UNIVERSITÀ
DEGLI STUDI
DI PADOVA

Road to Fluxonium implementation

Quantum information and Computing

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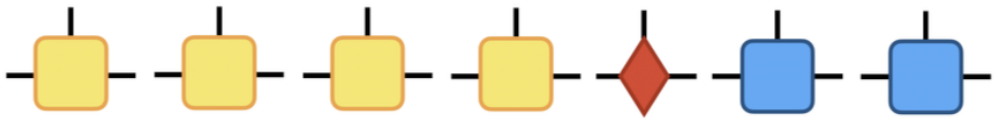
Table of contents

MPS and MPO

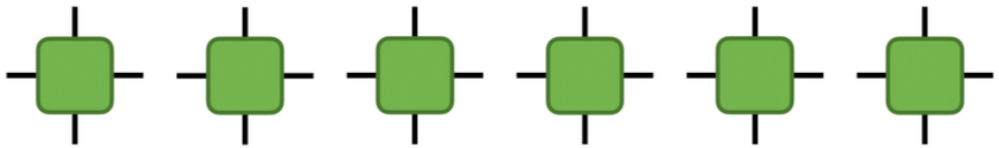
MPS:

$$|\psi\rangle = \sum_{\{\sigma_j\},\{a_j\}} A^{[1]\sigma_1}_{a_1} A^{[2]\sigma_2}_{a_1 a_2} \cdots A^{[N-1]\sigma_{N-1}}_{a_{N-2} a_{N-1}} A^{[N]\sigma_N}_{a_{N-1}} |\sigma_1 \sigma_2 \cdots \sigma_N\rangle$$



MPO:

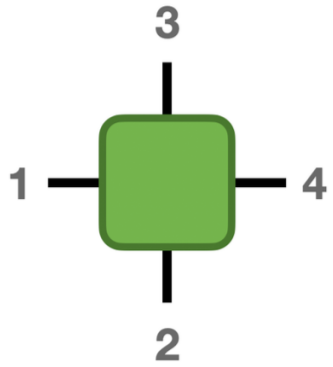
$$H = \sum_{\sigma'_1 \ldots \sigma'_N} \sum_{\sigma_1 \ldots \sigma_N} \sum_{b_1 \ldots b_{N-1}} H^{[\sigma'_1 \sigma_1]}_{b_1} H^{[\sigma'_2 \sigma_2]}_{b_1 b_2} \ldots H^{[\sigma'_N \sigma_N]}_{b_{N-1}} |\sigma'_1 \sigma'_2 \ldots \sigma'_N\rangle\langle\sigma_1 \sigma_2 \ldots \sigma_N|$$



How to build the MPO (1)

Ising Hamiltonian for a chain of spins:

$$\hat{H}^{tot}_{\text{Ising}} = -J \sum_{\langle i,j \rangle} \hat{S}^z_i \hat{S}^z_j - H \sum_i \hat{S}^x_i$$



Single tensor in the MPO:

$$H^{[\sigma'_i \sigma_i]}_{b_j b_{j+1}} = \begin{pmatrix} \hat{\mathbb{I}} & \hat{S}_z & -H\hat{S}_x \\ \hat{\mathbb{0}} & \hat{\mathbb{0}} & -J\hat{S}_z \\ \hat{\mathbb{0}} & \hat{\mathbb{0}} & \hat{\mathbb{I}} \end{pmatrix}$$

- 1 and 4: bond dim. (χ).
- 2 and 3: physical dim. (d).
- rank 4: $(\chi \times \chi \times d \times d)$.

How to build the MPO (2)

