Variational iMPS on Quantum Circuits

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Outline

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Quantum many-body challenges

generic quantum state with N sites, spin-d has d^N dimensional Hilbert space

$$|\psi\rangle = \sum_{s_1, s_2, \ldots, s_N} \psi_{s_1, s_2, \ldots, s_N} |s_1\rangle |s_2\rangle \ldots |s_N\rangle, s_n = 1, \ldots, d$$

In exact diagonalization, the number of quantum state parameters increases exponentially with N.

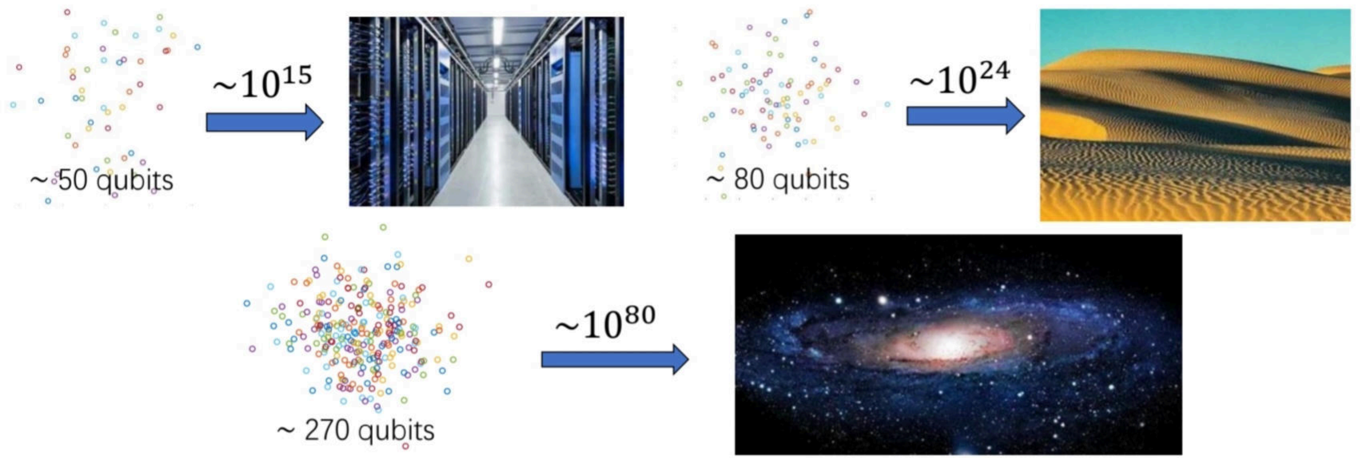

Figure is from Ran Shiju's lecture note.

Entanglement

Decompose a pure state into a superposition of product states through Schmidt decomposition:

$|\psi\rangle = \sum_\alpha \Lambda_\alpha \, |\alpha\rangle_A \otimes |\alpha\rangle_B$

with $\langle\alpha|\alpha'\rangle = \delta_{\alpha\alpha'}$ and $\sum_\alpha \Lambda_\alpha^2 = 1$

Entanglement entropy: $S = -\sum_\alpha \Lambda_\alpha^2 \log(\Lambda_\alpha^2)$

Area law: for ground states of gapped Hamiltonians in 1D system

$$S(L) = \text{const}$$

Eisert, J., Cramer, M., Plenio, M.B., 2010. Area laws for the entanglement entropy - a review. Rev. Mod. Phys. 82, 277-306. https://doi.org/10.1103/RevModPhys.82.277

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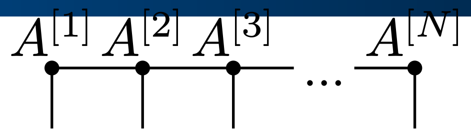
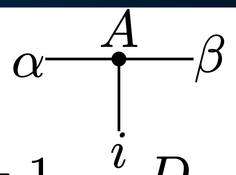
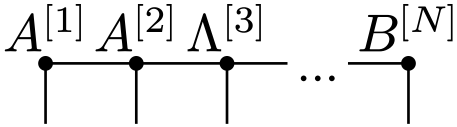
MPS

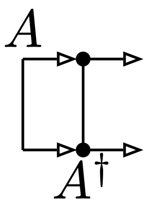
$|\psi\rangle =$ 

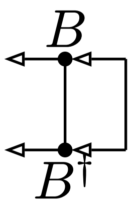
$A^i_{\alpha,\beta} =$ 

$$\alpha, \beta = 1, \ldots, D$$
$$i = 1, \ldots, d$$

Canonical form: Use the gauge degree of freedom to find a convenient representation





$= I$


$= I$ isometric condition

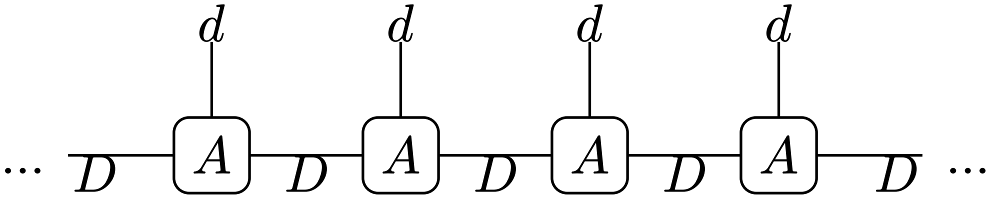
(1) Reduction of the number of variables: $d^N \to NdD^2$;

