Quantum Chemistry on Quantum Computers

#5 Variational Quantum Algorithms

Kenji Sugisaki[1,2,3]

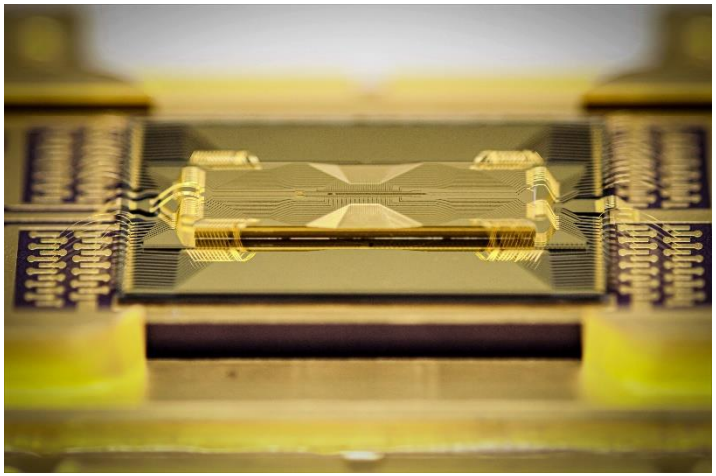
[1]*Department of Chemistry, Graduate School of Science, Osaka City University, Japan*
[2]*JST PRESTO, Japan*
[3]*CQuERE, TCG CREST, India*

NISQ devices

Noisy Intermediate-Scale Quantum devices

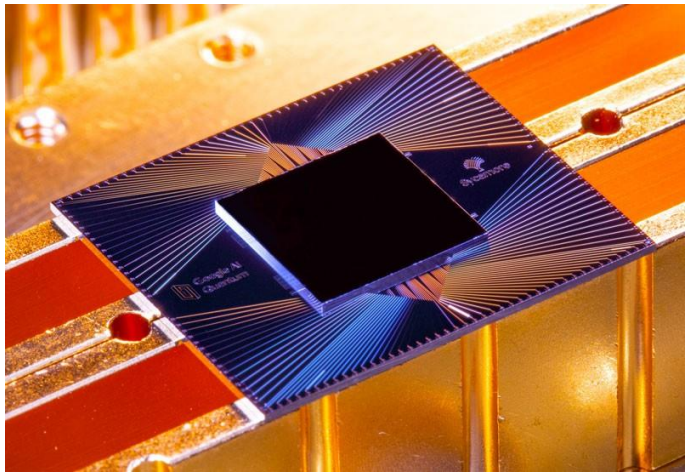
J. Preskill, *Quantum* **2018**, *2*, 79.

- About 50–100 qubits
- Too small to implement quantum error correction
- The number of executable coherent gates is at most 1,000



IonQ's EGT Series Ion Trap Chip
Photo taken from IonQ's website

https://ionq.com/news/august-25-2021-reconfigurable-multicore-quantum-architecture

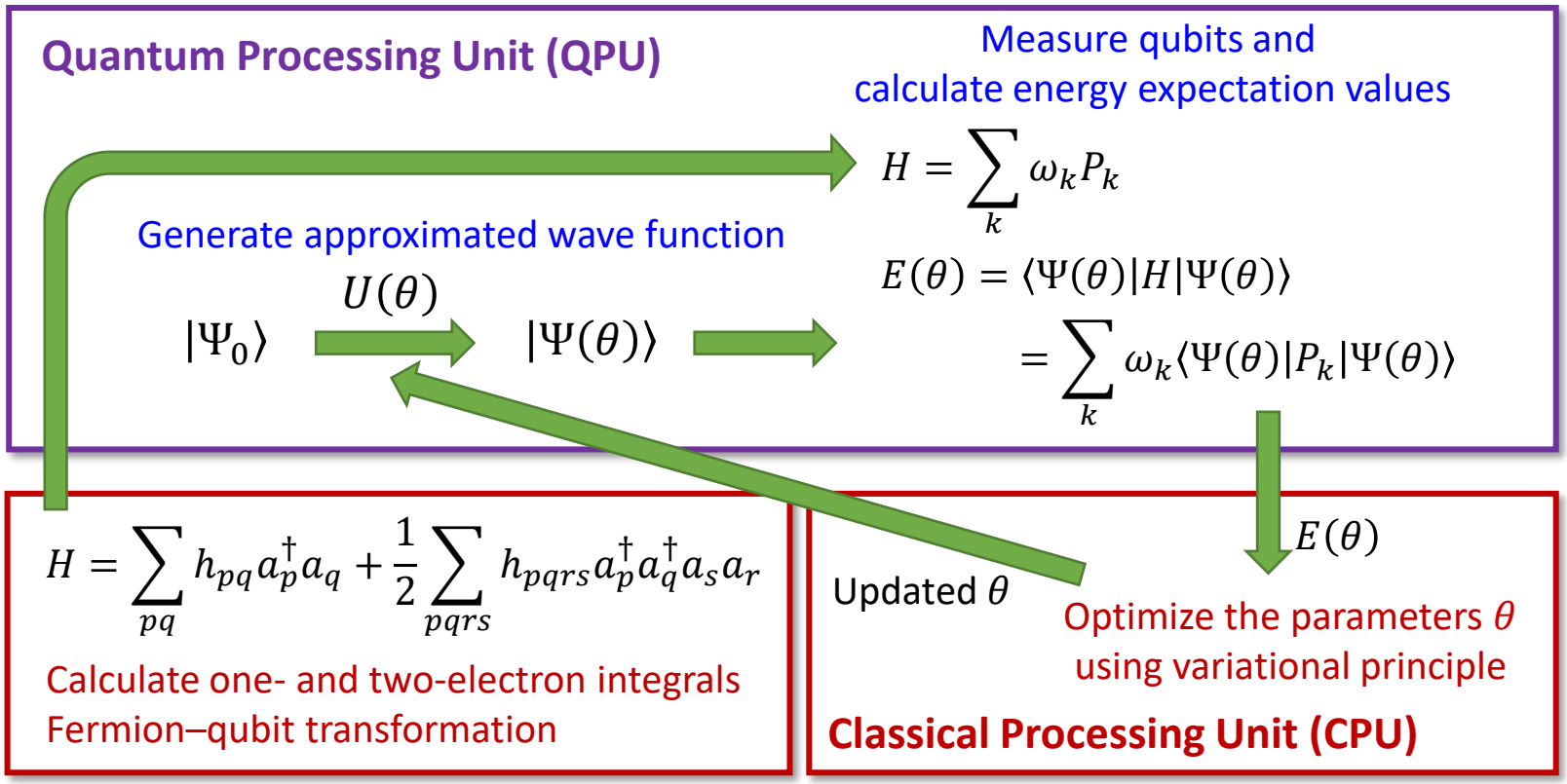


Google's 54-qubit quantum chip "Sycamore"
Photo taken from *Nature* **2019**, *574*, 461–462.

