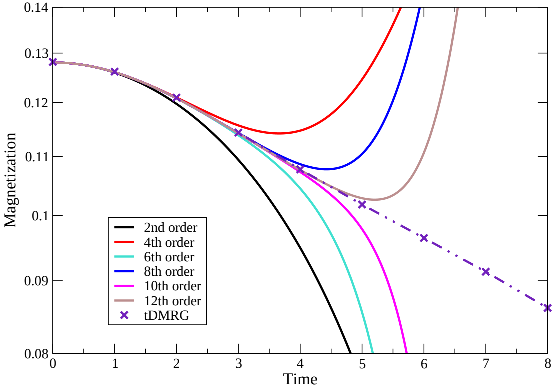
- truncation error: a property of the *algorithm*, not always well defined
- variance $\langle H\rangle^2 - \langle H^2\rangle$: a propery of the *state*, always well-defined



The limits of what is possible (in an hour or so):

$$A(t) = A + \frac{it}{\hbar}[H,A] - \frac{t^2}{2!\hbar^2}[H,[H,A]] - \frac{it^3}{3!\hbar^3}[H,[H,[H,A]]] + \cdots \, .$$

Relaxation of an impurity in the SIAM



$\Gamma = 0.1$, $U = 0.2$, $h_0 = 0.1$, $\epsilon_{d0} = 0.05$, on a log-discretized Wilson chain with $\Lambda = 1.8$.

At time $t = 0$, the Hamiltonian was switched to $h_1 = 0$ and $\epsilon_{d1} = -0.1$.

command line: `mp-expectation siam:"[H,[H,[H,[H,Sz(0)]]]]" psi`

DMRG in the infinite size limit (arxiv:0804.2509)

Infinite-size translationally invariant MPS

- The “infinite size” DMRG algorithm has existed since the year 0AD
- It doesn’t produce a translationally invariant MPS fixed point
- No prescription for constructing the initial wavefunction at next iteration
- Rarely used in the literature, and often incorrectly
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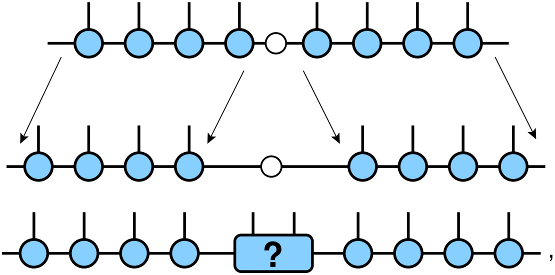
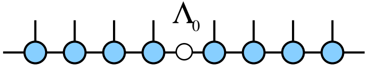
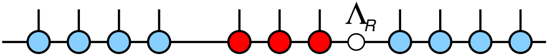


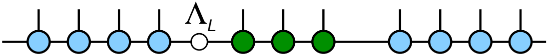
A recurrence relation for MPS

Suppose we can an initial state:



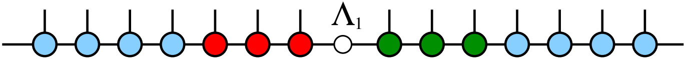
Suppose we also have the same MPS with an extra unit cell:





Note: Λ_L and Λ_R are not necessarily diagonal

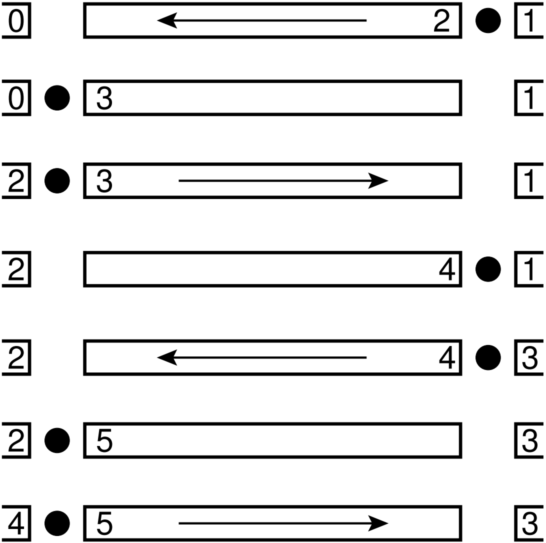
Now we can insert one more unit cell:



$$\Lambda_1 = \Lambda_R \, \Lambda_0^{-1} \, \Lambda_L$$

Variant of the finite system algorithm

- Different treatment of the boundaries



$$\Lambda_{23} = \Lambda_{21}\,\Lambda_{01}^{-1}\,\Lambda_{03}$$

$$\Lambda_{43} = \Lambda_{41}\,\Lambda_{21}^{-1}\,\Lambda_{23}$$

$$\Lambda_{45} = \Lambda_{43}\,\Lambda_{23}^{-1}\,\Lambda_{25}$$

Comparison with iTEBD

- Local minimization is *much* faster than imaginary time evolution
- Unit cell can be an arbitrary size $(1, 2, \ldots)$
- Efficiency is largely independent of unit cell size
- Scaling $\Delta\tau \to 0$ is not needed
- Not yet any scheme for krlov-based time evolution

iTEBD and iDMRG are the same algorithm, except the update works slightly differently

- iTEBD: evolve a single bond at the middle of the chain
- iDMRG: locally minimize the energy with respect to the Hamiltonian of the whole system

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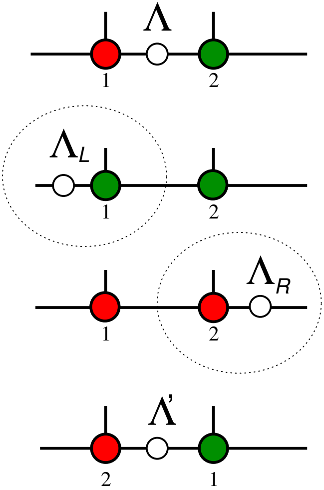
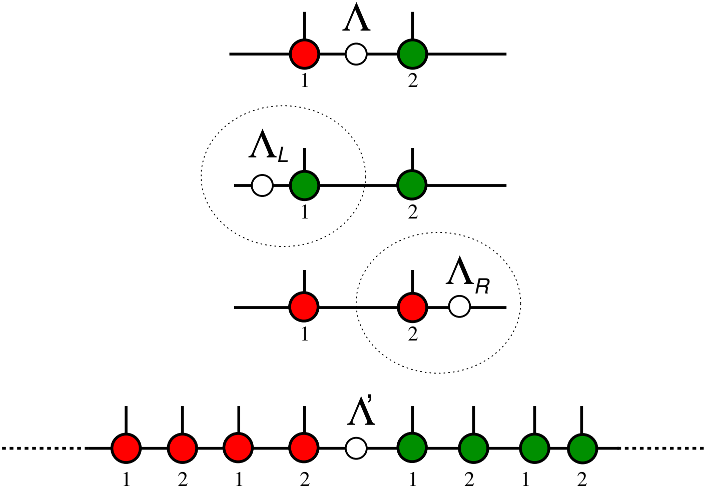


$\Lambda' = \Lambda_R \, \Lambda^{-1} \, \Lambda_L$ gives an initial state for the evolution

With respect to the whole lattice, the MPS is *always orthogonal*



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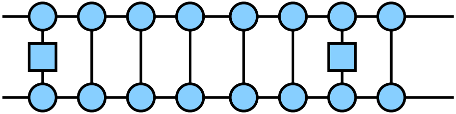
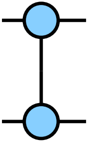
Expectation Values

