Quantum State Initialization:
Approximating Hamiltonian Eigenstates by One- and Two-Qubit Gates

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Outline

- Quantum many body system and Matrix Product State (MPS)
- From MPS to Quantum Circuit
- Variational Energy Optimization
- MPO Bond Dimension Scaling
- Numerical Results and Summary

Motivation : State Preparation Challenges

1. Dimension Scaling

- Hilbert space grows exponentially with the system size N, exponential Dimension Scaling d^N.

2. Non-Unitary Operation

- Physical quantum gates are unitary. However, algorithms like Imaginary Time Evolution (ITE), operator $e^{-H\tau}$ is not unitary.

Unitary Matrix: $U^{\dagger}U = I$

ITE: $U(\tau) = e^{-H\tau}$

$U^{\dagger}(\tau) = e^{-H\tau}$

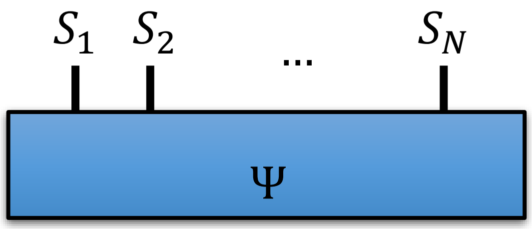
$U(\tau)^{\dagger}U(\tau) = e^{-2H\tau} \neq I$

➢ Tensor Network is used as a Solution.

Matrix Product State

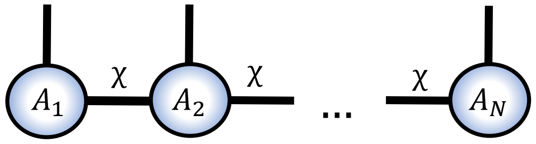
- Quantum many-body system of N particles $|\Psi\rangle = \sum_{s_1,s_2,\dots,s_N} \Psi_{s_1,s_2\dots,s_N} |s_1, s_2, \dots, s_N\rangle$

Total Dimension : d^N



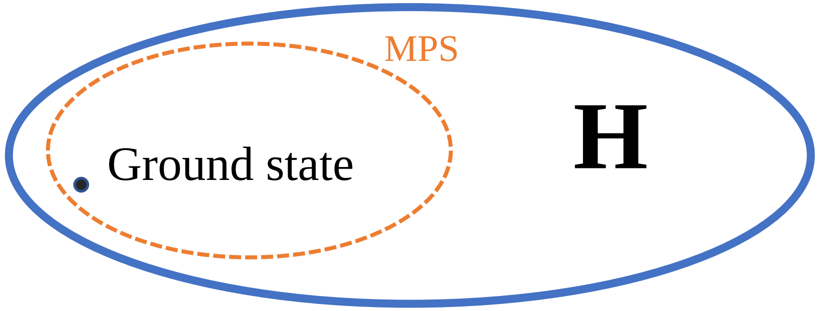
- Matrix Product State (MPS) $\Psi^{s_1 s_2 \dots s_N} = \sum_{\alpha_1,\alpha_2,\dots,\alpha_{N-1}} A^{(1)s_1}_{\alpha_1} A^{(2)s_2}_{\alpha_1\alpha_2} \dots A^{(N)s_N}_{\alpha_{N-1}}$

Total Dimension : $N \times d \times \chi^2$



- good approximation for ground state

- area laws of entanglement entropy



Hastings, Matthew B. *Journal of statistical mechanics: theory and experiment* 2007.08 (2007): P08024-P08024.

Ground State Preparation

◆ We want to prepare the ground state on quantum device, but the dimension of qubit is 2.

Ground State Representation (MPS) :

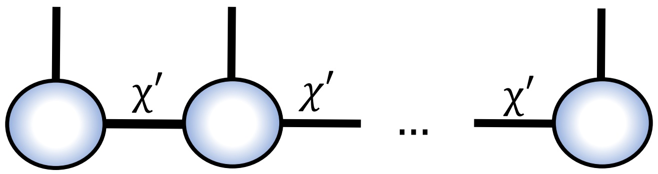
<u>High Bond Dimension MPS</u>

- can represent exact ground state
- cannot directly implement on quantum device

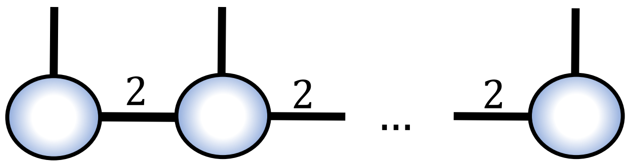
<u>MPS Bond Dimension = 2</u>

- has same dimension as qubit
- single layer is not enough to capture full ground state entanglement

$|\Omega\rangle_{\chi'}$ χ': large number



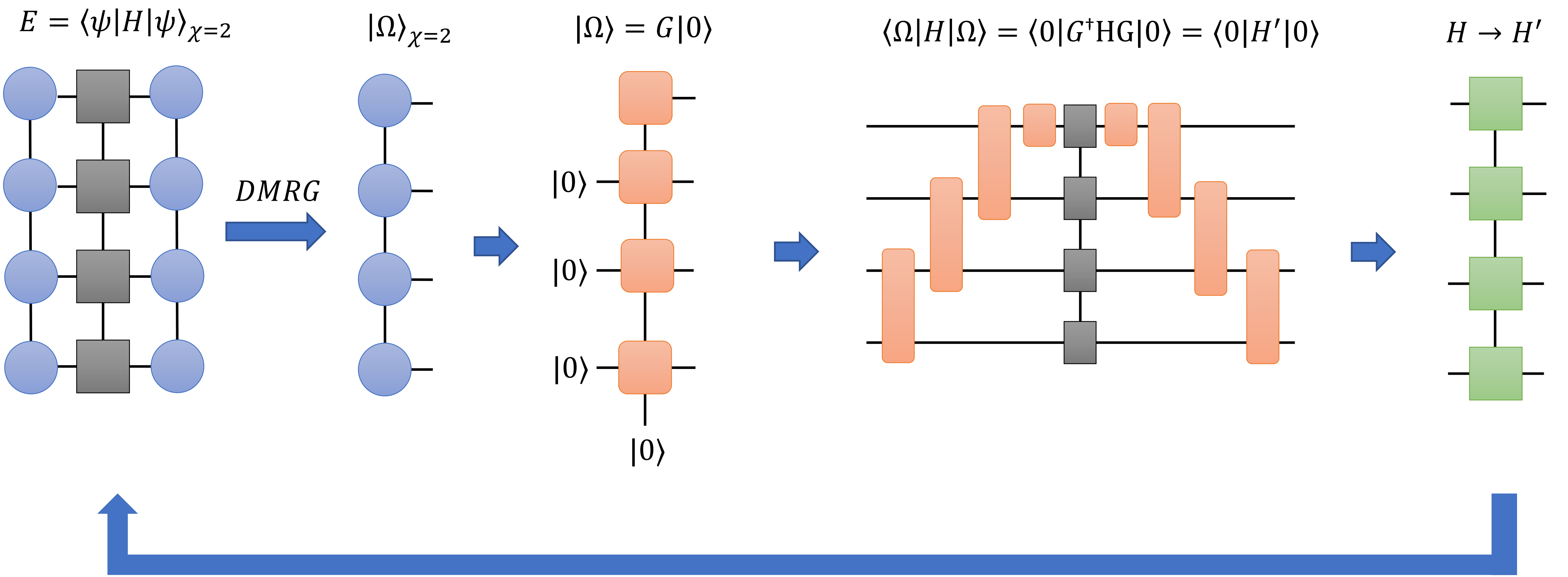
$|\Omega\rangle_{\chi=2}$



➢ Increasing circuit depth (with $\chi = 2$) to represent the high bond dimension ground state .

