APS March meeting 2023

Imaginary-time evolution with a single ancilla: first-quantized eigensolver for electronic structure calculation in quantum chemistry

Taichi Kosugi[1,2], Yusuke Nishiya[1,2],
Hirofumi Nishi[1,2], Yu-ichiro Matsushita[1,2,3]

[1] Tokyo Institute of Technology
[2] Quemix Inc.
[3] National Institutes for Quantum Science and Technology

Purpose

To obtain the ground state of a given Hamiltonian …

Imaginary-time evolution (ITE)

$$\underbrace{e^{-\mathcal{H}\tau}}_{\text{Nonunitary}} \underbrace{\sum_k c_k |\phi_k\rangle}_{\text{Initial state}} = \sum_k c_k e^{-E_k \tau} |\phi_k\rangle$$

Nonunitary   Initial state

- ✓ The weights of excited states decay rapidly.
- ✓ No need for an appropriate ansatz
- ✗ Nonunitarity : cannot be implemented directly in a quantum circuit

We propose a new framework using ITE for fault-tolerant quantum computers.

Probabilistic Imaginary-Time Evolution (PITE)

How to realize ITE operation in quantum circuits

Probabilistic imaginary-time evolution (PITE)

Space expansion & Measurement

$$\mathcal{M} = m_0 e^{-\mathcal{H}\Delta\tau} \qquad \mathcal{U}_{\mathrm{PITE}} \equiv \begin{pmatrix} \mathcal{M} & \sqrt{1-\mathcal{M}^2} \\ \sqrt{1-\mathcal{M}^2} & -\mathcal{M} \end{pmatrix}_a$$

$$\mathcal{U}_{\mathrm{PITE}}|\psi\rangle \otimes |0\rangle = \mathcal{M}|\psi\rangle \otimes |0\rangle + \sqrt{1-\mathcal{M}^2}|\psi\rangle \otimes |1\rangle$$

Ancillary qubit Success state

By measuring the ancillary qubit, the Success state is obtained with probability $\mathbb{P}_0 = \langle\psi|\mathcal{M}^2|\psi\rangle$

Kosugi, Nishiya, Nishi, and Matsushita,
Phys. Rev. Res. **4**, 033121 (2022)

PITE circuit

$$\mathcal{U}_{\mathrm{PITE}} \equiv \begin{pmatrix} \mathcal{M} & \sqrt{1-\mathcal{M}^2} \\ \sqrt{1-\mathcal{M}^2} & -\mathcal{M} \end{pmatrix}_a = (I_{2^n} \otimes W^\dagger) \begin{pmatrix} e^{i\kappa\Theta} & 0 \\ 0 & e^{-i\kappa\Theta} \end{pmatrix}_a (I_{2^n} \otimes WH)$$

$$W \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}$$

$$\approx (I_{2^n} \otimes W^\dagger)[I_{2^n} \otimes R_z(-2\theta)] \begin{pmatrix} e^{-i\mathcal{H}s\Delta\tau} & 0 \\ 0 & e^{i\mathcal{H}s\Delta\tau} \end{pmatrix}_a (I_{2^n} \otimes WH)$$

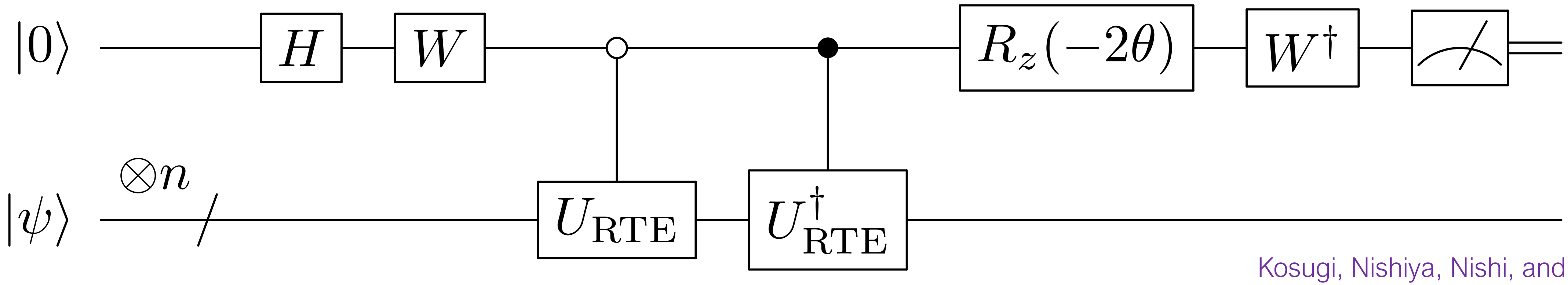
U_{RTE} $\quad U_{\mathrm{RTE}}^\dagger$

