



Variational ansatz inspired by quantum imaginary time evolution

Xiaoyang Wang

Peking University

collaborate with

Yahui Chai, Maria Demidik, Xu Feng,

Yibin Guo, Karl Jansen, Cenk Tüysüz

[arXiv:2303.11016]

[arXiv:2307.13598]

Content

- Background: VQE algorithm and QAOA ansatz
- Quantum Imaginary Time Evolution (QITE)
- Numerical results

Ground state preparation for Ising model

$$H_{\text{Ising}} = - \sum_{\langle i,j \rangle} Z_i Z_j \quad \text{Ground state: } \frac{1}{\sqrt{2}} (|000 \dots 0\rangle + |111 \dots 1\rangle)$$

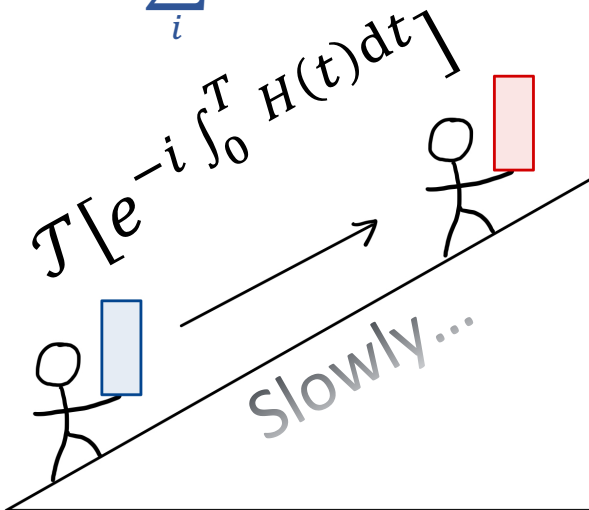
- Prepare ground state with an adiabatic process:

$$H(t) = \frac{t}{T} H(0) + \left(1 - \frac{t}{T}\right) H(T)$$

$$- \sum_i X_i \qquad \qquad \qquad - \sum_{\langle i,j \rangle} Z_i Z_j$$

$$- \sum_i X_i \text{ Ground state:}$$

$$\frac{1}{\sqrt{2^N}} (|0\rangle + |1\rangle)^{\otimes N} = |+\rangle^{\otimes N}$$



$$- \sum_{\langle i,j \rangle} Z_i Z_j \text{ Ground state:}$$

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$$\mathcal{T} \left[e^{-i \int_0^T H(t) dt} \right]$$

Initial state:

final state:

$$\frac{1}{\sqrt{2^N}} (|0\rangle + |1\rangle)^{\otimes N} = |+\rangle^{\otimes N} \quad \longrightarrow \quad e^{i\delta t \sum X} e^{i\delta t \sum ZZ} \dots e^{i\delta t \sum X} e^{i\delta t \sum ZZ} \quad \longrightarrow \quad \frac{1}{\sqrt{2}} (|000 \dots 0\rangle + |111 \dots 1\rangle)$$

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$\frac{T}{\delta t}$ layers, too many!

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$$\frac{1}{\sqrt{2^N}} (|0\rangle + |1\rangle)^{\otimes N} = |+\rangle^{\otimes N} \quad \longrightarrow \quad e^{i\theta_1 \sum X} e^{i\theta_2 \sum ZZ} e^{i\theta_3 \sum X} e^{i\theta_4 \sum ZZ} \quad \longrightarrow \quad \frac{1}{\sqrt{2}} (|000 \dots 0\rangle + |111 \dots 1\rangle)$$

