AKLT model and Matrix product states

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Introduction

- **AKLT Hamiltonian (spin-1 chain):**

$$H = \sum_{i=1}^{L-1} \left[\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \frac{1}{3} (\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \right]$$

where $\mathbf{S}_i = (S_i^x, S_i^y, S_i^z)$ is the collection of operators at site i.

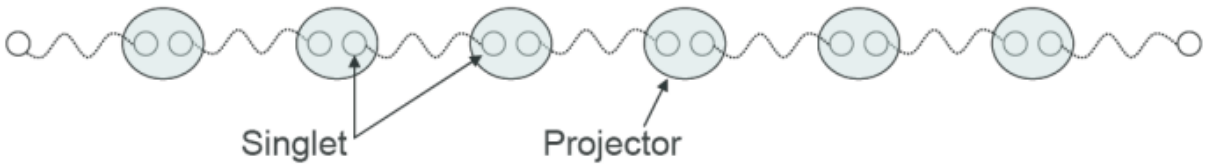
- Explicit matrix representation:

$$s^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad s^y = \frac{-i}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad s^z = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

- MPS were studied in the work by Affleck, Kennedy, Lieb and Tasaki (AKLT) where it was proven that the exact ground state of the spin-1 chain with the AKLT hamiltonian can be parametrized exactly by MPS

AKLT Chain: A Valence Bond Solid

- The AKLT hamiltonian is made of spin-1 sites which can be modeled as two spin1/2 particles symmetrized. We can build the full Hilbert space using the tensor product as $\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$
- Each site shares one of its virtual spin-1/2's with a neighboring site. These two virtual spins form a singlet state (spin-0), which creates the entangled valence bonds between sites.



The AKLT ground state is constructed by locally projecting the two virtual spin-1/2 particles at each site onto the physical spin-1 subspace via the projector [4]:

$$P = |-1\rangle(\frac{\langle 00| - \langle 11|}{\sqrt{2}}) + |0\rangle(\frac{\langle 01| + \langle 10|}{\sqrt{2}}) + |1\rangle(\frac{\langle 00| + \langle 11|}{\sqrt{2}})$$

- Where $\{|-1\rangle, |0\rangle, |1\rangle\}$ form the physical spin-1 basis at each site

Energy Spectrum and Symmetries

- We constructed the full Hamiltonian matrix explicitly using the `np.kron`:

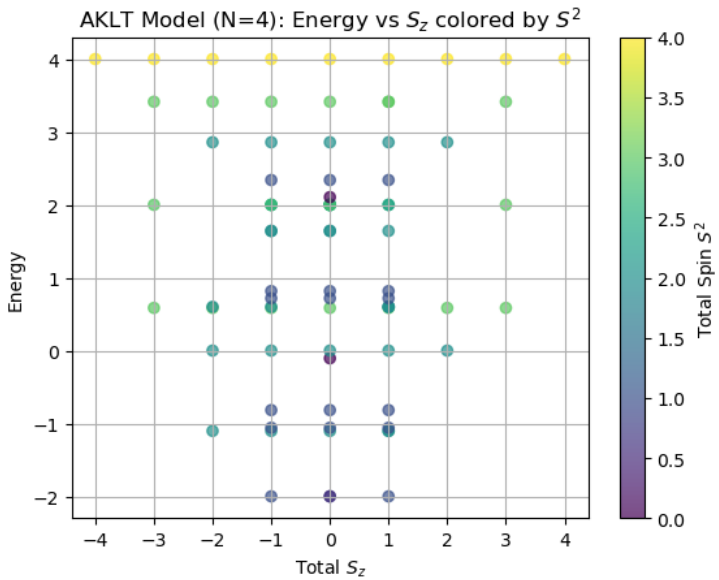
$$S_i^x S_{i+1}^x \Rightarrow \mathbb{I}_1 \otimes \cdots \otimes \mathbb{I}_{i-1} \otimes S^x \otimes S^x \otimes \mathbb{I}_{i+2} \otimes \cdots \otimes \mathbb{I}_N$$

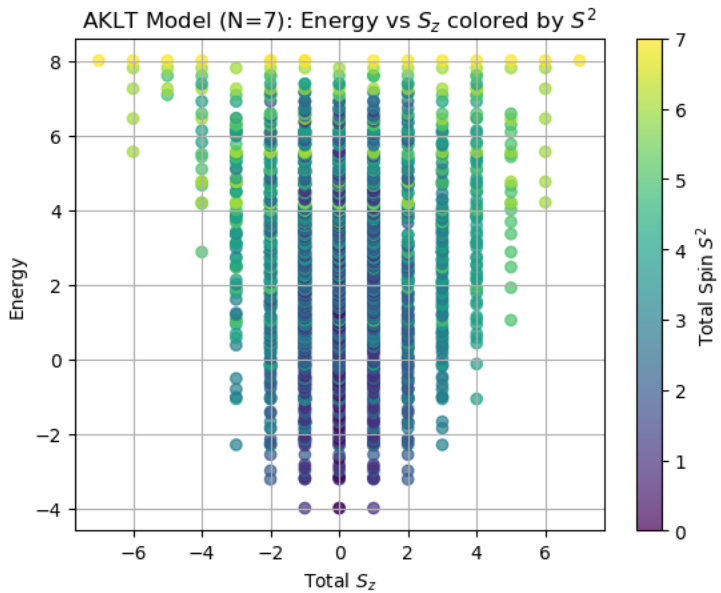
  and similarly for S^y, S^z
- Scalar product: $\mathbf{S}_i \cdot \mathbf{S}_{i+1} = S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z$ The previous for each term and summing into the Hamiltonian for the $(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2$ term we just did the matrix multiplication with the previously built term $\mathbf{S}_i \cdot \mathbf{S}_{i+1}$
- AKLT Hamiltonian commutes with:
  $S^z_{\text{tot}} = \sum_i S_i^z$ and $\mathbf{S}^2_{\text{tot}} = \left(\sum_i \mathbf{S}_i\right)^2$
- Hilbert space block-decomposes into spin sectors:
  $\mathscr{H}_{\text{AKLT}} = \bigoplus_{S,S^z} \mathscr{H}_{S,S^z}$
- Diagonalization performed within each sector $\Rightarrow$ reduced computational cost

