APS March Meeting 2023
Y72.00002

Improving success probability of imaginary-time evolution on a quantum computer

arXiv:2212.13816

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Background

One of the motivations: ground state calculation of quantum chemistry

Imaginary-time evolution (ITE) method on a quantum computer

Difficulty：Implementation of nonunitary is not straightforward

Methodologies developed so far：

- ✓ Variational imaginary-time evolution: VQE-based

  [X. Yuan et al., Quantum 3, 191 (2019)]

- ✓ Quantum imaginary-time evolution

  [Motta et al., Nat. Phys. 16(2) 205 (2020)], [Nishi et al. npj QI 7, 85 (2021).]

- ✓ Probabilistic imaginary-time evolution (PITE)

  [Kosugi, Nishi, et. al., Phys. Rev. Res. 4, 033121 (2022)]

  Solving the difficulty by introducing ancilla bit and measurement

  Advangage: reduction of number of measurements

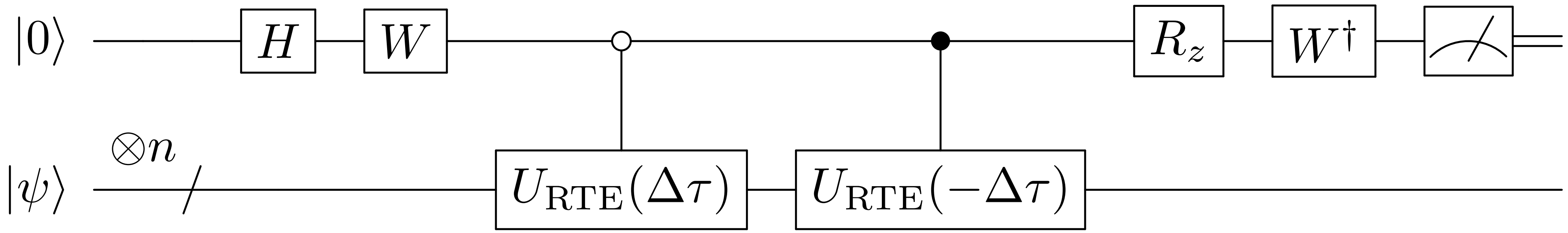
NISQ ↕ FTQC

Probabilistic Imaginary-Time Evolution (PITE)

Y72.00007 9:12am-9:24am: Kosugi, Nishi, et. al., Phys. Rev. Res. 4, 033121 (2022)

Approximate PITE circuit within first order of imaginary-time step Δτ

ancilla



Feature: Express ITE operator with real-time evolution operators (U_{RTE})

Input **Output**

$$|\psi\rangle \otimes |0\rangle \longrightarrow \mathcal{M}|\psi\rangle \otimes |0\rangle + \sqrt{1-\mathcal{M}^2}|\psi\rangle \otimes |1\rangle \qquad \mathcal{M} = \gamma e^{-\mathcal{H}\Delta\tau}$$

ancilla bit **success state probabilistically obtained**

Goal of this study

Y72.00007 9:12am-9:24am: Kosugi, Nishi, et. al., Phys. Rev. Res. 4, 033121 (2022)