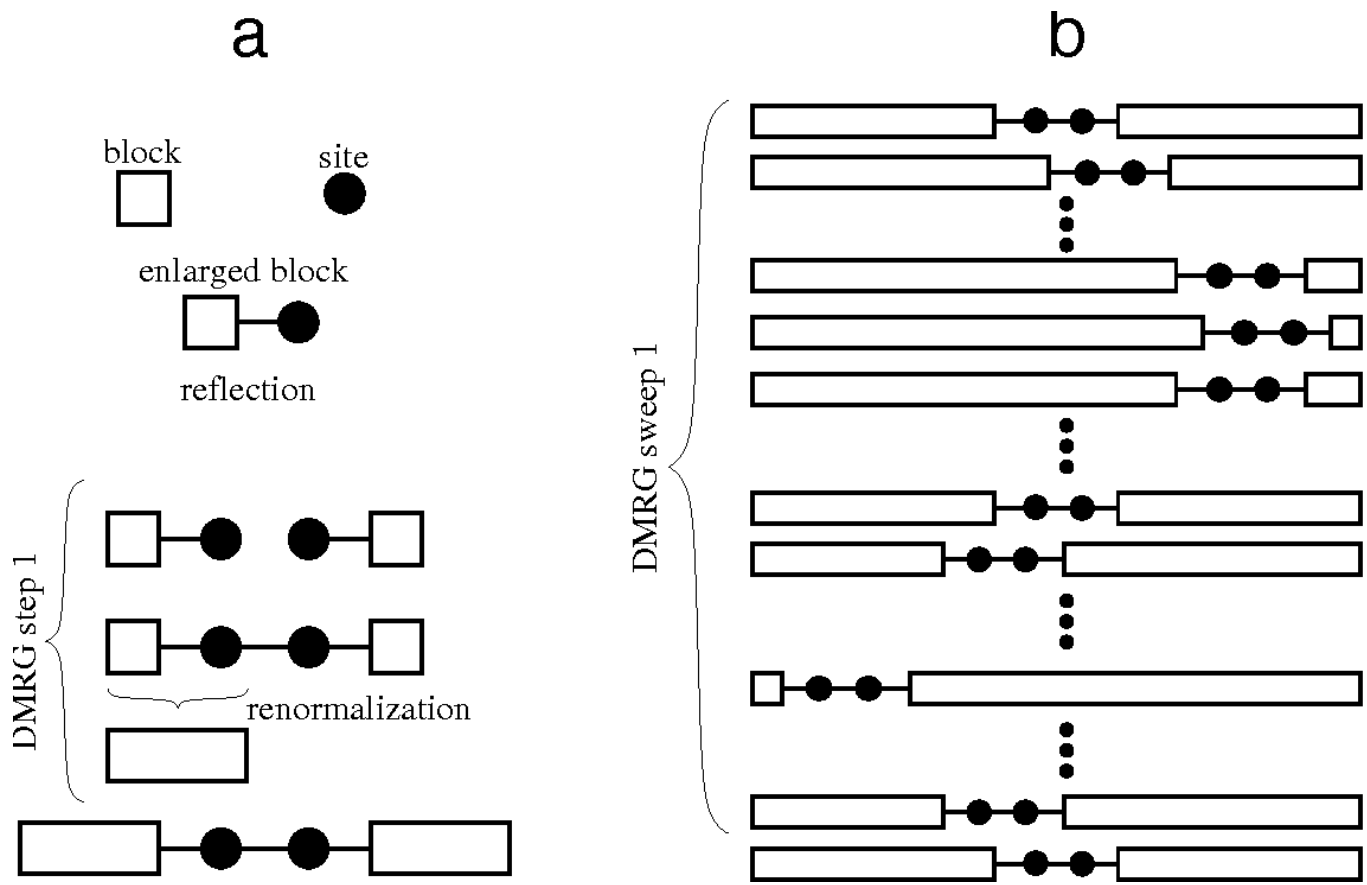
In the case of Open Boundary Condition (OBC) the first and the last tensor need to be contracted as shown below:

$$\begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{\mathbb{I}} & \hat{S}_z & -H\hat{S}_x \\ \hat{\mathbb{O}} & \hat{\mathbb{O}} & -J\hat{S}_z \\ \hat{\mathbb{O}} & \hat{\mathbb{O}} & \hat{\mathbb{I}} \end{pmatrix} \begin{pmatrix} \hat{\mathbb{I}} & \hat{S}_z & -H\hat{S}_x \\ \hat{\mathbb{O}} & \hat{\mathbb{O}} & -J\hat{S}_z \\ \hat{\mathbb{O}} & \hat{\mathbb{O}} & \hat{\mathbb{I}} \end{pmatrix} \dots \begin{pmatrix} \hat{\mathbb{I}} & \hat{S}_z & -H\hat{S}_x \\ \hat{\mathbb{O}} & \hat{\mathbb{O}} & -J\hat{S}_z \\ \hat{\mathbb{O}} & \hat{\mathbb{O}} & \hat{\mathbb{I}} \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

The product of the matrices should yield the exact Hamiltonian of the system

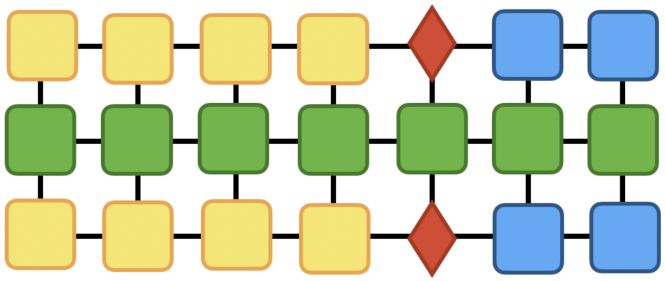
Infinite vs Finite DMRG

Infinite(a) vs Finite(b) DMRG



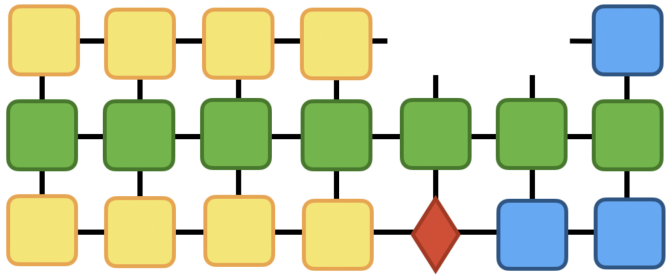
Finite DMRG (1)

1) The initial network is shown below, where the initial MPS is randomly generated.