Research Steps Flowchart

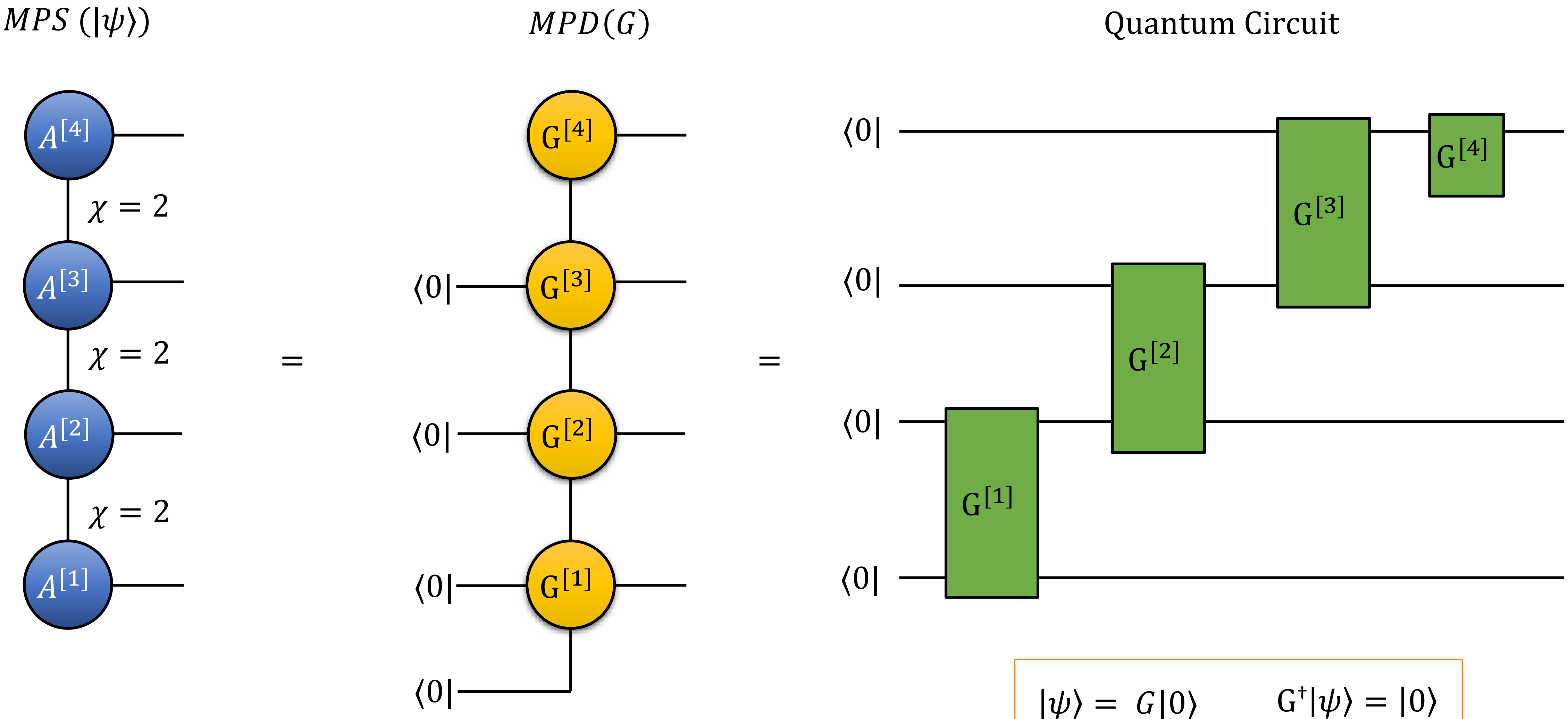
$|0\rangle$: *Product State* $|\Omega\rangle$: *Correspond to Ground State*



How to prepare MPS on quantum device?

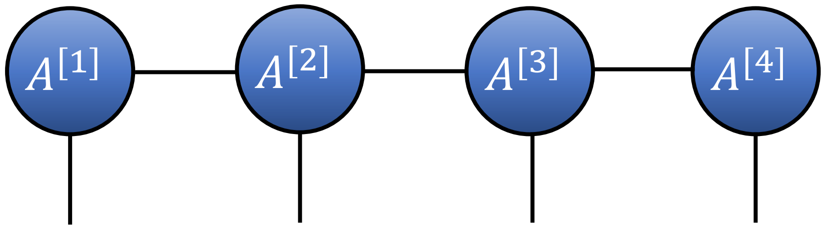
- Apply $G^{[N]}$ with inputs set to $|0\rangle$, we reconstruct the original tensor $A^{[N]}$.
- MPD disentangle the target MPS into product state $|0\rangle$.

$|0\rangle$: *Product State*

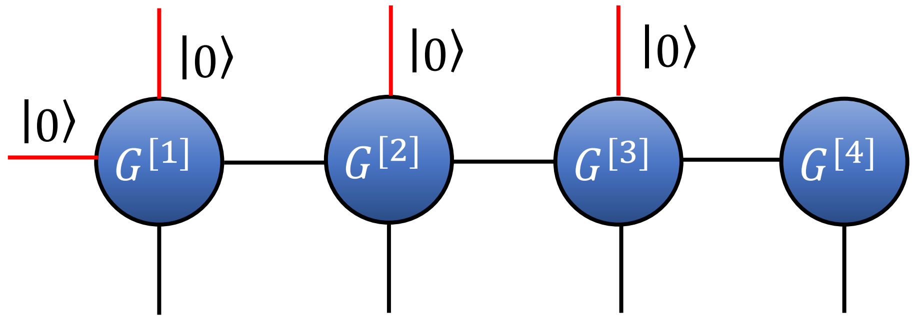


$|\psi\rangle = G|0\rangle \qquad G^{\dagger}|\psi\rangle = |0\rangle$

MPS (orthogonalized):

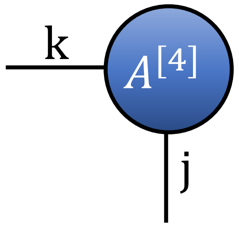


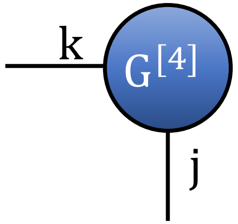
MPD:



For the last tensor (N=4) :

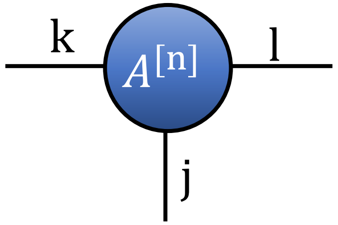
$$A^{[4]}_{jk} = G^{[4]}_{jk}$$

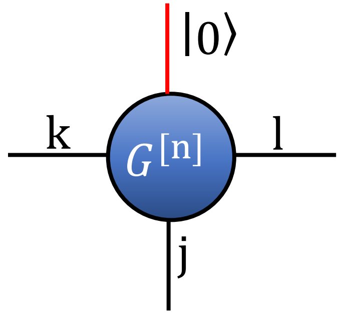




For tensor 1 < n < N :

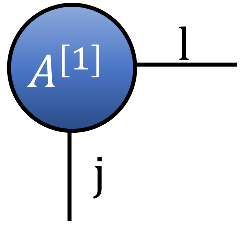
$$A^{[n]}_{jkl} = G^{[n]}_{0jkl}$$

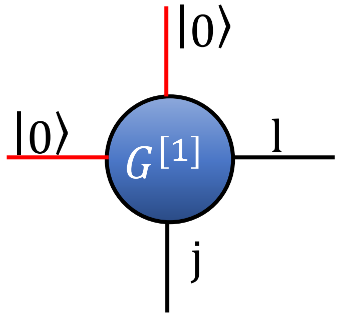




For tensor n = 1 :