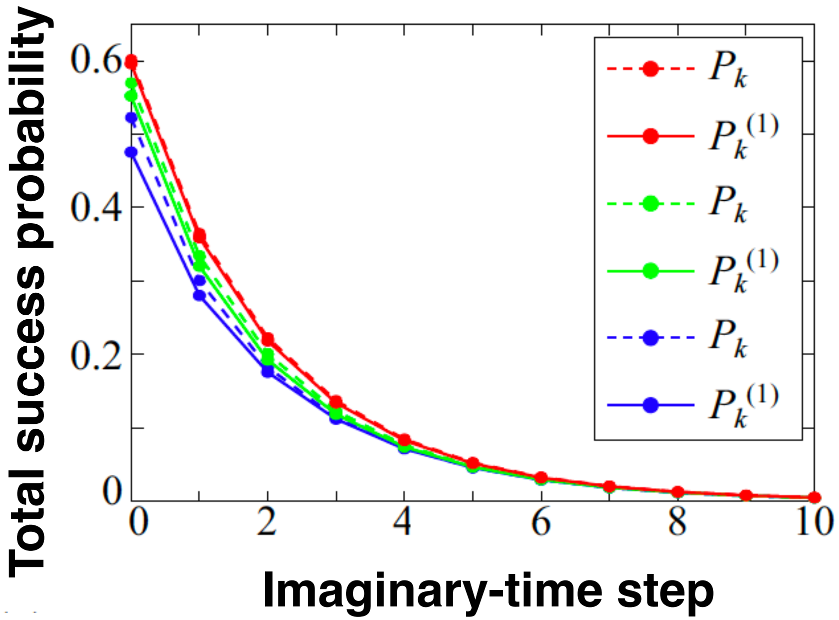
Problems of PITE method：

1. Success probability ≠ 100%
2. Exponential decay of total success probability according to ITE steps increasing

Input Output

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

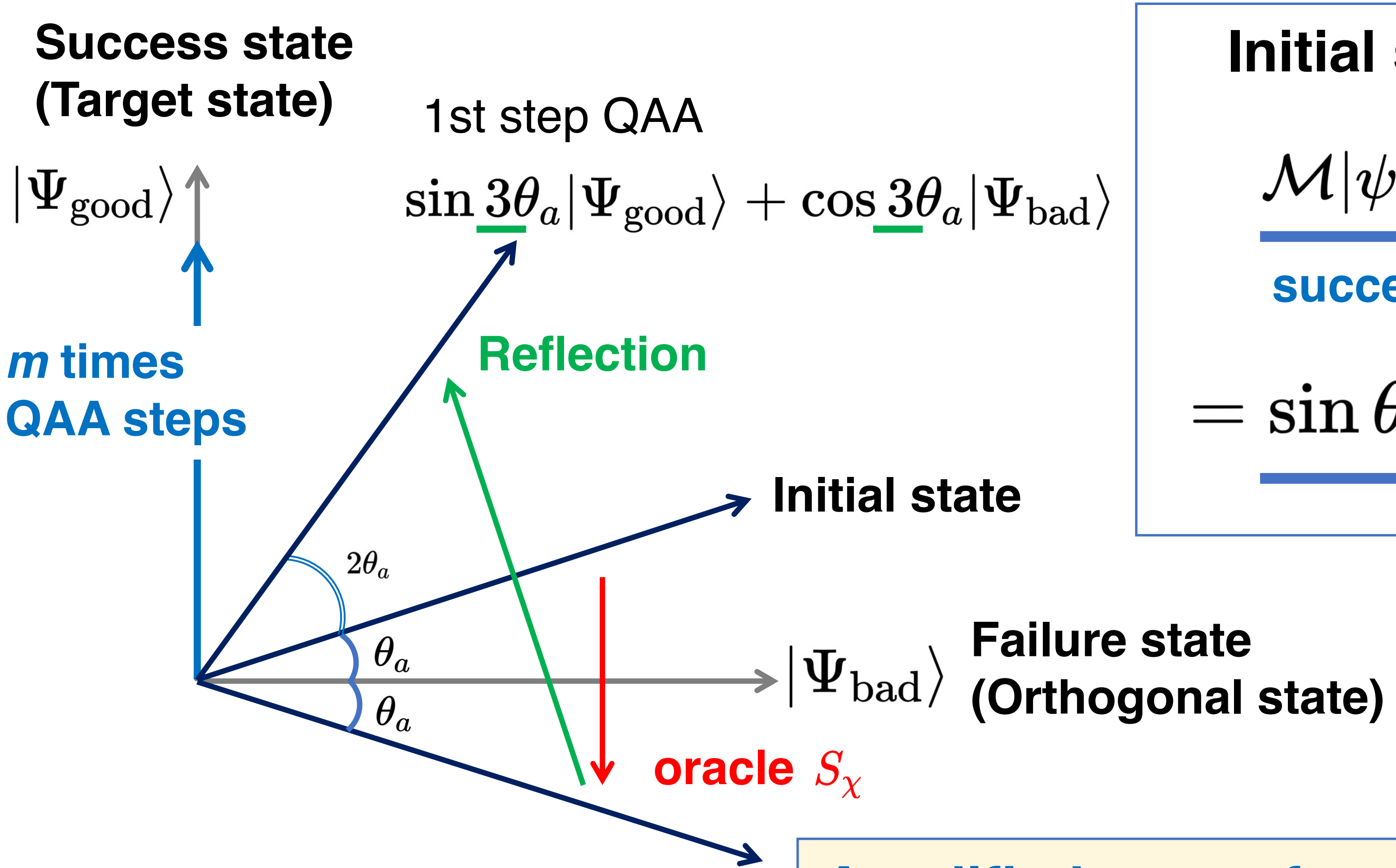
ancilla bit success state probabilistically obtained



