Quantum Imaginary-Time Evolution

Prepare ITE state with polynomial resources in time

Preprint
(v3 updated soon)

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Dec 10th , 2025

Imaginary-time evolution (ITE)

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Problem For Hamiltonian H, given initial state $|\phi(0)\rangle$, prepare the normalized solution of imaginary-time Schrödinger equation

$$\partial_\tau |\phi(\tau)\rangle = -H |\phi(\tau)\rangle \text{ with } |\phi\rangle = |\phi(0)\rangle$$

$$\Longrightarrow |\phi(\tau)\rangle = e^{-\tau H} |\phi\rangle \,/\, \left\| e^{-\tau H} |\phi\rangle \right\|$$

τ	imaginary evolution time
$\vert\phi(\tau)\rangle$	normalized imaginary-time evolved state (ITE state)
$\vert\phi\rangle \to \vert\phi(\tau)\rangle$	imaginary-time evolution operator (ITE operator)

Imaginary-time evolution

Application

- Ground state preparation $|\psi_0\rangle \propto \lim_{\tau\to\infty} \boldsymbol{e^{-\tau H}}|\phi(0)\rangle$ if $|\langle\psi_0|\phi(0)\rangle| > 0$
- Thermal state preparation [1] $\rho = \boldsymbol{e^{-\tau H}} / \mathrm{Tr}(e^{-\tau H})$
- Open-system simulation [2] $e^{\mathcal{L}t}[\rho] = V\rho V^\dagger,\ V = \lim_{N\to\infty}\left(e^{-itH_1/N}\boldsymbol{e^{-tH_2/N}}\right)^N$
- Others:
  - computing Hamiltonian-related properties [3]
  - data classification [4], optimization [5]
  - quantum mechanics [6], quantum field theory [7]

[1] Motta, Mario, et al. "Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution." *Nature Physics* 16.2 (2020): 205-210.
[2] Kamakari, Hirsh, et al. "Digital quantum simulation of open quantum systems using quantum imaginary–time evolution." *PRX quantum* 3.1 (2022): 010320.
[3] Wang, Xiaoyang, et al. "Computing n-Time Correlation Functions without Ancilla Qubits." *Physical Review Letters* 135 (2025): 230602.
[4] Ye, Qi, et al. "Quantum automated learning with provable and explainable trainability." *arXiv preprint arXiv:2502.05264* (2025).
[5] Wang, Xiaoyang, et al. "Imaginary Hamiltonian variational Ansatz for combinatorial optimization problems." *Physical Review A* 111.3 (2025): 032612.
[6] Wick, Gian-Carlo. "Properties of Bethe-Salpeter wave functions." *Physical Review* 96.4 (1954): 1124.
[7] Lancaster, Tom, and Stephen J. Blundell. *Quantum field theory for the gifted amateur*. OUP Oxford, 2014.

Existing works

Routine 1

Fix one $|\phi\rangle$. Find a physical unitary U such that $U|\phi\rangle = |\phi(\tau)\rangle$.

① (PQC scheme) find θ^* such that $U(\theta^*) \approx U$ [1]

② (Manifold scheme) find $V \in \mathrm{SU}(2^n)$ such that $V \approx U$ [2]

③ (Trotter scheme) compute $\{(t_j, A_j)\}$ such that $\prod_j e^{-iA_j t_j} \approx U$ [3]

✓ polynomial resource complexity in system size
✓ execute without failure
× one solution cannot be converted to the other that has unknown initial state
× unclear relation between τ and precision, possibly an exponential dependency

[1] McArdle, Sam, et al. "Variational ansatz-based quantum simulation of imaginary time evolution." npj Quantum Information 5.1 (2019): 75.
[2] Gluza, Marek, et al. "Double-bracket quantum algorithms for quantum imaginary-time evolution." arXiv preprint arXiv:2412.04554 (2024).
[3] Motta, Mario, et al. "Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution." Nature Physics 16.2 (2020): 205-210.

Existing works

Routine 2

Unknown $|\phi\rangle$. Find a physical operation $\mathcal{E}$ such that $\mathcal{E}(\phi) = \phi(\tau)$ or FAILURE.