Turn the evolution time into arbitrary rotation angles

$$\theta_1, \theta_2, \theta_3, \theta_4$$

Ground state preparation for Ising model

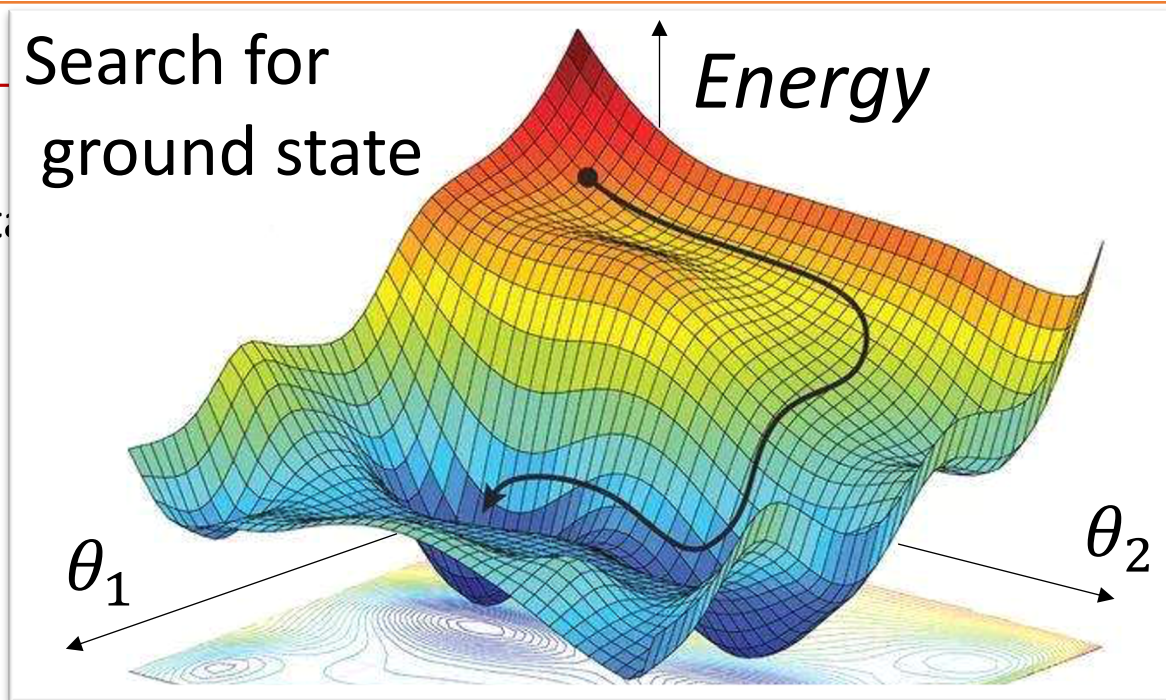
$$H_{\text{Ising}} = -$$

Search for
ground state

Energy

$|11 \dots 1\rangle\rangle$

- Prepare ground state



Initial state:

final state:

$$\frac{1}{\sqrt{2^N}} (|0\rangle + |1\rangle)^{\otimes N} = |+\rangle^{\otimes N}$$



$$e^{i\theta_1 \sum X} e^{i\theta_2 \sum ZZ} e^{i\theta_3 \sum X} e^{i\theta_4 \sum ZZ}$$



$$\frac{1}{\sqrt{2}} (|000 \dots 0\rangle + |111 \dots 1\rangle)$$

Variational Quantum Eigensolver (VQE) with QAOA ansatz [E. Farhi et al. 2014]

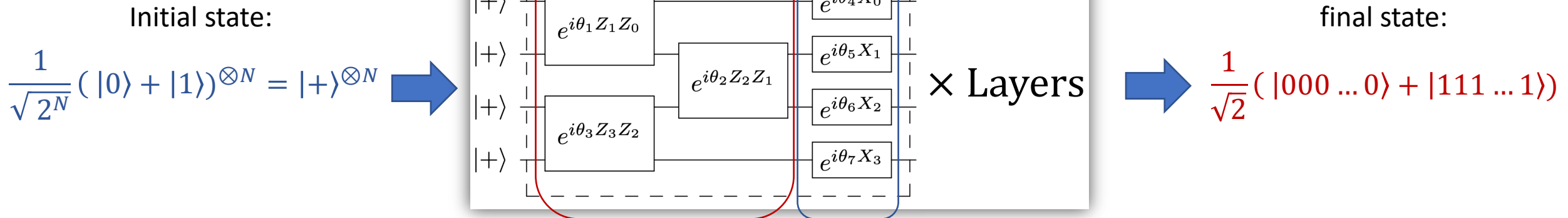
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- Prepare ground state with an adiabatic process:

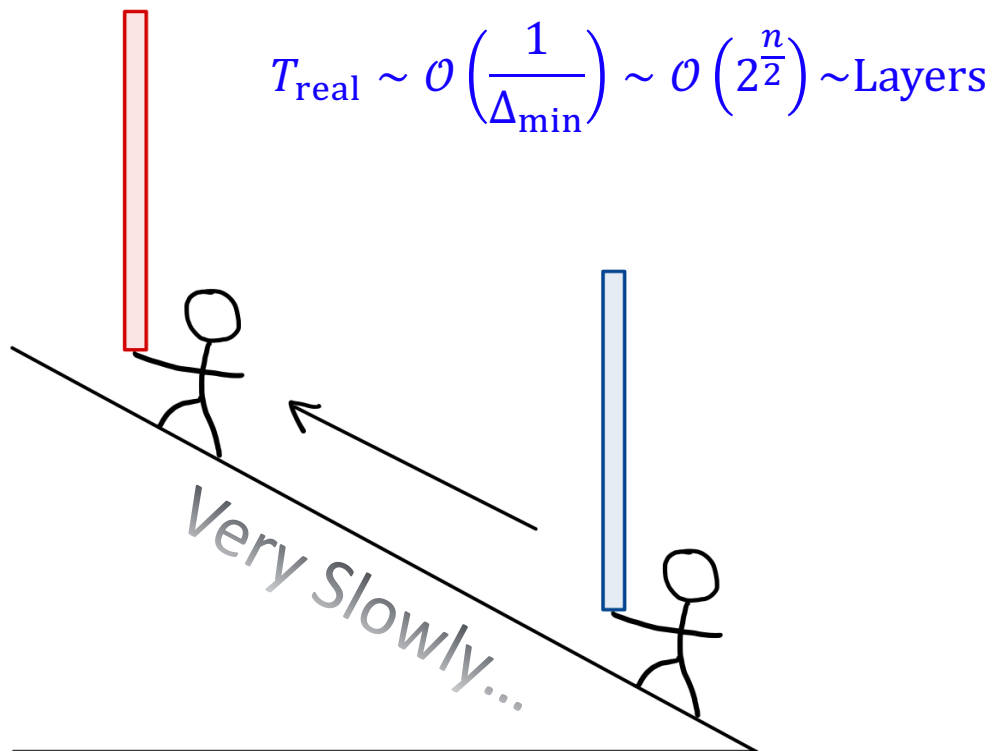
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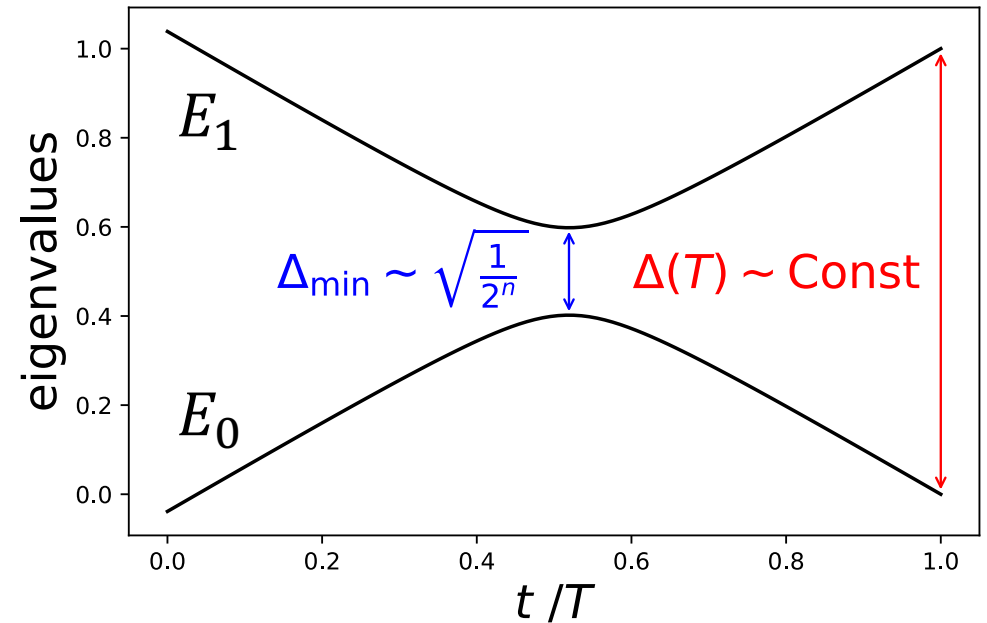
Adiabatic process is too slow!

- In **some models** H_P [E. Farhi et al. 2000], the evolution time T_{real} grows exponentially with the system size n



$$H(t) = \frac{t}{T}H(0) + \left(1 - \frac{t}{T}\right)H_P$$

Illustration of $H(t)$ mass gap
 $\Delta(t) = E_1(t) - E_0(t)$



Adiabatic process is too slow!

- In some models H_P [E. Farhi et al. 2000], the evolution time T_{real} grows exponentially with the system size n

$$T_{\text{real}} \sim \mathcal{O}\left(\frac{1}{\Delta_{\text{min}}}\right) \sim \mathcal{O}\left(2^{\frac{n}{2}}\right) \sim \text{Layers}$$