Goal：Improve success probability of PITE method combined with QAA

QAA (Quantum Amplitude Amplification)

Quantum Amplitude Amplification (QAA)



$$S_\chi = I_{2^n} \otimes \sigma_x \sigma_z \sigma_x$$

Initial state

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

success state — failure state

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

Amplified state after *m* steps of QAA

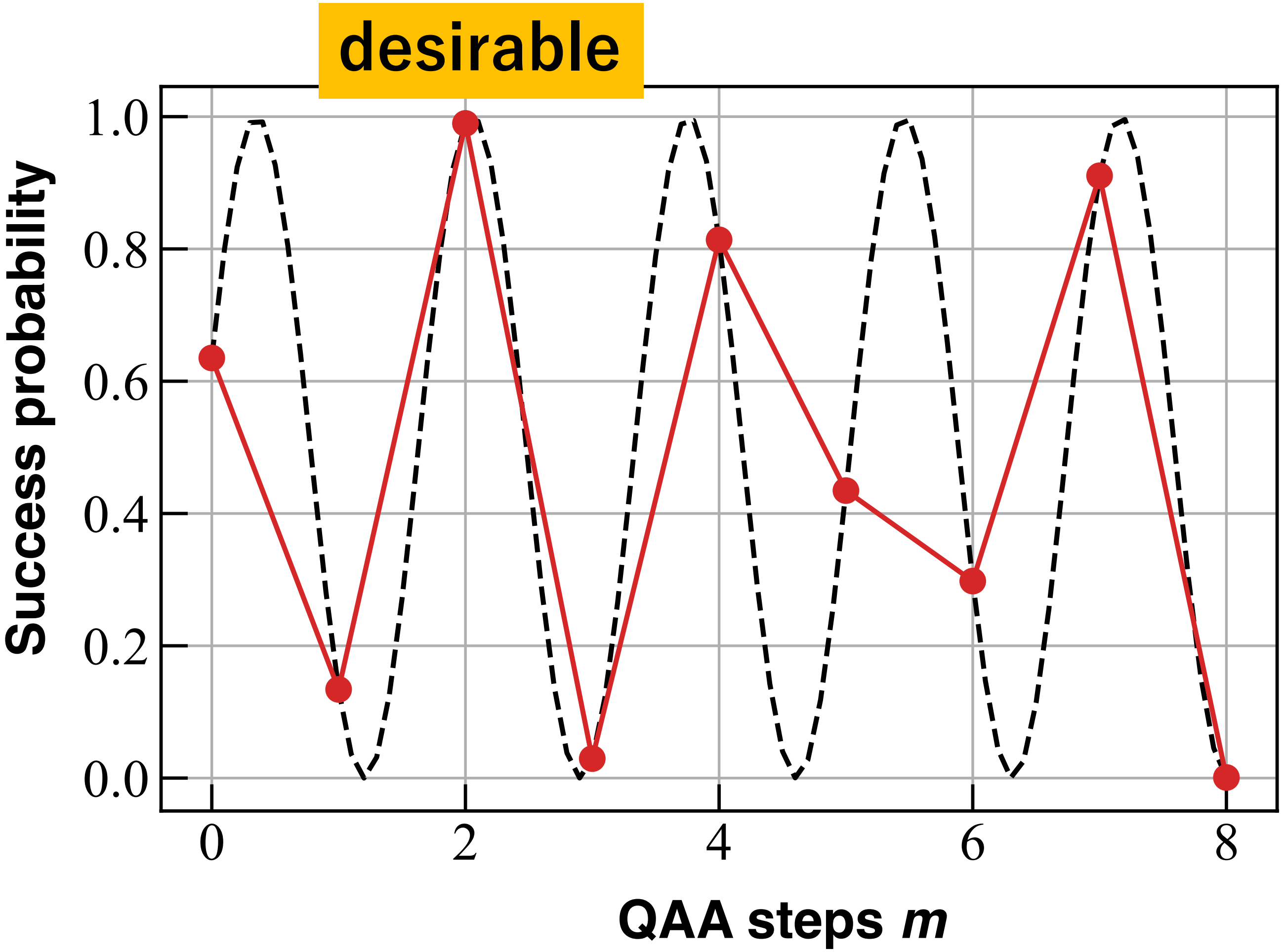
$$\sin(2m+1)\theta_a|\Psi_{\rm good}\rangle + \cos(2m+1)\theta_a|\Psi_{\rm bad}\rangle$$