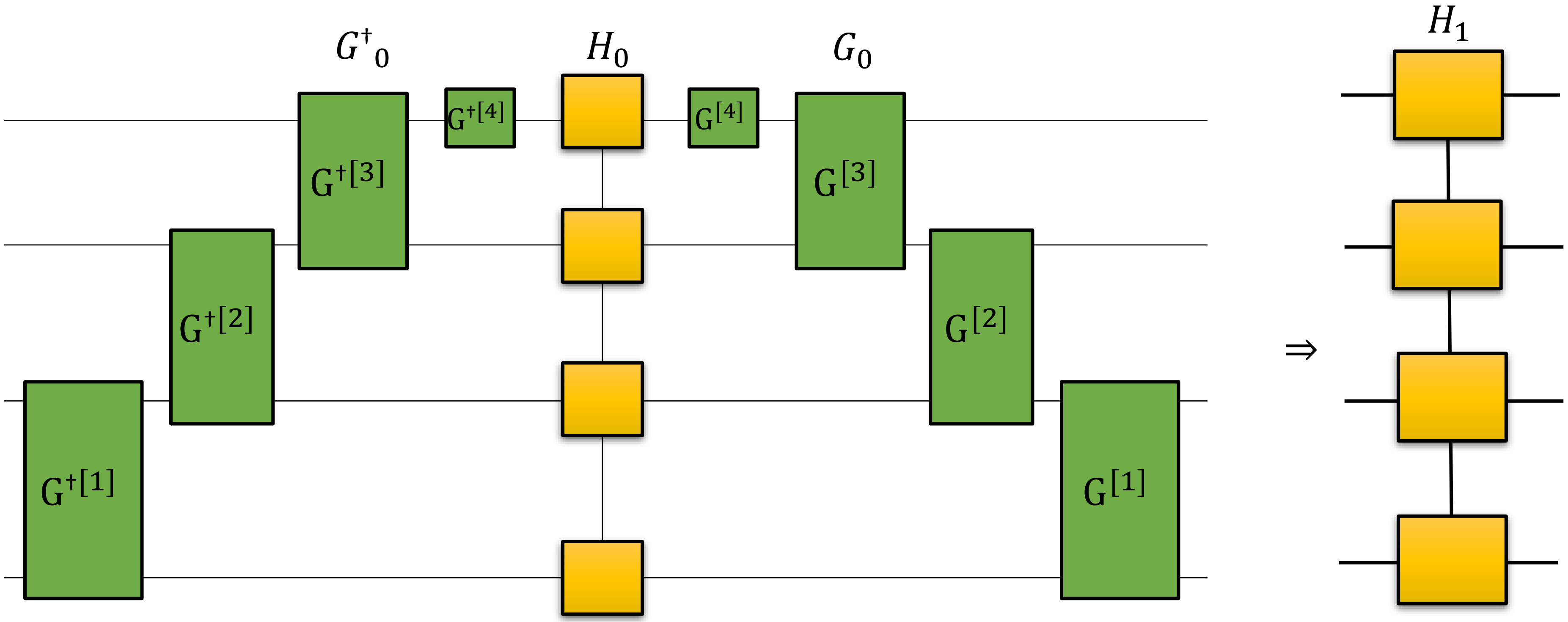
$$A^{[1]}_{jl} = G^{[1]}_{00jl}$$

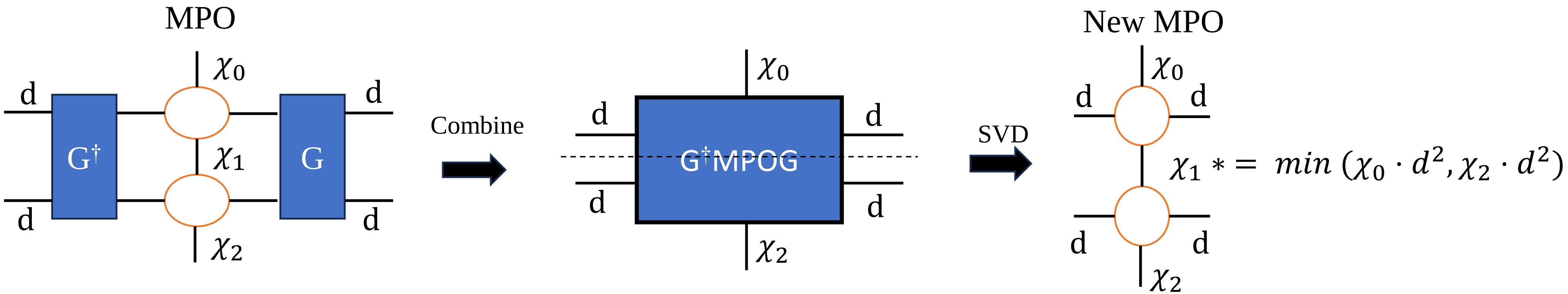




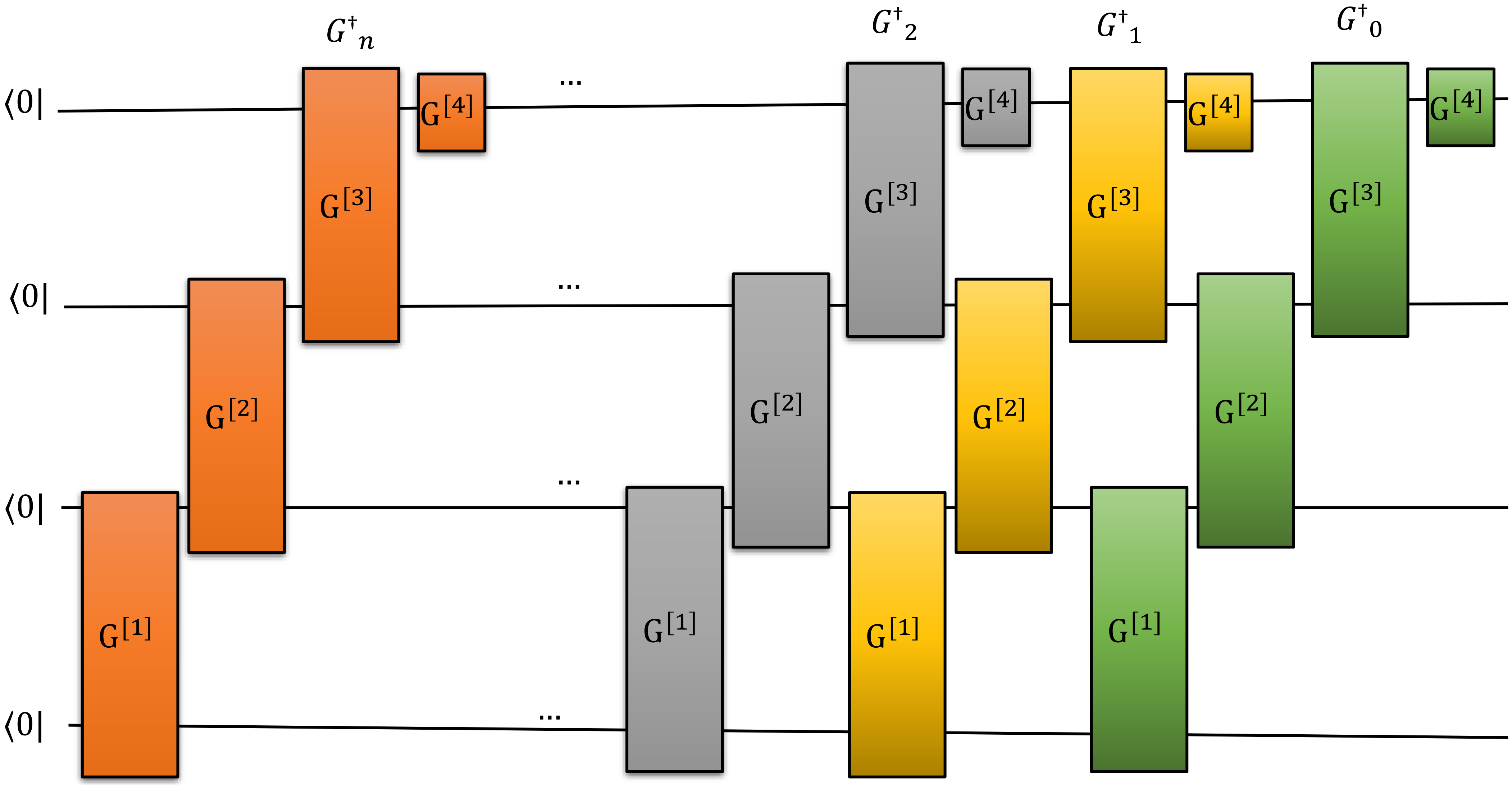
Variational Energy Optimization – Optimize Hamiltonian

$E_0 = \langle \Omega_0 | H_0 | \Omega_0 \rangle_{\chi=2} = \langle 0 | G^{\dagger}{}_0 H_0 G_0 | 0 \rangle \quad \Rightarrow \quad \langle 0 | H_1 | 0 \rangle$ $|\Omega\rangle$: *Correspond to Ground State* $|0\rangle$: *Product State*





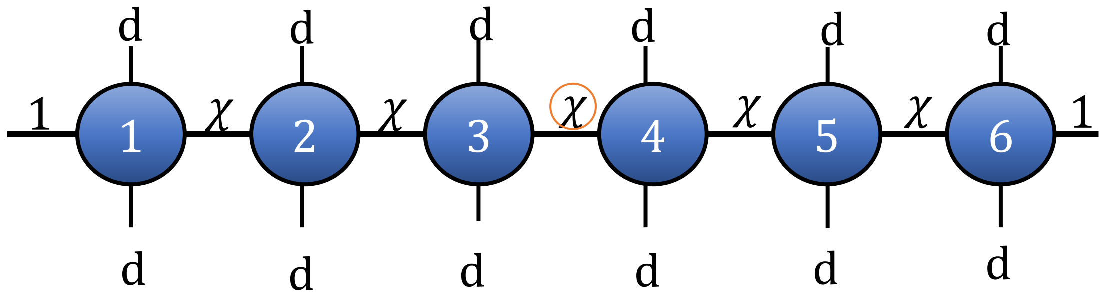
$$E_n = \langle 0| G^\dagger{}_n \ldots G^\dagger{}_3 G^\dagger{}_2 G^\dagger{}_1 G^\dagger{}_0 \; H_0 \; G_0 G_1 G_2 G_3 \ldots G_n |0\rangle$$



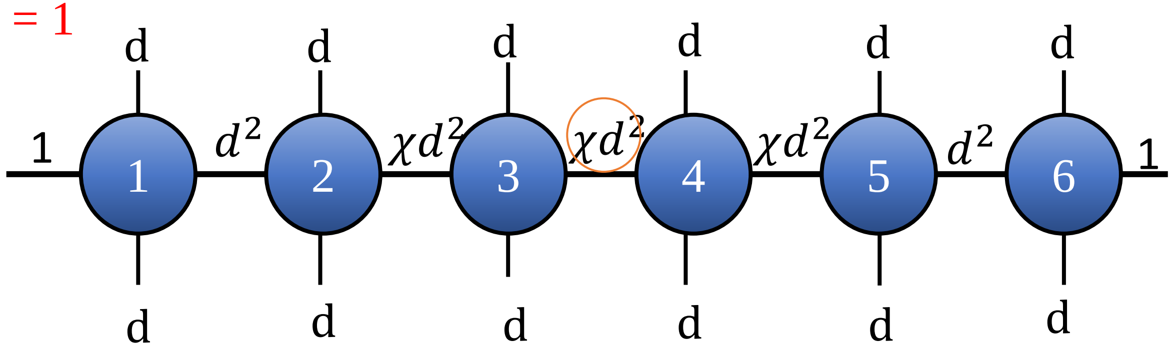
MPO Bond Dimension Scaling – Taking N=6 as an example