Quantum circuit for QPE-based full-CI is too deep to execute on NISQ devices!!

Variational quantum eigensolver

A quantum–classical hybrid approach that is executable on noisy intermediate-scale quantum (NISQ) devices



M.-H. Yung et al, *Sci. Rep.* **2014**, *4*, 3589; A. Peruzzo et al, *Nat. Comm.* **2014**, *5*, 4213.

VQE with UCC ansatz

ARTICLE

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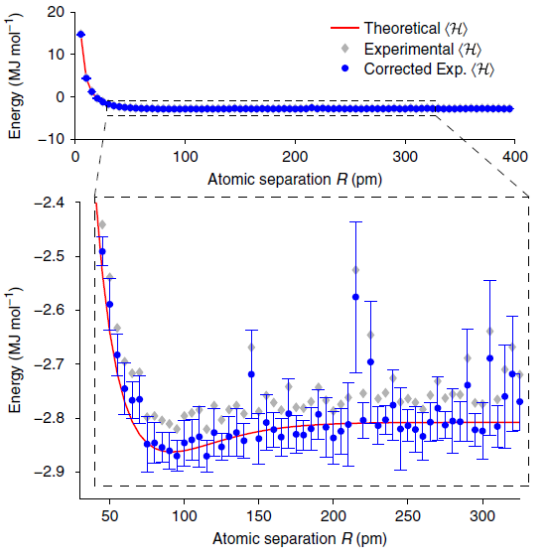
A variational eigenvalue solver on a photonic quantum processor

Alberto Peruzzo[1,*,†], Jarrod McClean[2,*], Peter Shadbolt[1], Man-Hong Yung[2,3], Xiao-Qi Zhou[1], Peter J. Love[4], Alán Aspuru-Guzik[2] & Jeremy L. O'Brien[1]

- Use photonic quantum computer
- Potential energy curve of the electronic ground state of HeH^+ molecule
- Unitary coupled cluster ansatz, UCCSD/STO-3G
- Two qubits for wave function storage



Unitary coupled cluster ansatz

☆ Coupled Cluster (CC) Method

Nonlinear expansion by using exponentials

$$|\Psi_{\mathrm{CCSD}}\rangle = \exp(T_1 + T_2)|\Psi_{\mathrm{HF}}\rangle$$

T_1 ⋯ One-electron excitation operators
T_2 ⋯ Two-electron excitation operators

☆ Unitary Coupled Cluster (CC) Method

$$|\Psi_{\mathrm{UCCSD}}\rangle = \exp(\tau)|\Psi_{\mathrm{HF}}\rangle = \exp\left(T - T^\dagger\right)|\Psi_{\mathrm{HF}}\rangle$$
$$= \exp\left(T_1 - T_1^\dagger + T_2 - T_2^\dagger\right)|\Psi_{\mathrm{HF}}\rangle$$

T_1 ⋯ One-electron excitation operators
$T_1^\dagger$ ⋯ One-electron de-excitation operators
T_2 ⋯ Two-electron excitation operators
$T_2^\dagger$ ⋯ Two-electron de-excitation operators

Number of variables: $O\left(N_{\mathrm{occ}}^2 N_{\mathrm{vir}}^2\right)$

A. G. Taube, R. J. Bartlett, *Int. J. Quantum Chem.* **2006**, *106*, 3393–3401.
A. Anand et al, arXiv:2109.15176.

Unitary coupled cluster ansatz

☆ **Unitary Coupled Cluster (CC) Method**

$$|\Psi_{\mathrm{UCC}}\rangle = \exp(\tau)|\Psi_{\mathrm{HF}}\rangle = \exp\left(T - T^{\dagger}\right)|\Psi_{\mathrm{HF}}\rangle$$

UCC energy: $E_{\mathrm{UCC}} = \dfrac{\langle\Psi_{\mathrm{UCC}}|H|\Psi_{\mathrm{UCC}}\rangle}{\langle\Psi_{\mathrm{UCC}}|\Psi_{\mathrm{UCC}}\rangle} = \dfrac{\langle\Psi_{\mathrm{HF}}|e^{-\tau}He^{\tau}|\Psi_{\mathrm{HF}}\rangle}{\langle\Psi_{\mathrm{HF}}|e^{-\tau}e^{\tau}|\Psi_{\mathrm{HF}}\rangle} = \langle\Psi_{\mathrm{HF}}|e^{-\tau}He^{\tau}|\Psi_{\mathrm{HF}}\rangle$

$$= \left\langle\Psi_{\mathrm{HF}}\right| \left(H + [H,\tau] + \frac{1}{2}[[H,\tau],\tau] + \frac{1}{3!}\Big[[[H,\tau],\tau],\tau\Big] + \cdots\right) \left|\Psi_{\mathrm{HF}}\right\rangle$$

- BCH expansion does not terminate for UCC, because τ contains de-excitation operators as well as excitation operators. To solve UCC on a classical computer, we have to truncate the BCH expansion at certain order.
- $\exp(\tau)$ is a unitary operator. Construction of quantum circuit for $\exp(\tau)$ is rather straightforward, as discussed below.
- By using a quantum computer, we can calculate the UCC energy expectation value. We can use the Rayleigh–Ritz variational principle to optimize the UCC wave function.