(2) Efficient to get expectation values

$\Rightarrow$ suited variational ansatz

Cirac, I., Perez-Garcia, D., Schuch, N., Verstraete, F., 2021. Matrix Product States and Projected Entangled Pair States: Concepts, Symmetries, and Theorems.

infinite uniform MPS



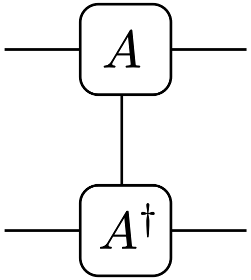
- Properties:
  - Translational invariance: The same local tensor A is repeated across all sites. $\Rightarrow$ Efficient parameterization: Describes an infinite system with a finite number of parameters.
  - The whole state only depend on tensor A, which reflect the bulk properties of the system.
  - Allow to work directly in the thermodynamic limit.

Vanderstraeten, L., Haegeman, J., Verstraete, F., 2019. Tangent-space methods for uniform matrix product states. SciPost Phys. Lect. Notes 7. https://doi.org/10.21468/SciPostPhysLectNotes.7

infinite uniform MPS

- Transfer matrix:

$$E = \sum_{s=1}^{d} A^s \otimes (A^s)^\dagger =$$



In generic case, leading eigenvalue is non-degenerate.(Perron-Frobenius theorem: If degenerate, there exist phase transition, not a equilibria state.)

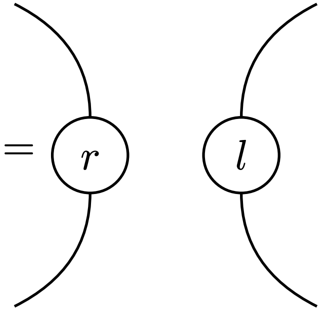
- Spectral decomposition:

$$E = \lambda_0 \, |r\rangle\langle l| + \sum_i \lambda_i \, |r_i\rangle\langle l_i|$$

λ_0 is the leading eigenvalue, which should be scaled to 1 by normalizing the MPS tensor $A \to \frac{A}{\sqrt{\lambda_0}}$. Thus the rest eigenvalues $\lambda_i < 1$

infinite uniform MPS

$$\lim_{N\to\infty} E^N = \lambda_0^N \, |r\rangle\langle l| + \sum_i \lambda_i^N \, |r_i\rangle\langle l_i| =$$



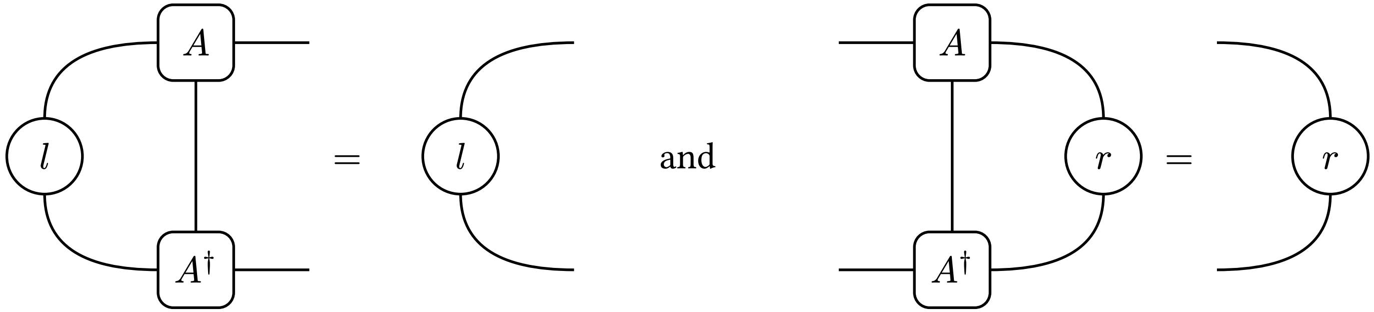
- fixed point equation:

$$E^N \, |l\rangle = |r\rangle\langle l|l\rangle = |r\rangle \Rightarrow E(E^N \, |l\rangle) = E \, |r\rangle = |r\rangle$$

$$\langle r| \, E^N = \langle r|r\rangle\langle l| = \langle l| \Rightarrow (\langle l| \, E^N)E = \langle l| \, E = \langle l|$$

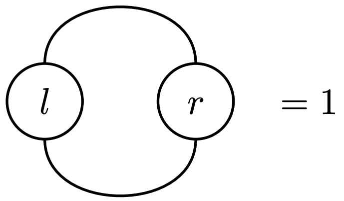
infinite uniform MPS

represent by tensor network:

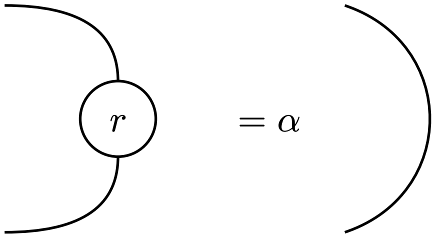


l is left environment, r is right environment.