Energy Spectrum and symmetries

- It also allows to classify eigenstates according to the spin operators S^z_{tot} and $\mathbf{S}^2_{\text{tot}}$ by contructing the operators and the diagonalizing the full matrix then we compute the expectation values for each state vector with each operator as $\langle\psi|S^z_{\text{tot}}|\psi\rangle$ and $\langle\psi|\mathbf{S}^2_{\text{tot}}|\psi\rangle$

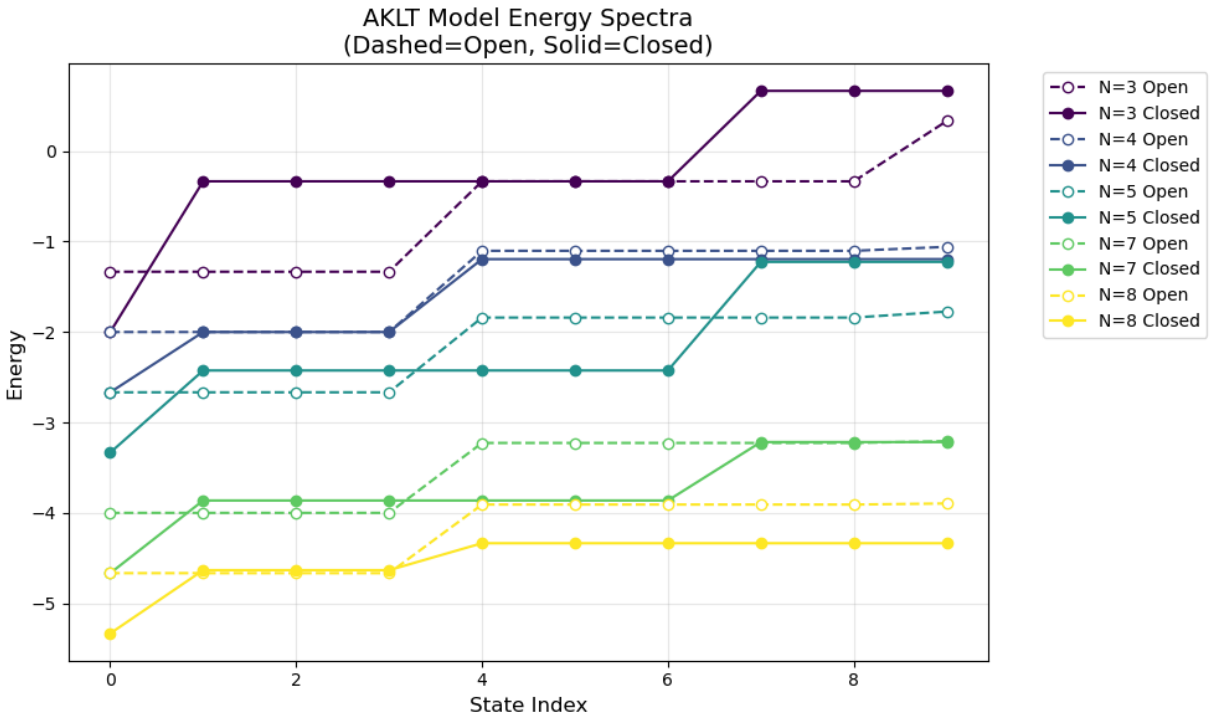
Figures reproduced based on [1]





Boundary conditions

When the chain has open boudary conditions the spin-1/2 particles at the two ends remain unpaired, forming free edge spins. Each can be in either $|\uparrow\rangle$ or $|\downarrow\rangle$, leading to a fourfold ground state degeneracy:
$|\uparrow\rangle|\uparrow\rangle, |\uparrow\rangle|\downarrow\rangle, |\downarrow\rangle|\uparrow\rangle, |\downarrow\rangle|\downarrow\rangle$
For periodic Boundary conditions, the chain forms a closed loop. All spin-1/2 particles pair into singlets, leaving no unpaired edge spins.



Matrix Product States (MPS) and SVD

An arbitrary quantum state on a lattice of L sites with local Hilbert space of dimension d (spanned by basis states $\{|\sigma_i\rangle\}$) can be written as:

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} c_{\sigma_1\ldots\sigma_L} |\sigma_1,\ldots,\sigma_L\rangle.$$

By successively applying Singular Value Decomposition (SVD), we can factorize the tensor $c_{\sigma_1\ldots\sigma_L}$ into Matrix Product State (MPS) representation. This process:

- Encodes the state in a form that emphasizes its local structure.
- Preserves non-local quantum correlations via the singular values.