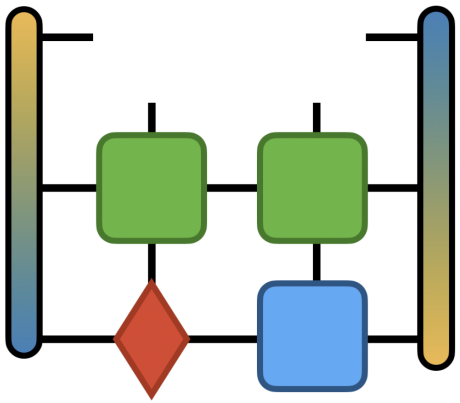
The initial MPS must be in the canonical form with the orthogonality center (red diamond) in the i-th position.

2) Select the i-th and (i+1)-th sites, one of which must be the center of orthogonality. Remove those sites with a partial derivative, so that the network can be variationally optimized.



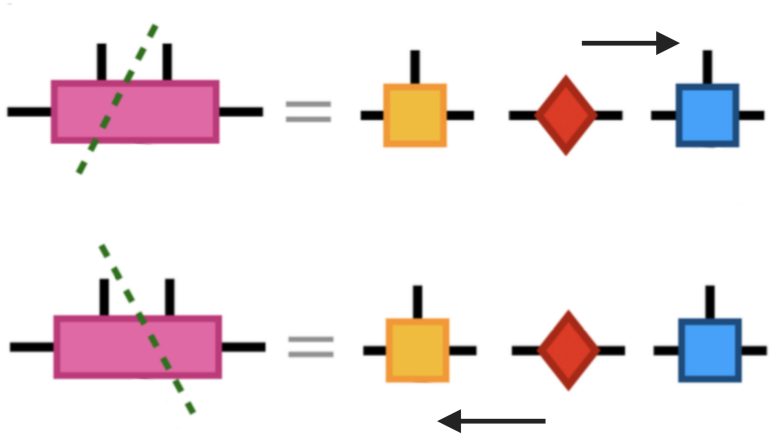
Finite DMRG (2)

3) Contract the tensors. The tensor on the left represents the left environment. Same thing for the right.



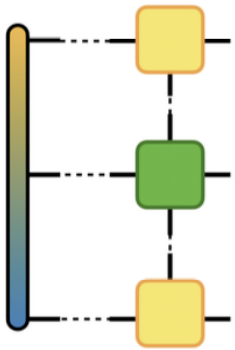
4) Apply Lanczos to update the tensors (discussed later).

5) Apply the SVD to the output of the Lanczos algorithm. And move the orthogonality center on the right/left (depending on the sweep).



Finite DMRG (3)

6) Substitute the optimized tensors in the previous MPS and update the left/right environment (if you are moving to the right/left).



7) Repeat 2,3,4,5 and 6 scanning back and forth across the lattice until a set number of iterations (called sweeps) or until some relevant quantities reach convergence.

Lanczos algorithm (1)

Start with a random vector: $|\psi_1\rangle \in \mathbb{C}^n$.

For $i = 1$:

$$\alpha_1 = \langle\psi_1|\mathcal{H}|\psi_1\rangle \qquad \beta_1 = 0$$

$$\phi_1 = \mathcal{H}|\psi_1\rangle - \alpha_1|\psi_1\rangle$$

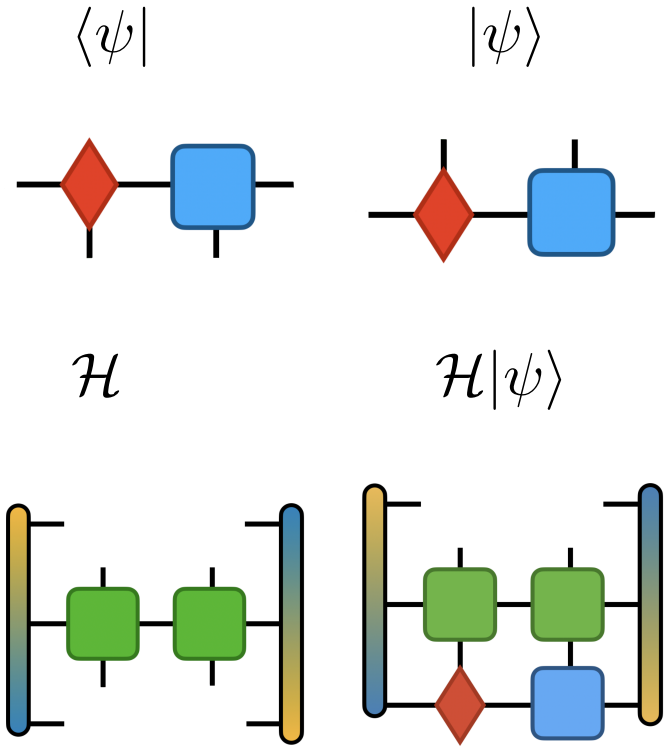
For $i = 2, ..., m$:

$$\beta_i^2 = \langle\phi_{i-1}|\phi_{i-1}\rangle$$

$$|\psi_i\rangle = |\phi_{i-1}\rangle/\beta_i$$

$$\alpha_i = \langle\psi_i|\mathcal{H}|\psi_i\rangle$$

$$\phi_i = \mathcal{H}|\psi_i\rangle - \alpha_i|\psi_i\rangle - \beta_i|\psi_{i-1}\rangle$$