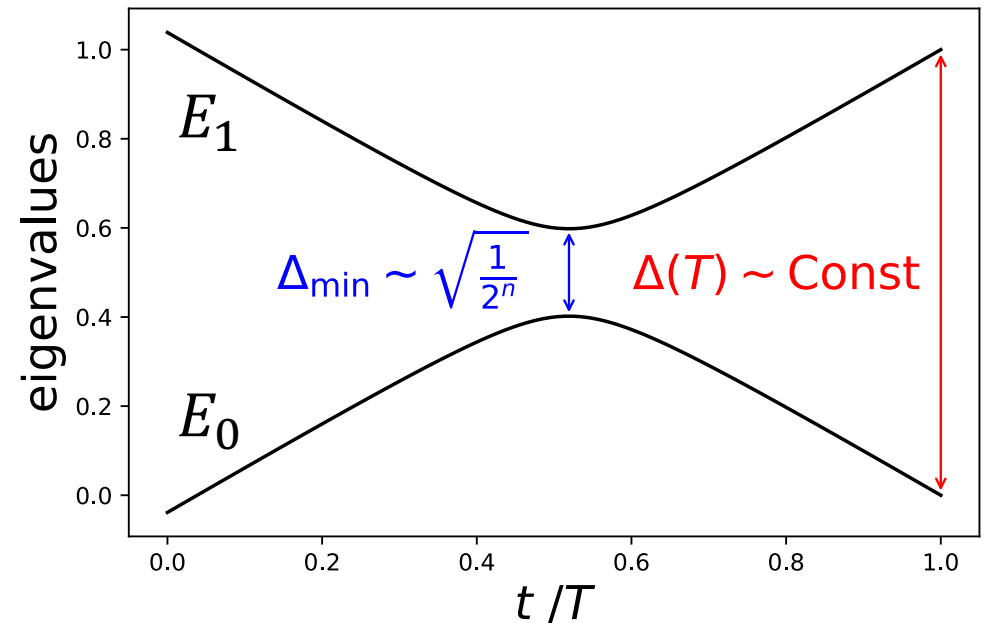
$$e^{-T_{\text{imag}} H_P}$$

- In contrast, the **imaginary time evolution** needs evolution time:

$$T_{\text{imag}} \sim \mathcal{O}\left(\frac{1}{\Delta(T)}\right) \sim \mathcal{O}(\text{Const}) \sim \text{Layers}$$

$$H(t) = \frac{t}{T} H(0) + \left(1 - \frac{t}{T}\right) H_P$$

Illustration of $H(t)$ mass gap
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Imaginary time evolution on quantum computer

- Euclidean correlation function:

$$\lim_{T \rightarrow \infty} \frac{1}{Z_T} \text{Tr} \left[\underbrace{e^{-(T-t)H} O_2 e^{-tH}}_{\text{}} O_1 \right] = \sum_n \langle 0 | O_2 | n \rangle \langle n | O_1 | 0 \rangle e^{-tE_n}$$

- Quantum **Imaginary Time Evolution** (QITE) [M. Motta et al. 2020]:

$$\frac{e^{-\Delta\tau H}}{\sqrt{\langle \psi | e^{-2\Delta\tau H} | \psi \rangle}} |\psi\rangle = e^{i\Delta\tau \sum_i a_i \sigma_i} |\psi\rangle = \prod_i e^{i\Delta\tau a_i \sigma_i} |\psi\rangle + \mathcal{O}(\Delta\tau^2)$$

Decomposed into
CNOT, R_X , R_Y , R_Z
quantum gates

Completeness
of Pauli-basis

Trotter
decomposition



eg: $\sigma_i = X \otimes Y \otimes Z \otimes I$

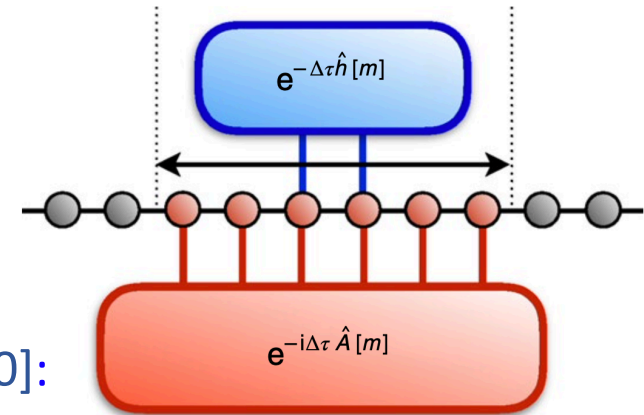
Imaginary time evolution on quantum computer

Number of Paulis is a constant if:

- H is **local**
- $|\psi\rangle$ is **finite correlated**

[M. Motta et al. 2020]

- Quantum Imaginary Time Evolution (QITE) [M. Motta et al. 2020]:



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Variational ansatz inspired by QITE

$$e^{i\Delta\tau a_i \sigma_i} \rightarrow e^{i\theta_i \sigma_i},$$
$$\forall a_i \neq 0$$

Which $e^{i\Delta\tau a_i \sigma_i}$ has non-zero a_i ?
Use symmetry [1]!

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$$H_{\text{Ising}} = \sum_l Z_l Z_{l+1}$$

$$e^{-\epsilon ZZ} \propto e^{ia_1 \epsilon II} \times e^{ia_2 \epsilon IX} \times e^{ia_3 \epsilon IY} \times e^{ia_4 \epsilon IZ}$$

$$\times e^{ia_5 \epsilon XI} \times e^{ia_6 \epsilon XX} \times e^{ia_7 \epsilon XY} \times e^{ia_8 \epsilon XZ}$$

$$\times e^{ia_9 \epsilon YI} \times e^{ia_{10} \epsilon YX} \times e^{ia_{11} \epsilon YY} \times e^{ia_{12} \epsilon YZ}$$

$$\times e^{ia_{13} \epsilon ZI} \times e^{ia_{14} \epsilon ZX} \times e^{ia_{15} \epsilon ZY} \times e^{ia_{16} \epsilon ZZ}$$