MPS and SVD

Step 1: Reshape the state vector (with d^L components) into a matrix Ψ of shape (d, d^{L-1}):

$$\Psi_{\sigma_1,(\sigma_2 \ldots \sigma_L)} = c_{\sigma_1 \ldots \sigma_L}.$$

Step 2: Perform SVD on Ψ:

$$\Psi = U \Sigma V^\dagger,$$

where: U is a $d \times d$ unitary matrix, Σ is a diagonal matrix with singular values, $V^\dagger$ is a $d^{L-1} \times d^{L-1}$ unitary matrix.

Step 3: Absorb Σ into $V^\dagger$ and reshape again into a vector, then U is reshaped into the a tensor $A^{\sigma_1}_{a_1} = U_{\sigma_1, a_1}$

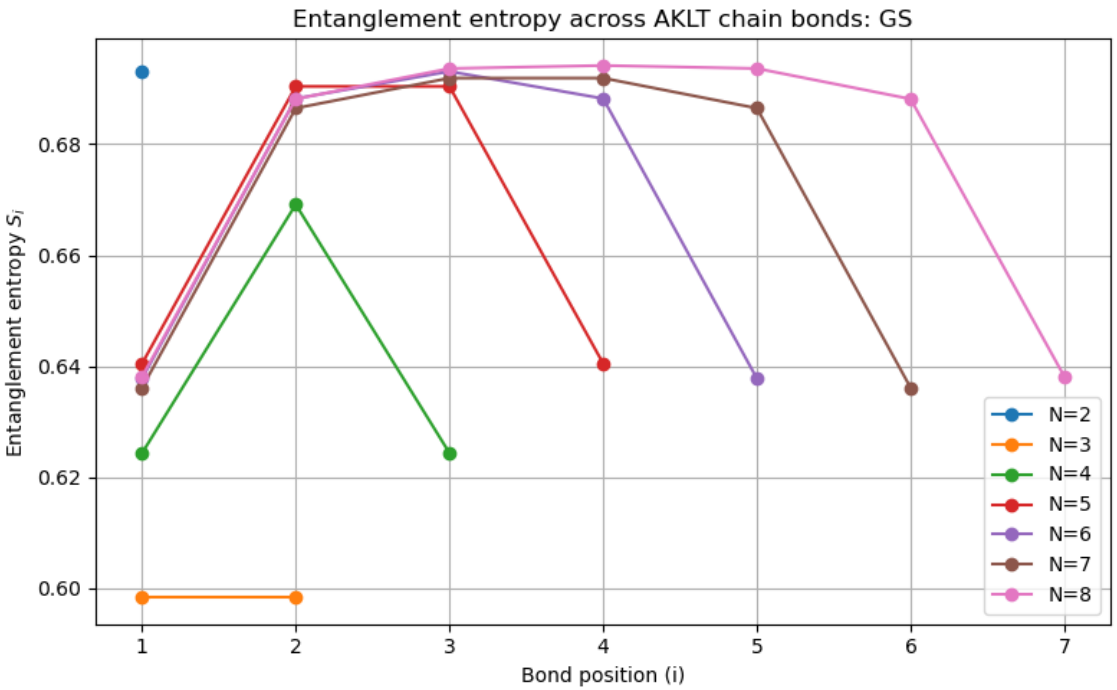
Repeat this procedure recursively to build the full MPS

$$|\psi\rangle = \sum_{\sigma_1 \ldots \sigma_L} A^{\sigma_1} A^{\sigma_2} \ldots A^{\sigma_L} |\sigma_1, \ldots, \sigma_L\rangle.$$

Computational cost: For the full tensor it was $\mathcal{O}(d^L)$ for the MPS with bond dimension m then $\mathcal{O}(Ldm^2)$

Entanglement

The AKLT Hamiltonian structure naturally leads to a Matrix Product State (MPS) representation with finite bond dimension $D = 2$. Since each internal bond cuts one singlet, the entanglement entropy across any internal cut is equal to the maximal entropy of a singlet pair, which corresponds to $\log 2$.



TeNPy library

TeNPy (Tensor Network Python) is a Python library for the simulation of strongly correlated quantum systems with tensor networks.
We used:

- From `tenpy.models` the AKLT model
- From `tenpy.networks.mps` we use the MPS and the MPO
- From `tenpy.algorithms` we use the TEBD and the DMRG

Philosophy of the library: good readability and usability for newcomers, and at the same time powerful algorithms and fast development of new algorithms for experts. [2]

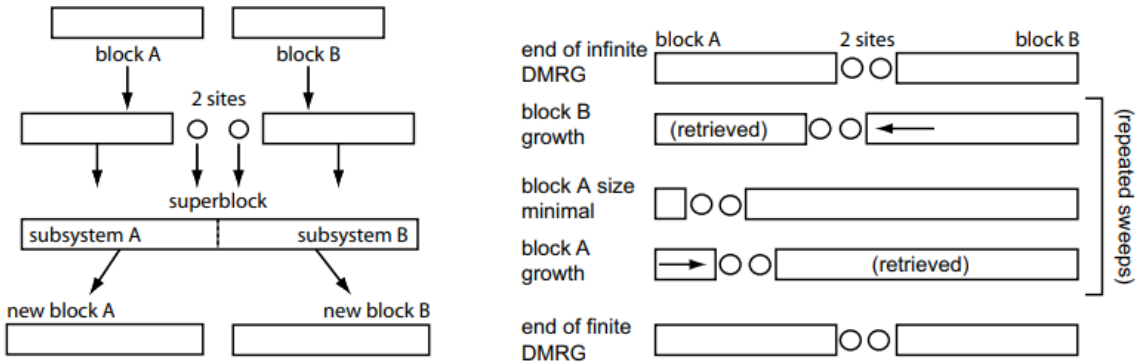


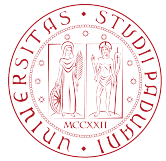
Figure: iDMRG and DMRG diagram from [3]