✓ polynomial resource complexity in system size
✓ theoretically analyzed; work for any initial state
× success probability decrease exponentially with τ

exponential decay problem

Short Conclusion

- For long imaginary evolution, algorithms are either
  - heuristic or
  - theoretically infeasible

⇒ NEED ITE algorithm for $\tau \gg 0$

Transformation of quantum data

- A unitary U applies rotations with respect to its eigenspaces.

eigenphase: angle of the rotation

$$U = \sum_j e^{i\lambda_j} |\psi_j\rangle\langle\psi_j|$$

eigenvalue: amplitude of the rotation

eigenbasis: basis of the rotation

Transformation of quantum data

- Transformation of U in terms of function $f: \mathbb{R} \rightarrow \mathbb{C}$ can be described as

eigenphase: angle of the rotation

$$\boldsymbol{f}(\boldsymbol{U}) = \sum_{j} \boldsymbol{f}(\overline{\boldsymbol{\lambda}_j}) |\boldsymbol{\psi}_j\rangle\langle\boldsymbol{\psi}_j|$$

eigenvalue: amplitude of the rotation

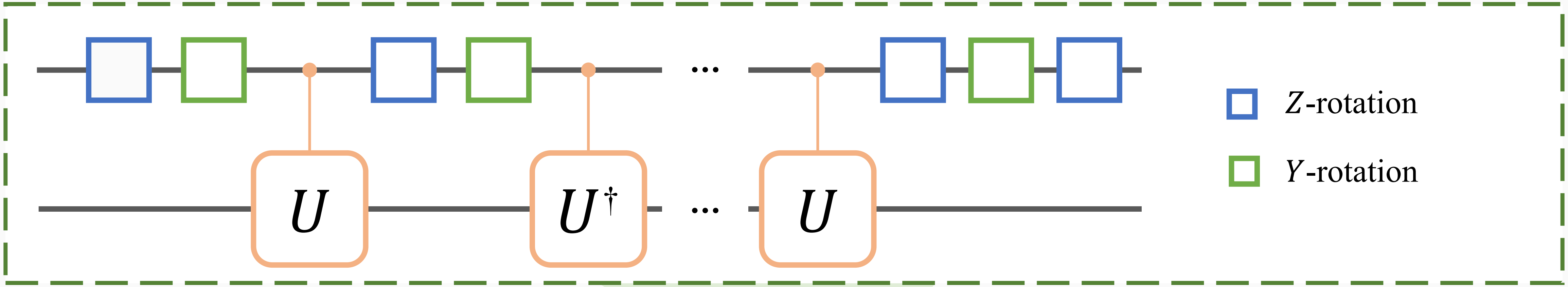
eigenbasis: basis of the rotation

- Quantum algorithms using unitaries deal with eigen-information procession.
  - Extract the target eigenphase/value – Shor, HHL, QAE
  - Amplify the target eigenphase/value – Hamiltonian simulation, Grover

Transformation of quantum data

Core Idea 1

Use quantum phase processing (QPP) [1] , a QSP-based structure to simulate transformation



$$\begin{pmatrix} P(U) & -Q(U) \\ Q^*(U) & P^*(U) \end{pmatrix}$$

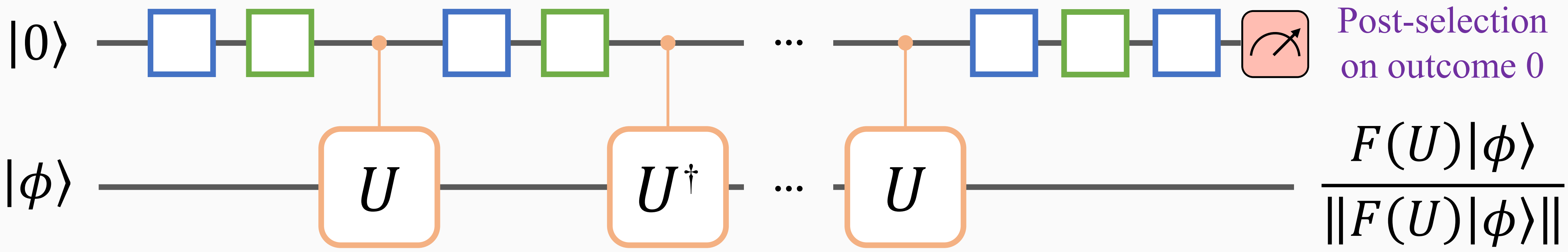
P, Q satisfy $\begin{cases} P, Q \in \mathbb{C}[e^{-ix/2}, e^{ix/2}], \\ \deg P = \deg Q \\ P, Q \text{ has the same parity} \end{cases}$

[1] Wang, Youle, et al. "Quantum phase processing and its applications in estimating phase and entropies." *Physical Review A* 108.6 (2023): 062413.