N : system size, n : number of iteration

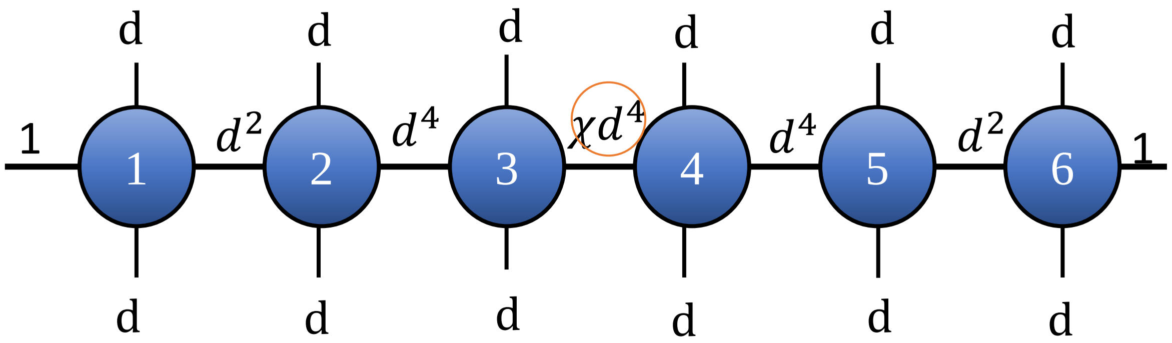
n = 0



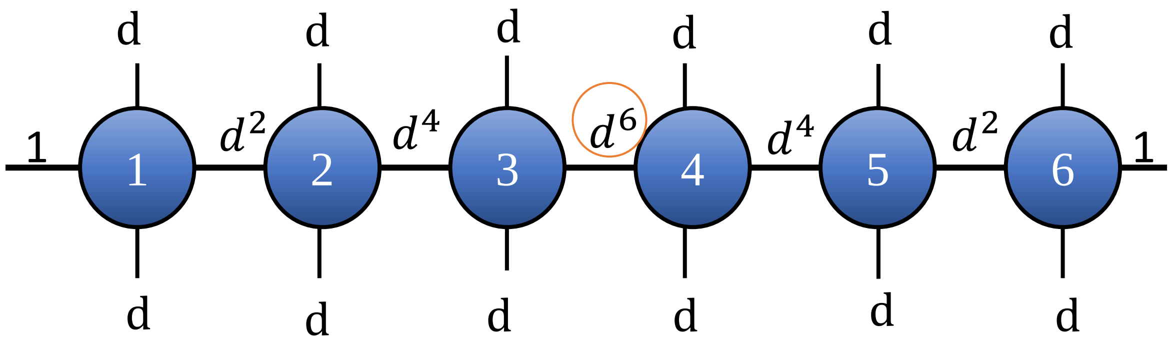
n = 1



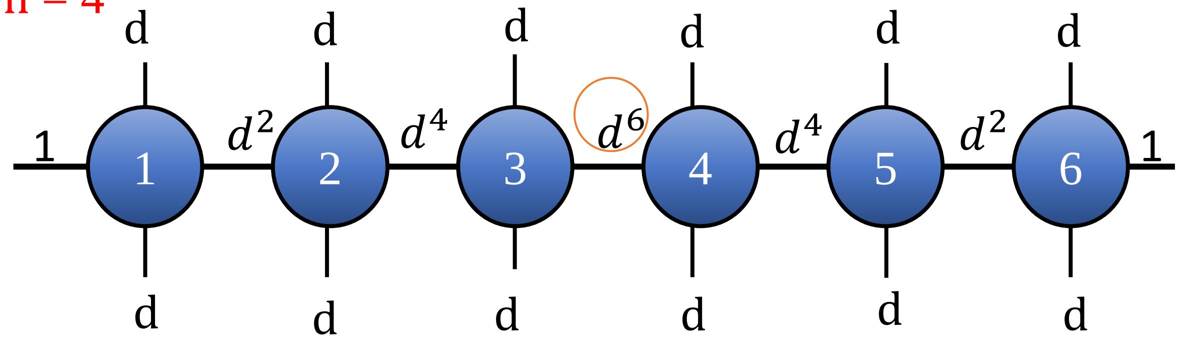
n = 2



n = 3



n = 4

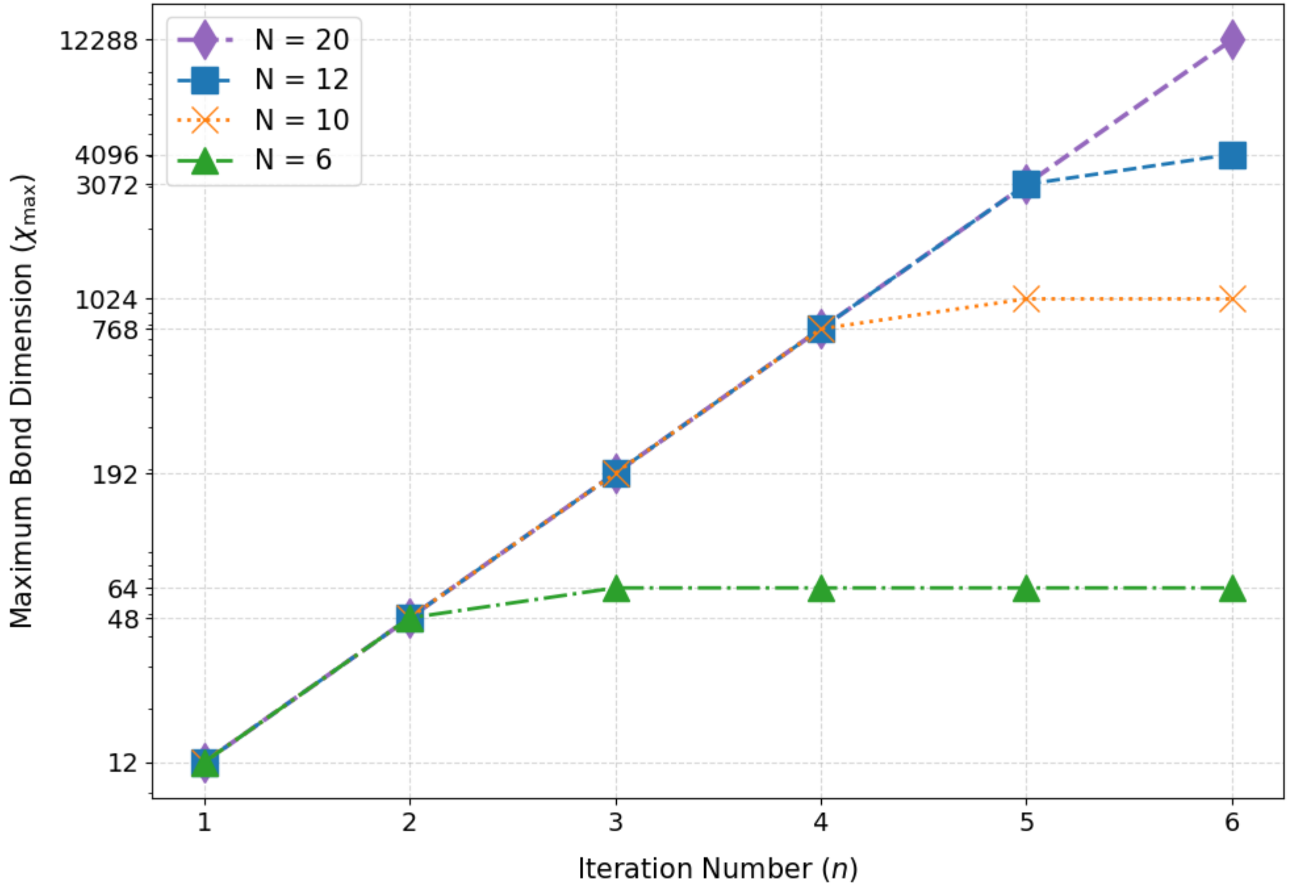


When $n < \frac{N}{2}$, the maximum bond dimension grows d^{2n}.

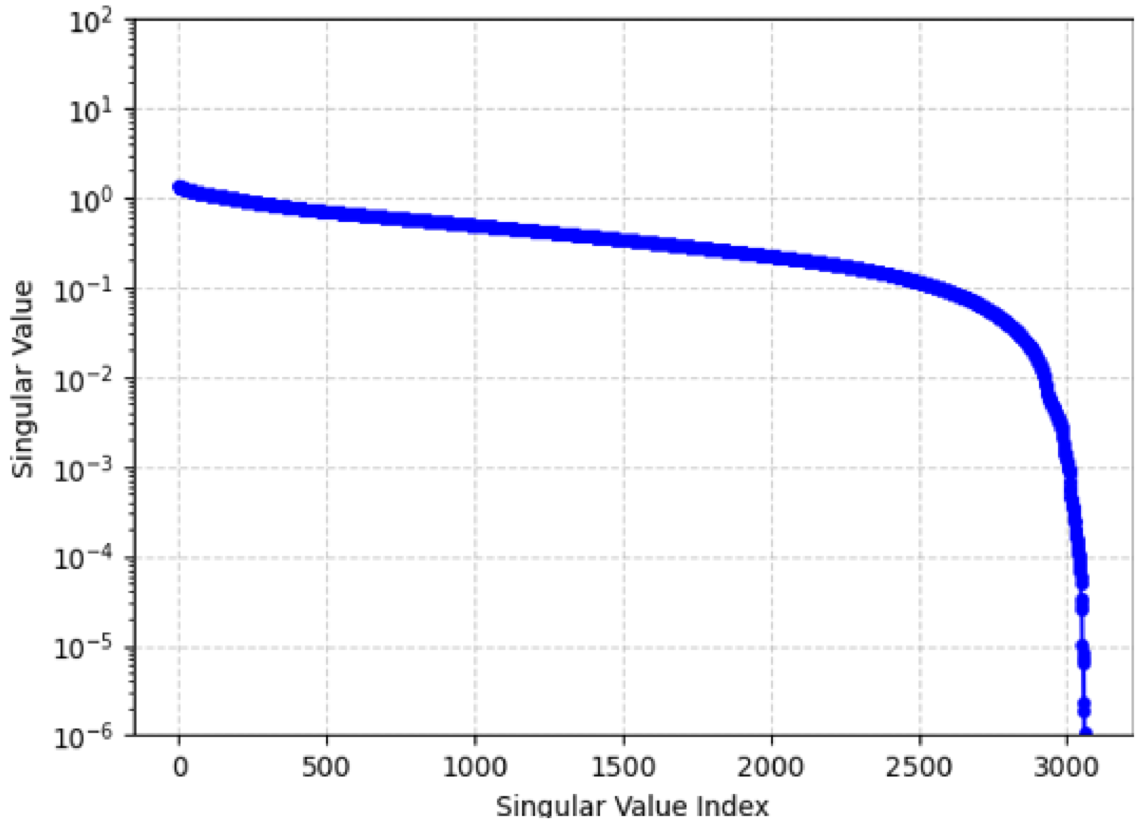
$n \geq \frac{N}{2}$, the maximum bond dimension frozen at d^N.