Correlation functions



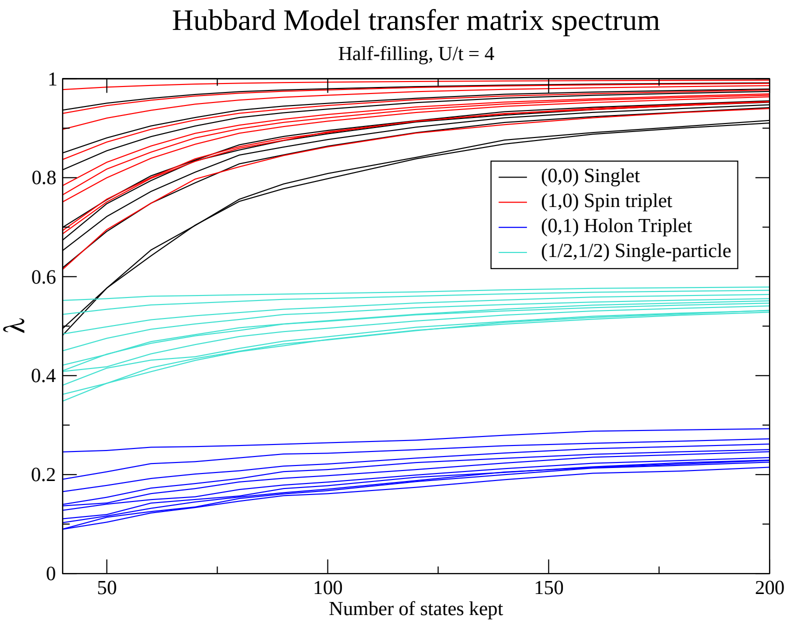
The form of correlation functions are determined by the eigenvalues of the *transfer operator*



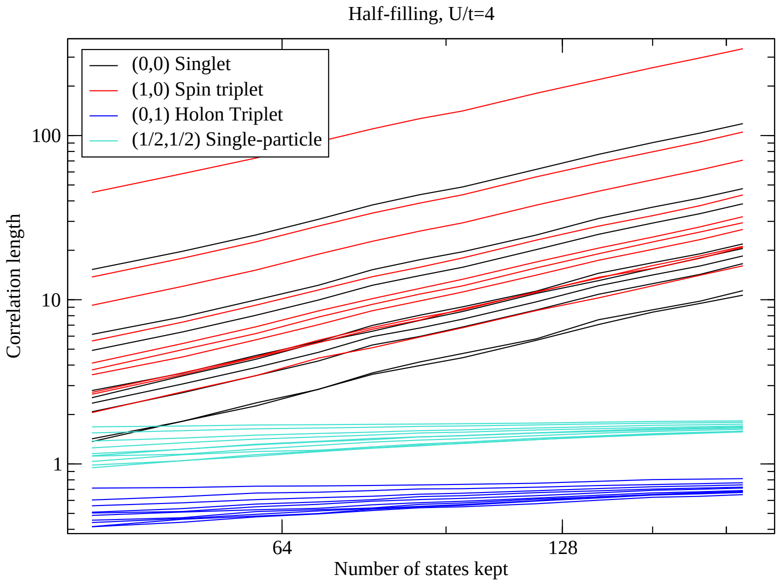
- All eigenvalues ≤ 1
- One eigenvalue equal to 1, corresponding to the identity operator

Expansion in terms of eigenspectrum λ_i:

$$\langle O(x) O(y) \rangle = \sum_i a_i \, \lambda_i^{|y-x|}$$


Hubbard Model transfer matrix spectrum
Half-filling, U/t = 4
λ
1
0.8
0.6
0.4
0.2
0
50
100
150
200
Number of states kept
(0,0) Singlet
(1,0) Spin triplet
(0,1) Holon Triplet
(1/2,1/2) Single-particle

Hubbard model transfer matrix spectrum



CFT Parameters

For a critial mode, the correlation length increases with number of states m as a power law,

$$\xi \sim m^{\kappa}$$

[T. Nishino, K. Okunishi, M. Kikuchi, Phys. Lett. A **213**, 69 (1996)
M. Andersson, M. Boman, S. Östlund, Phys. Rev. B **59**, 10493 (1999)
L. Tagliacozzo, Thiago. R. de Oliveira, S. Iblisdir, J. I. Latorre, Phys. Rev. B **78**, 024410 (2008)]

This exponent is a function *only* of the central charge,

$$\kappa = \frac{6}{\sqrt{12c} + c}$$

[Pollmann et al, arxiv:0812.2903, see poster in foyer]

Can we find an expression for the scaling dimension?

Suppose we have a two-point correlator that has a power-law at large distances

$$\langle O(x)O(y)\rangle = |y - x|^{-2\Delta}$$

As we increase the number of states kept m the correlation length increases, so the region of validity of the power law increases.