Transformation of quantum data

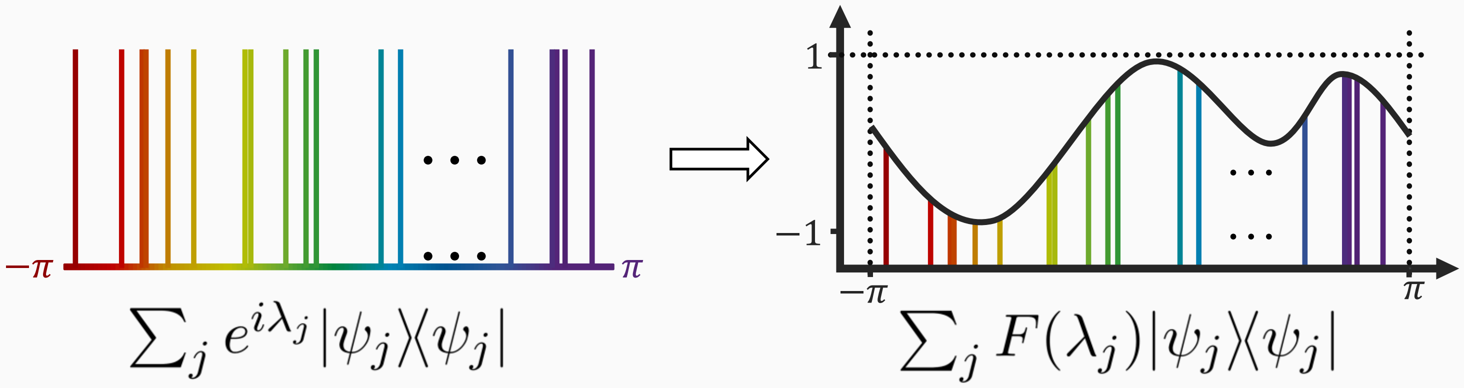
Core Idea 1

Use quantum phase processing (QPP), a QSP-based structure to simulate transformation F



How to simulate $f(U)$?

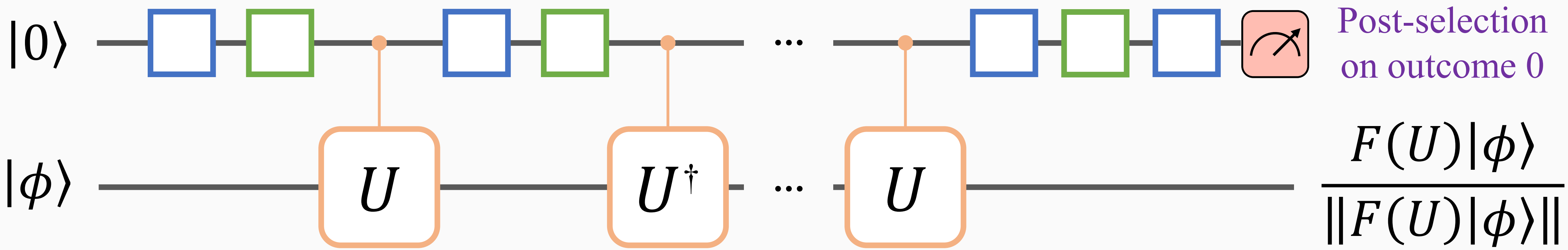
① Assume access to control $-U$
② Compute f's Fourier approximation F
③ Compute rotation angles for □ □
④ Construct the QPP circuit
⑤ Post-select the ancilla qubit



Transformation of quantum data

Core Idea 1

Use quantum phase processing (QPP) to simulate transformation



For ITE problem, choose $U = e^{-iH}$

$F(x) \approx e^{\tau x}/e^{\tau}$, then

output state $\approx |\phi(\tau)\rangle$ with success probability $\mathcal{O}\left(e^{-2\tau}\right)$

Naïve choice raises exponential decay problem

Adaptive normalization

Core Idea 2

Choose an exponential transformation with adaptive normalization factor λ. Consider function

$$\sout{F(x) \approx e^{\tau x}} \Longrightarrow F(x) \approx \begin{cases} \alpha e^{\tau(x-\lambda)}, & x \in [-\pi, \lambda] \\ \xi_{\tau,\lambda}(x), & x \in (\lambda, \pi] \end{cases}$$

where $\alpha, \xi_{\tau,\lambda}$ ensure approximation error decays *super-polynomially* with the degree of approximation.

Lemma 1 *Let $C \geq \tau(\lambda - |\lambda_0|) \geq 0$. Under Assumptions (i,iv,v), the output state $|\widetilde{\phi}(\tau)\rangle$ from the ITE circuit $V^{\epsilon}_{f_{\tau,\lambda}}(U_H)$ is obtained with success probability lower bounded by $\alpha^2\gamma^2 e^{-2C} - \epsilon$. Moreover, the state fidelity between the output state and the ITE state is approximately lower bounded as*

$$|\langle\phi(\tau)|\widetilde{\phi}(\tau)\rangle| \gtrsim 1 - \mathcal{O}(\alpha^{-1}\epsilon \cdot e^{C}). \tag{5}$$

⟹ Finding $\lambda \in [|\lambda_0|, |\lambda_0| + \tau^{-1}]$ outputs an approximated ITE state with success probability nearly lower bounded by a CONSTANT $\alpha^2 e^{-2}\gamma^2$