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

Quantum Amplitude Amplification (QAA)

Amplified state after *m* steps of QAA

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



Determine QAA steps *m* s.t. success prob. is maximized

$$m_{\text{opt}} = \frac{\pi}{4\theta_a}(2n-1) - \frac{1}{2}$$

***n*: integer**

Estimate θ_a by QAE

Optimized m_{opt} depends on θ_a, which is derived from initial state, Smaller value of optimized m_{opt} is preferable

Deterministic Imaginary-Time Evolution

In order to reduce the optimized m, look back again PITE

$$m_{\mathrm{opt}} = \frac{\pi}{4\theta_a}(2n-1) - \frac{1}{2}$$

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

$$\mathcal{M} = \gamma e^{-\mathcal{H}\Delta\tau}$$

Focus: PITE has a freely choosing parameter γ (in the range 0<γ<1, γ≠1/√2)

Initial success prob.:

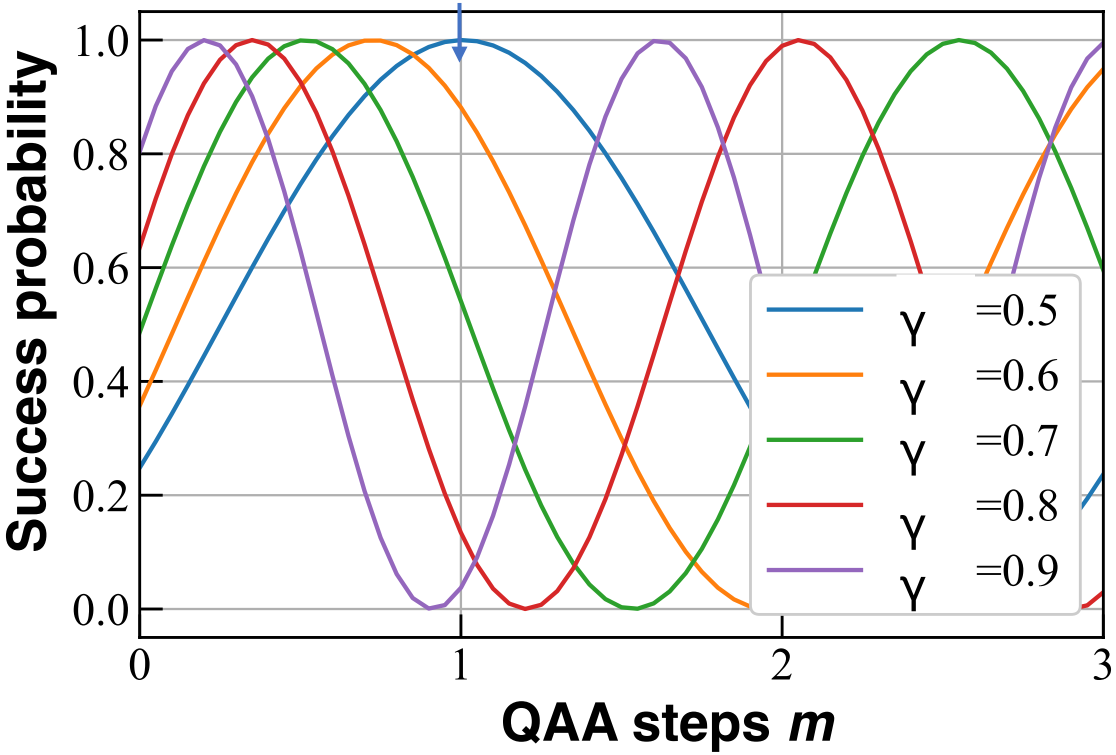
$$\sin^2\theta_a = \gamma^2 \langle\psi| e^{-2\Delta\tau\mathcal{H}} |\psi\rangle$$

θ_a depends on parameter γ

γ is an degree of freedom to tune the initial success prob., leading to smaller value of the optimized m_{opt}.