UCC ansatz: Quantum circuit construction

☆ **Unitary Coupled Cluster (CC) Method**

$$|\Psi_{\mathrm{UCC}}\rangle = \exp(\tau)|\Psi_{\mathrm{HF}}\rangle = \exp\left(T - T^{\dagger}\right)|\Psi_{\mathrm{HF}}\rangle$$

$$= \exp\left\{\sum_{ia} t_{ia}\left(a_a^{\dagger}a_i - a_i^{\dagger}a_a\right) + \sum_{ijab} t_{ijab}\left(a_a^{\dagger}a_b^{\dagger}a_j a_i - a_i^{\dagger}a_j^{\dagger}a_b a_a\right)\right\}|\Psi_{\mathrm{HF}}\rangle$$

(UCCSD case)

$$t_{ia}\left(a_a^{\dagger}a_i - a_i^{\dagger}a_a\right) \xrightarrow{\mathrm{JWT}} \frac{i}{2} t_{ia}\left(X_a Z_{a-1} Z_{a-2} \cdots Z_{i+1} Y_i - Y_a Z_{a-1} Z_{a-2} \cdots Z_{i+1} X_i\right)$$

$$\exp\left\{t_{ia}\left(a_a^{\dagger}a_i - a_i^{\dagger}a_a\right)\right\} \xrightarrow{\mathrm{JWT}} \exp\left\{\frac{i}{2} t_{ia}\left(X_a Z_{a-1} Z_{a-2} \cdots Z_{i+1} Y_i - Y_a Z_{a-1} Z_{a-2} \cdots Z_{i+1} X_i\right)\right\}$$

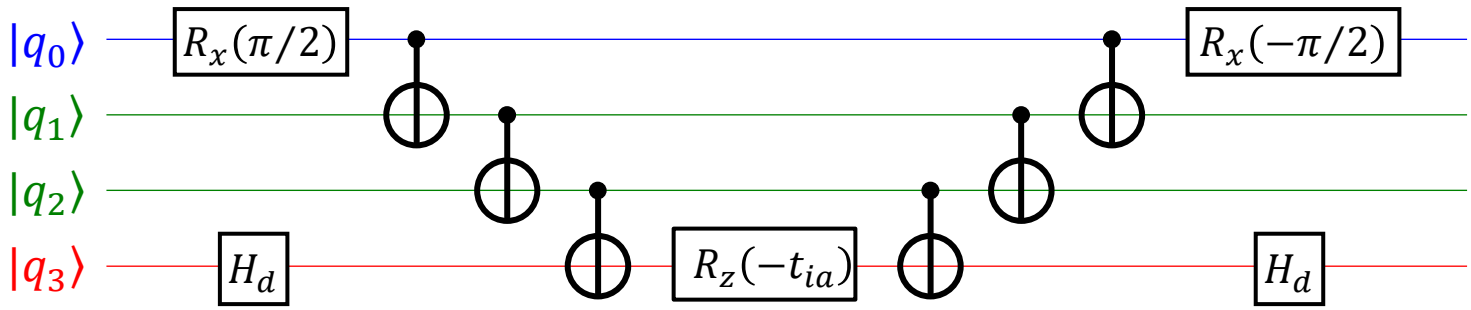
$$\approx \exp\left\{\frac{i}{2} t_{ia}\left(X_a Z_{a-1} Z_{a-2} \cdots Z_{i+1} Y_i\right)\right\} \times \exp\left\{-\frac{i}{2} t_{ia}\left(Y_a Z_{a-1} Z_{a-2} \cdots Z_{i+1} X_i\right)\right\}$$

(Trotter decomposition)

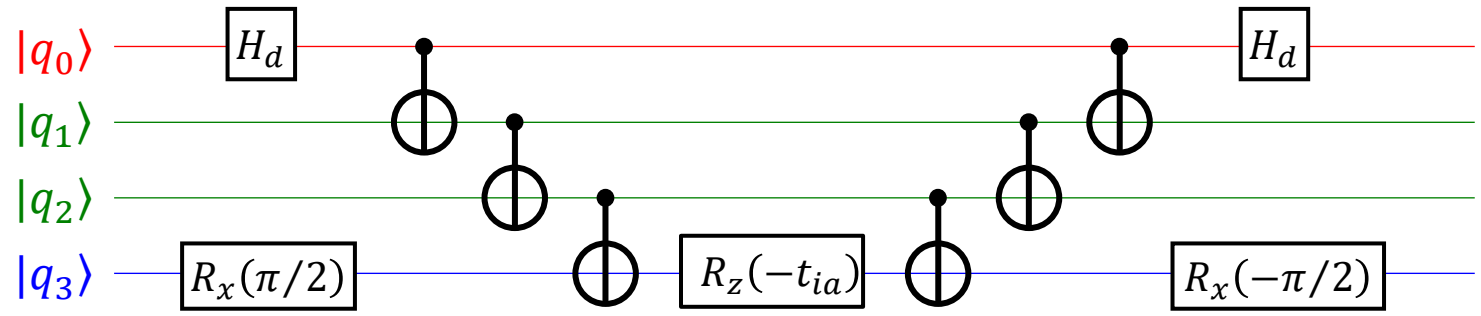
UCC ansatz: Quantum circuit construction

$\exp\left\{\frac{i}{2}t_{ia}(X_3Z_2Z_1Y_0)\right\}$ term

$$R_z(\theta) = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$$



$\exp\left\{\frac{i}{2}t_{ia}(Y_3Z_2Z_1X_0)\right\}$ term



Calculation of an energy expectation value

$$H = g_1\mathbf{1} + g_2Z_0 + g_3Z_1 + g_4Z_0Z_1 + g_5X_0X_1 + g_6Y_0Y_1$$

$$E = g_1 + g_2\langle\Psi|Z_0|\Psi\rangle + g_3\langle\Psi|Z_1|\Psi\rangle + g_4\langle\Psi|Z_0Z_1|\Psi\rangle + g_5\langle\Psi|X_0X_1|\Psi\rangle + g_6\langle\Psi|Y_0Y_1|\Psi\rangle$$

Hamiltonian terms containing only Pauli-*Z* operators

Measurement results: 1000 shots

Measurement outcome	Frequency
00	15
01	124
10	823
11	38

$$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$Z \otimes Z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$g_2\langle\Psi|Z_0|\Psi\rangle$ term

$$\langle\Psi|Z_0|\Psi\rangle = \frac{1\times(15+124) - 1\times(823+38)}{1000} = -0.722$$

$g_3\langle\Psi|Z_1|\Psi\rangle$ term

$$\langle\Psi|Z_1|\Psi\rangle = \frac{1\times(15+823) - 1\times(124+38)}{1000} = 0.676$$