Avoids the exponential decay problem

Main results

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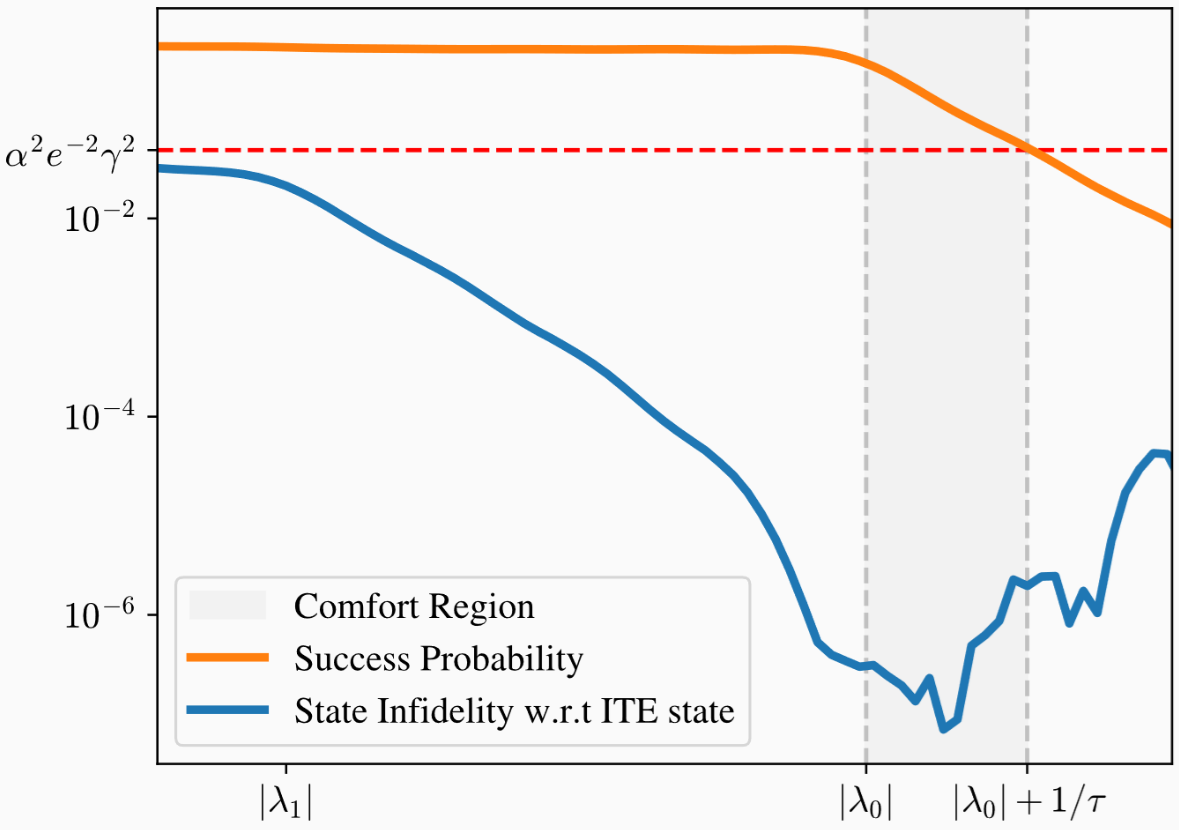
$\lambda \in [|\lambda_0|, |\lambda_0| + \tau^{-1}]$

Error of ITE state preparation: $\mathcal{O}(10^{-5})$

Success probability $\gtrsim \alpha^2 e^{-2} \gamma^2$



Assumptions without loss of generality

i) eigenvalues of H is within $[-1, 1]$, and ground-state energy λ_0 is negative

iv) imaginary-time evolution is long i.e., $\tau \gg 0$

v) the overlap between input state $|\phi(0)\rangle$ and the ground state is non-zero

Lemma 1 *Let* $C \geq \tau(\lambda - |\lambda_0|) \geq 0$. *Under Assumptions (i,iv,v), the output state* $|\widetilde{\phi}(\tau)\rangle$ *from the ITE circuit* $V^{\epsilon}_{f_{\tau,\lambda}}(U_H)$ *is obtained with success probability lower bounded by* $\alpha^2\gamma^2 e^{-2C} - \epsilon$. *Moreover, the state fidelity between the output state and the ITE state is approximately lower bounded as*

$$|\langle\phi(\tau)|\widetilde{\phi}(\tau)\rangle| \gtrsim 1 - \mathcal{O}(\alpha^{-1}\epsilon \cdot e^{C}). \quad (5)$$

* Some modifications are not shown on arXiv and will be updated in the version 3 soon

Main results

Assumptions that are specific to this problem

vii) the overlap between input state $|\phi(0)\rangle$ and the ground state is at least $\mathcal{O}\big(\mathrm{poly}(n^{-1})\big)$

viii) the gap Δ between the ground-state energy λ_0 and the first-excited-state energy λ_1 is not zero

ix) Δ satisfies $e^{\tau\Delta}$ is at least $\mathcal{O}\big(\mathrm{poly}(\tau)\big)$