DMRG using MPS with TeNPy

With TeNPy: Not required to build finite DMRG from iDMRG

1. Start from a random MPS: Defined a chain of products as `psi = [0.0] * L`, got the MPS using `MPS.from_product_state()`, evolved randomly the state using `RandomUnitaryEvolution()`
2. Model definition: Constructed with `AKLTChain({'L': L, 'bc_MPS': 'finite'})`
3. Initialize the DMRG parameters
4. We used the Two site DMRG model

Search of 1st excited state



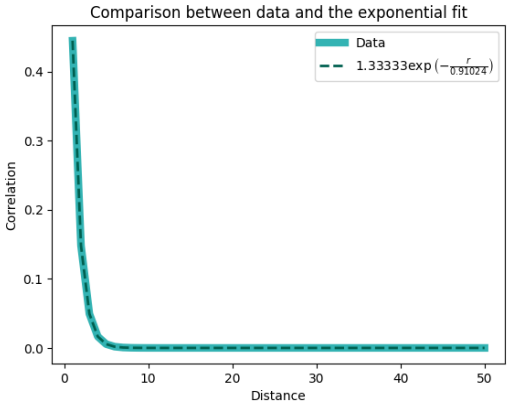
- Start from a biased initial state: end spins random and bulk are 0

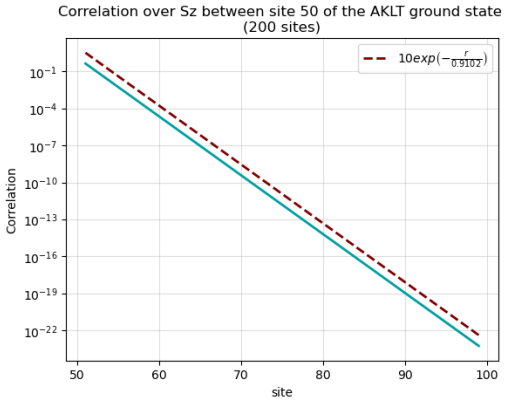
```
biased_states = [i]+["0.0"] * (L - 2)+[j]
```

- Run the DMRG with initial state using the biased MPS to find low-energy states.
  - If the resulting state has energy close to the expected ground state energy, we store it as a ground state candidate and keep looking while asking for orthogonality
  - Eventually, DMRG is forced to find a state orthogonal to all known ground states. DMRG always sees to minimize energy, but under the orthogonality constraint, it converges to the lowest excited state
- **Some results:** with open boundary conditions (OBC) the ground state energy is $-\frac{2}{3} \cdot (L-1)$ for the 1st excited state is GS + 0.7, which is exactly what we found for the gap energy

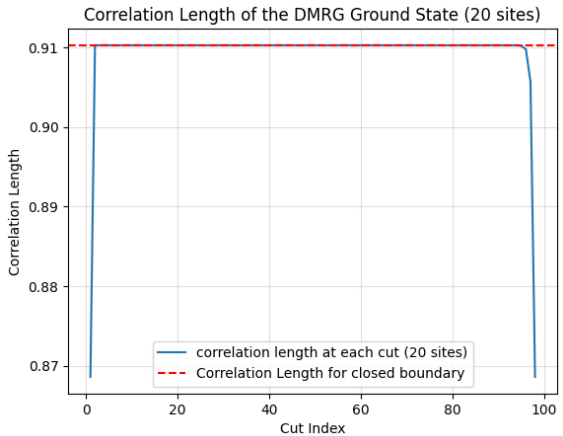
Correlation length

- Calculated using the correlation function $\langle S_i^z, S_j^z \rangle$ from the middle to the outside end of the chain

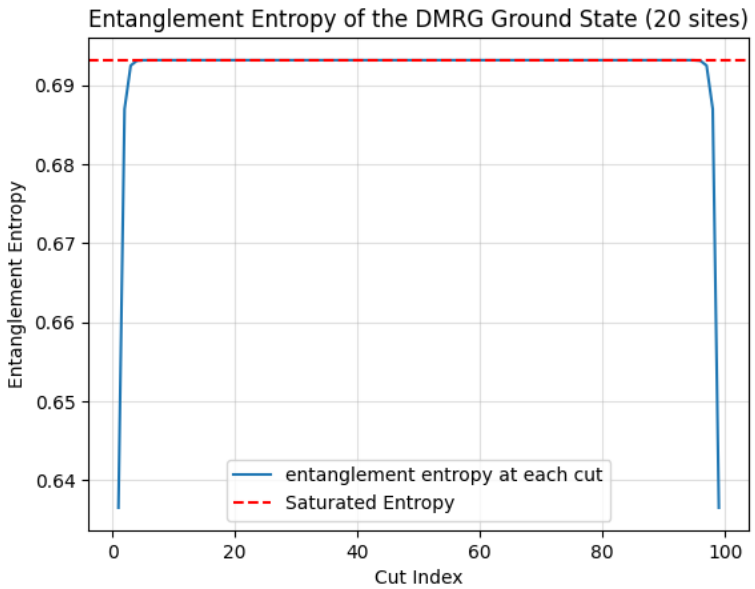




- Getting the transfer matrix for each of the MPS matrices



Entanglement entropy



Time evolving block decimation (TEBD)