$g_4\langle\Psi|Z_0Z_1|\Psi\rangle$ term

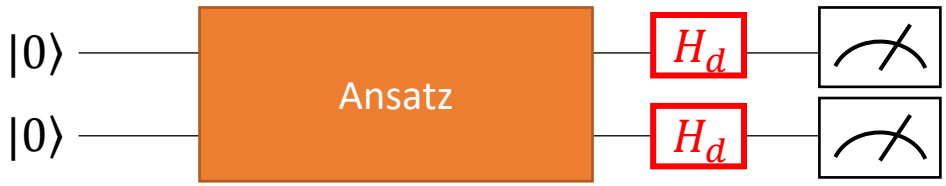
$$\langle\Psi|Z_1Z_2|\Psi\rangle = \frac{1\times(15+38) - 1\times(124+823)}{1000} = -0.894$$

Calculation of an energy expectation value

$$H = g_1\mathbf{1} + g_2 Z_0 + g_3 Z_1 + g_4 Z_0 Z_1 + g_5 X_0 X_1 + g_6 Y_0 Y_1$$

$$E = g_1 + g_2\langle\Psi|Z_0|\Psi\rangle + g_3\langle\Psi|Z_1|\Psi\rangle + g_4\langle\Psi|Z_0 Z_1|\Psi\rangle + g_5\langle\Psi|X_0 X_1|\Psi\rangle + g_6\langle\Psi|Y_0 Y_1|\Psi\rangle$$

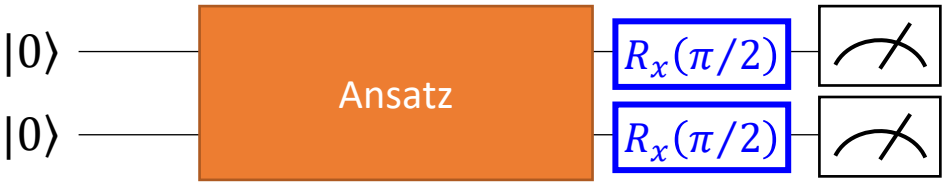
$g_5\langle\Psi|X_0 X_1|\Psi\rangle$ term



Measurements of quantum states are carried out in the *Z*-basis.

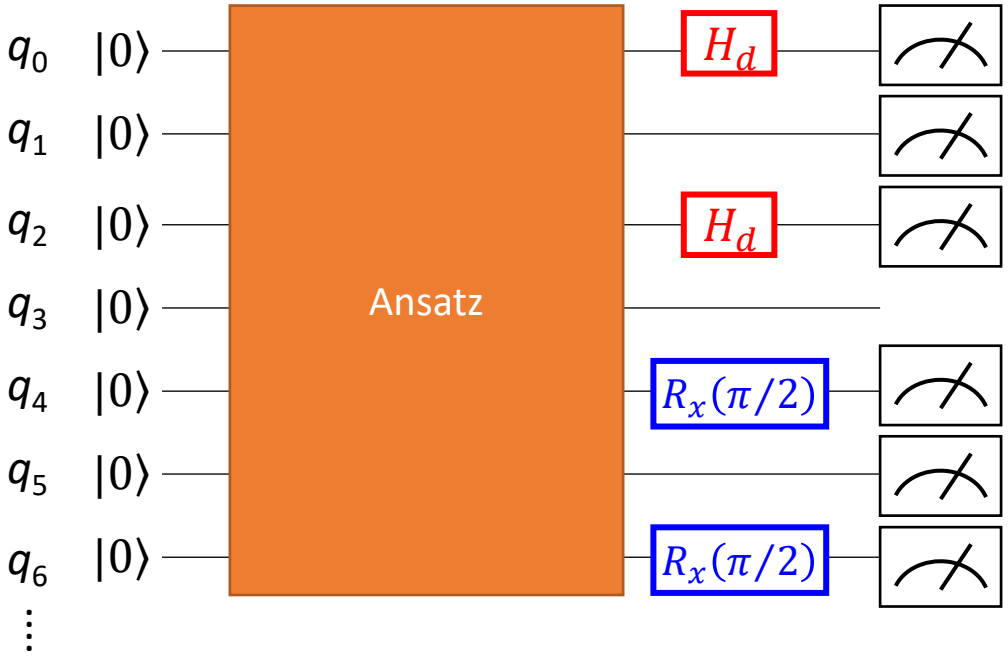
Hadamard gates are introduced before the measurement to change *X*-basis to *Z*-basis.

$g_6\langle\Psi|Y_0 Y_1|\Psi\rangle$ term



Calculation of an energy expectation value

In case of evaluating $g\langle\Psi|X_0 Z_1 X_2 Y_4 Z_5 Y_6|\Psi\rangle$ term, the quantum circuit for the expectation value calculation will be



* Measurement of q_3 is not necessary.

Calculation of an energy expectation value

In principle, expectation values of mutually commute Pauli strings can be evaluated simultaneously.

Pauli strings containing Pauli-Z only.

$$Z_0,\ Z_1,\ Z_2,\ Z_3,\ Z_0Z_1,\ Z_0Z_2,\ Z_0Z_1Z_2Z_3,\ \text{etc}$$

Pauli strings having no identical qubit indices

$$X_0X_1,\ \ Y_2Y_3$$

Hamiltonian term grouping is very important to reduce the measurement cost in VQE!

$$H = \sum_k w_k P_k$$

Group 1: P_0, P_1, P_4, P_6, ...

Group 2: P_2, P_5, P_9, ...

Group 3: P_3, P_7, P_8, ...