$$\Theta \equiv \arccos \frac{\mathcal{M} + \sqrt{1-\mathcal{M}^2}}{\sqrt{2}} \xrightarrow{\text{Taylor expansion}} \kappa\Theta = \theta - \mathcal{H}s\Delta\tau + \mathcal{O}(\Delta\tau^2)$$

$$\kappa \equiv \mathrm{sgn}\left(m_0 - 1/\sqrt{2}\right)$$

$$\theta \equiv \kappa \arccos \frac{m_0 + \sqrt{1-m_0^2}}{\sqrt{2}}$$

$$s \equiv \frac{m_0}{\sqrt{1-m_0^2}}$$



Kosugi, Nishiya, Nishi, and Matsushita, Phys. Rev. Res. **4**, 033121 (2022)

PITE for quantum chemistry

First-quantized Hamiltonian of n_e electrons

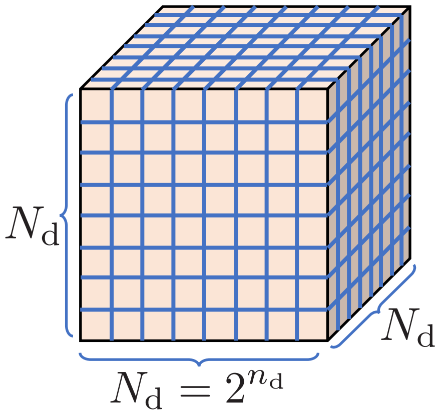
cf. Kassal et al., PNAS **105**, 18681 (2008)
for real-time dynamics

$$\mathcal{H} = \underbrace{\sum_{\ell=0}^{n_e-1} \frac{\hat{\boldsymbol{p}}_\ell^2}{2m_e}}_{\equiv \hat{T}} + \underbrace{\frac{1}{2} \sum_{\substack{\ell,\ell'=0 \\ (\ell \neq \ell')}}^{n_e-1} v\left(|\hat{\boldsymbol{r}}_\ell - \hat{\boldsymbol{r}}_{\ell'}|\right)}_{\equiv \hat{V}_{ee}} + \underbrace{\sum_{\ell=0}^{n_e-1} v_{\mathrm{ext}}\left(\hat{\boldsymbol{r}}_\ell\right)}_{\equiv \hat{V}_{\mathrm{ext}}}$$

Encoding of wave functions

Discretize wave function by using $3n_\mathrm{d}n_e$ qubits

$$|\psi\rangle = \Delta V^{n_e/2} \sum_{\boldsymbol{k}_0,\ldots,\boldsymbol{k}_{n_e-1}} \psi(\boldsymbol{r}^{(\boldsymbol{k}_0)}, \ldots, \boldsymbol{r}^{(\boldsymbol{k}_{n_e-1})}) |\boldsymbol{k}_0\rangle \otimes \cdots \otimes |\boldsymbol{k}_{n_e-1}\rangle$$



$|\boldsymbol{k}\rangle$: Position eigenstate of an electron at $(k_x\boldsymbol{e}_x+k_y\boldsymbol{e}_y+k_z\boldsymbol{e}_z)\Delta x$