Theorem 3 *Under Assumptions (i,iii,iv,v,vi,vii,viii,ix), one can prepare the ITE state* $|\phi(\tau)\rangle$ *up to fidelity* $1 - \mathcal{O}\big(L^2\Lambda^2\,\mathrm{poly}(\tau^{-1})\big)$*, using the following cost:*

- $\widetilde{\mathcal{O}}(L\,\mathrm{poly}(n\tau))$ *queries to controlled Pauli rotations,*
- $\mathcal{O}(\mathrm{poly}(n))$ *copies of* $|\phi\rangle$*,*
- $\widetilde{\mathcal{O}}(L\,\mathrm{poly}(\tau))$ *maximal query depth, and*
- *one ancilla qubit initialized in the zero state,*

where L *is the number of Pauli terms and* $\Lambda = \max_j |h_j|$.

Main Result Approximates the target state to polynomially small errors in inverse imaginary time using polynomially many elementary quantum gates and a single ancilla qubit.

Comparison with theoretical works

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Methods	Circuit depth	Expected circuit runs	Ancilla	H in Pauli form?
Manifold-based, k steps [23]	$\mathcal{O}(3^k n)$	1	0	No
Grover-based [25]	$\mathcal{O}(\tau)$	\	$\mathcal{O}(n)$	No
TE-based [26]	$\mathcal{O}(\tau)$	\	1	No
QSP-based [27, 28]	$\widetilde{\mathcal{O}}(\tau)$	\	1	No
QSP-based with AN (Theorem 2)	$\widetilde{\mathcal{O}}(\tau)$	$\mathcal{O}(\gamma^{-2})$	1	No
QSP-based with AN (Theorem 3)	$\widetilde{\mathcal{O}}(L\,\mathrm{poly}(\tau))$	$\mathcal{O}(\mathrm{poly}(n))$	1	Yes

adaptive normalization

holds for reasonable ground-state overlap

proves **ITE state can be prepared in polynomial resource**
in terms of evolution time

[23] Gluza, Marek, et al. "Double-bracket quantum algorithms for quantum imaginary-time evolution." *arXiv preprint arXiv:2412.04554* (2024).
[25] Liu, Tong, Jin-Guo Liu, and Heng Fan. "Probabilistic nonunitary gate in imaginary time evolution." *Quantum Information Processing* 20.6 (2021): 204.
[26] Kosugi, Taichi, et al. "Imaginary-time evolution using forward and backward real-time evolution with a single ancilla: First-quantized eigensolver algorithm for quantum chemistry." *Physical Review Research* 4.3 (2022): 033121.
[27] Silva, Thais L., et al. "Fragmented imaginary-time evolution for early-stage quantum signal processors." Scientific Reports 13.1 (2023): 18258.
[28] Chan, Hans Hon Sang, David Muñoz Ramo, and Nathan Fitzpatrick. "Simulating non-unitary dynamics using quantum signal processing with unitary block encoding." arXiv preprint arXiv:2303.06161 (2023).

* This table is not shown on arXiv and will be updated in the version 3 soon

Summary for the ITE part

Ground-state energy estimation
of precision $\mathcal{O}(\tau^{-1})$

→

ITE state preparation
of precision $\mathcal{O}\left(\mathrm{poly}(\tau^{-1})\right)$

Why ITE state can be prepared in polynomial resource?

① Multi-qubit QSP circuits are independent of system size

② Exponential transformation can be approximated via super-polynomial Fourier convergence

③ Assumption on reasonable ground state overlap (otherwise may not be scalable in system size)

↳ not scalable for directly applying to Gibbs state preparation ☹

Application

- Ground state preparation and ground-state energy estimation

Application to Ground-state problems

- Given a non-degenerate Hamiltonian

$$H = \sum_j \lambda_j |\psi_j\rangle\langle\psi_j|, \text{ with } \lambda_0 < \lambda_1 \leq \cdots$$

find

λ_0 → Ground-state energy estimation

$|\psi_0\rangle$ → Ground-state preparation

- Common query model $U(t) = e^{iHt}$

Application to Ground-state problems

Lemma 4 *Under Assumptions (iii, vi),*

$$|\langle\psi_0|\phi(\tau)\rangle| \geq \gamma/\sqrt{e^{-2\tau\Delta}+\gamma^2}.$$

Moreover, the lower bound is tight for some Hamiltonians.

- ITE state converges to the ground state as $\tau \to \infty$
- The rate of convergence is at least polynomial if $e^{\tau\Delta} = \Omega(\text{poly}(\tau))$

If τ satisfies $e^{\tau\Delta} = \Omega(\text{poly}(\tau))$:

Ground-state energy estimation of precision $\mathcal{O}(\tau^{-1})$ → ITE state preparation of precision $\mathcal{O}\left(\text{poly}(\tau^{-1})\right)$ → Ground-state preparation of precision $\mathcal{O}\left(\text{poly}(\tau^{-1})\right)$

How to find such τ ?