Lanczos algorithm (2)

At the end of the procedure, the Hamiltonian in the Krylov subspace takes the tridiagonal form (in our case, only 2 iterations are needed):

$$\mathcal{M} = \begin{pmatrix} \alpha_1 & \beta_2 & 0 & \cdots \\ \beta_2 & \alpha_2 & \beta_3 & \cdots \\ 0 & \beta_3 & \alpha_3 & \ddots \\ \vdots & \vdots & \ddots & \ddots \end{pmatrix}$$

$$\mathcal{M} = U\mathbf{D}U^{\dagger}$$

$$|\psi_{GS}^{optimized}\rangle = (U_{[1,1]})^*|\psi_1\rangle + (U_{[2,1]})^*|\psi_2\rangle + \cdots + (U_{[m,1]})^*|\psi_m\rangle$$

Ising implementation

Ising model Hamiltonian

$$\hat{H}^{\text{n.n.}}_{\text{Ising}} = \underbrace{-J \sum_i \hat{S}^z_i \hat{S}^z_{i+1}}_{\text{nearest neighbor}} \underbrace{- H \sum_i \hat{S}^x_i}_{\text{local}}$$

The Ising interaction is short-range due to nearest neighbor (n.n.)

Ising implementation

Ising model Hamiltonian

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The Ising interaction is short-range due to nearest neighbor (n.n.)

Ising model MPO

$$\text{MPO} = \begin{pmatrix} \hat{\mathbb{I}} & \hat{S}_z & -H\hat{S}_x \\ \hat{\mathbb{0}} & \hat{\mathbb{0}} & -J\hat{S}_z \\ \hat{\mathbb{0}} & \hat{\mathbb{0}} & \hat{\mathbb{I}} \end{pmatrix}$$

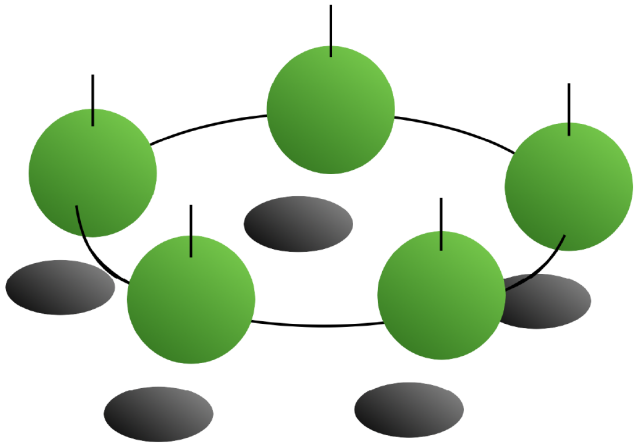
MPO bond dimensions are small (dim = 3) due to the Hamiltonian form

PBC (1)

Periodic Boundary Conditions (PBC):

- MPS non-physical dimension is constant

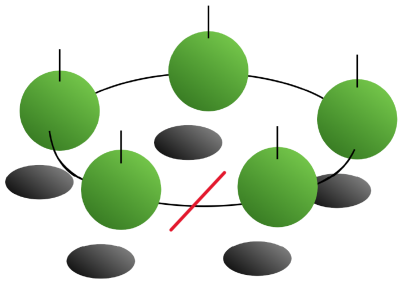
- MPS closed in a loop



PBC (2)

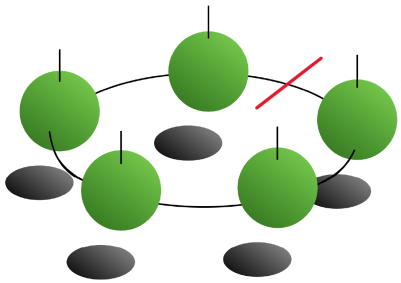
Operative way:

1. Cut the MPS in a specific position



2. Optimize the MPS using the normal Finite DMRG

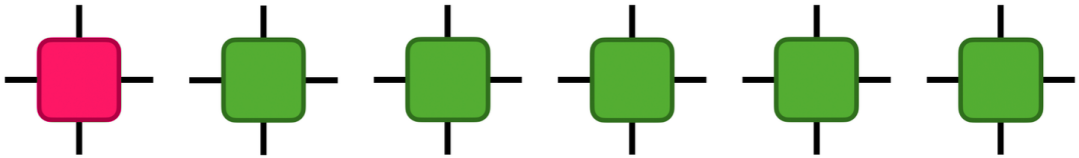
3. Cut the MPS in another (different) position



4. Repeat cut and optimize until energy converges

PBC and MPO (1)

To address the interaction between the initial and final links in the chain it is necessary to modify the MPO