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$$H_{\text{Ising}} = \sum_l Z_l Z_{l+1}$$


$$e^{-\epsilon ZZ} \propto e^{ia_1 \epsilon I I} \times e^{ia_2 \epsilon I X} \times e^{ia_3 \epsilon I Y} \times e^{ia_4 \epsilon I Z}$$

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$$\times e^{ia_{13} \epsilon Z I} \times e^{ia_{14} \epsilon Z X} \times e^{ia_{15} \epsilon Z Y} \times e^{ia_{16} \epsilon Z Z}$$

 :Time-reversal symmetry

 : \mathcal{Z}_2 symmetry, $[H_{\text{Ising}}, \prod X_i] = 0$

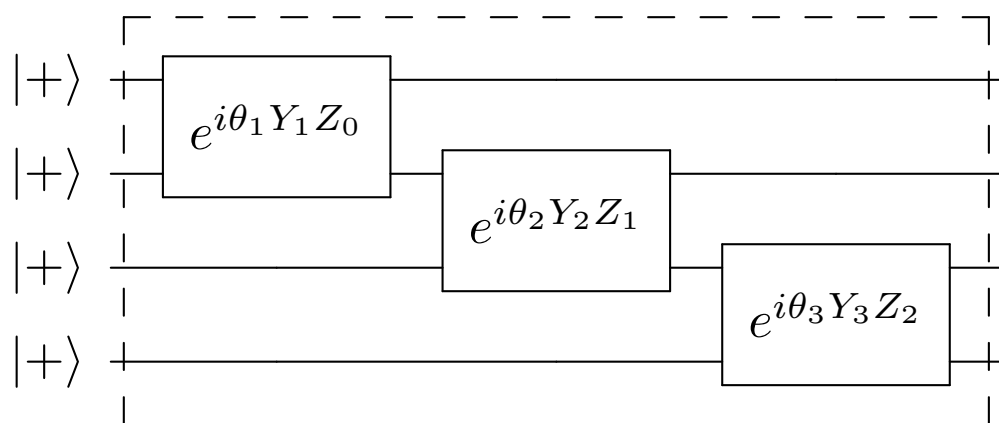
Variational ansatz inspired by QITE

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QITE-inspired ansatz for Ising model



$$e^{-\epsilon ZZ} \propto e^{ia_1 \epsilon I I} \times e^{ia_2 \epsilon I X} \times e^{ia_3 \epsilon I Y} \times e^{ia_4 \epsilon I Z}$$

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Which $e^{i\Delta\tau a_i \sigma_i}$ has non-zero a_i ?
Use symmetry [1]!

Local U(1) symmetry \Rightarrow **Gauss law is kept in Schwinger model** (No penalty terms)

$$e^{i\theta_1 \sigma_1} |\text{vac}\rangle = \cos\theta_1 |\text{vac}\rangle + \sin\theta_1 |\text{positron} \rightarrow \text{electron}\rangle$$

$$e^{i\theta_2 \sigma_2} |\text{vac}\rangle = \cos\theta_2 |\text{vac}\rangle - \sin\theta_2 |\text{electron} \leftarrow \text{positron}\rangle$$

electric field

Electric field line emitted from the positron and absorbed by the electron

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Gibbs state preparation on QITE-inspired ansatz

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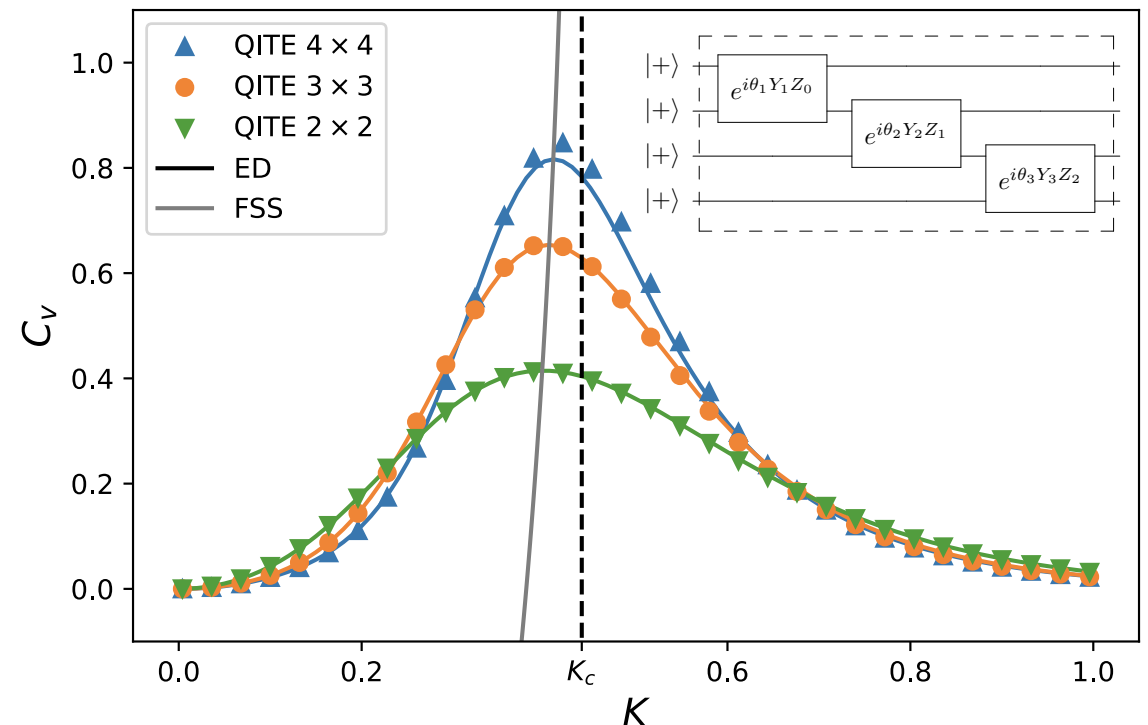
Gibbs state:

$$\rho = \frac{e^{-KH_{\text{Ising}}}}{Z}, \quad \langle \hat{O} \rangle = \text{Tr}(\rho \hat{O})$$

Calculate the heat capacity C_v :

$$C_v = \frac{K^2}{|\Lambda|} (\langle H^2 \rangle - \langle H \rangle^2)$$

- Heat capacity as a function of inverse temperature K . [1]

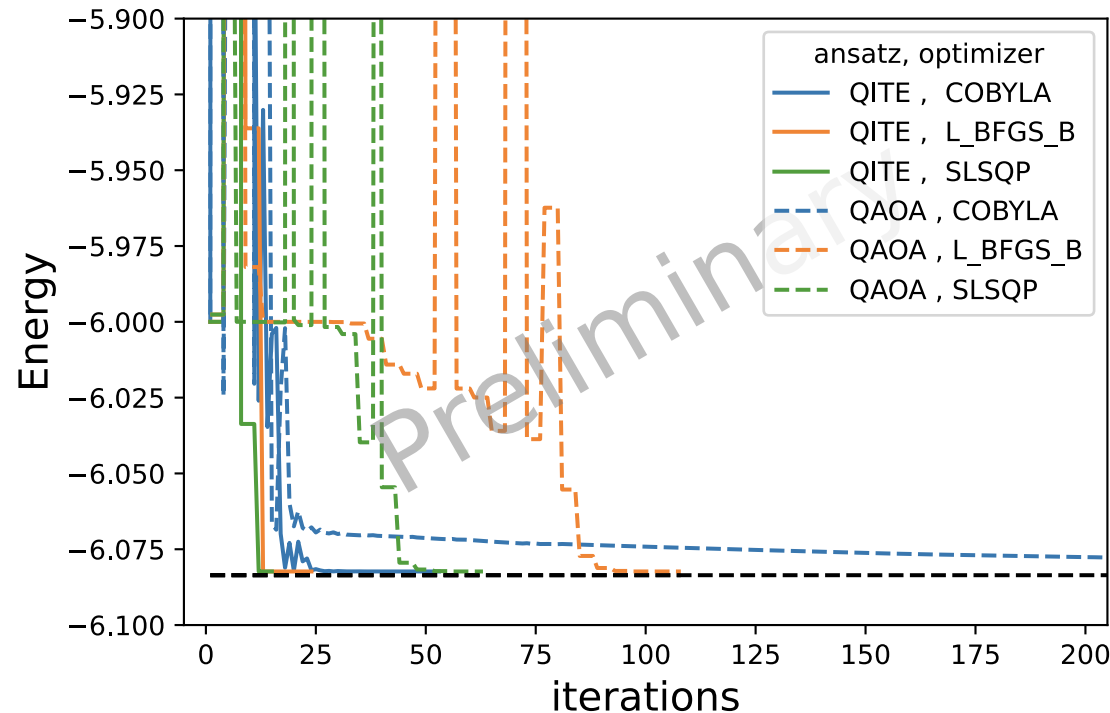


Schwinger model

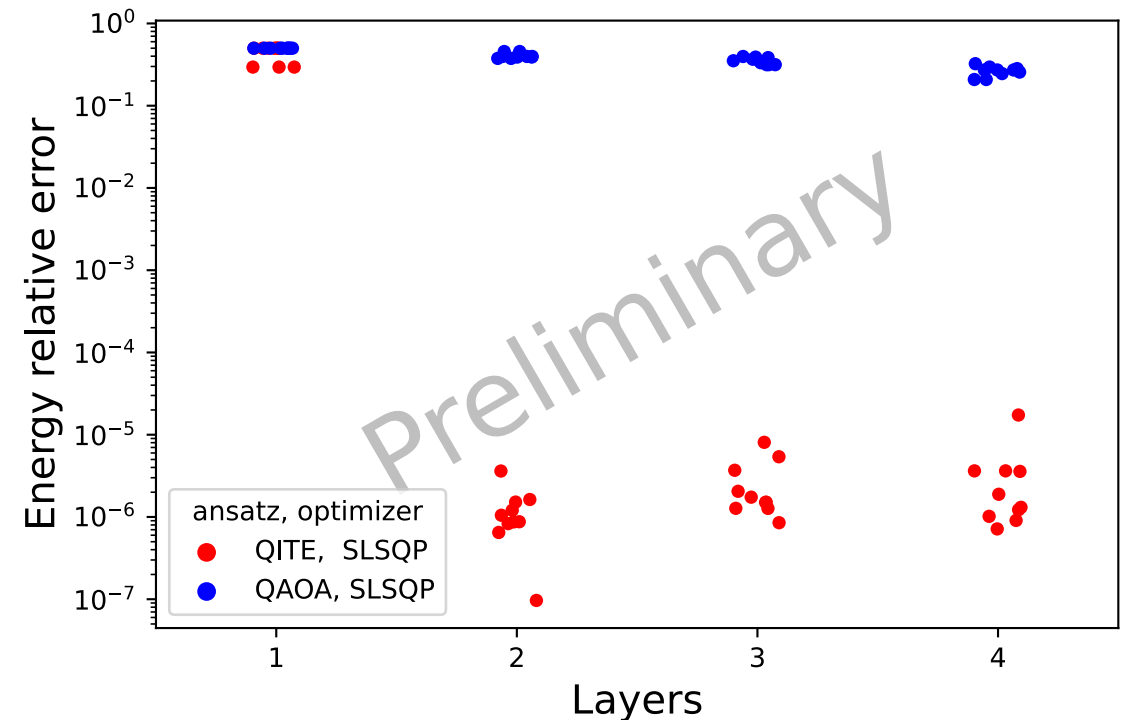
Hamiltonian with Wilson fermion [1]

$$\begin{aligned}
 W = & ix(r-1) \sum_{n=1}^{N-1} (\sigma_{2n}^- \sigma_{2n+1}^+ - \sigma_{2n}^+ \sigma_{2n+1}^-) \\
 & + ix(r+1) \sum_{n=1}^{N-1} (\sigma_{2n-1}^+ \sigma_{2n}^z \sigma_{2n+1}^z \sigma_{2n+2}^- - \sigma_{2n-1}^- \sigma_{2n}^z \sigma_{2n+1}^z \sigma_{2n+2}^+) \\
 & + \sum_{n=1}^{N-1} \left(l_0 + \sum_{k=1}^n Q_k \right)^2 + 2i \left(\frac{m_{\text{lat}}}{g} \sqrt{x} + xr \right) \sum_{n=1}^N (\sigma_{2n-1}^- \sigma_{2n}^+ - \sigma_{2n-1}^+ \sigma_{2n}^-).
 \end{aligned}$$

- QITE-inspired ansatz converges faster to the ground state



- QITE-inspired ansatz requires less layers:

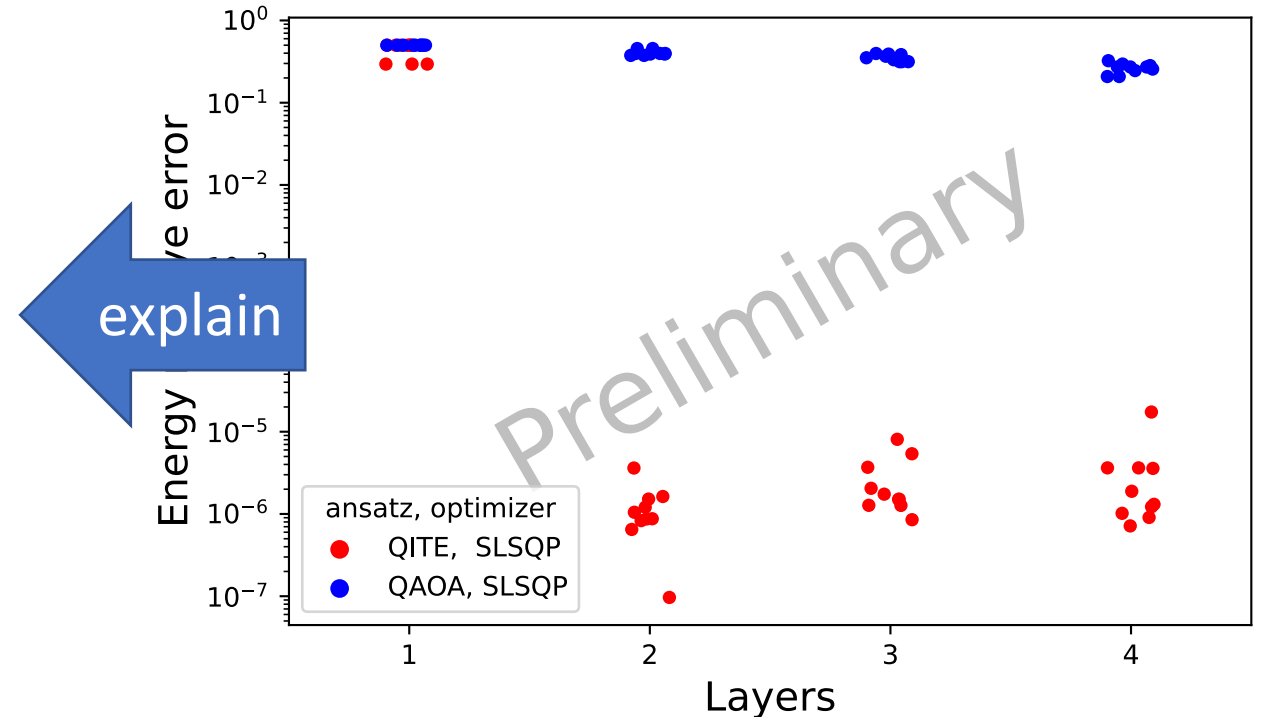
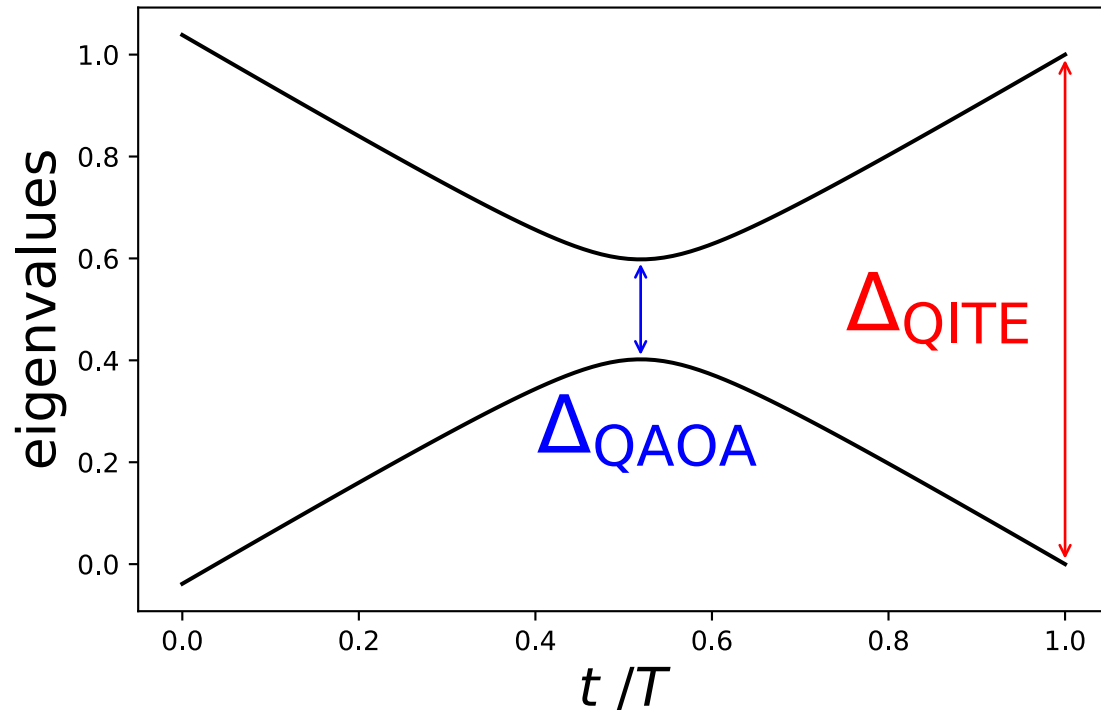


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 \end{aligned}$$

- **QITE-inspired ansatz** requires less layers:



Variational ansatz inspired by QITE

$$e^{i\Delta\tau a_i \sigma_i} \rightarrow e^{i\theta_i \sigma_i},$$
$$\forall a_i \neq 0$$

Advantages of **QITE-inspired ansatz**:

1. symmetry preserving
2. good at Gibbs state preparation (better than hardware-efficient ansatz [1])
3. converging faster to the ground state
4. requiring fewer layers than QAOA

Conclusion

- We propose an ansatz design strategy inspired by quantum imaginary time evolution.
- The ansatz is suitable for **Gibbs state preparation**, and performs better than the hardware-efficient ansatz.
- The ansatz could perform better than the QAOA ansatz in the **ground state preparation**.

Thanks for listening!