Accelerating ground state calculation using probabilistic imaginary-time evolution and quantum amplitude amplification

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See also Contributed talk [C06-1-03]
2:20PM - 2:40PM Sun. Arg. 6 301 (3F)

Background

Ground state preparation

Quantum Phase Estimation (QPE):
A standard algorithm for estimating the ground-state energy. The computational cost of QPE depends on the initial state, which scales as $O(1/(|c_1|^2 \varepsilon))$.

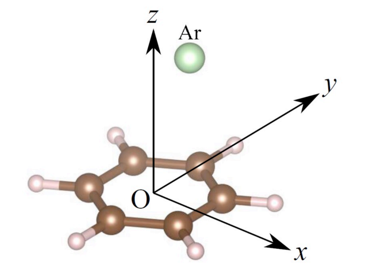
$|c_1|^2$: the probability weight of the ground state in the initial state, ε: a statistical error

Imaginary-time evolution (ITE) operator on a quantum computer is one promising way for ground state preparation. The ITE operator is probabilistically realized on a quantum computer (PITE method), comprising single ancilla qubit and forward- and backward-controlled real time evolution (RTE).

T. Kosugi et al, Phys. Rev. Res., **4**(3) 033121(2022).

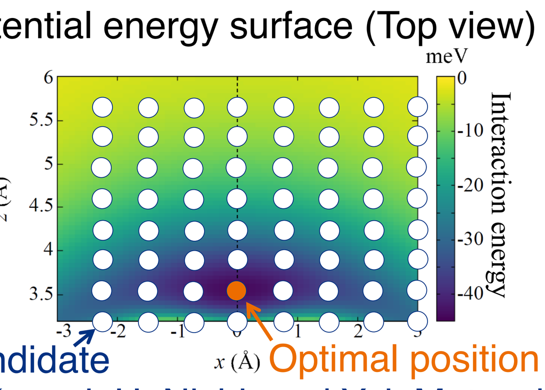
Application of the PITE method: Exhaustive search among all candidate geometries

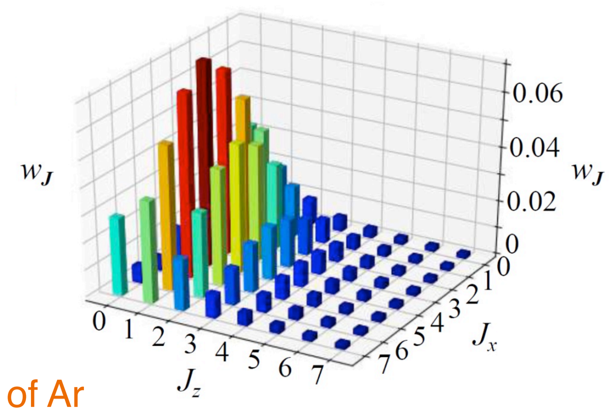
Ar atom above a benzene molecule



After 19th step of PITE, the most stable geometry has the highest probability

Potential energy surface (Top view)





Candidate — Optimal position of Ar

T. Kosugi, H. Nishi, and Y.-i. Matsushita, arXiv:2210.09883 (2022).

Aim of this study

(1) Investigate the computational cost of the PITE method

Ground state preparation is classified as complexity-class quantum Merlin-Arthur (analogy of complexity-class NP on a quantum computer). Exponential computational cost is required in the PITE method.

(2) Realize quantum acceleration in ground state preparation

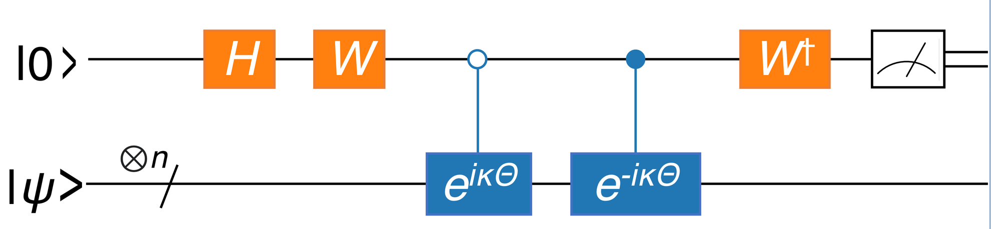
Ground state is probabilistically obtained in the PITE method. Combining quantum amplitude amplification is remedy for probabilistic nature, which also bring us quantum acceleration.