Steps:
1. Initialization: start from a random normalized MPS with shapes $(1, d, \chi)...(\chi, d, \chi)...(\chi, d, 1)$ where d is the site dimension and χ the bond dimension
2. Evolve: Uses the methods:

- *time_evolution_operator* which builds $U(t) = \exp(-Ht)$
- *Trotter-Suzuki Decomposition:* Second order Trotter-Suzuki decomposition $e^{(V+W)\delta} = e^{V\delta/2}e^{W\delta}e^{V\delta/2} + \mathcal{O}(\delta^3)$. This method applied the decomposition to each bond using the Update method
- *Update:* For each bond the U(t) operator is applied to two contracted neighboring sites (A and B). Then SVD is applied, then truncation (max bond dimension =2), and then we update the evolved A and B

NOTE: The AKLT Hamiltonian applies the same projector on each bond — it's uniform and translationally invariant no even/odd splitting needed.
NOTE: We use imaginary-time evolution (non-unitary), so the canonical form is not preserved $\Rightarrow$ re-canonicalize at every step.

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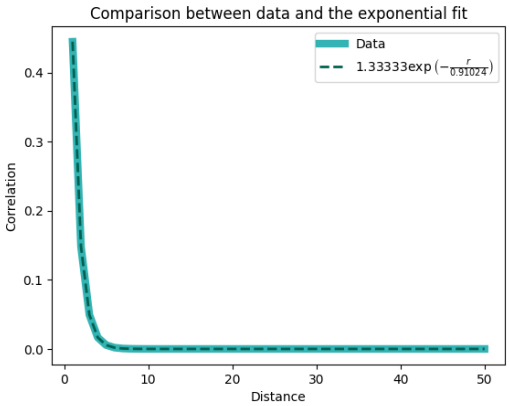