For simplicity, let us suppose $D = d = 2$, and the MPS is normalized and in right canonical form. Thus we have



and

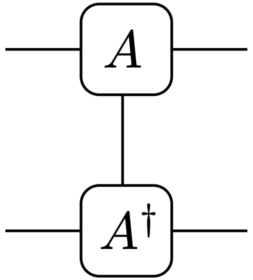


Vanderstraeten, L., Haegeman, J., Verstraete, F., 2019. Tangent-space methods for uniform matrix product states. SciPost Phys. Lect. Notes 7. https://doi.org/10.21468/SciPostPhysLectNotes.7

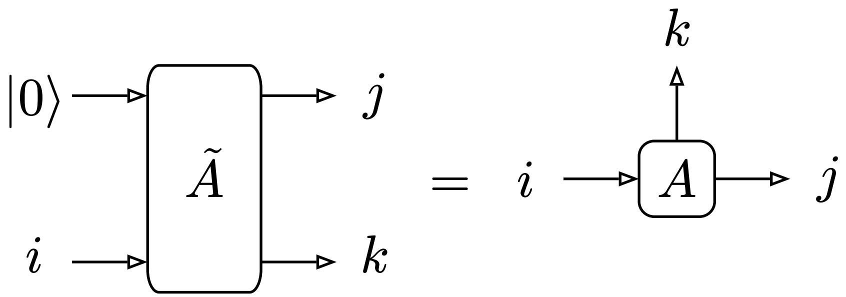
Mapping to circuits

A plays the role of Kraus operator. The transfer matrix plays the role of quantum channel.

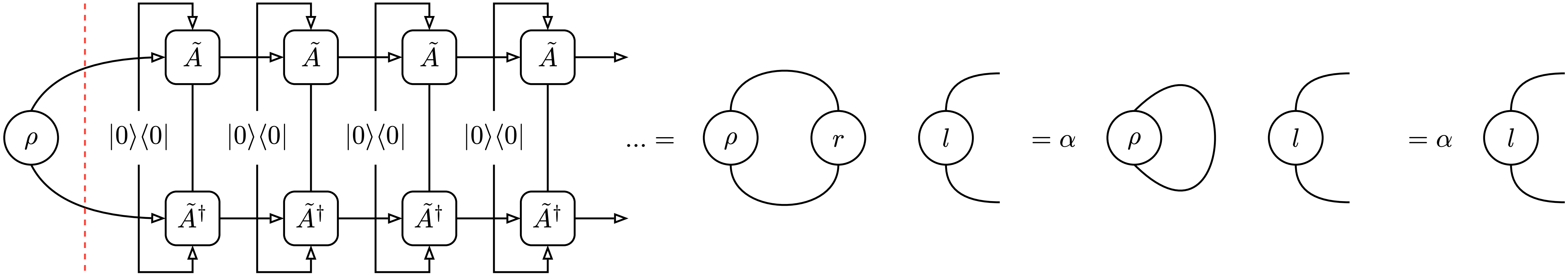
$$E = \sum_{s=1}^{d} A^s \otimes (A^s)^\dagger =$$



Since A is right canonical, we can always define a unitary matrix $\tilde{A}$ such that:

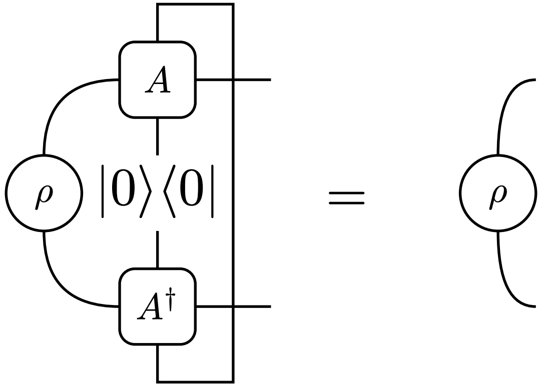


Mapping to circuits



$$\mathrm{Tr}(\rho) = 1, r = \alpha \mathbb{I}$$

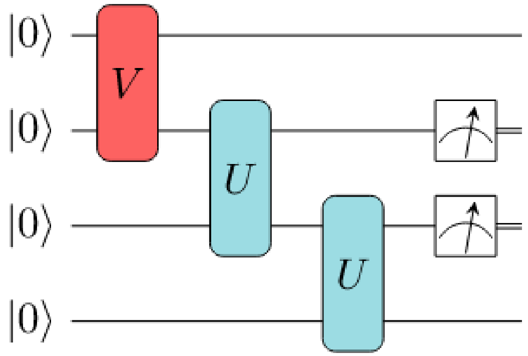
Fixed point equation of channel: $\varepsilon(\rho_*) = \rho_*$.



Thus $\rho_* = \alpha l$.