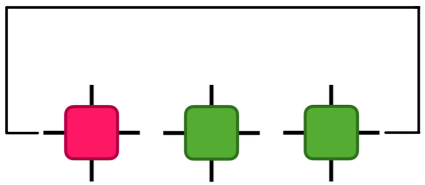


Let us consider the MPO for 3 sites:

$$= \begin{pmatrix} ? \end{pmatrix} \begin{pmatrix} \hat{\mathbb{I}} & \hat{S}_z & -H\hat{S}_x \\ \hat{\mathbb{0}} & \hat{\mathbb{0}} & -J\hat{S}_z \\ \hat{\mathbb{0}} & \hat{\mathbb{0}} & \hat{\mathbb{I}} \end{pmatrix} \begin{pmatrix} \hat{\mathbb{I}} & \hat{S}_z & -H\hat{S}_x \\ \hat{\mathbb{0}} & \hat{\mathbb{0}} & -J\hat{S}_z \\ \hat{\mathbb{0}} & \hat{\mathbb{0}} & \hat{\mathbb{I}} \end{pmatrix}$$

PBC and MPO (2)

The trace of the full contracted MPO must represent the correct Hamiltonian of the system (chain of 3 spins):



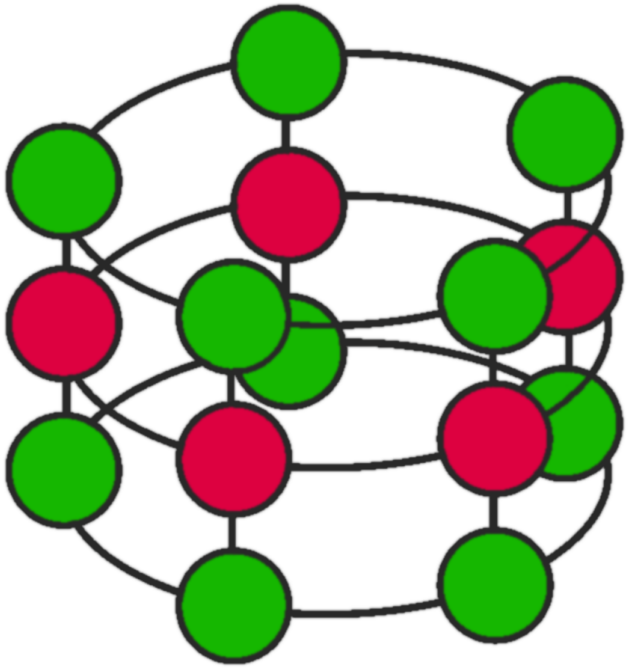
$$= -J\hat{S}_z^1\hat{S}_z^2 - J\hat{S}_z^2\hat{S}_z^3 - J\hat{S}_z^3\hat{S}_z^1 - H\hat{S}_x^1 - H\hat{S}_x^2 - H\hat{S}_x^3$$

$$\begin{pmatrix} \hat{\mathbb{O}} & \hat{\mathbb{O}} & \hat{\mathbb{O}} \\ -J\hat{S}_z & \hat{\mathbb{O}} & \hat{\mathbb{O}} \\ \hat{\mathbb{I}} & \hat{S}_z & -H\hat{S}_x \end{pmatrix} \begin{pmatrix} \hat{\mathbb{I}} & \hat{S}_z & -H\hat{S}_x \\ \hat{\mathbb{O}} & \hat{\mathbb{O}} & -J\hat{S}_z \\ \hat{\mathbb{O}} & \hat{\mathbb{O}} & \hat{\mathbb{I}} \end{pmatrix} \begin{pmatrix} \hat{\mathbb{I}} & \hat{S}_z & -H\hat{S}_x \\ \hat{\mathbb{O}} & \hat{\mathbb{O}} & -J\hat{S}_z \\ \hat{\mathbb{O}} & \hat{\mathbb{O}} & \hat{\mathbb{I}} \end{pmatrix}$$

$$\begin{pmatrix} \hat{\mathbb{O}} & \hat{\mathbb{O}} & \hat{\mathbb{O}} \\ -J\hat{S}_z^1 & -J\hat{S}_z^1\hat{S}_z^3 & J\hat{S}_z^1(H\hat{S}_x^3 + H\hat{S}_x^2 + J\hat{S}_z^2\hat{S}_z^3) \\ \hat{\mathbb{I}} & -J\hat{S}_z^3 & -H\hat{S}_x^3 - H\hat{S}_x^2 - H\hat{S}_x^1 - J\hat{S}_z^1\hat{S}_z^2 - J\hat{S}_z^2\hat{S}_z^3 \end{pmatrix}$$

The ANSATZ is correct.

PBC and MPO (3)