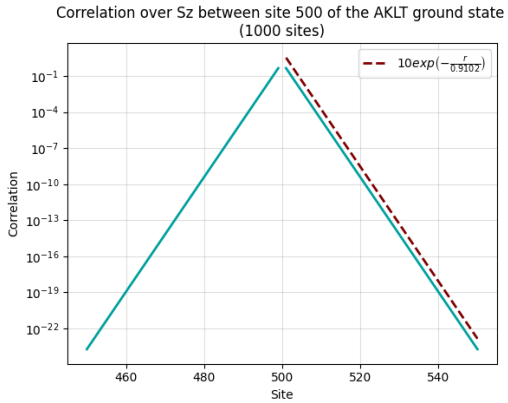

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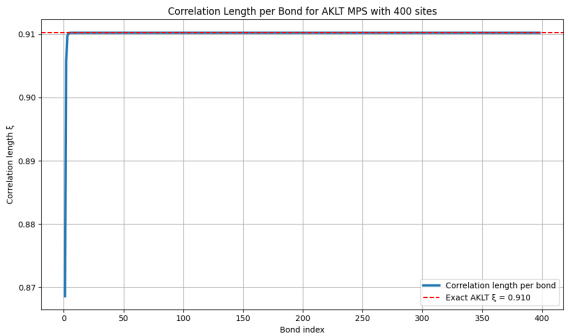
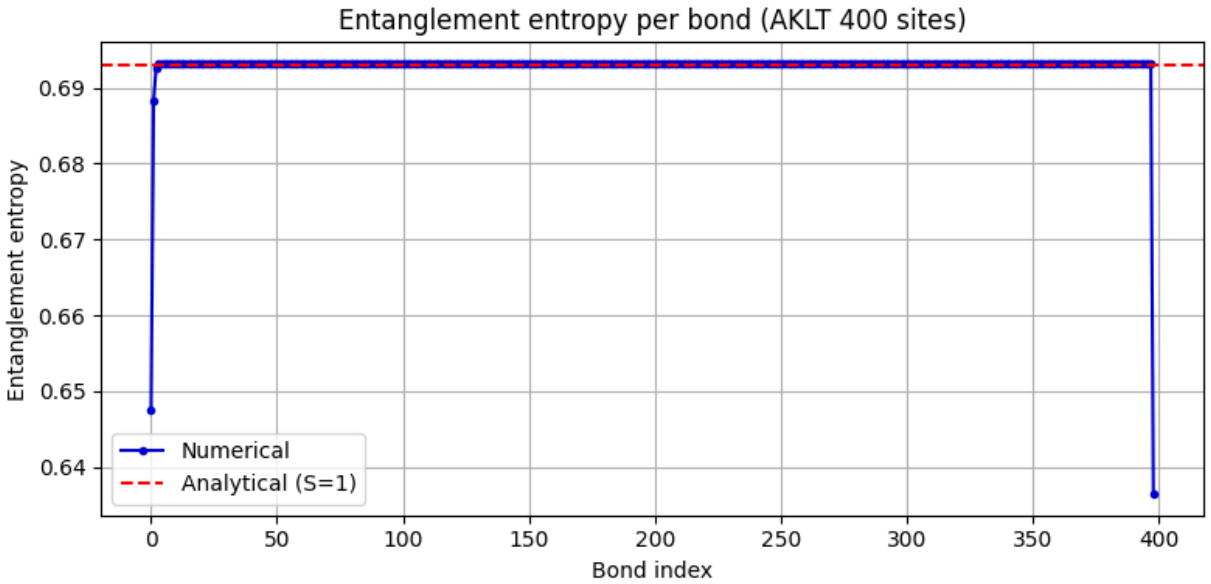
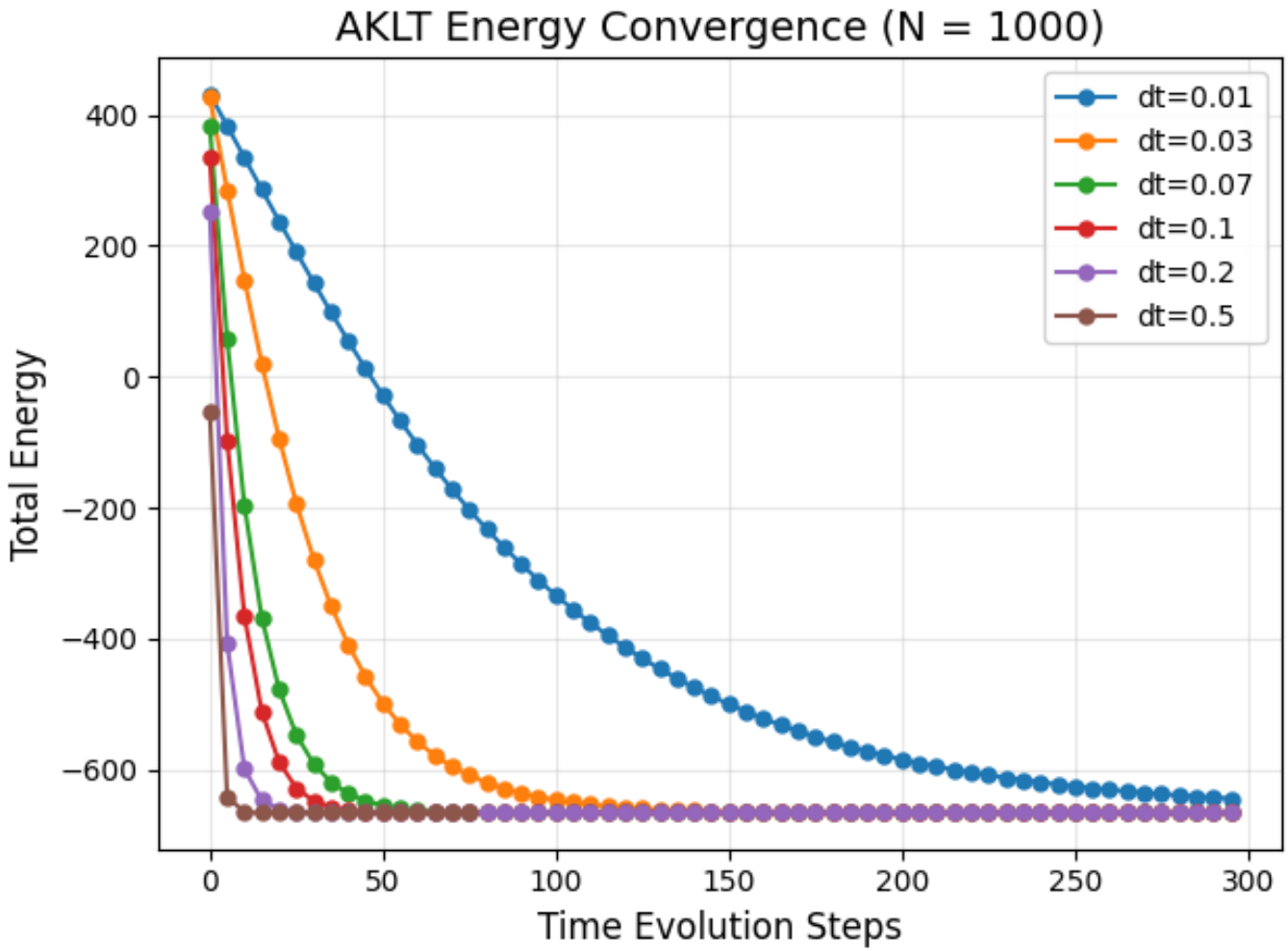