- The maximum bond dimension grows exponentially until it reaches the system limit of 2^N.

- Singular values decay very slowly.
- Keep all elements to next iteration.



- *Growth of maximum bond dimension* χ_{max} *across different system sites* (N).



- Singular values spectrum - TFIM : N=20 iteration=5 number of singular values=3072

Result

1. Transverse Field Ising Model

2. Heisenberg Model

3. XY Model

- Truncate the current state to $\chi = 2$.

$$|\psi_n\rangle_\chi \to |\tilde{\psi}_n\rangle_{\chi=2}$$

- Transform into MPD layer.

$$|\tilde{\psi}_n\rangle \to G_n$$

- Apply MPD to the current state to disentangle it for next iteration.

$$|\psi_{n+1}\rangle = G_n|\psi_n\rangle$$

- Relative Energy Error (ΔE)

$$\Delta E = \frac{|E - E_{\chi=64}|}{|E_{\chi=64}|}$$

- Infidelity ($F_{n,\chi}$)

$$F_{n,\chi} = -\frac{ln\langle\psi_\chi|G_n \ldots G_0|0\rangle}{N}$$

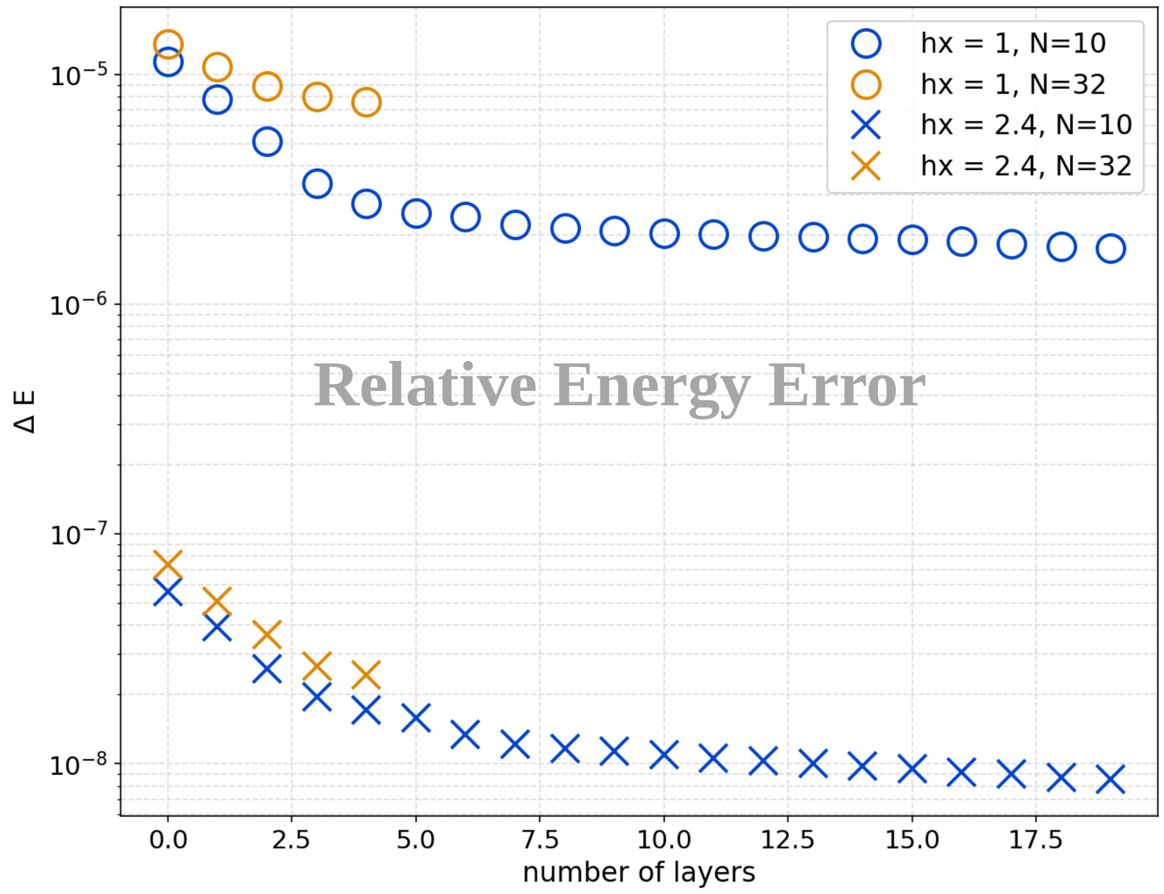
- Comparison

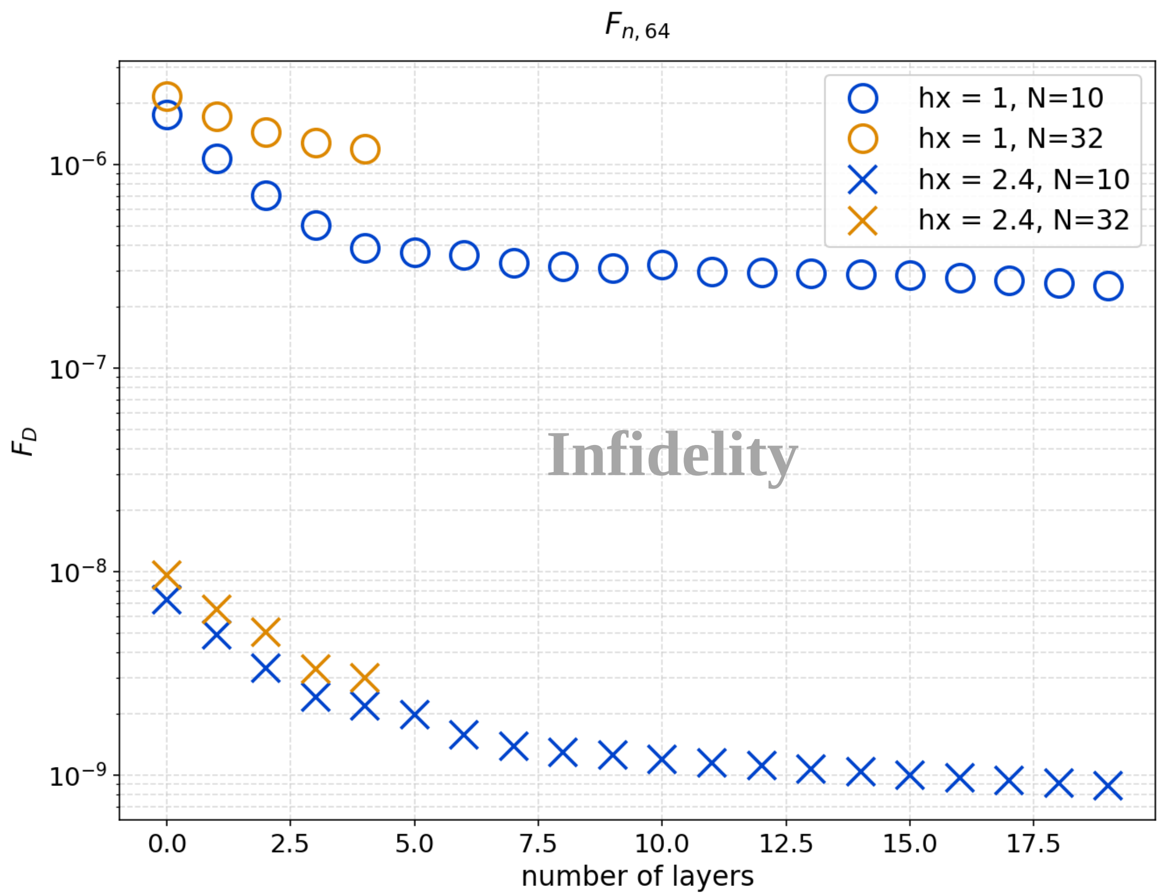
Ran, Shi-Ju. *Physical Review A* 101.3 (2020): 032310.