⋮

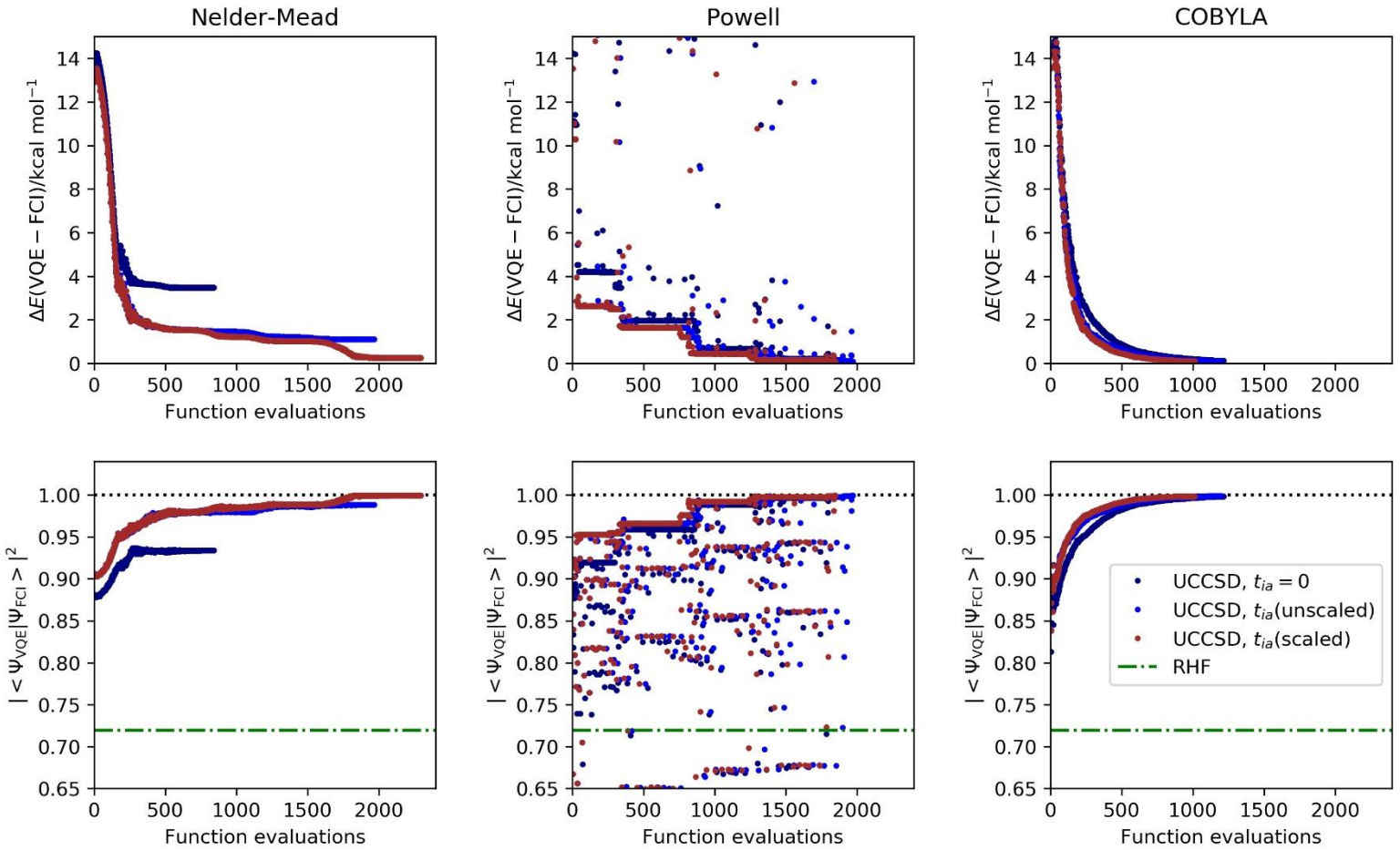
$[P_i, P_j] = 0$ for any i and j within the group.

Hamiltonian has $O(N^4)$ terms, but the measurement cost becomes $O(N^3)$ by grouping.

P. Gokhale et al, *IEEE Trans. Quantum Eng.* **2020**, *1*, 3102324.

Parameter optimization on classical computer

LiH molecule, R(Li–H) = 3.0 Å, VQE-UCCSD/STO-3G



K. Sugisaki et al, ChemRxiv-2021-w7n78

Parameter shift rule for analytical gradient

$$|\Psi\rangle = e^{-i\frac{\theta_n}{2}P_n} \cdots e^{-i\frac{\theta_k}{2}P_k} \cdots e^{-i\frac{\theta_0}{2}P_0}|\Psi_0\rangle$$

$$E = \underbrace{\left\langle \Psi_0 \middle| e^{i\frac{\theta_0}{2}P_0} \cdots}_{\langle\psi|} e^{i\frac{\theta_k}{2}P_k} \underbrace{\cdots e^{i\frac{\theta_n}{2}P_n} H e^{-i\frac{\theta_n}{2}P_n} \cdots}_{A} e^{-i\frac{\theta_k}{2}P_k} \underbrace{\cdots e^{-i\frac{\theta_0}{2}P_0} \middle| \Psi_0 \right\rangle}_{|\psi\rangle} = \left\langle \psi \middle| e^{i\frac{\theta_k}{2}P_k} A e^{-i\frac{\theta_k}{2}P_k} \middle| \psi \right\rangle$$

$$\frac{\partial E}{\partial \theta_k} = \frac{i}{2}\left\langle \psi \middle| P_k e^{i\frac{\theta_k}{2}P_k} A e^{-i\frac{\theta_k}{2}P_k} - e^{i\frac{\theta_k}{2}P_k} A e^{-i\frac{\theta_k}{2}P_k} P_k \middle| \psi \right\rangle$$

$$= \frac{i}{2}\left\langle \psi \middle| \left[P_k, \underbrace{e^{i\frac{\theta_k}{2}P_k} A e^{-i\frac{\theta_k}{2}P_k}}_{B} \right] \middle| \psi \right\rangle = \frac{i}{2}\langle \psi | [P_k, B] | \psi \rangle$$

$$[P_k, B] = -i\left(e^{i\frac{\pi/2}{2}P_k} B e^{-i\frac{\pi/2}{2}P_k} - e^{i\frac{-\pi/2}{2}P_k} B e^{-i\frac{-\pi/2}{2}P_k}\right)$$

$$= -i\left(e^{i\frac{\theta_k+\pi/2}{2}P_k} A e^{-i\frac{\theta_k+\pi/2}{2}P_k} - e^{i\frac{\theta_k-\pi/2}{2}P_k} A e^{-i\frac{\theta_k-\pi/2}{2}P_k}\right)$$

$$\frac{\partial E}{\partial \theta_k} = \frac{1}{2}\left\{\left\langle \psi \middle| e^{i\frac{\theta_k+\pi/2}{2}P_k} A e^{-i\frac{\theta_k+\pi/2}{2}P_k} \middle| \psi \right\rangle - \left\langle \psi \middle| e^{i\frac{\theta_k-\pi/2}{2}P_k} A e^{-i\frac{\theta_k-\pi/2}{2}P_k} \middle| \psi \right\rangle\right\}$$