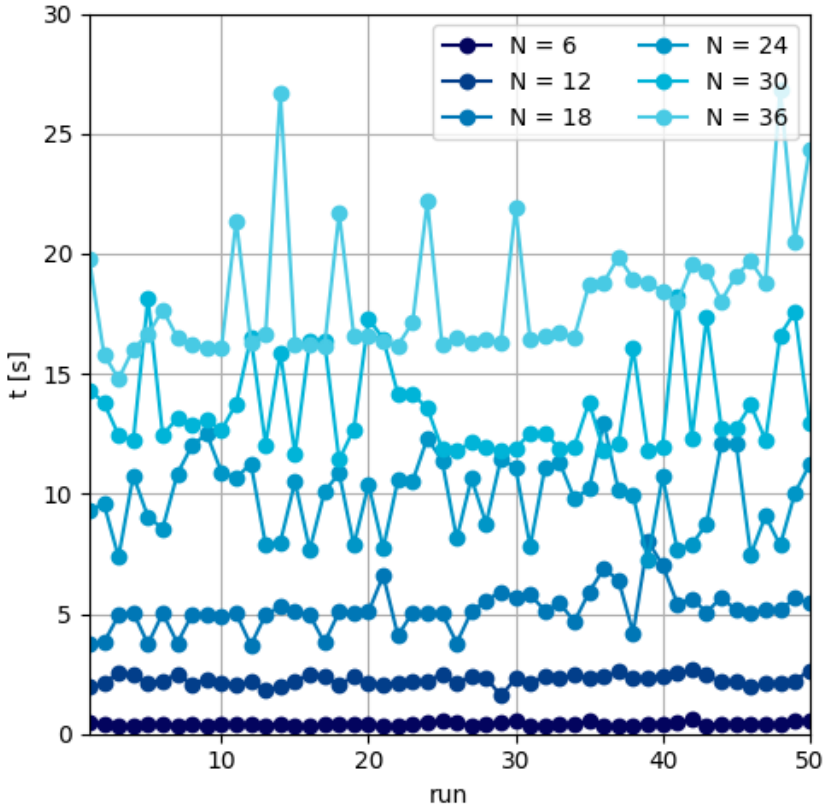
$\langle \psi_{tot} | \mathcal{H} | \psi_{tot} \rangle$

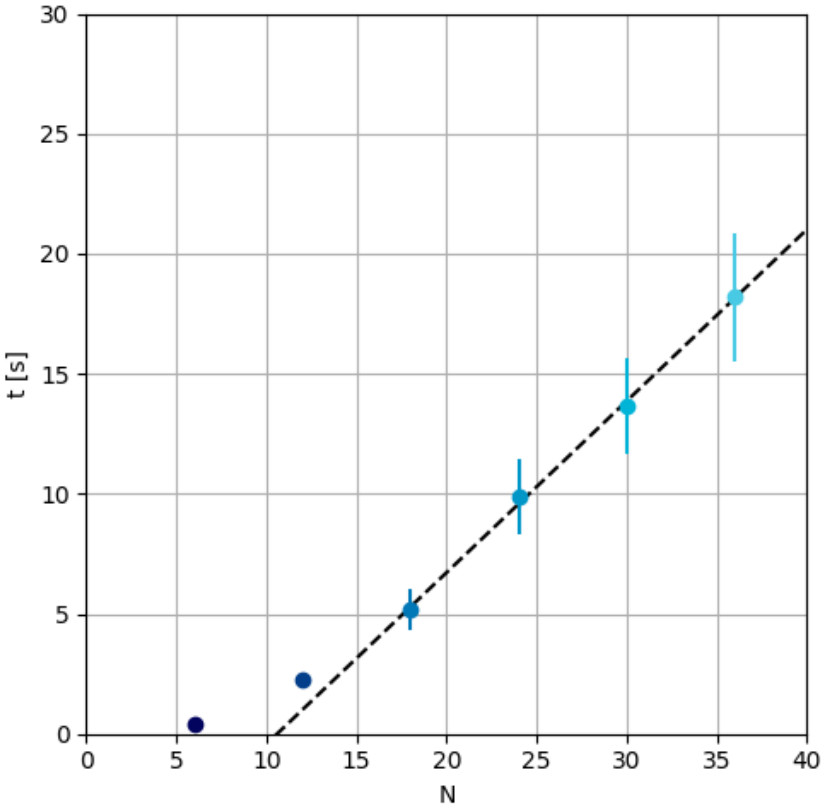
To verify the convergence of energy:

- Combine the MPS in one cycle (green)
- Normalize the MPS in this form
- Merge the modified MPO into one cycle (red)
- Contract everything

DMRG Results (Time)