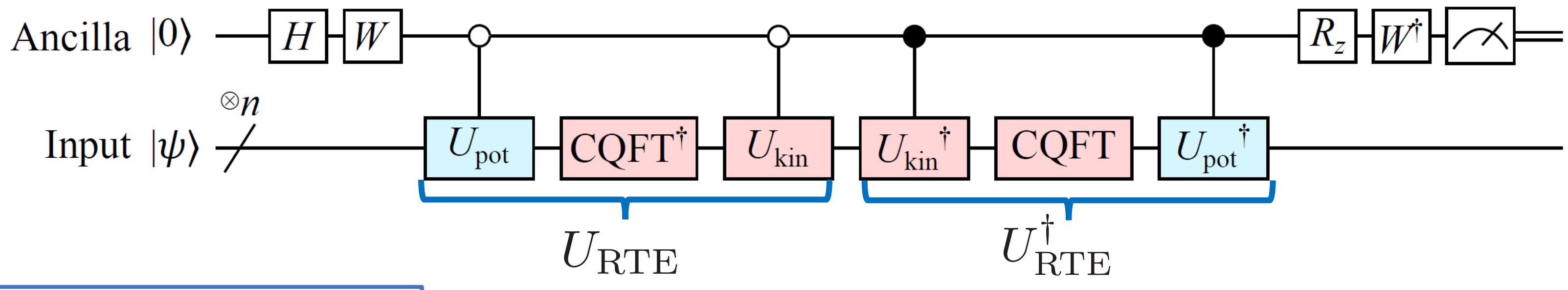
Implementation of RTE

1st-order Suzuki-Trotter : $e^{-i\mathcal{H}\Delta t} \approx e^{-i\hat{T}\Delta t} e^{-i(\hat{V}_{ee}+\hat{V}_{\mathrm{ext}})\Delta t}$