Application to Ground-state problems

Lemma 4 *Under Assumptions (iii, vi),*

$$|\langle \psi_0 | \phi(\tau) \rangle| \geq \gamma / \sqrt{e^{-2\tau\Delta} + \gamma^2}.$$

Moreover, the lower bound is tight for some Hamiltonians.

- ITE state converges to the ground state as $\tau \to \infty$
- The rate of convergence is at least polynomial if $e^{\tau\Delta} = \Omega(\mathrm{poly}(\tau))$

Problem to be solved For Hamiltonian H, find

1. $\tau \gg 0$ s.t. $e^{\tau\Delta} = \Omega(\mathrm{poly}(\tau))$ (**ITE state ≈ ground state**)

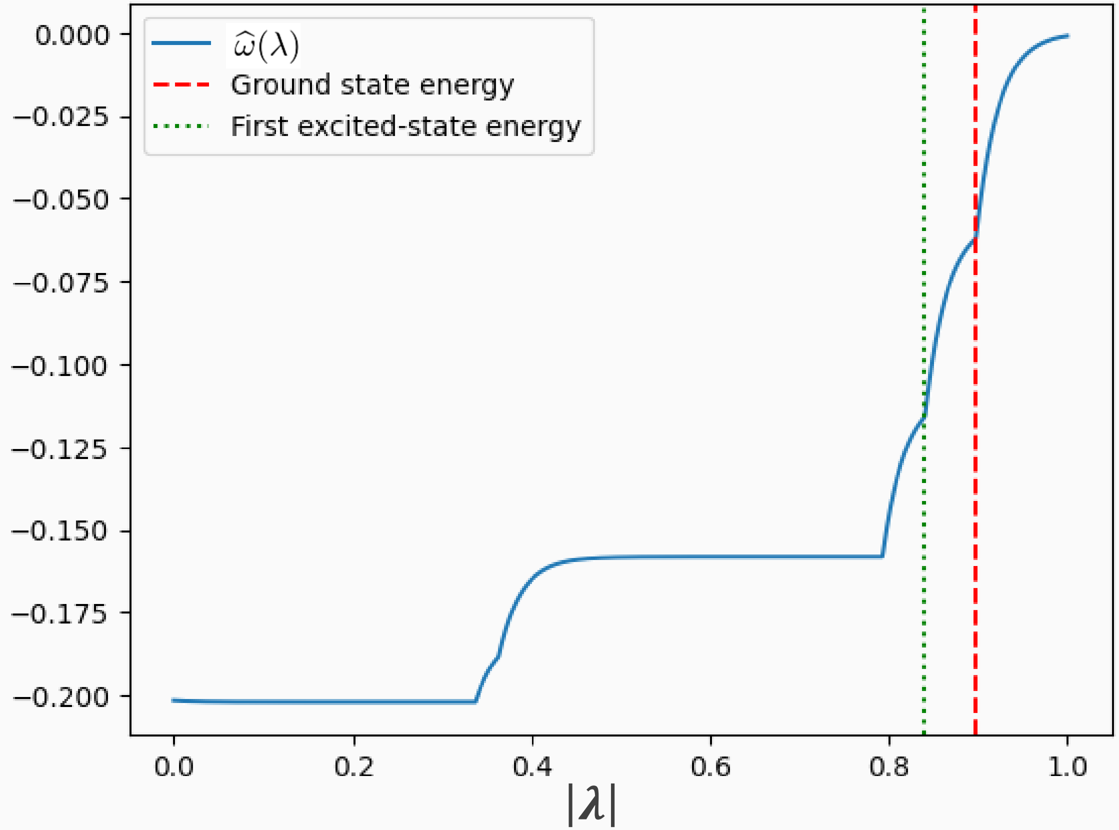
2. $\lambda \in [|\lambda_0|, |\lambda_0| + \tau^{-1}]$ (**efficient ITE state preparation**)

3. E, an estimation of ITE state's expectation value w.r.t. H (**ground-state energy estimation**)

Our work

Expectation value of circuit wrt. *H*

$$\widehat{\omega}(\lambda) = \langle\phi| f_{\tau,\lambda}(U_H)^\dagger \, H \, f_{\tau,\lambda}(U_H) |\phi\rangle$$



Algorithm Sketch

1. Start with a guess time t, and a search interval $[\lambda_l, \lambda_r]$
2. Measure QPP circuits that prepare ITE states, which will give an estimation E_i and the interval where λ_0 lies.
3. If search interval is small enough and the estimation sequence $\{E_i\}_i$ converges, return t, λ_r, E_{-1}
4. Otherwise, update guess time, search interval, and go back to Step 1.