Importantly,
by using QAA, make success prob. = 1
Realize deterministic ITE

Success prob. is almost one even when *m*=1



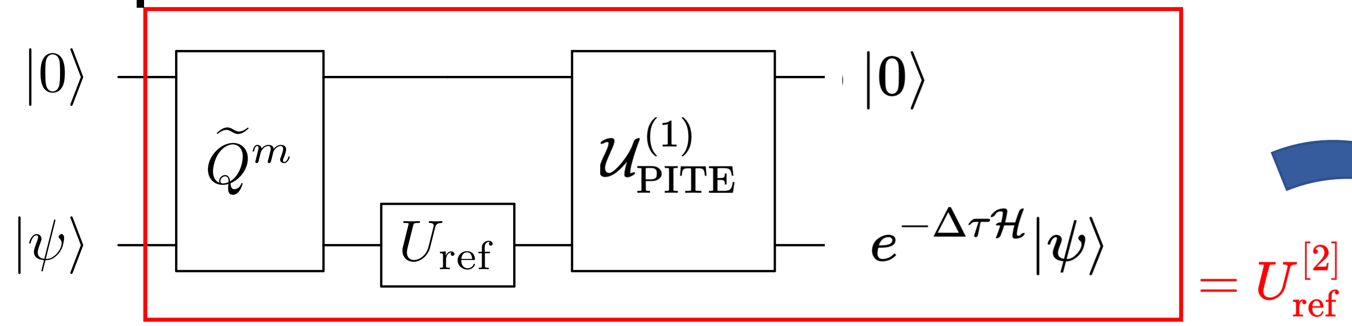
Deterministic Imaginary-Time Evolution

By adopting the optimized γ_{opt} and m_{opt}, the success state is always realized (deterministic PITE)

$$\mathcal{U}_{\mathrm{PITE+ref}}\widetilde{Q}^{m}\left(|0\rangle^{\otimes n}\otimes|0\rangle\right)=e^{-\Delta\tau\mathcal{H}}|\psi\rangle\otimes|0\rangle$$

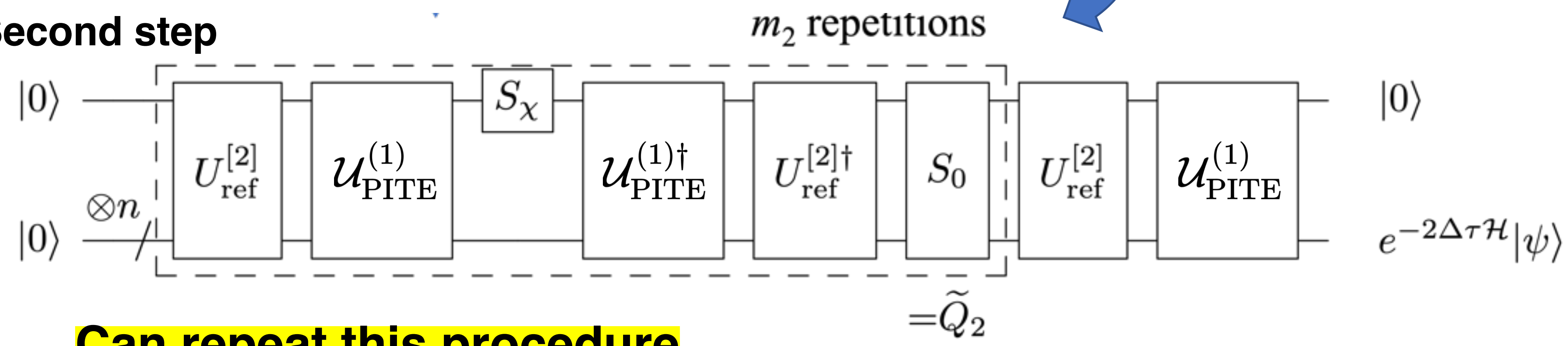
No need to observe the ancilla bit anymore