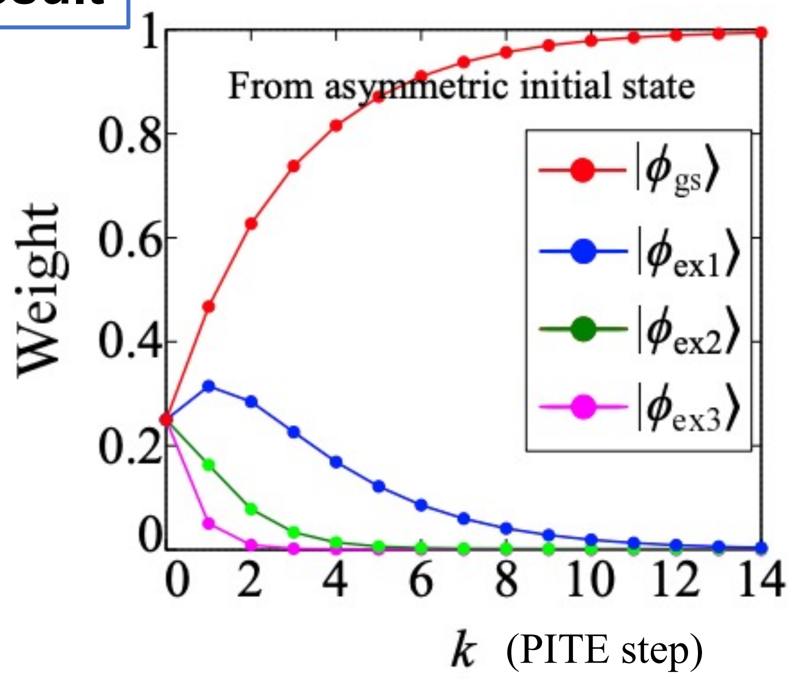
Numerical simulation

Model : Single particle in 1D space

$$\mathcal{H} = \frac{p^2}{2m} + V(x)$$ Harmonic potential



Simulation result

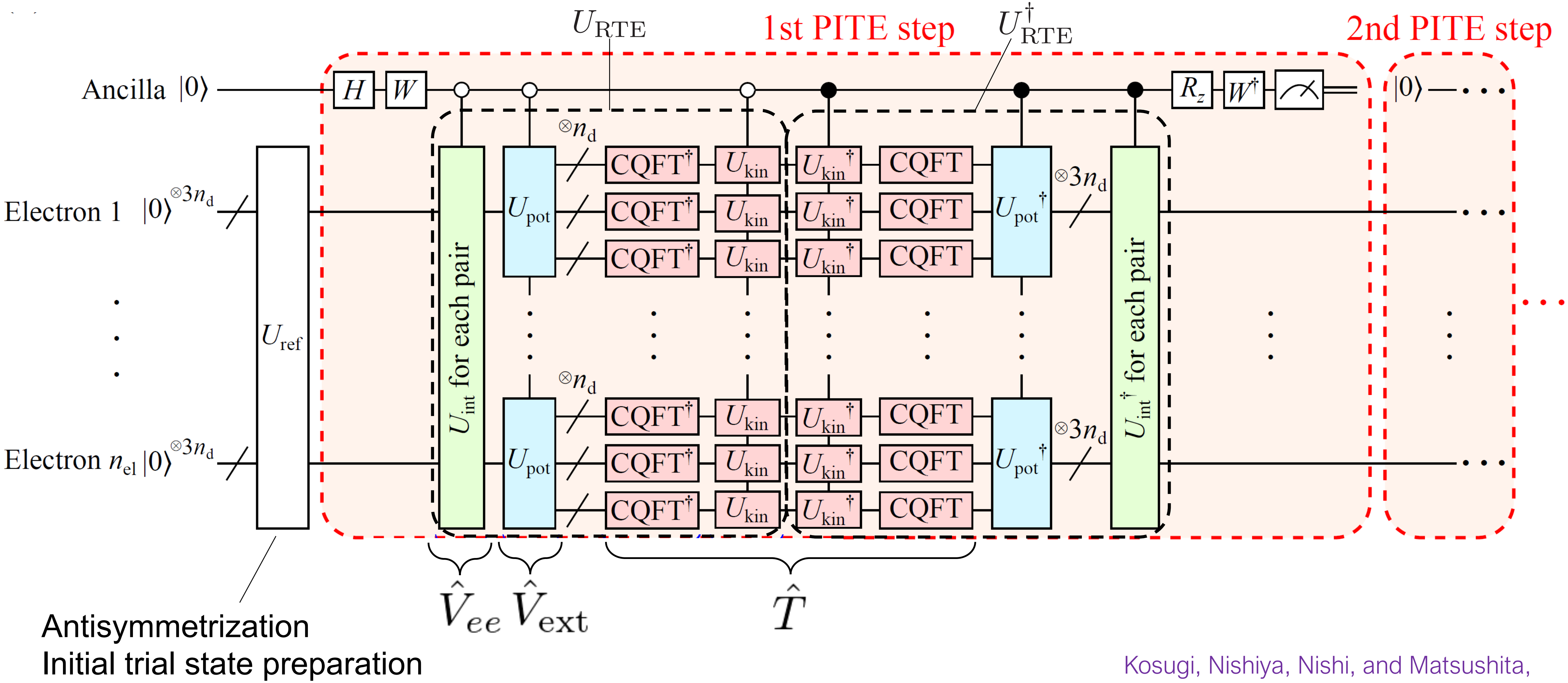


Approaching the ground state as step proceeds

Kosugi, Nishiya, Nishi, and Matsushita,
Phys. Rev. Res. **4**, 033121 (2022)

First-quantized Eigensolver (FQE)

Circuit : Interacting many-electron system in 3D space



Kosugi, Nishiya, Nishi, and Matsushita,
Phys. Rev. Res. **4**, 033121 (2022)

Scaling

Comparison with 2nd-quantized formalism

Kosugi, Nishiya, Nishi, and Matsushita, Phys. Rev. Res. **4**, 033121 (2022)

	1st-quantized	2nd-quantized
# of qubits for a many-electron state	$O(n_e \log n_e)$	$O(n_e)$
# of oprs at each PITE step	$O(n_e^2 (\log n_e)^{p'})$ p': degree of polynomial for e-e interactions	$O(n_e^4)$

Better scaling of 1st-quantized formalism !

Optimization of molecular geometry

Quantum mechanical electrons & classical nuclei

Kosugi, Nishi, and Matsushita,
arXiv:2210.09883

$$\mathcal{H}\left(\{\boldsymbol{R}_\nu\}_\nu\right) = \underbrace{\sum_{\ell=0}^{n_e-1} -\frac{1}{2m_e}\nabla_\ell^2}_{\equiv \hat{T}} + \underbrace{\frac{1}{2}\sum_{\ell=0}^{n_e-1}\sum_{\ell'=0}^{n_e-1} v\left(|\hat{\boldsymbol{r}}_\ell - \hat{\boldsymbol{r}}_{\ell'}|\right)}_{\equiv \hat{V}_{ee}} + \underbrace{\sum_{\ell=0}^{n_e-1}\sum_{\nu=0}^{n_{\mathrm{nucl}}-1} -Z_\nu v\left(|\hat{\boldsymbol{r}}_\ell - \boldsymbol{R}_\nu|\right)}_{\equiv \hat{V}_{en}}$$