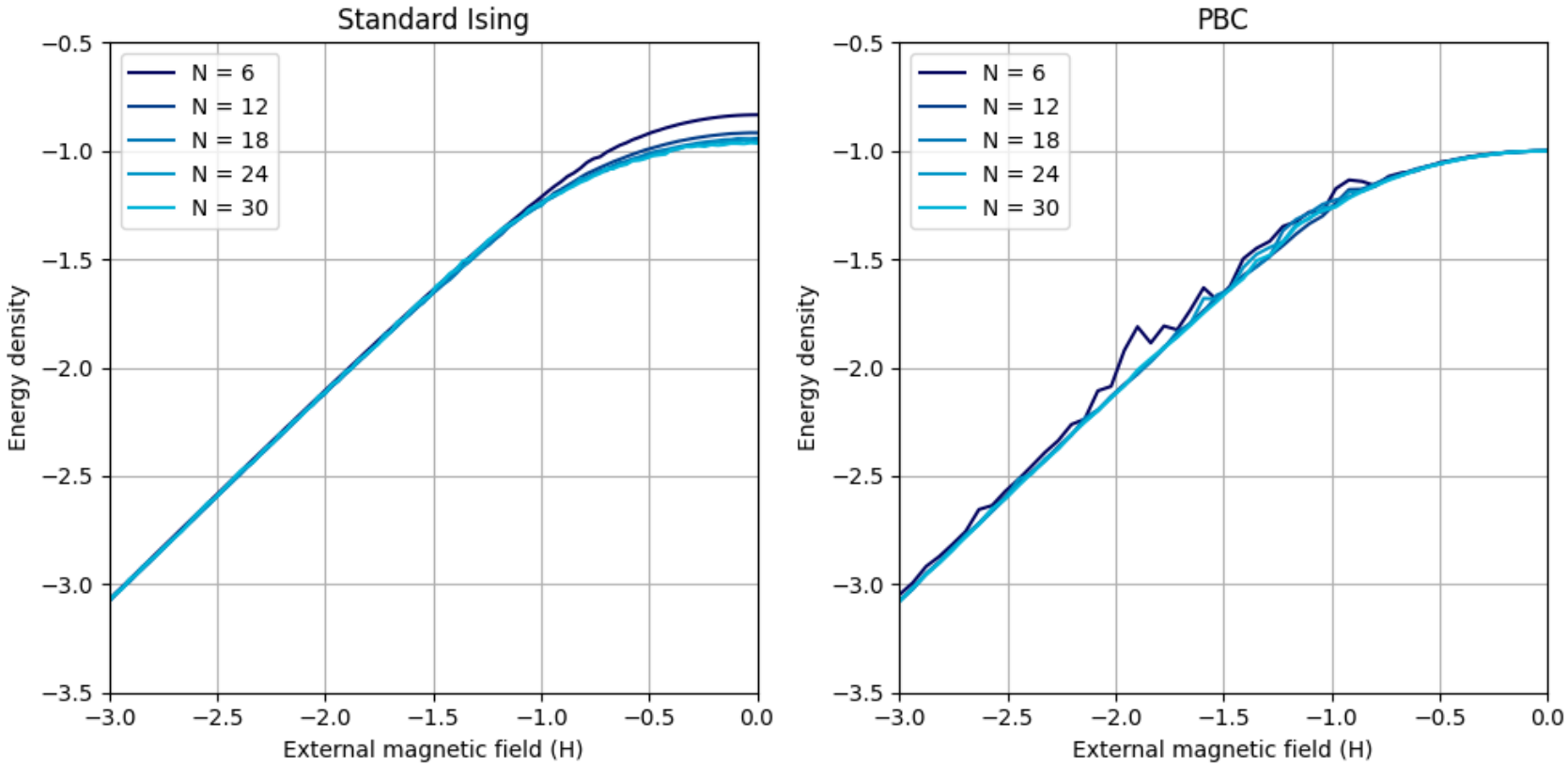
Time taken for the algorithm to run: linear behavior





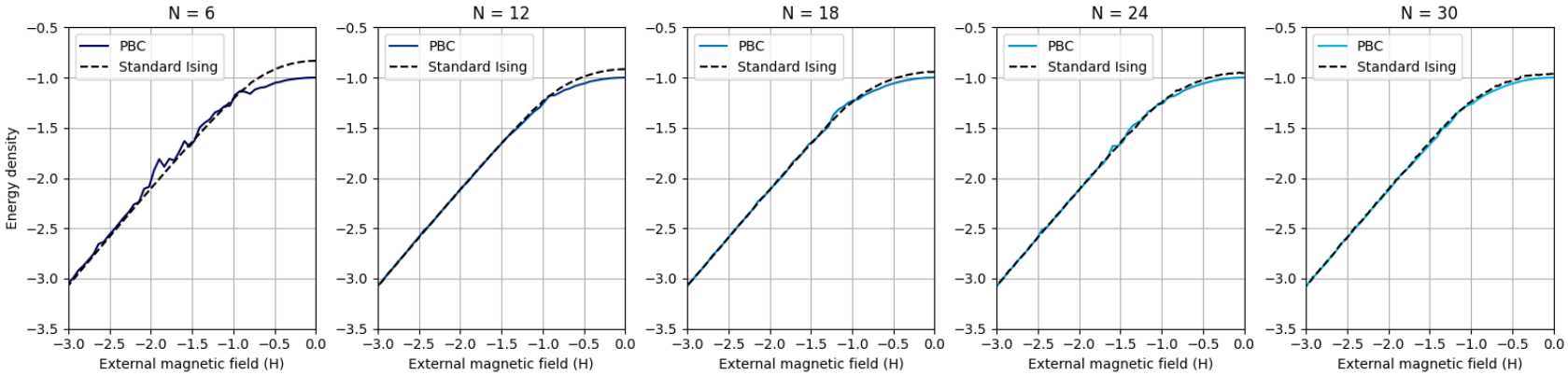
DMRG Results (Correctness)

Ground state energy for different values of the external field: go beyond the writable hamiltonian limit



DMRG Results (Correctness)

Comparison between the ground state with and without the PBC

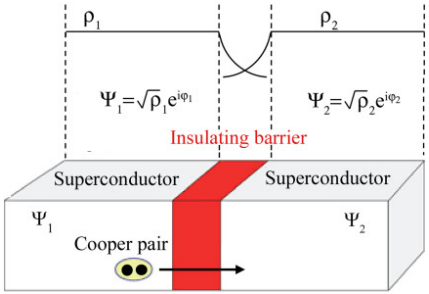


Attention: the results suffer of "over-oprimization" if the convergence limit $\epsilon = E_{new} - E_{old}$ is too small in the sweep optimization (impossible to eliminate for small N)