Entropy

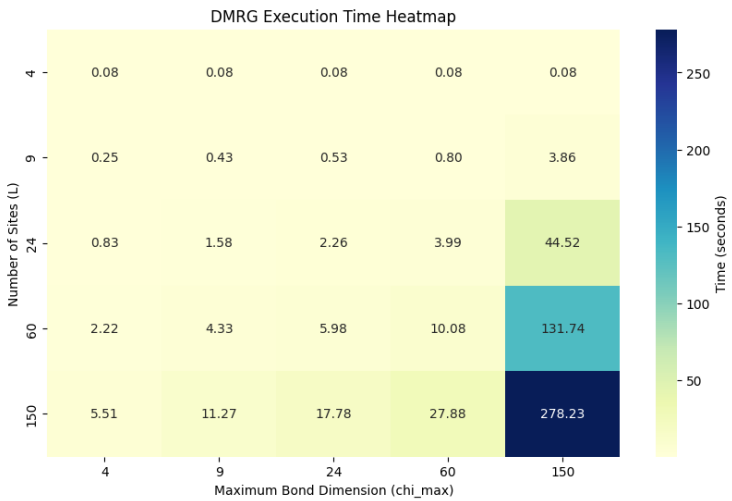


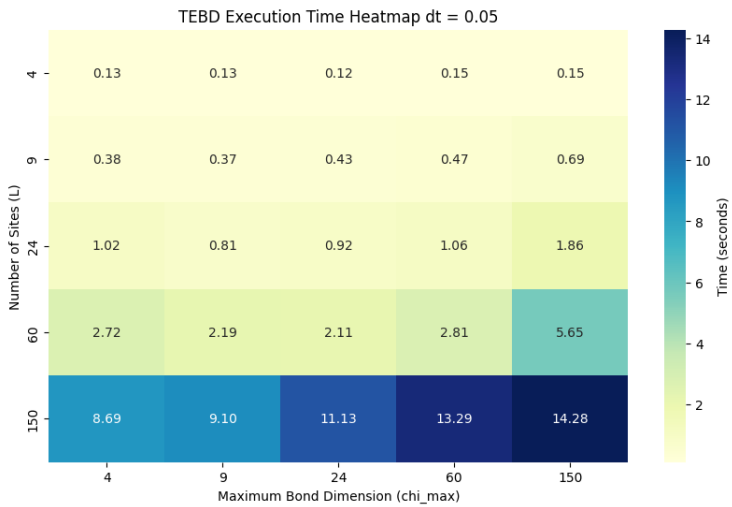
Ground state energy convergence



Computational cost

- The computational cost of the DMRG scales as $\mathcal{O}(ND^3)$, where N is the number of sites in the system and D is the bond dimension of the MPS.
- For the TEBD applied to a finite system, the computational cost per time step similarly scales as $\mathcal{O}(ND^3)$, assuming nearest-neighbor interactions and a second-order Trotter decomposition.





References

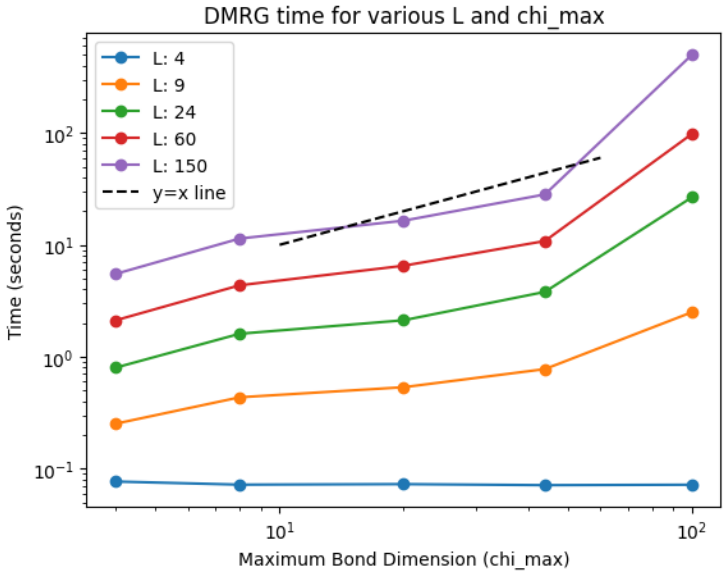
[1] A. Akhtar and N. Regnault. A Practical Introduction to Quantum Many-Body Simulation and Matrix Product States.

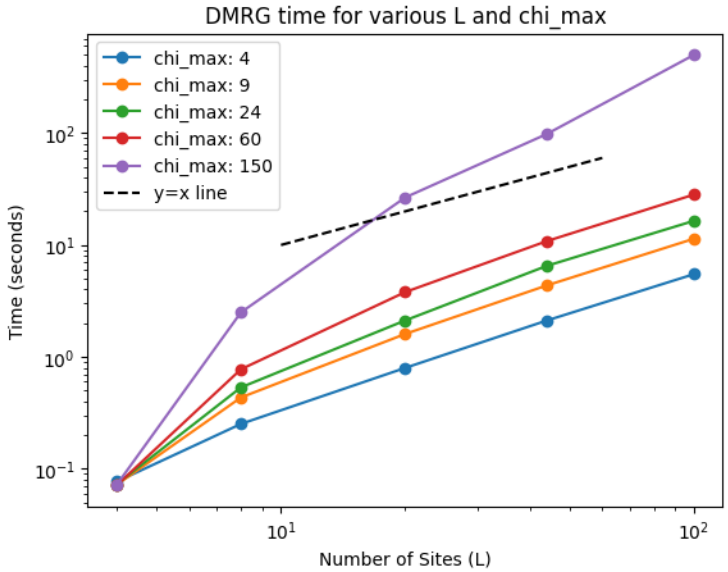
[2] J. Hauschild, J. Unfried, S. Anand, and et al. Tensor network Python (TeNPy) version 1. *SciPost Physics Codebases*, Nov. 2024. Publisher: Stichting SciPost.

[3] U. Schollwoeck. The density-matrix renormalization group in the age of matrix product states. *Annals of Physics*, 326(1):96–192, Jan. 2011. arXiv:1008.3477 [cond-mat].

[4] F. Verstraete, J. I. Cirac, and V. Murg. Matrix Product States, Projected Entangled Pair States, and variational renormalization group methods for quantum spin systems. *Advances in Physics*, 57(2):143–224, Mar. 2008. arXiv:0907.2796 [quant-ph].