Probabilistic Imaginary-Time Evolution and Quantum Amplitude Amplification

Exact PITE

Embed the nonunitary as a submatrix into a unitary

$$\mathcal{U}_{\mathcal{M}} \equiv \begin{pmatrix} \mathcal{M} & \sqrt{1-\mathcal{M}^2} \\ \sqrt{1-\mathcal{M}^2} & -\mathcal{M} \end{pmatrix}$$



$$\mathcal{M} = \gamma e^{-\mathcal{H}\Delta\tau}$$
$$\Theta \equiv \arccos \frac{\mathcal{M} + \sqrt{1-\mathcal{M}^2}}{\sqrt{2}}$$
$$\kappa \equiv \mathrm{sgn}(\|\mathcal{M} - 1/2\|)$$

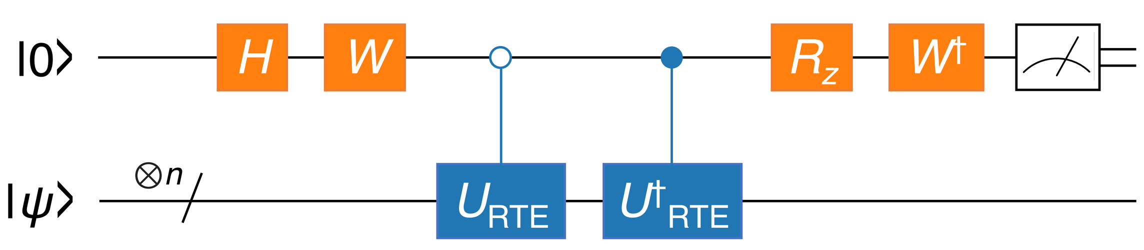
$$|\psi\rangle \otimes |0\rangle \longrightarrow \mathcal{M}|\psi\rangle \otimes |0\rangle + \sqrt{1-\mathcal{M}^2}|\psi\rangle \otimes |1\rangle$$

ancilla bit — Success state: probabilistically obtained

Approximated PITE

The arccos function is expanded up to the first order of $\Delta\tau$

$$\kappa\Theta = \theta - \mathcal{H}s\Delta\tau + \mathcal{O}(\Delta\tau^2)$$



Feature: Express ITE operator with RTE operators

After K operations of the approximated PITE, observing all ancilla state as |0> state leads to collapse from the entangled state to

$$|\Psi_K(\tau)\rangle = \frac{1}{\sqrt{P_K}} F_K(\mathcal{H})|\psi\rangle$$

$$F_K(\mathcal{H}) \equiv \prod_{k=1}^{K} f_k(\mathcal{H})$$

Approximated ITE operator

The normalization constant (Total success probability):

$$P_K = \langle\psi|F_K^2(\mathcal{H})|\psi\rangle$$

Computational cost

Total success probability: when the F_K is well design to decay unwanted state

$$P_K = \frac{1}{1-\delta}|c_1|^2$$

Every quantum algorithm that decays unwanted state by non-unitary operation shows same scaling

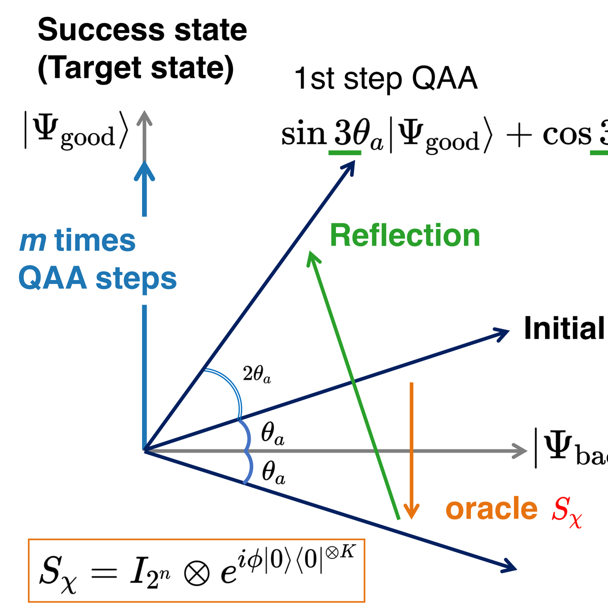
Computational cost for PITE:

$$\frac{d_{\mathrm{CRTE}}K}{P_K} = \mathcal{O}\left(\frac{d_{\mathrm{CRTE}}}{|c_1|^2} \ln\left(\frac{(1-\delta)\left(1-|c_1|^2\right)}{\delta|c_1|^2}\right)\right)$$