1st step



We can continue subsequent 2nd step of PITE without measurement

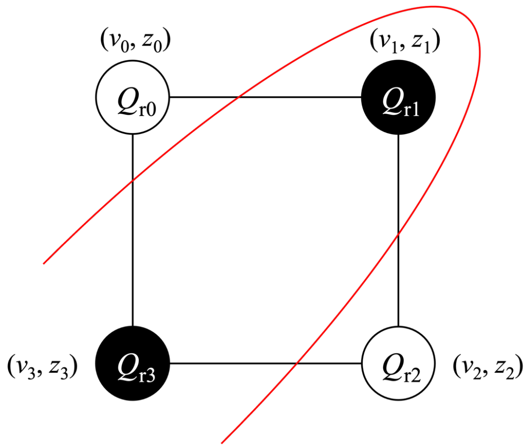
Second step



Can repeat this procedure

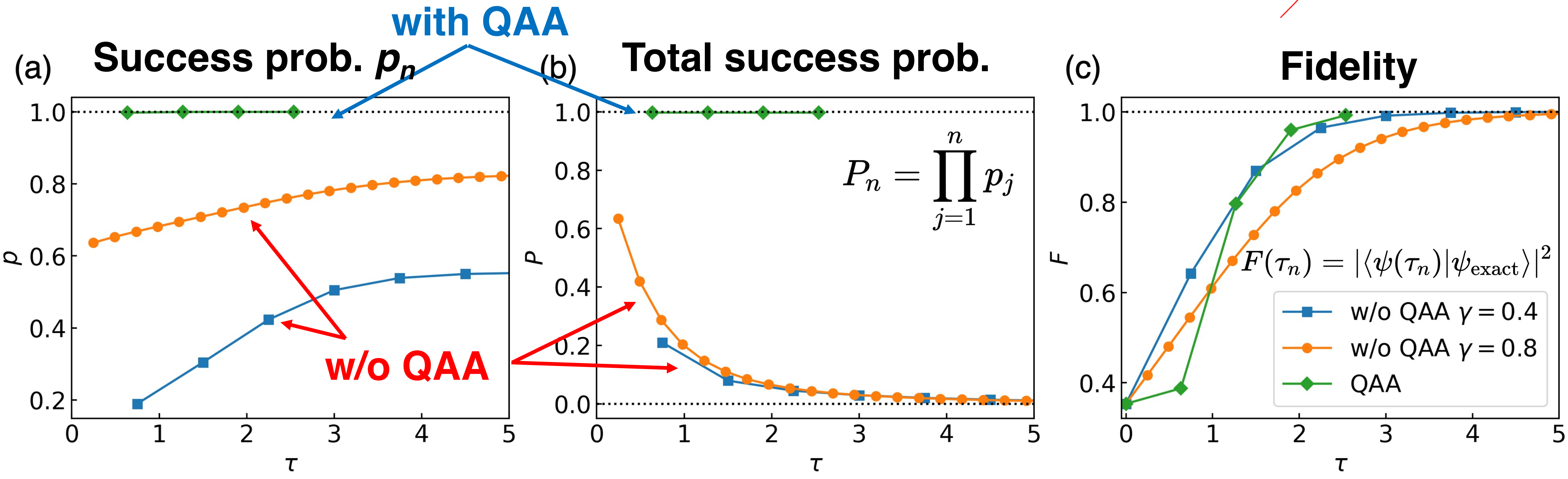
Numerical Results

$$H_{\mathrm{C}} = \frac{1}{2} \sum_{(i,j)\in E} (Z_i \otimes Z_j - 1)$$



Setup:

Max-cut problem (Ising Hamiltonian)



✓ **Dramatically improve the total success probability**

Summary

- ✓ Improved success probability of the PITE method by QAA
- ✓ Realized deterministic ITE by optimizing an parameter γ included in the PITE

  Nishi,et al., arXiv:2212.13816

See Also

1. For details of PITE

   Y72.00007 9:12am-9:24am

2. Geometric optimization using PITE method

   TK, Nishi, et al., arXiv:2210.09883, YY03.00005 Wed. March 22, 2023 (Virtual)

3. Electron states under a uniform magnetic field using PITE method,

   TK, Nishi, et. al., arXiv:2212.13800.