Algorithm 1: Ground state preparation and energy estimation via ITE

Input : Hamiltonian H, initial state $|\phi\rangle$, step size Δt, lower bound B, a boolean function $\mathcal{X}$ for testing convergence

Output: τ, λ, E in Problem 1

```
Guess t ≫ 0;
E_0 ← 0, i ← 0;
λ_l ← 0, λ_r ≈← max{ λ : |ω(λ)| > B };
while λ_r − λ_l > t^{-1} or X({E_i}_i) = False do
    Measurement shots # ← 8LΛ^2 t^3 B^{-2};
    δ ← (λ_r − λ_l)/3, λ_lm ← λ_l + δ, λ_rm ← λ_r − δ;
    Estimate ω(λ_lm), ω(λ_r);
    r ← (ω(λ_lm) − ω(λ_r)) / ω(λ_r);
    if |r − (e^{4τδ} − 1)| > τ^{-1}(e^{4τδ} + 1) then
        E_i ← selected samples that estimate ω(λ_r);
        [λ_l, λ_r] ← [λ_lm, λ_r];
    else
        E_i ← selected samples that estimate
         ω(λ_lm), ω(λ_r);
        [λ_l, λ_r] ← [λ_l, λ_rm];
    t ← t + Δt, i ← i + 1;
return τ ← t, λ_r, E_i;
```

Our work

Theorem 6 *Suppose Assumptions (i,ii,v,vi,vii,viii,x) hold. Algorithm 1 returns a time τ that satisfies Assumption (ix), an estimate $\lambda \in [|\lambda_0|, |\lambda_0| + \tau^{-1}]$, and an estimate of λ_0 within precision $\mathcal{O}(B\gamma^{-1}\tau^{-1})$, with failure probability $\mathcal{O}(e^{-\tau}\log\tau)$. Moreover, there are at most $\mathcal{O}(L\log\tau)$ distinct circuit constructed in Algorithm 1, and each circuit takes at most:*

- *$\mathcal{O}(\tau)$ queries to controlled-U_H and its inverse,*
- *$\mathcal{O}(\tau)$ query depth of U_H,*
- *1 ancilla qubit, and*
- *$\mathcal{O}(L\Lambda^2 B^{-2}\tau^3)$ measurement shots,*

where L is the number of Pauli terms and $\Lambda = \max_j |h_j|$.

Algorithm Sketch

1. Start with a guess time τ, and a search interval $[\lambda_l, \lambda_r]$
2. Measure QPP circuits that prepare ITE states, which will give an estimation E_i and the location where λ_0 lies.
3. If search interval is small enough and the estimation sequence $\{E_i\}_i$ converges, return τ, λ_r, E_{-1}
4. Otherwise, update guess time, search interval, and go back to Step 1.

Algorithm 1: Ground state preparation and energy estimation via ITE

Input : Hamiltonian H, initial state $|\phi\rangle$, step size Δt, lower bound B, a boolean function $\mathcal{X}$ for testing convergence

Output: τ, λ, E in Problem 1

Guess $t \gg 0$;
$E_0 \leftarrow 0$, $i \leftarrow 0$;
$\lambda_l \leftarrow 0$, $\lambda_r \overset{\approx}{\leftarrow} \max\{\lambda : |\omega(\lambda)| > B\}$;
while $\lambda_r - \lambda_l > t^{-1}$ *or* $\mathcal{X}(\{E_i\}_i) =$ False **do**
  Measurement shots # $\leftarrow 8L\Lambda^2 t^3 B^{-2}$;
  $\delta \leftarrow (\lambda_r - \lambda_l)/3$, $\lambda_{lm} \leftarrow \lambda_l + \delta$, $\lambda_{rm} \leftarrow \lambda_r - \delta$;
  Estimate $\omega(\lambda_{lm})$, $\omega(\lambda_r)$;
  $r \leftarrow (\omega(\lambda_{lm}) - \omega(\lambda_r))/\omega(\lambda_r)$;
  if $|r - (e^{4\tau\delta} - 1)| > \tau^{-1}(e^{4\tau\delta} + 1)$ **then**
    $E_i \leftarrow$ selected samples that estimate $\omega(\lambda_r)$;
    $[\lambda_l, \lambda_r] \leftarrow [\lambda_{lm}, \lambda_r]$;
  else
    $E_i \leftarrow$ selected samples that estimate $\omega(\lambda_{lm}), \omega(\lambda_r)$;
    $[\lambda_l, \lambda_r] \leftarrow [\lambda_l, \lambda_{rm}]$;
  $t \leftarrow t + \Delta t$, $i \leftarrow i + 1$;
return $\tau \leftarrow t$, λ_r, E_i;