If we do not know even the approximated ground state at all, e.g., $|c_1|=1/N$, the computational cost of at least one success scales as $O(N)$. No quantum acceleration.

H. Nishi, K. Hamada, Y. Nishiya, T. Kosugi, and Y.-i. Matsushita, arXiv:2305.04600 (2023).

Quantum Amplitude Amplification (QAA)



Initial state

$$F_K(\mathcal{H})|\psi\rangle \otimes |0\rangle^{\otimes K} + (\text{other state})$$

success state — failure state

$$= \sin\theta_a|\Psi_{\mathrm{good}}\rangle + \cos\theta_a|\Psi_{\mathrm{bad}}\rangle$$

Amplified state after m steps of QAA

$$\sin(2m+1)\theta_a|\Psi_{\mathrm{good}}\rangle + \cos(2m+1)\theta_a|\Psi_{\mathrm{bad}}\rangle$$

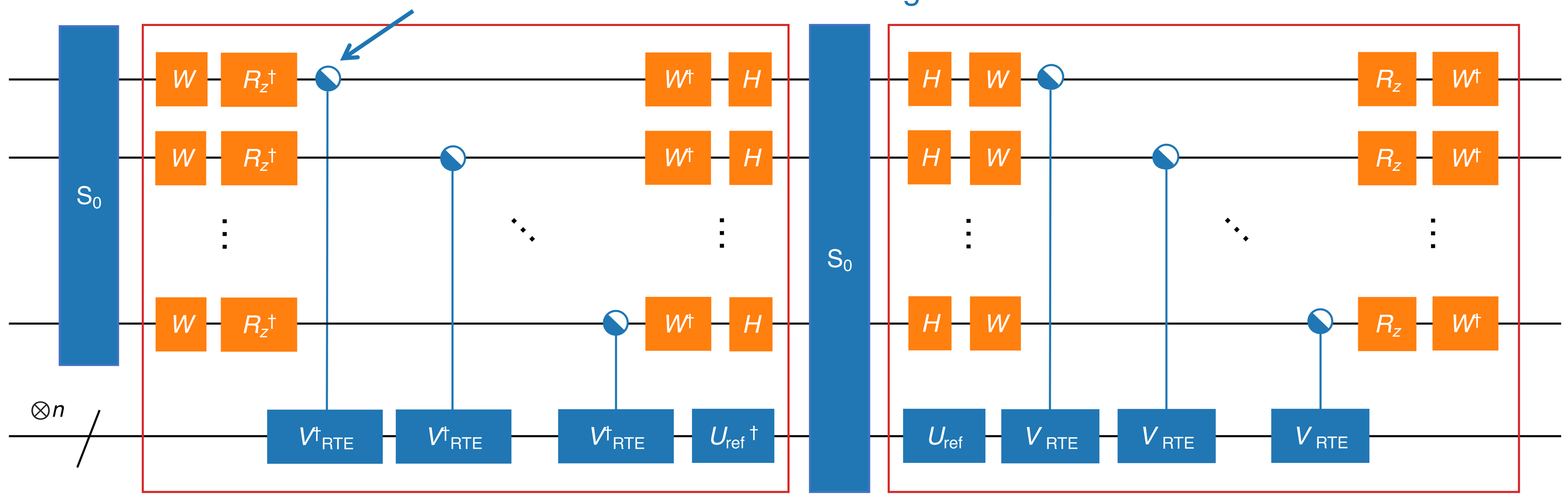
Optimal number of repetitions of QAA: $m^* = \left\lfloor \frac{(2n+1)\pi}{4\sin^{-1}\sqrt{P_K}} \right\rfloor$