Past method

Cholesky decomposition of ρ: $\rho = VV^\dagger$, $\mathrm{tr}(\rho) = 1$

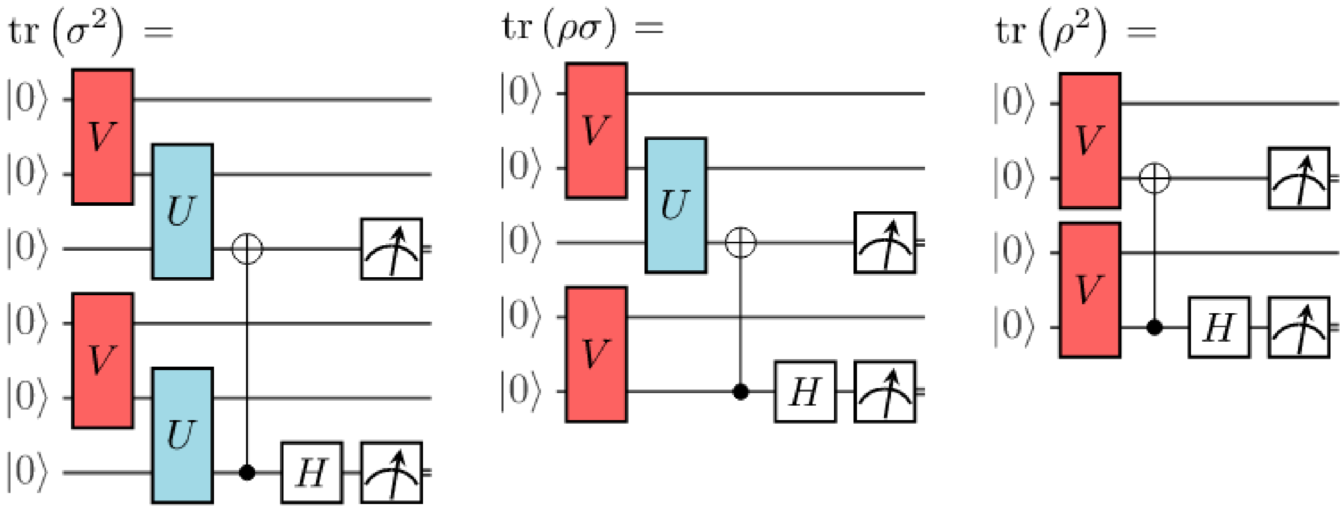


V has also been parameterized.

Judge whether $VV^\dagger$ is left environment by swap test.

Barratt, F., Dborin, J., Bal, M., Stojevic, V., Pollmann, F., Green, A.G., 2021. Parallel Quantum Simulation of Large Systems on Small Quantum Computers. npj Quantum Inf 7, 79. https://doi.org/10.1038/s41534-021-00420-3