K. Mitarai et al, *Phys. Rev. A* **2018**, *98*, 032309.

ADAPT ansatz

ARTICLE

https://doi.org/10.1038/s41467-019-10988-2 OPEN

Nat. Comm. **2019**, *10*, 3007

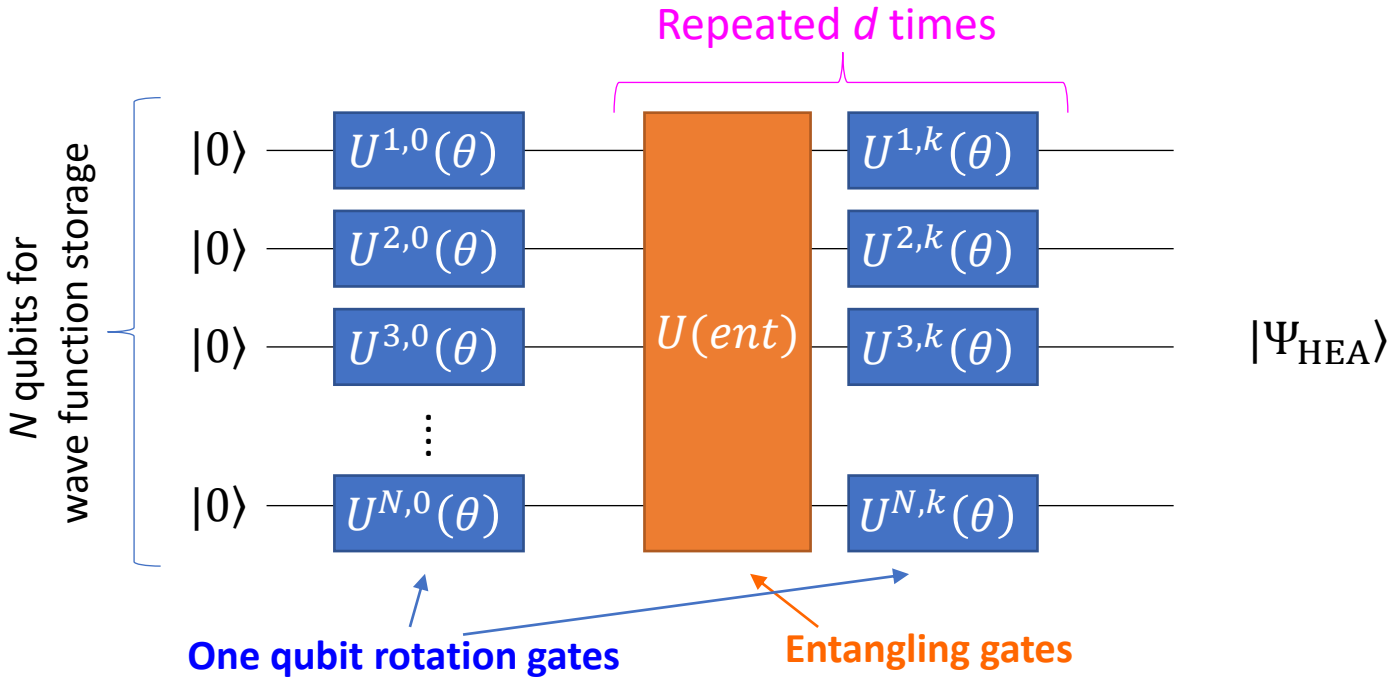
An adaptive variational algorithm for exact molecular simulations on a quantum computer

Harper R. Grimsley[1], Sophia E. Economou[2], Edwin Barnes[2] & Nicholas J. Mayhall[1]

1) Define an "operator pool", which is a collection of operator definitions.
2) Select operators from "pool".
3) Prepare a trial state $\left|\Psi^{(n)}\right\rangle$ with the current ansatz.
4) Calculate the gradient $\frac{\partial E^{(n)}}{\partial \theta_j} = \left\langle \Psi^{(n)} \middle| \left[H, A_j\right] \middle| \Psi^{(n)} \right\rangle$ for each operator in the pool
5) Exit if the norm of the gradient vector is smaller than the threshold, otherwise go to step (6)
6) Identify the operator having the largest gradient, and add the operator to the left of the ansatz.
7) Perform VQE to re-optimize all parameters in the ansatz.
8) Return to step (3)

Hardware-efficient ansatz

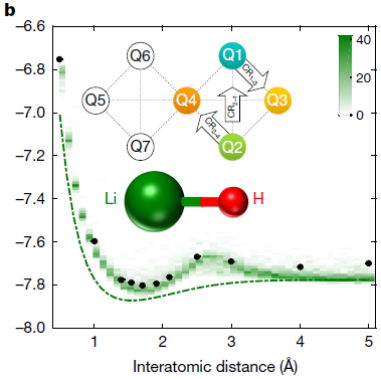
Wave function is entangled states. If we can generate arbitrary entangled states, it can be regarded as the approximated wave function.



- Quantum circuit is shallower than that based on the UCCSD ansatz
- Quantum gates do not necessary to have a correspondence to electron excitations/de-excitations
- The energy-lowest state of the given Hamiltonian is obtained.
- Even if we try to compute the neutral state, VQE-HEA can converge to the anionic state, if anionic state is more stable than the neutral state.

Constrained VQE

Appearance of the “kink” implies that the energy-lowest state at the qubit mean field changes.



Snapshot taken from *Nature* **2017**, *549*, 242.

Use $H' = H + \left| \boldsymbol{S}^2 - S_{\text{target}}(S_{\text{target}} + 1) \right|$ as a cost function.

Spin quantum number of the target electronic state

Spin S-squared operator giving an eigenvalue $S(S + 1)$.

- $|\Psi_{S = Sa}\rangle$ with $S_a < S_{\text{target}}$ does not contribute as the spin contaminants, if the quantum chemical calculation is performed for $M_S = S_{\text{target}}$. Spin contaminants are electronic states with $S = S_a > S_{\text{target}}$ only.
- Penalty term should be included in the parameter optimization step only. For the final energy evaluation, one should use original Hamiltonian H.