Brassard, Gilles, et al. "Quantum amplitude amplification and estimation." Contemporary Mathematics 305, 53 (2002)

Quantum circuit for QAA combined with multistep PITE

Quantum circuit for the amplitude amplification operator of the PITE method

Forward- and backward- controlled RTE gates



$= \mathcal{U}^\dagger_{\mathrm{PITE+ref}}$ $= \mathcal{U}_{\mathrm{PITE+ref}}$

Computational cost for PITE combined with QAA (multi-step PITE)

$$d_{\mathrm{CRTE}}Km^* = \mathcal{O}\left(\frac{d_{\mathrm{CRTE}}}{|c_1|} \ln\left(\frac{(1-\delta)(1-|c_1|^2)}{\delta|c_1|^2}\right)\right)$$

Quadratic speedup owing to combining QAA

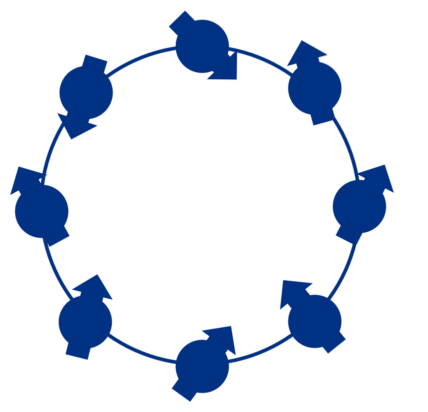
H. Nishi, Y. Nishiya, T. Kosugi, and Y.-i. Matsushita, in preparation.

Result: Numerical Simulations

Setup

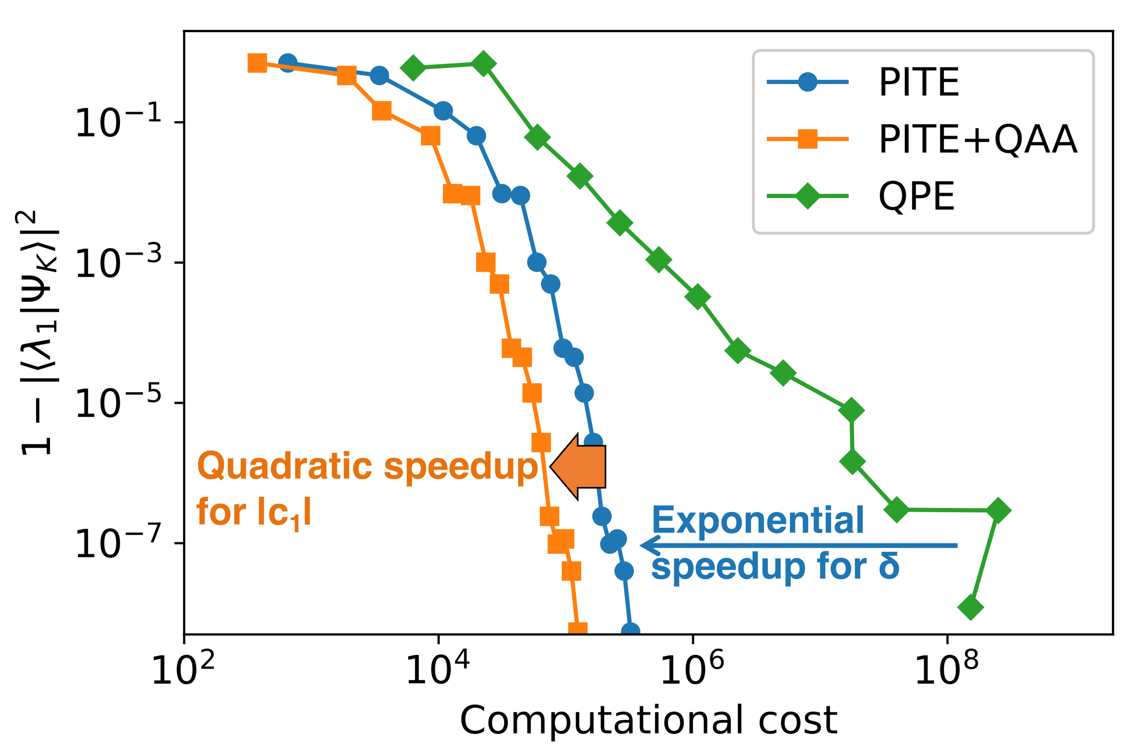
The Heisenberg model

$$\mathcal{H} = \sum_{\langle j,k\rangle} \vec{\sigma}_j \cdot \vec{\sigma}_k + \sum_j h_j \sigma_j^z$$

