ETRI Electronics and Telecommunications Research Institute

Variational Quantum Eigensolver

백경현
한국전자통신연구원
양자컴퓨팅실

(2023.08.09 고려대학교)

양자 시뮬레이션
Quantum simulation

Quantum simulation

- Richard Feynman’s memorable words:

  “Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy.”

  “자연은 고전이 아니다, 젠장. 만약 당신이 자연을 모사하고 싶다면 그것을 양자 역학으로 만들어야 좋을 것이다. 이는 쉽지 않기에, 아름다운 문제이다.

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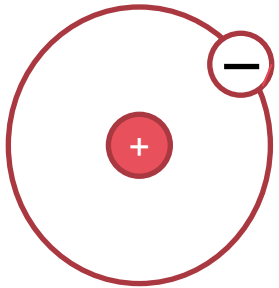
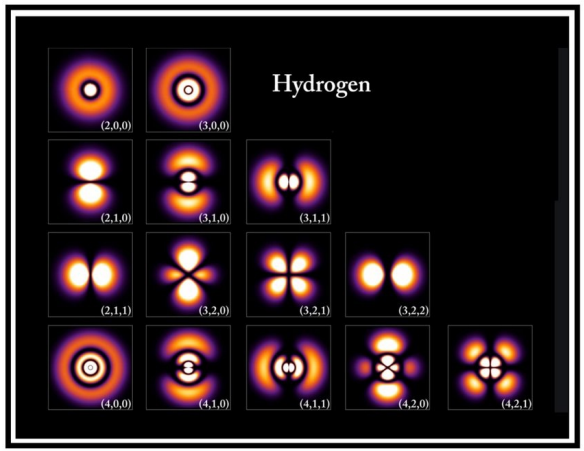


Hydrogen atom



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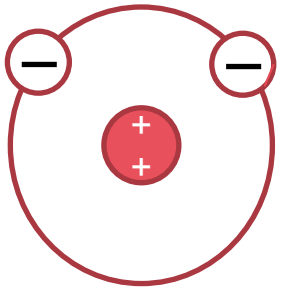
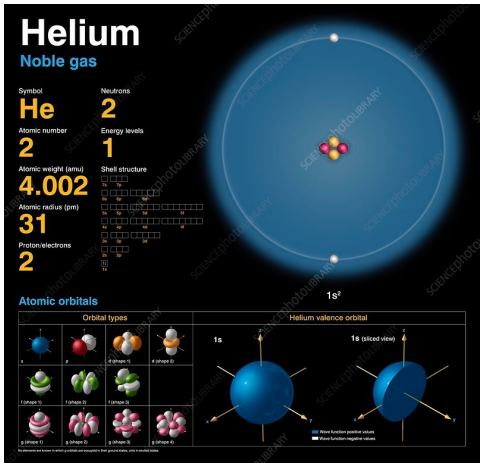


Helium atom



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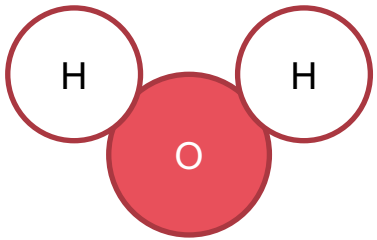