Transverse Field Ising Model

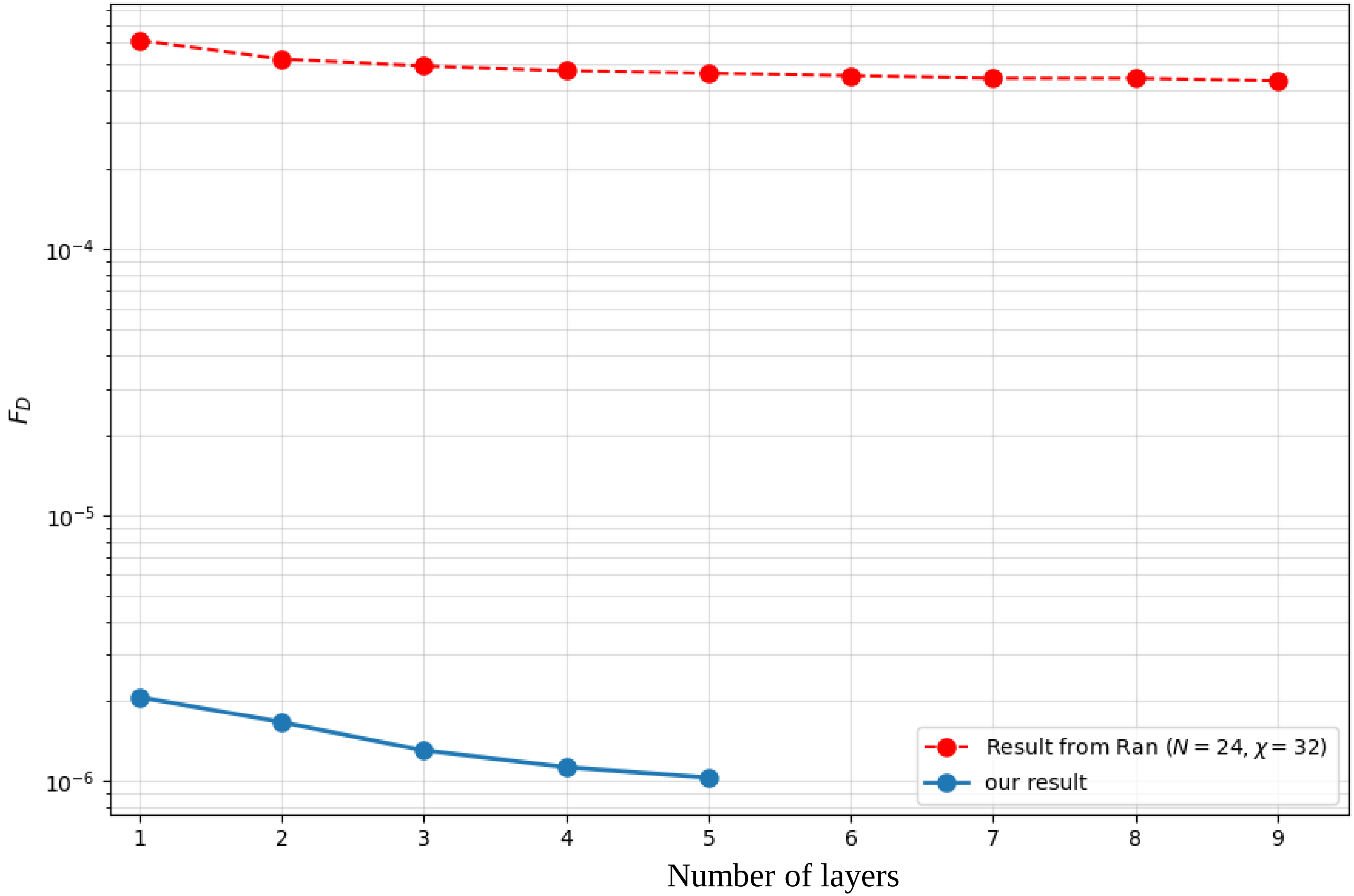
$$\mathcal{H}_{\mathrm{TFIM}} = \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - h_x \sum_i \sigma_i^x$$

- *critical point* : $h_x = 1$





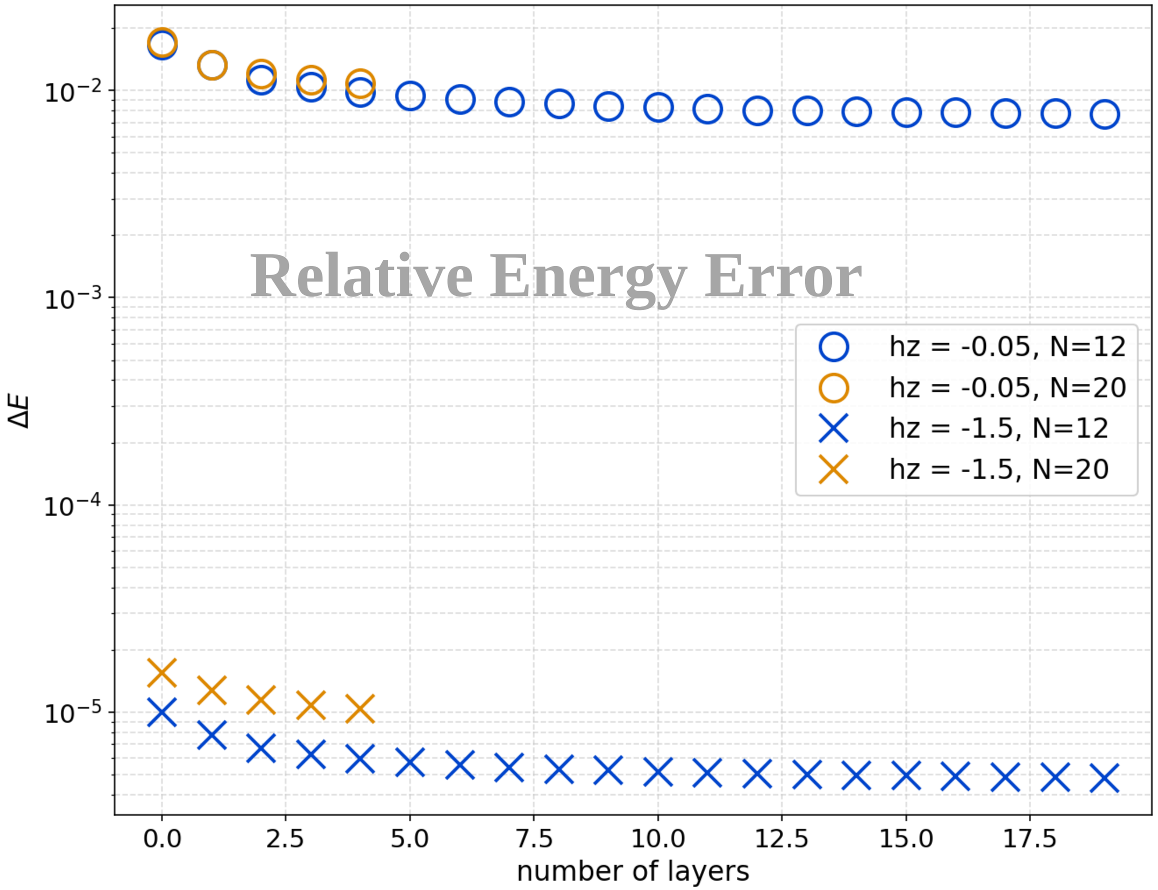
- In the first 5 iterations, our algorithm has achieved better results.