I. G. Ryabinkin, S. N. Genin, A. F. Izmaylov, *J. Chem. Theory Comput.* **2019**, *15*, 249–255.

Symmetry-preserving quantum circuits

In the JWT, CNOT gate will change the number of electrons

$$\text{CNOT}|00\rangle = |00\rangle$$
$$\text{CNOT}|01\rangle = |01\rangle$$
$$\text{CNOT}|10\rangle = |11\rangle$$
$$\text{CNOT}|11\rangle = |10\rangle$$

If we use the *A* gate as the entangling gate, the number of electrons is preserved.

$$A(\theta,\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & e^{i\phi}\sin\theta & 0 \\ 0 & e^{-i\phi}\sin\theta & -\cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$A(\theta,\phi)|00\rangle = |00\rangle$$
$$A(\theta,\phi)|01\rangle = \cos\theta|01\rangle + e^{i\phi}\sin\theta\,|10\rangle$$
$$A(\theta,\phi)|10\rangle = e^{-i\phi}\sin\theta\,|01\rangle - \cos\theta\,|10\rangle$$
$$A(\theta,\phi)|11\rangle = |11\rangle$$

B. T. Gard et al, *npj Quantum Info.* **2020**, *6*, 10.

Error mitigations

Applying quantum error correction is quite difficult on NISQ devices.

Instead, one can mitigate errors by performing additional measurements and postprocessing.

Measurement error mitigation

https://qiskit.org/textbook/ch-quantum-hardware/measurement-error-mitigation.html

Measurement outcome	Initial state			
	00	01	10	11
00	8049	240	325	9
01	80	7886	5	325
10	63	3	7755	233
11	0	63	233	7625

$$C_{noisy} = MC_{ideal} \qquad M = \frac{1}{8192}\begin{pmatrix} 8049 & 240 & 325 & 9 \\ 80 & 7886 & 5 & 325 \\ 63 & 3 & 7755 & 233 \\ 0 & 63 & 233 & 7625 \end{pmatrix}$$

$$\boldsymbol{C_{ideal} = M^{-1}C_{noisy}}$$

Symmetry verifications

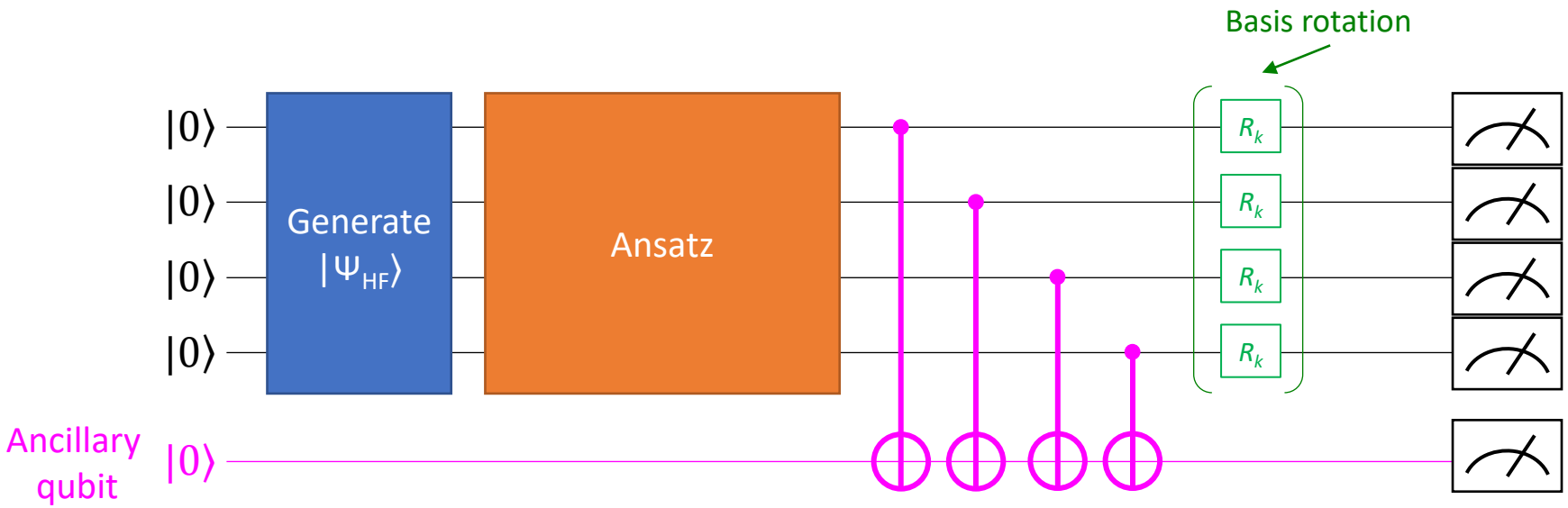
In the JWT, bit flip error will change the number of electrons

$$|\Psi\rangle = c_0|1100\rangle + c_1|0011\rangle \xrightarrow{\text{Bit flip on the rightmost qubit}} c_0|1101\rangle + c_1|0010\rangle$$

Neutral state

Anionic

Cationic



Situation	Measurement outcome of ancilla
No bit flip error	N_{elec} (mod 2)
Presence of a bit flip error	(N_{elec} + 1) (mod 2)

X. Bonet-Monroig, R. Sagastizabal, M. Singh, T. E. O'Brien, *Phys. Rev. A* **2018**, *98*, 062339.

Excited states calculations: Use orthogonality

Quantum **2019**, *3*, 156; arXiv:1805.08138.

Variational Quantum Computation of Excited States

Oscar Higgott[1,2], Daochen Wang[1,3], and Stephen Brierley[1]

[1] Riverlane, 3 Charles Babbage Road, Cambridge CB3 0GT

[2] Department of Physics and Astronomy, University College London, London, WC1E 6BT

[3] Joint Center for Quantum Information and Computer Science, University of Maryland, College Park, MD 20742

July 1, 2019

(1) Calculate ground state using conventional VQE

(2) Calculate the first excited state by minimizing $E_1' = \langle\Psi_1|H|\Psi_1\rangle + \lambda|\langle\Psi_0|\Psi_1\rangle|^2$

Energy of the first excited state

0 if $|\Psi_0\rangle$ and $|\Psi_1\rangle$ are orthogonal

⋮

(*n*+1) Calculate the *n*-th excited state by minimizing $E_n' = \langle\Psi_n|H|\Psi_n\rangle + \sum_{k=0}^{n-1}\lambda|\langle\Psi_k|\Psi_n\rangle|^2$

Square overlaps between wave functions $|\langle\Psi_k|\Psi_n\rangle|^2$ can be evaluated by the SWAP test

Excited states calculations: Subspace expansion

An approach similar to MR-CI, where reference wave function is computed by using VQE.