$$+ \underbrace{\frac{1}{2}\sum_{\nu=0}^{n_{\mathrm{nucl}}-1}\sum_{\nu'=0}^{n_{\mathrm{nucl}}-1} Z_\nu Z_{\nu'} v\left(|\boldsymbol{R}_\nu - \boldsymbol{R}_{\nu'}|\right)}_{\equiv E_{\mathrm{nn}}} + \underbrace{\sum_{\ell=0}^{n_e-1} v_{\mathrm{ext}}\left(\hat{\boldsymbol{r}}_\ell\right)}_{\equiv \hat{V}_{\mathrm{ext}}}$$

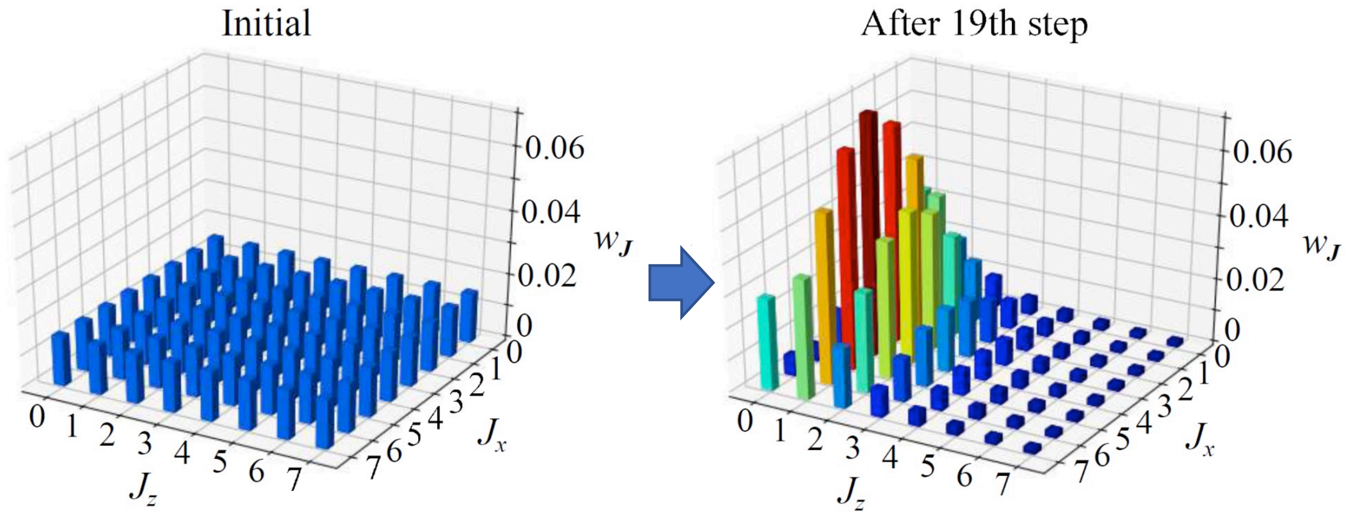
Input register

$$|\Psi\rangle = \sum_{\boldsymbol{J}} \sqrt{w_{\boldsymbol{J}}}\,|\psi[\boldsymbol{J}]\rangle \otimes |\boldsymbol{J}\rangle$$

Nuclear positions

Many-electron state

Sum over possible geomatries



Most stable structure in the candidates
(the ground state of the Hamiltonian above)

In detail …
March 22, 10:00~
@Virtual room 3

Conclusions

Summary

- Generic construction of PITE circuit with a single ancilla and RTE oprs.
- FQE : a new framework for quantum chemistry
- FQE for an electronic system exhibits better scaling than 2nd-quantized formalism.

This talk

Kosugi, Nishiya, Nishi, and Matsushita, Phys. Rev. Res. **4**, 033121 (2022)

Related studies

Structural search with PITE

Kosugi, Nishi, and Matsushita, arXiv:2210.09883

Under a magnetic field

Kosugi, Nishi, and Matsushita, arXiv:2212.13800

With amplitude amplification

Nishi, Kosugi, Nishiya and Matsushita, arXiv:2212.13816