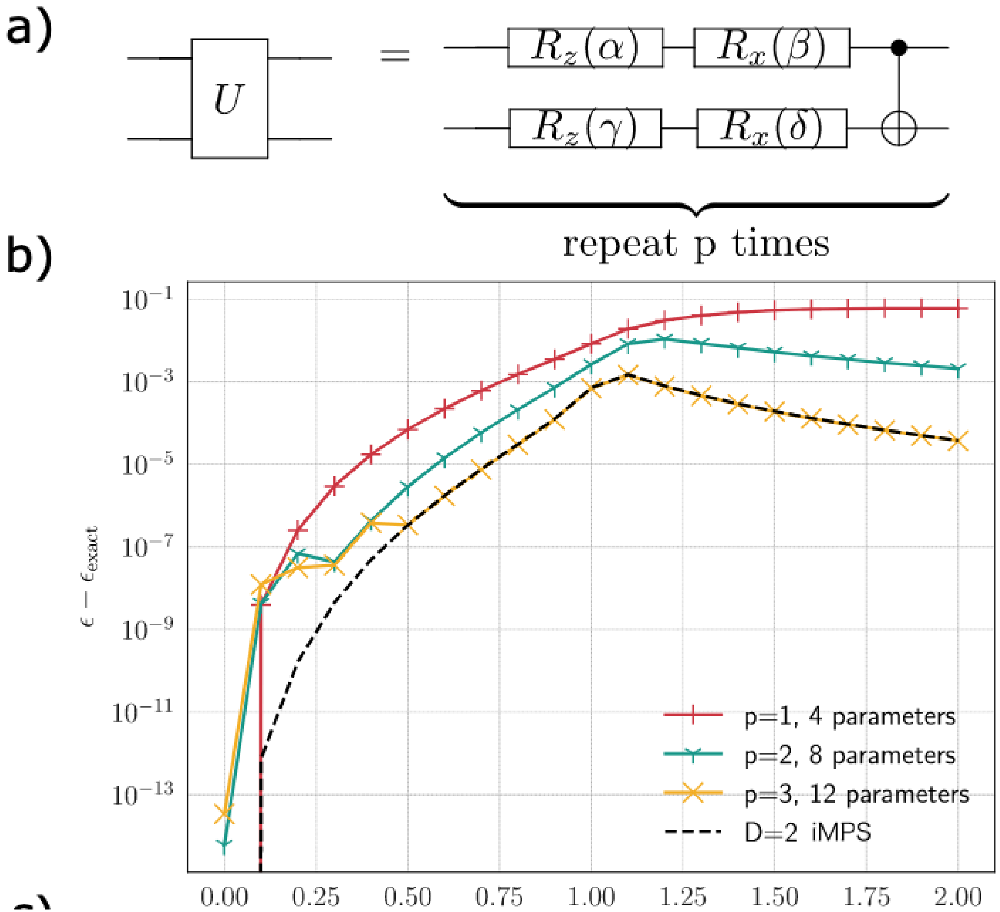
Past method



$\mathrm{tr}\big((\rho-\sigma)^\dagger(\rho-\sigma)\big)$ would be minized at $\rho=\sigma$.

Garcia-Escartin, J.C., Chamorro-Posada, P., 2013. The SWAP test and the Hong-Ou-Mandel effect are equivalent. Phys. Rev. A 87, 052330. https://doi.org/10.1103/PhysRevA.87.052330

TFIM ground state:



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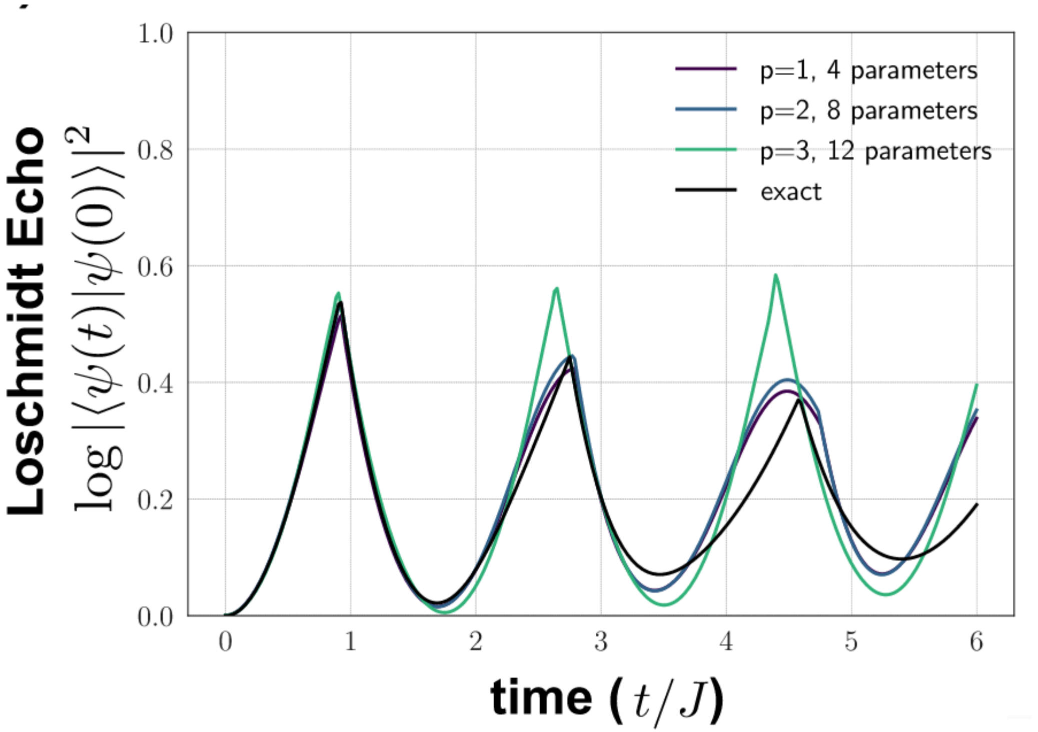
Time evolution:



Disadvantages: need so many circuits, more variables, high complexity.