- Take two different calculations with m_1 and m_2
- Correlation lengths ξ_1 and ξ_2
- We expect: $\dfrac{O(\xi_2)}{O(\xi_1)} = \left(\dfrac{\xi_2}{\xi_1}\right)^{\Delta}$
- We have: $O(x) \sim a\,\lambda^x$ (with $\xi = -1/(1-\lambda)$)
- Prefactor a is overlap of operator O with next-leading eigenvector of transfer operator
- $\cdots$ algebra $\cdots$

$$a = (1 - \lambda)^{\Delta}$$

This gives directly the operator scaling dimensions by direct fit

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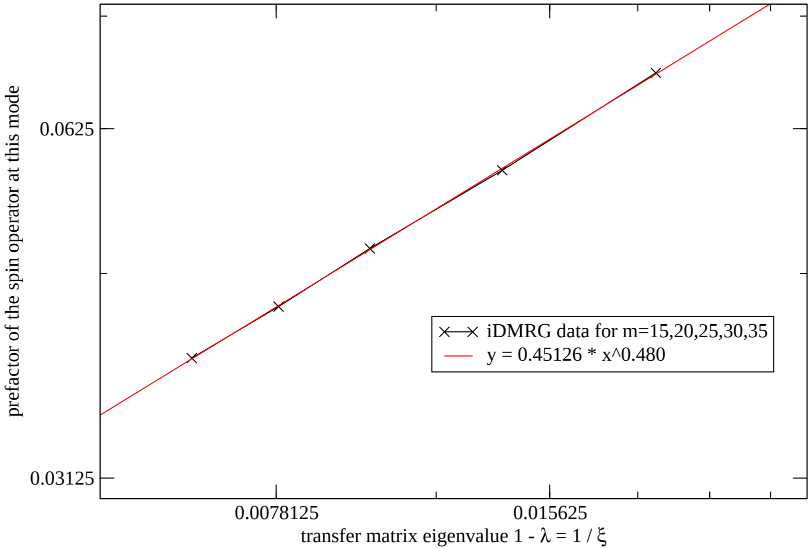
Heisenberg model fit for the scaling dimension

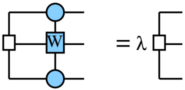


Expectation values of MPO's

We have seen that we can write many interesting operators in the form of a matrix product operator

- Can we evaluate the expectation value of an arbitrary MPO?

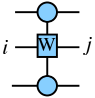
If the MPO has no Jordan structure, this is a simple eigenvalue problem



For a lower triangular MPO, this doesn't work.

- But we can make use of the triangular structure
- index by index, each component is a function only of the previously calculated terms

Choose bond indices i, j of W_{ij}, and denote $T_{W_{ij}}$



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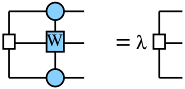

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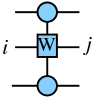

At the n^{th} iteration, we have

$$\tilde{E}_i[n] = T_{W_{ii}}(\tilde{E}_i[n-1]) + \underbrace{\sum_{j>i} T_{W_{ij}}(\tilde{E}_j[n-1])}_{\text{const. operator}}$$

Case 1: $W_{ii} = 0$

- $\tilde{E}_i =$ const

Case 2: $W_{ii} = xI$ (proportional to identity operator)

- A geometric series with respect to transfer matrix eigenvalues. $\sum_i c_i \sum_n \lambda_i^n$. Component in the direction of the identity operator diverges linearly, remaining components can be solved efficently:

$$(1-T)\tilde{E}_i = \text{const. operator}$$

Similar scheme works if x is complex

Case 3: W_{ii} unitary

- similar, keep track of diverging component giving long-range string order

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Summary

- MPO's are convienent in practical applications
- Variance $\langle H \rangle^2 - \langle H^2 \rangle$ as a general purpose measure of accuracy, scales similarly to the truncation error in DMRG
- Perturbative expansions, commutators, higher moments, ...

- iDMRG is a very efficient method to construct translationally invariant thermodynamic states
- All expectation values can be expressed in terms of the eigenmodes of the transfer matrix
- Scaling with respect to m (or D, or χ) can give power laws
- Easy to extract scaling dimensions of operators
- For a critical state, can we extract the primary fields and the operator algebra of the CFT? Analogies to finite-width transfer matrix spectra.