Comparison with existing works

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Methods	Query depth	Expected circuit runs	Ancilla
Conventional QPE [31]	$\Omega(\gamma^{-1}\tau)$	$\mathcal{O}(\gamma^{-2}\tau)$	$\Omega(\log(\gamma^{-1}\tau))$
Semi-classical QPE [32, 33]	$\Omega(\gamma^{-3}\tau)$	$\mathcal{O}(\gamma^{-2}\tau)$	1
QET-based [34] (state preparation)	$\Omega(\gamma^{-1}\tau)$	$\tilde{\mathcal{O}}(\gamma^{-2}\tau)$	3
QET-based [34] (energy estimation)	$\Omega(\gamma^{-1}\tau)$	$\tilde{\mathcal{O}}(\gamma^{-2}\tau)$	1
HT-based [35] (energy estimation)	$\Omega\left((1-\gamma^2)^{1/2}\gamma^{-1}\tau\right)$	$\tilde{\mathcal{O}}(\gamma^{-4}\tau)$	1
ITE-based [3, 7]	\	\	0
ITE-based (Theorem 6)	$\mathcal{O}(\tau)$	$\Omega(\gamma^{-4}\tau^3)$	1

Obtain shorter circuit depth as a trade-off of more queries to U_H

[3] Motta, Mario, et al. "Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution." *Nature Physics* 16.2 (2020): 205-210.
[7] McArdle, Sam, et al. "Variational ansatz-based quantum simulation of imaginary time evolution." *npj Quantum Information* 5.1 (2019): 75.
[31] Kitaev, A. Yu. "Quantum measurements and the Abelian stabilizer problem." *arXiv preprint* quant-ph/9511026 (1995).
[32] Griffiths, Robert B., and Chi-Sheng Niu. "Semiclassical Fourier transform for quantum computation." *Physical Review Letters* 76.17 (1996): 3228.
[34] Dong, Yulong, Lin Lin, and Yu Tong. "Ground-state preparation and energy estimation on early fault-tolerant quantum computers via quantum eigenvalue transformation of unitary matrices." *PRX Quantum* 3.4 (2022): 040305.
[35] Ding, Zhiyan, and Lin Lin. "Even shorter quantum circuit for phase estimation on early fault-tolerant quantum computers with applications to ground-state energy estimation." *PRX Quantum* 4.2 (2023): 020331.

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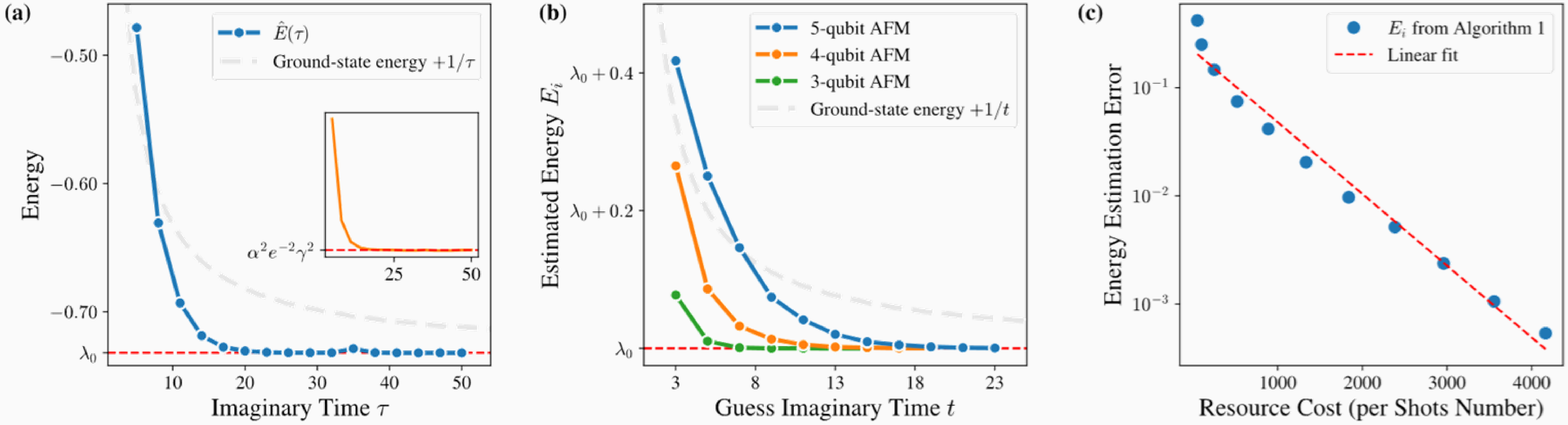
Experiments

Hamiltonian Type Antiferromagnetic Heisenberg Model (AFM) $H \propto \sum_{j=0}^{n}(X_jX_{j+1} + Y_jY_{j+1} + Z_jZ_{j+1} - I)$



Complete tasks with imaginary-time evolution time up to 50

Summary

- The first ITE algorithm proved to have
  polynomial resource dependence in evolution time
- Applying ITE to ground-state problems can reduce circuit depth
- Potential caveats
  - Does not consider classical machine error

Thank you

Research Group

Preprint
(v3 updated soon)

Code Repo