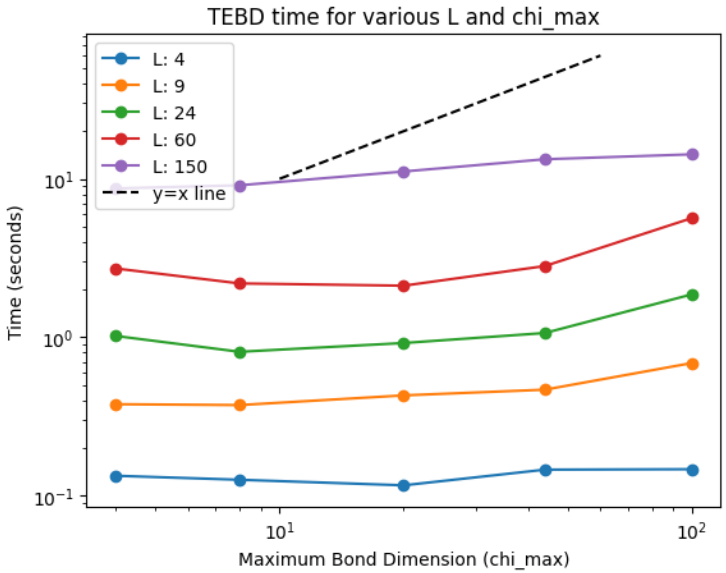
Backup slides (complexity)

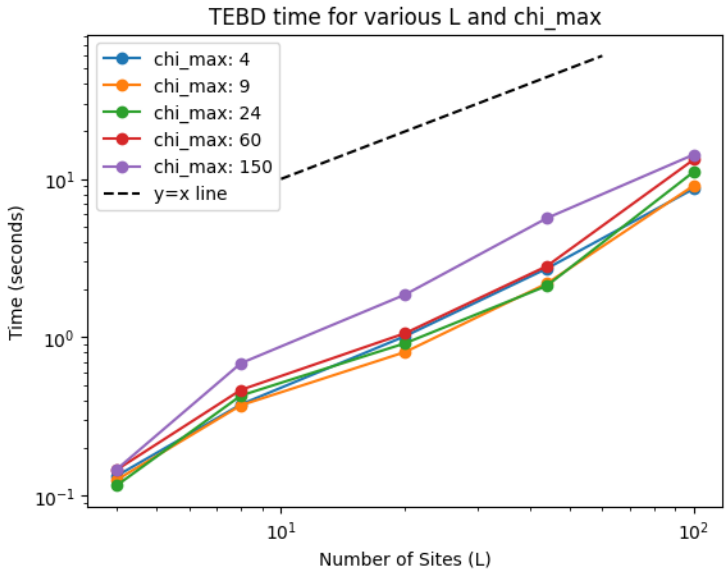




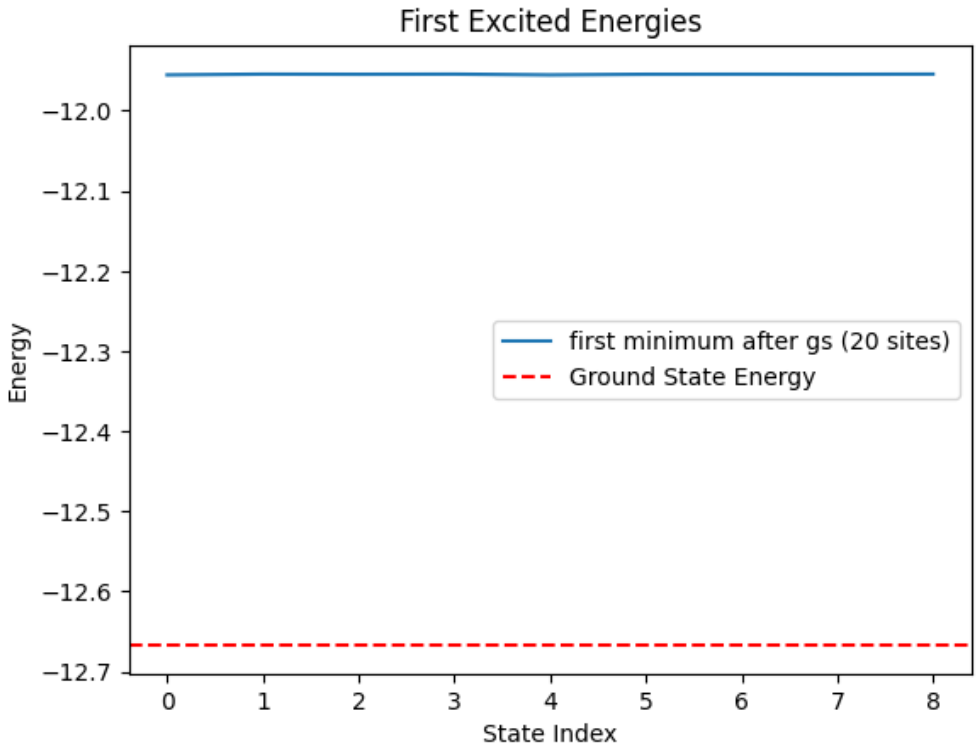
- There are two main reasons for not seeing the scaling with the bond dimension.
- The singular values are constantly being discarded and bond dimension reduced.
- Higher bond dimensions allow for better cpu utilization.

Backup slides (complexity)





Backup slides (1st excited)



- The energy gap between the ground state and the first excited state was found to be around 0.7, varying with the total number of sites