Outline

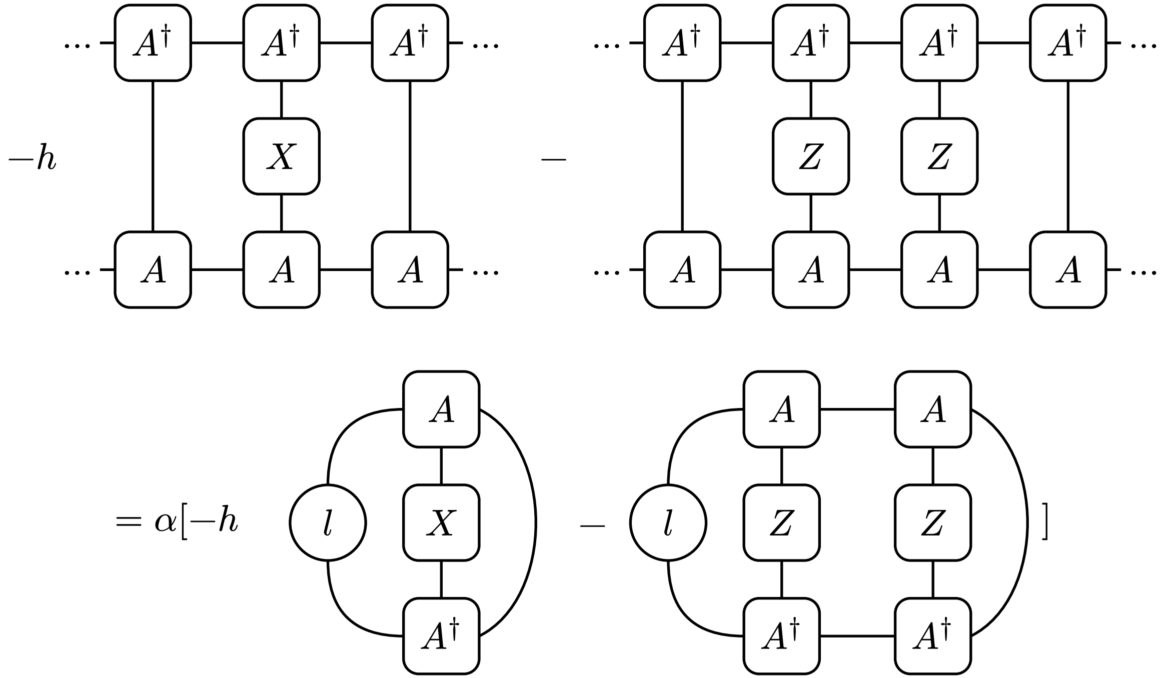
Goal

Hamiltonian of transverse field Ising model on an infinite chain:

$$H = -\sum_i Z_i Z_{i+1} - g \sum_i X_i$$

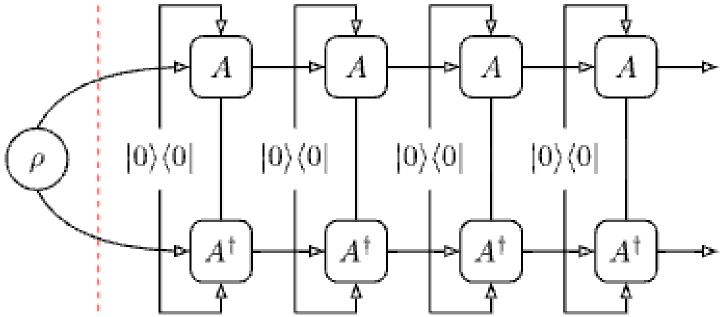
where Z_i is the Pauli-Z operator on the i-th site, X_i is the Pauli-X operator on the i-th site, and g is the transverse field. The goal is to find the ground state using infinite uniform MPS as variational ansatz.

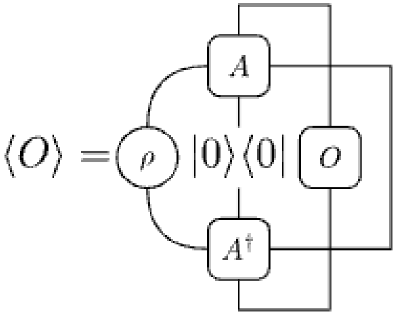
Energy per site of 1D TFIM can be evaluated as:



The contraction complexity is: $O(D^3)$

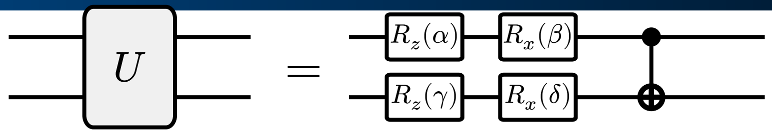
As we said before, we can get left environment by iterating channel, after it satisfy fixed point equation, we can get observables by measuring the physical qubits and trace the ancilla qubits.