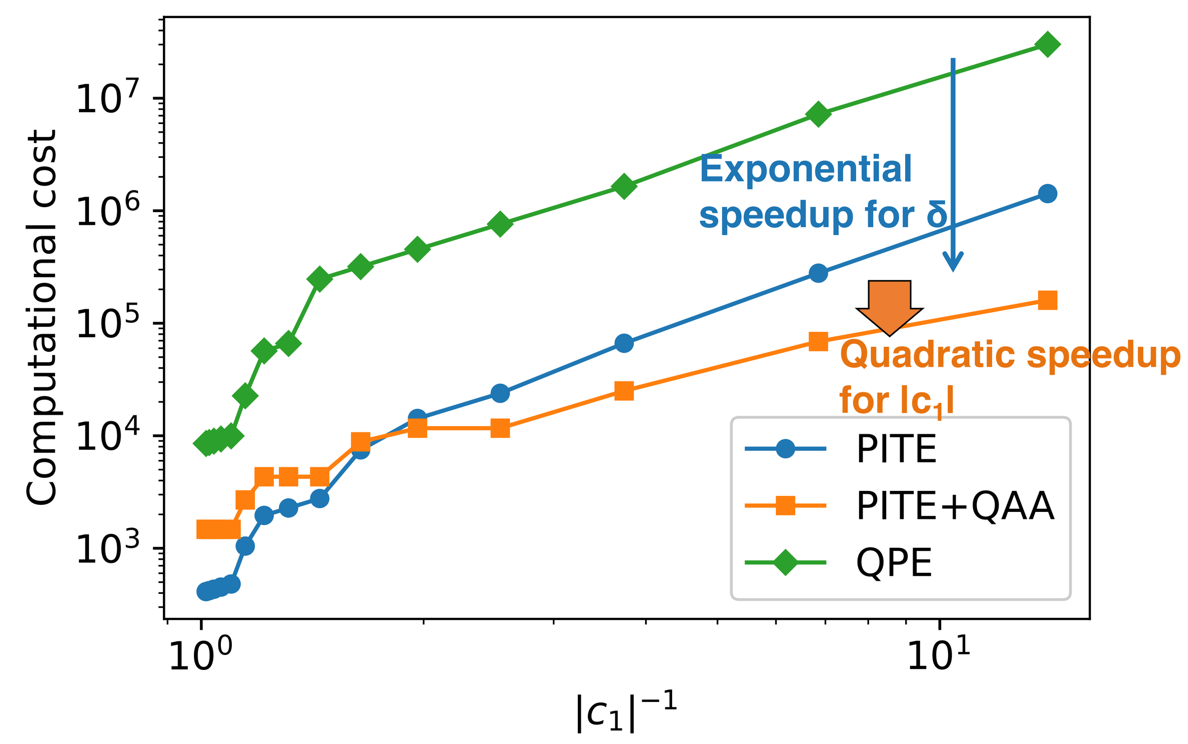


<j,k> represents the combination of the nearest neighbors of the closed one-dimensional chain.
Random magnetic field h_j are randomly chosen from uniform distribution as $h_j \in [-1, 1]$.

The controlled RTE gate is implemented by the fourth-order Trotter-Suzuki decomposition for even-odd group of the Hamiltonian.



The initial state is uniform probability weights of each eigenvector: $|c_j|^2=1/N$



Computational cost was estimated when the infidelity was below $\delta=10^{-4}$.
QAA is efficient for $|c_1|<1/2$ due to overhead of QAA.

Conclusion

1. Investigated the computational cost of the PITE method that implements a nonunitary ITE operator on a quantum computer with a single ancilla qubit.

2. Proposed a quantum algorithm combining QAA with PITE for ground-state preparation that present quadratic speedup overt he classical one.