$|\Psi(\theta)\rangle = U(\theta)|\Psi_0\rangle$ Optimize θ to minimize $E(\theta) = \langle\Psi(\theta)|H|\Psi(\theta)\rangle$ using VQE.

$H_{ij} = \langle\Psi(\theta)|O_i^\dagger H O_j|\Psi(\theta)\rangle,\ S_{ij} = \langle\Psi(\theta)|O_i^\dagger O_j|\Psi(\theta)\rangle$ O_i and O_j are excitation operators

$HC = SCE$ **Solve generalized eigenvalue problem on classical computer**

- Think effects of errors and noises as contaminations from other electronic states.
- If O_i and O_j are one-electron excitation operators, expectation values of $O_i^\dagger H O_j$ can be calculated by evaluating up to four-body RDM.
- Diagonalization of CI matrix → Not only the ground state but also the excited states can be obtained.

J. R. McClean et al, *Phys. Rev. A* **2017**, *95*, 042308.

Transition probability calculations

(1) Calculate $|\Psi_0\rangle$ and $|\Psi_1\rangle$.

(2) Evaluate the expectation values of **A**, where **A** is an operator we want to calculate off-diagonal terms.

$$\langle \mathbf{A} \rangle_0 = \langle \Psi_0 | \mathbf{A} | \Psi_0 \rangle, \langle \mathbf{A} \rangle_1 = \langle \Psi_1 | \mathbf{A} | \Psi_1 \rangle$$

(3) Evaluate the expectation values of A using $|\Phi_+\rangle$ and $|\Phi_-\rangle$.

$$|\Phi_+\rangle = \frac{1}{\sqrt{2}}(|\Psi_0\rangle + |\Psi_1\rangle) \qquad |\Phi_-\rangle = \frac{1}{\sqrt{2}}(|\Psi_0\rangle - |\Psi_1\rangle)$$

$$\langle \mathbf{A} \rangle_{\Phi_+} = \frac{1}{2}(\langle \Psi_0 | \mathbf{A} | \Psi_0 \rangle + \langle \Psi_1 | \mathbf{A} | \Psi_1 \rangle + \langle \Psi_0 | \mathbf{A} | \Psi_1 \rangle + \langle \Psi_1 | \mathbf{A} | \Psi_0 \rangle)$$

$$\langle \mathbf{A} \rangle_{\Phi_-} = \frac{1}{2}(\langle \Psi_0 | \mathbf{A} | \Psi_0 \rangle + \langle \Psi_1 | \mathbf{A} | \Psi_1 \rangle - \langle \Psi_0 | \mathbf{A} | \Psi_1 \rangle - \langle \Psi_1 | \mathbf{A} | \Psi_0 \rangle)$$

$$\langle \Psi_0 | \mathbf{A} | \Psi_1 \rangle = \frac{1}{2}\left(\langle \mathbf{A} \rangle_{\Phi_+} - \langle \mathbf{A} \rangle_{\Phi_-}\right)$$

R. M. Parrish et al, *Phys. Rev. Lett.* **2019**, *122*, 230401.

Barren plateaus problem

ARTICLE

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Barren plateaus in quantum neural network training landscapes

Jarrod R. McClean[1], Sergio Boixo[1], Vadim N. Smelyanskiy[1], Ryan Babbush[1] & Hartmut Neven[1]

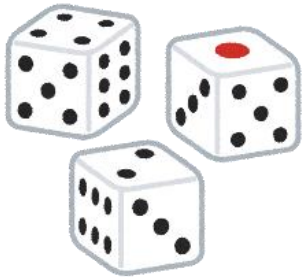
For a wide class of random quantum circuits,

- The expectation values of observables concentrate to their average over Hilbert space
- The probability that the gradient along any reasonable direction is nonzero to some fixed precision is exponentially small as a function of the number of qubits.

Nat. Comm. **2018**, *9*, 4812.

Measurement cost

Energy expectation value is computed statistically.
Statistical errors are unavoidable!



Number of measurements: $O(w_{max}^2/\varepsilon^2)$

Norm of Hamiltonian terms: w_{max}

Energy precision: ε

- If we want to make energy precision to be half, we must perform four time larger number of measurements.
- w_{max} becomes very large for molecules with heavier atoms due to strong nuclear–electron attraction.
- Most of the theoretical studies on VQE use a statevector simulator, which corresponds to infinite number of repetitive measurements.

Computational cost of VQE

Wave function preparation (Depth of parametrized quantum circuit)

★ UCCSD ansatz

Number of parameters: $O\left(N_{occ}^2 N_{vir}^2\right)$

Quantum circuit construction: $O(N)$ for JWT and $O(\log N)$ for BKT

★ Hardware-efficient ansatz

Number of parameters: $O(NL)$ (L denotes number of layers)

Energy expectation value evaluation (measurements)

Number of operator groups: $O(N^3)$

Parameter optimization (number of iterations to achieve convergence)

Strongly depend on the molecular systems, optimization algorithm being used, and initial parameters. Empirically, $O(N)$ or greater

Note that the computational cost of CCSD on classical computer is $O(N^6)$

Misconceptions on VQE

By using a quantum computer, quantum chemical calculations can be performed exponentially faster than the classical counterpart.

Quantum chemical calculations can be accelerated by using VQE.

	VQE	Classical computer
Approximated methods (such as CCSD and UCCSD)	Polynomial	Polynomial
Exact calculations (at the full-CI level)	Exponential	Exponential

Obtaining variationally best wave function (full-CI) is difficult, because the number of variables increases exponentially against the system size.

VQE calculates the wave function by variational optimizations of the parameters those number possibly scales exponentially against the system size.

Summary: Comparison of QPE and VQE

	Quantum phase estimation (QPE)	Variational quantum eigensolver (VQE)
Classification of algorithm	Fault-tolerant quantum computer (FTQC) algorithm	Noisy intermediate-scale quantum (NISQ) algorithm
Wave function	Full-CI or CAS-CI	UCC or heuristic ones
Energy	Eigenvalue	Expectation value
Quantum circuit	Deep	Shallow
Computational cost scaling against the energy precision ε	$1/\varepsilon$	$\lvert H\rvert^2/\varepsilon^2$
Exponential speedup against classical counterpart	Yes	Unknown