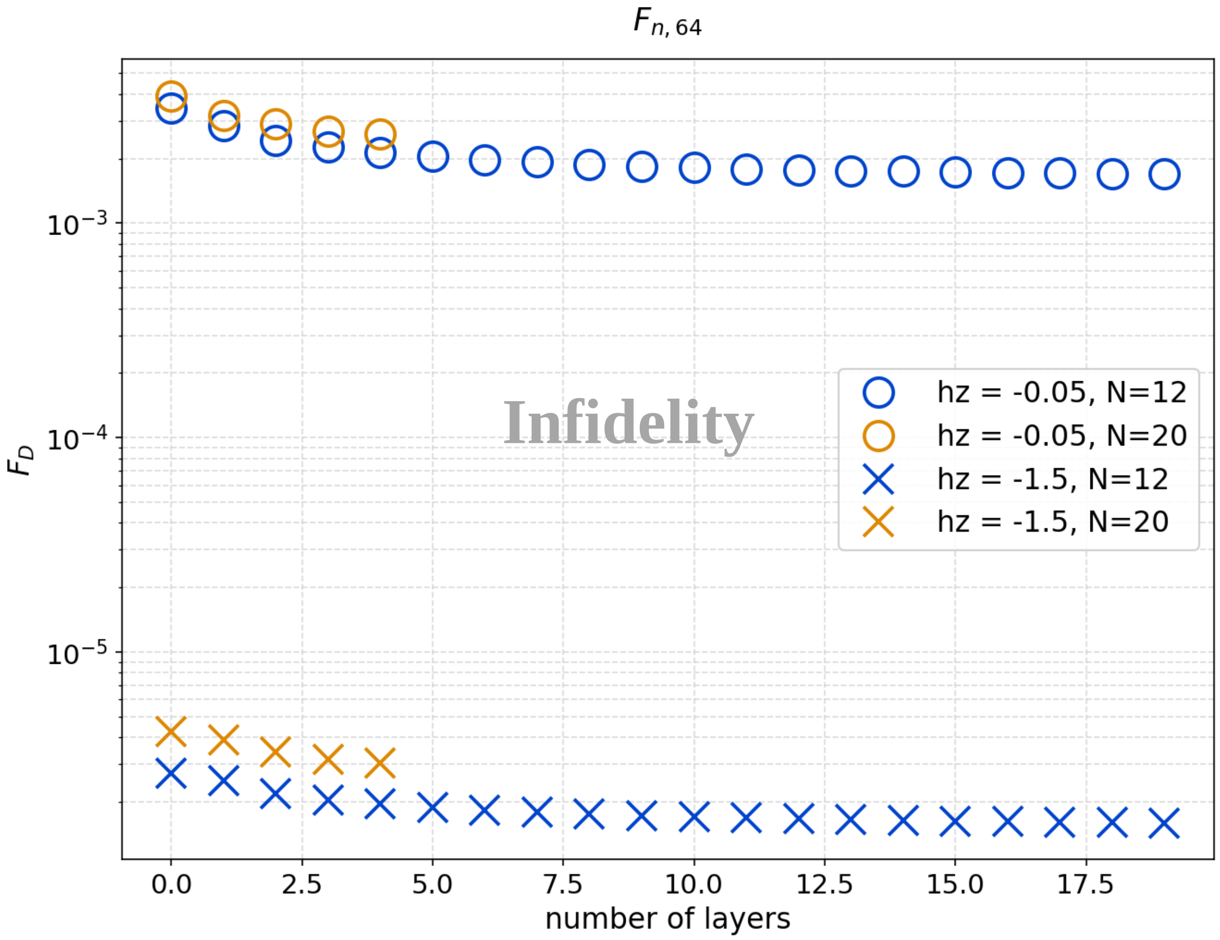


Heisenberg Model

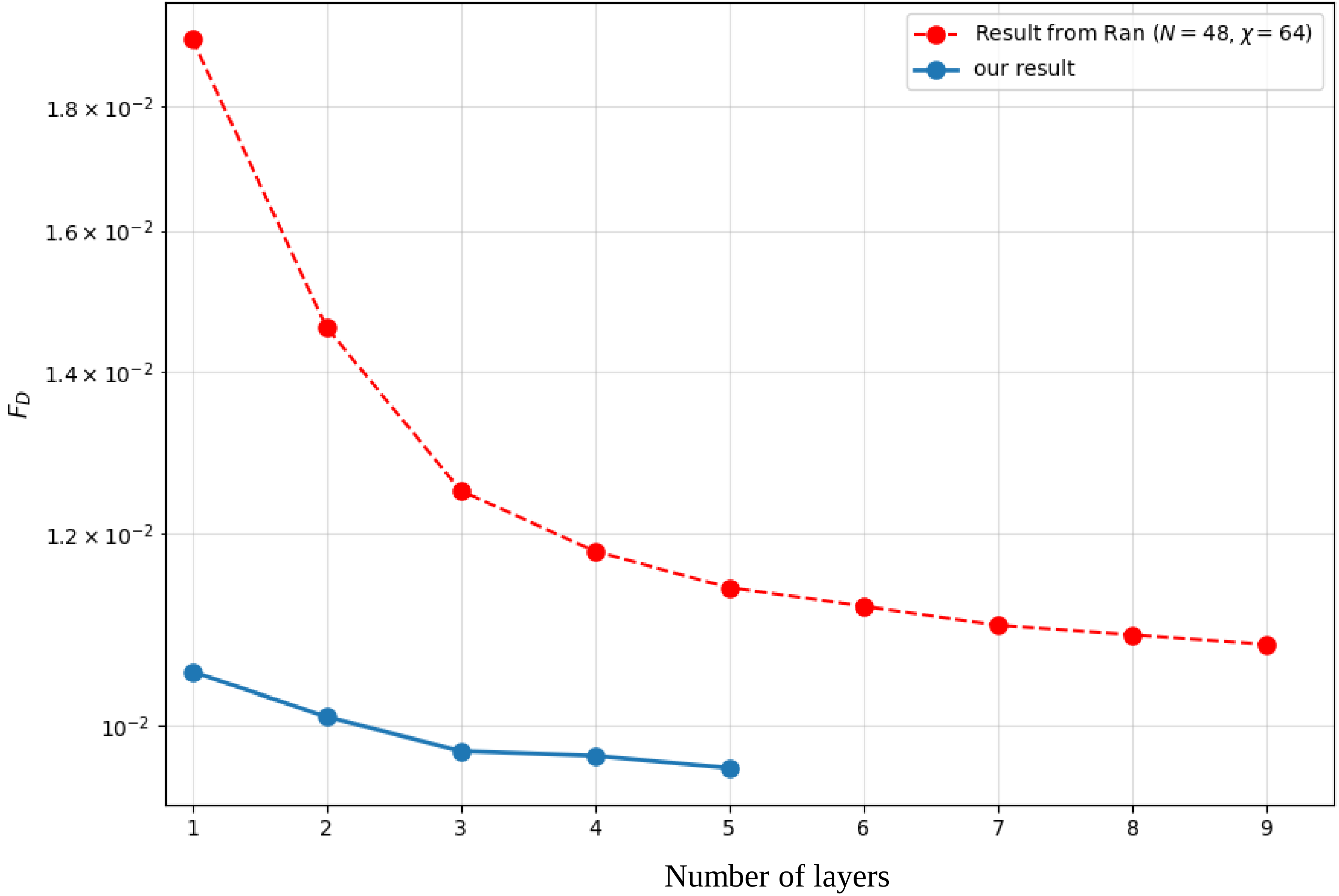
$$\mathcal{H}_{\text{Heisenberg}} = -\frac{1}{2}\sum_i \left(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \sigma_i^z\sigma_{i+1}^z\right) - h_x\sum_i \sigma_i^x - h_z\sum_i \sigma_i^z$$

- $critical\ point: h_z = 0$





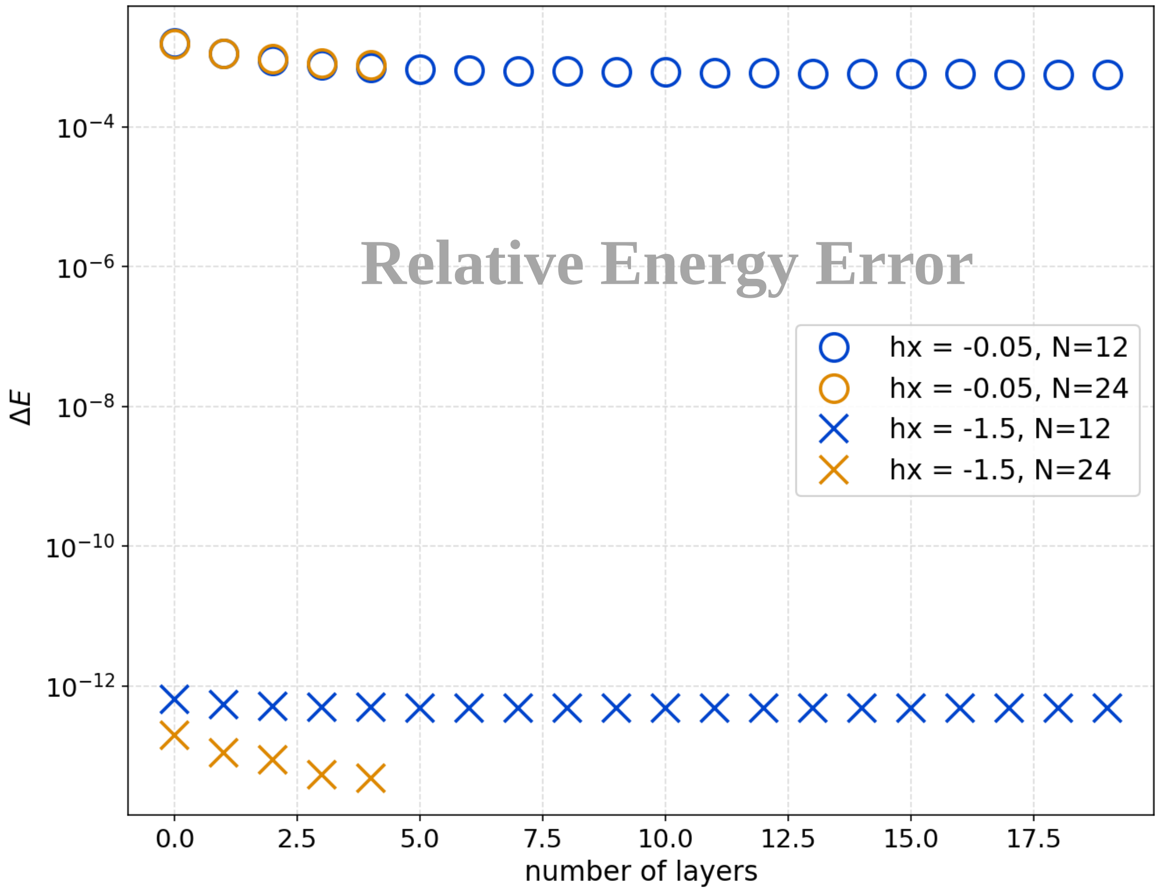
- Even though his results decrease very fast, at the 9th iteration they are still not as good as our results.