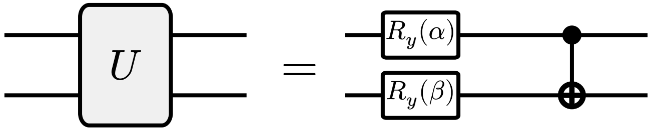


The complexity is $O(N_{\text{measure}})$

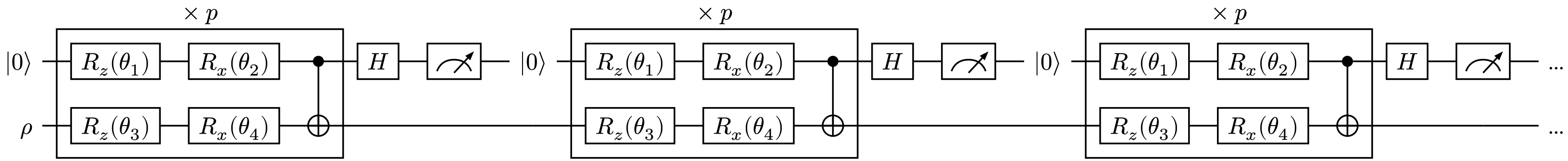
Compilation



or



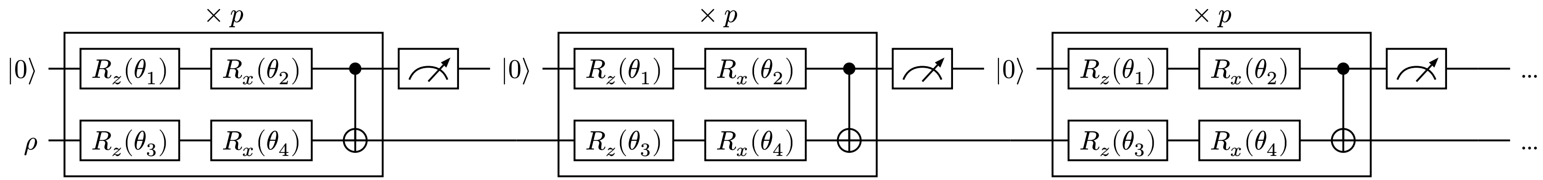
(1) $\langle X \rangle$:



p is repeat times

(2) $\langle ZZ \rangle$:

Compilation



Converged condition: $\langle X\rangle_n \approx \langle X\rangle_{n-1}$, $\langle Z_i Z_{i+1}\rangle_n \approx \langle Z_i Z_{i+1}\rangle_{n-1}$, n means the channel applying iteration.

(3) update θ:

$$\langle H(\theta)\rangle = -g\langle X(\theta)\rangle - J\langle Z_i(\theta) Z_{i+1}(\theta)\rangle$$

$$\frac{\partial}{\partial\theta_i}\langle H(\theta)\rangle \Rightarrow \theta \to \theta + \delta\theta$$

Iterate until it reach converged condition:

$\langle H(\theta_n)\rangle - \langle H(\theta_{n-1})\rangle \leq 10^{-8}$, n means the n-th update iteration.