Attention: bond dimension $\chi = 1$ is sufficient to retrieve the ground state energy results

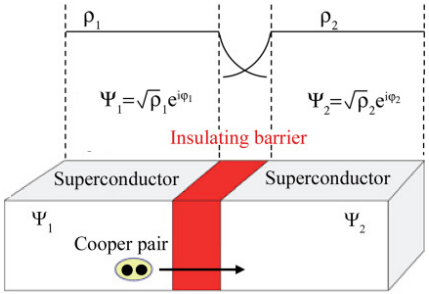
Fluxonium

Josephson Junction (JJ):



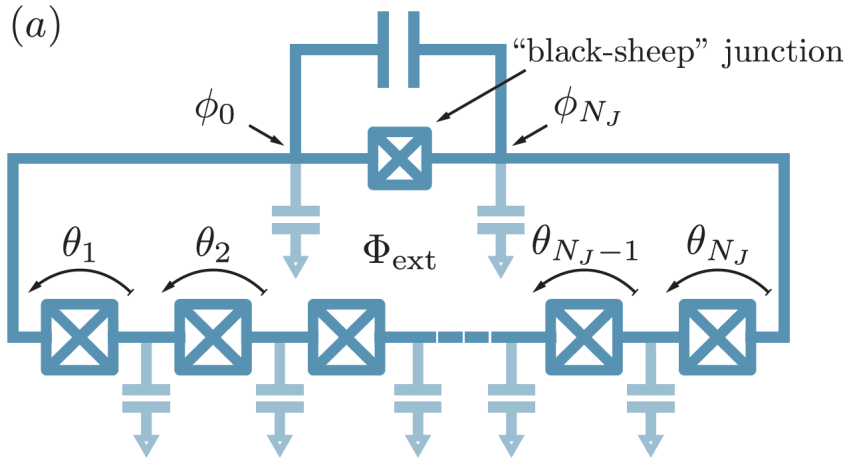
Fluxonium

Josephson Junction (JJ):



Fluxonium components:

- N Josephson Junctions
- Black-sheep Josephson Junction
- Shunted capacitances



Fluxonium

Strengths:

- big anharmonicity
- resistance to charge noise
- better control

Drowbacks:

- hard to compute theoretically
- hard to simulate

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Fluxonium Hamiltonian:

$$H = \sum_{i=1}^{N_j} H_{0,i} + \sum_{j} h g_{ij} \hat{n}_i \hat{n}_j - E_{J_B} \cos\left(\sum_{i=1}^{N_j} \theta_i + \phi_{\text{ext}}\right)$$

$$H_{0,i} = 4E_{C_i} \hat{n}_i^2 + E_{J_i} \cos(\theta_i)$$

Circuit quantization

Canonical quantization:

$$\begin{cases} \Phi \to \hat{\Phi} \\ Q \to \hat{Q} \end{cases} \to \begin{cases} \hat{\phi} = 2\pi\hat{\Phi}/\Phi_0 \\ \hat{n} = \hat{Q}/2e \end{cases}$$

Classical energy:

$$\text{Capacitance} \to C\dot{\Phi}^2/2$$

$$\text{Inductance} \to \dot{\Phi}^2/2L$$

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Classical energy:

$$\text{Capacitance} \to C\dot{\Phi}^2/2$$
$$\text{Inductance} \to \dot{\Phi}^2/2L$$

Fluxonium Lagrangian:

$$L(\phi,\dot{\phi}) = \frac{C_{J_B}}{2}(\dot{\phi}_N - \dot{\phi}_0)^2 + \sum_{i=1}^{N_j} C_{ij}(\dot{\phi}_i - \dot{\phi}_{i-1})^2 + \sum_{i=0}^{N_j} \frac{C_{0_i}}{2}\dot{\phi}_i^2 + \sum_{i=1}^{N_j} E_{J_i} \cos\left(\frac{\phi_i - \phi_{i-1}}{\phi_0}\right) + E_{J_B}\cos\left(\frac{\phi_N - \phi_0 + \phi_{\text{ext}}}{\phi_0}\right)$$

Fluxonium MPO

Fluxonium Hamiltonian:

$$H = \sum_{i=1}^{N_j} H_{0,i} + \underbrace{\sum_{j} h g_{ij} \hat{n}_i \hat{n}_j}_{\text{All-to-all}} - E_{J_B} \cos\left(\sum_{i=1}^{N_j} \theta_i + \phi_{\text{ext}} \right)$$

We were not able to implement the all-to-all connection in an optimized way

Conclusions

Topics of our project:

- How to write MPS and orthogonality center handling
- How to write MPO with and without PBC
- Finite DMRG algorithm using Lanczos in both the canonical way and the tensor network implementation
- Circuit quantization and fluxonium description

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Further developments:

- How to shrink the MPO operator for the all-to-all connection
- Implement Block-Lanczos in DMRG algorithm

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