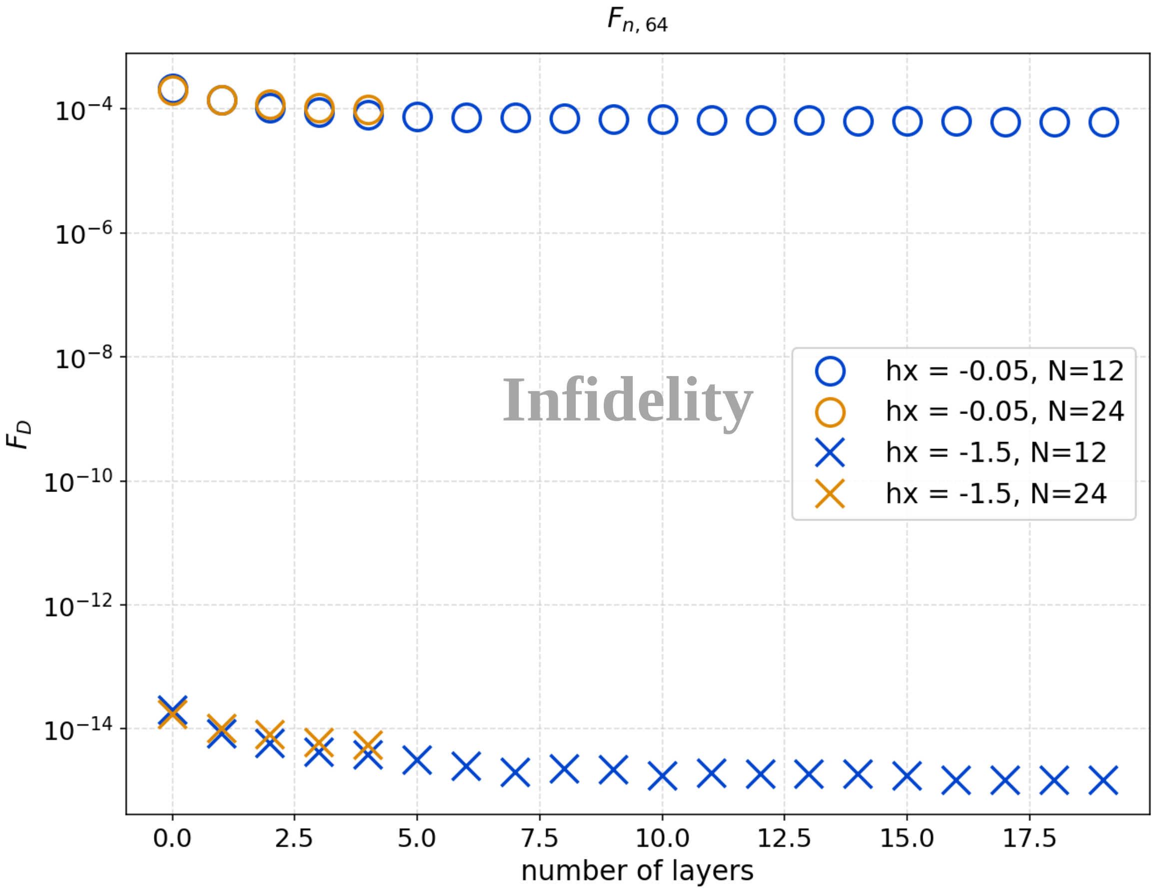


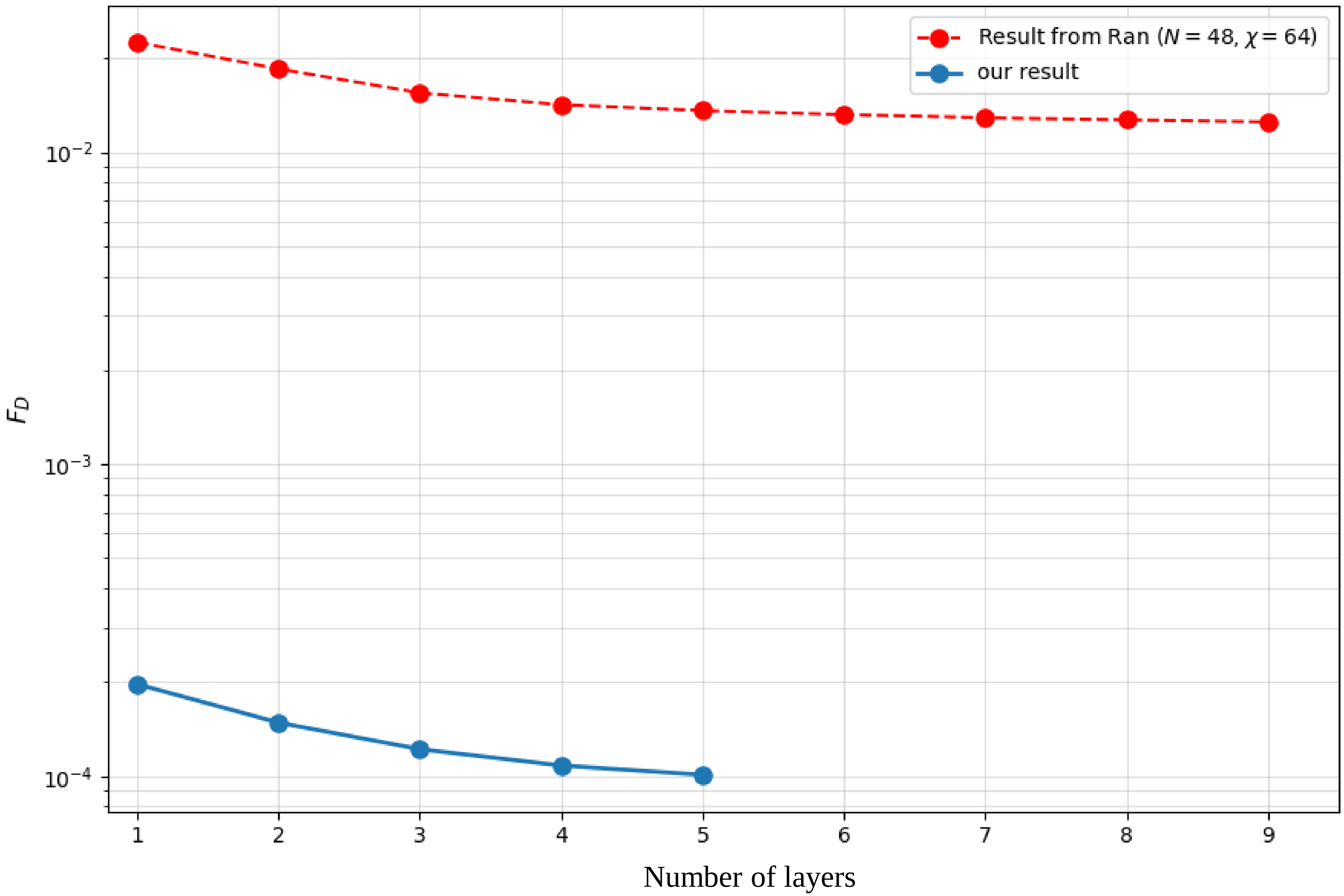
XY Model

$$\mathcal{H}_{\mathrm{XY}} = -\frac{1}{2}\sum_i(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y) + h_x\sum_i \sigma_i^x$$

- *critical point* : $h_x = 0$







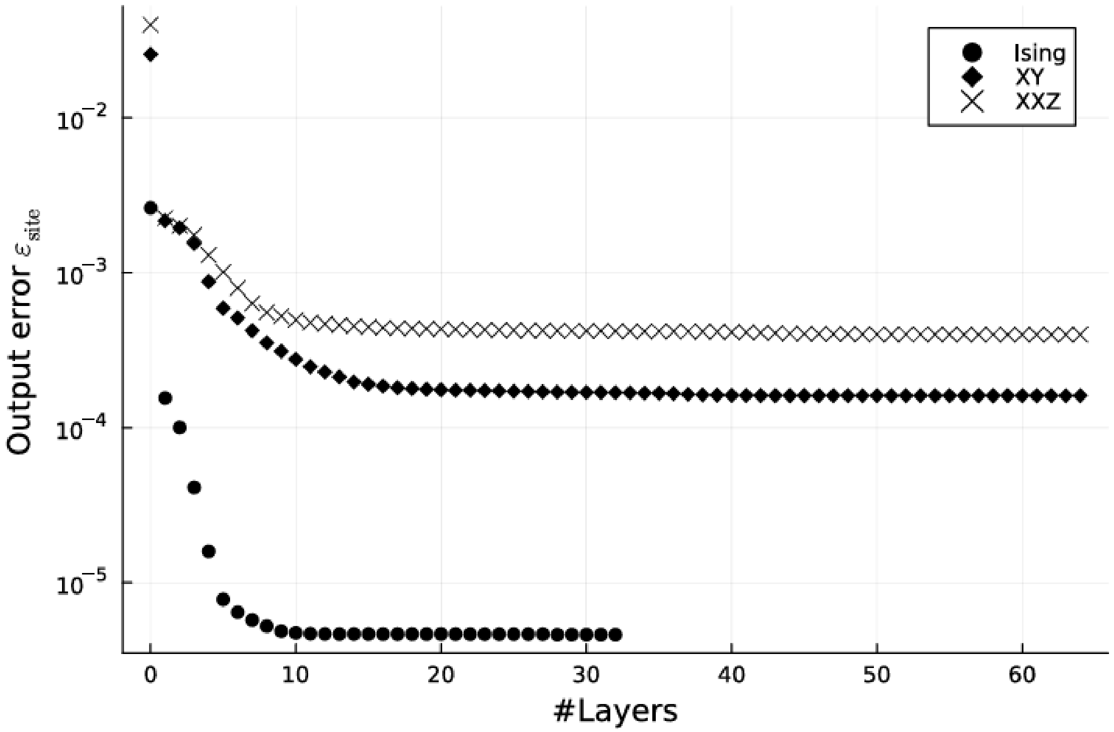
Result from Ran ($N = 48$, $\chi = 64$)
our result
10^{-2}
10^{-3}
10^{-4}
F_D
1
2
3
4
5
6
7
8
9
Number of layers

Summary and Future Work

- Previous Study : Optimize the state, Our Study : Optimize the Hamiltonian.
- Our algorithm achieves better results without requiring a large number of layers.
- The variational energy approaches the ground state with each layer, and the infidelity decreases.
- Use other methods to increase the number of iterations after our algorithm.

Back Up

Mansuroglu, Refik, and Norbert Schuch. "Preparation circuits for matrix product states by classical variational disentanglement." *Physical Review A* 113.4 (2026): 042430.



(b) Energy