Algorithm Box

Algorithm 1: Variational iMPS Ground State Optimization

procedure $\textsc{Variational-iMPS}(\theta_0,\ g,\ J,\ \text{maxiter})$

▷ Initialize parameters and convergence criteria

$\theta \leftarrow \theta_0, p$

$\text{iter} \leftarrow 0$

while iter < maxiter && f_tol > 1e-8 **do**

▷ Construct parameterized quantum circuit

$U(\theta) \leftarrow \text{ConstructCircuit}(\theta)$

▷ Iterate quantum channel to fixed point

$\rho \leftarrow \text{IterateChannel}(U(\theta))$

▷ Evaluate energy expectation

$\langle X \rangle \leftarrow \text{Expectation}(\rho_L, X)$

$\langle ZZ \rangle \leftarrow \text{Expectation}(\rho_L, Z \otimes Z)$

Algorithm Box

$E \leftarrow -g \cdot \langle X \rangle - J \cdot \langle ZZ \rangle$

$\triangleright$ Update parameters

$\theta \leftarrow \text{NelderMead}(\theta, E)$

iter $\leftarrow$ iter + 1

end

return θ, E

end

Outline

Exact contraction

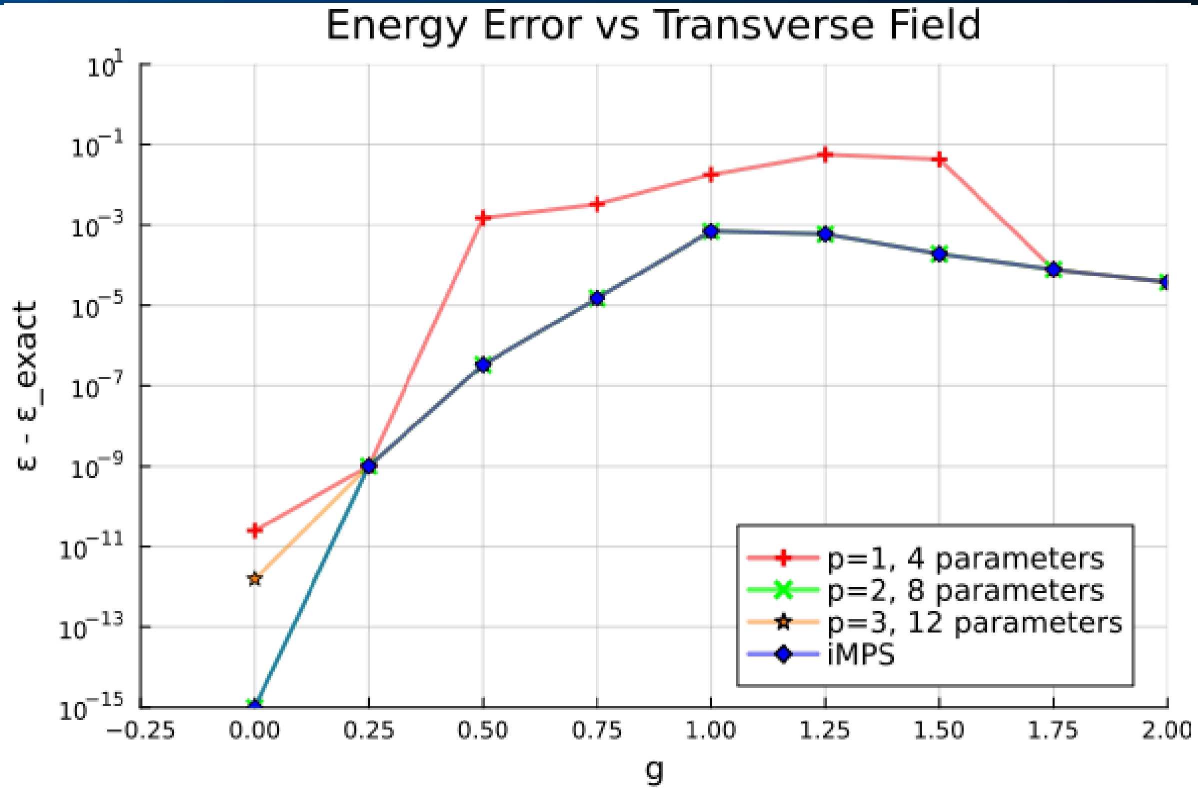


Fig. 1 Energy error v.s. transverse field strength for different circuit depths. iMPS: analytical results of $d = 2, D = 2$ infinite MPS from MPSKit.jl.

Measurement

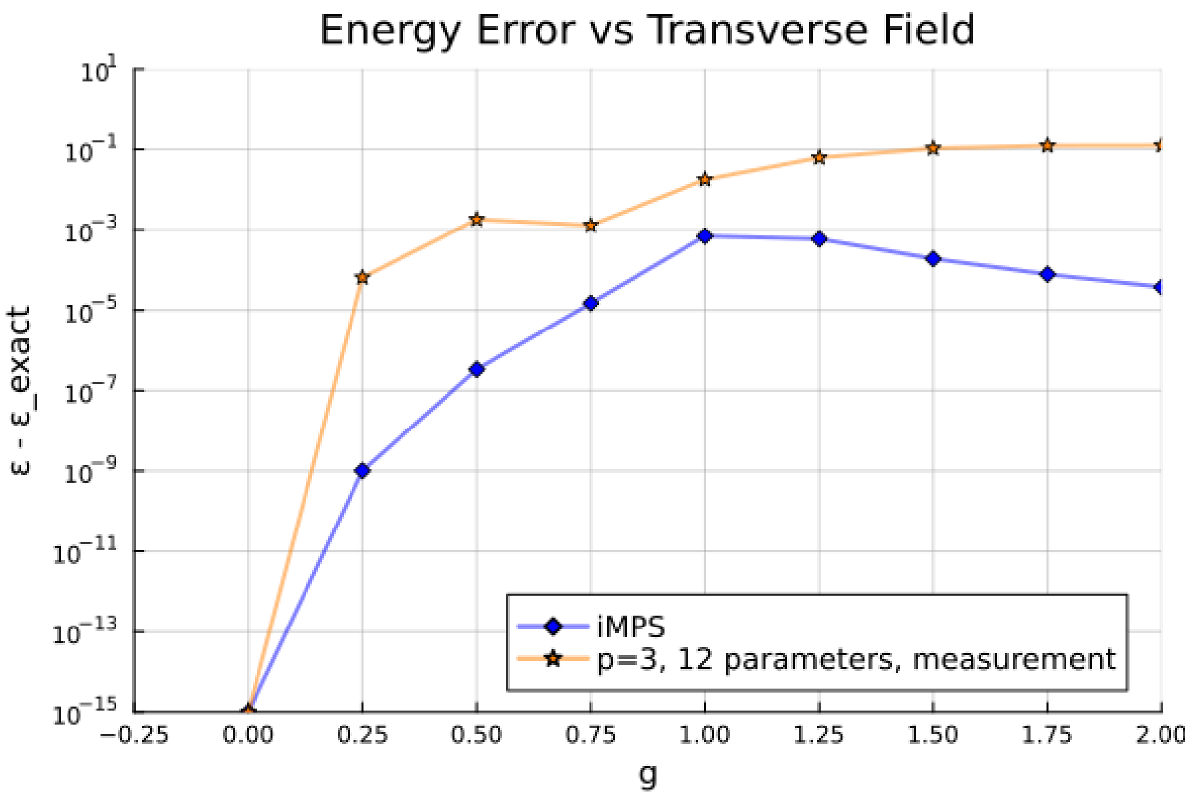


Fig. 2 Energy error v.s. transverse field strength for p=3 through measurement

The phase diagram of the 1D TFIM has a critical point at $g = 1$, with a corresponding infinite correlation length, where a finite depth circuit of nearest-neighbor gates will be unable to exactly prepare this state. It explains why at $g = 1$ the simulation result is the worst.

Besides, the correlation length $\varepsilon = -\frac{1}{\log(\lambda_1)}$, where λ_1 is the second largest magnitude eigenvalue of the ground state transfer matrix. If ε diverges, $\lambda_1 = 1 = \lambda_0$, the eigenvalue is degenerate.

Outline

1. Simple circuit;
2. Less variables;
3. Easy to implement on current hardware.

Future work:

1. Larger virtual dimension;
2. How to get gradient of infinite circuit;
3. Variational compilation.