Water molecule

Quantum simulation

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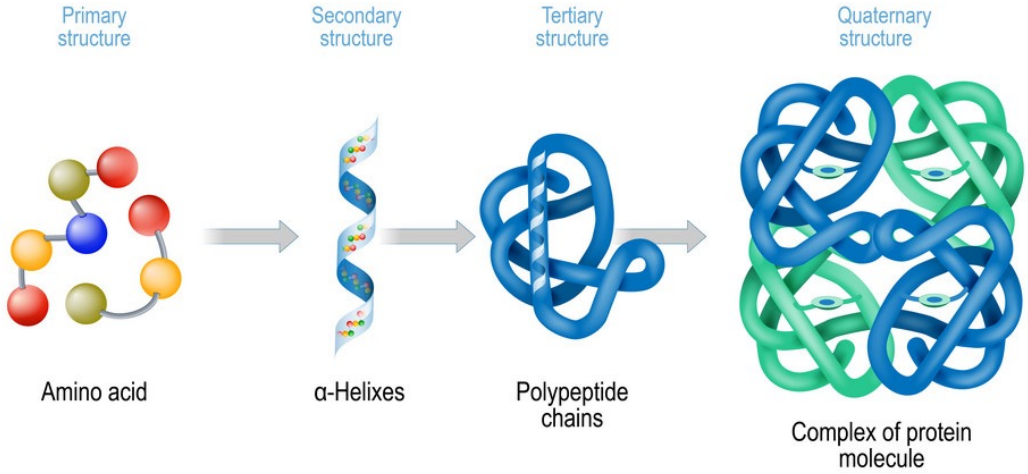
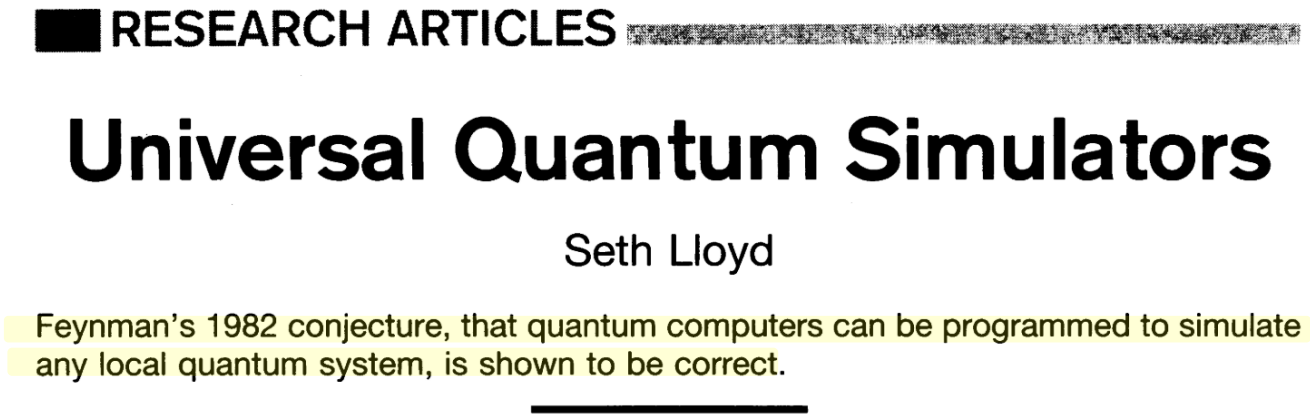


Quantum simulation

- Universal quantum simulators (1996)



RESEARCH ARTICLES

Universal Quantum Simulators

Seth Lloyd

Feynman's 1982 conjecture, that quantum computers can be programmed to simulate any local quantum system, is shown to be correct.

Quantum simulation

- Universal quantum simulators (1996)
  - 해밀토니안

$$H = \sum_{i=1}^{l} H_i$$

H_i 은 국소적인 상호작용을 기술하는 로컬 해밀토니안이다.

  - 해밀토니안 시뮬레이션 (Trotter approximation)

$$e^{iHt} \sim (e^{iH_1 t/n} \cdots e^{iH_l t/n})^n$$

국소 해밀토니안은 양자 컴퓨터에서 효율적으로 모사가 가능하다.

Quantum simulation

- 해밀토니안 바닥상태를 찾기 위한 양자 알고리즘

VOLUME 83, NUMBER 24 PHYSICAL REVIEW LETTERS 13 DECEMBER 1999

Quantum Algorithm Providing Exponential Speed Increase for Finding Eigenvalues and Eigenvectors

Daniel S. Abrams*
Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California 91109-8099

Seth Lloyd†
d'Arbeloff Laboratory for Information Sciences and Technology, Department of Mechanical Engineering, MIT 3-160, Cambridge, Massachusetts 02139
(Received 27 July 1998)

We describe a new polynomial time quantum algorithm that uses the quantum fast Fourier transform to find eigenvalues and eigenvectors of a local Hamiltonian, and that can be applied in cases (commonly found in *ab initio* physics and chemistry problems) for which all known classical algorithms require exponential time. Applications of the algorithm to specific problems are considered, and we find that classically intractable and interesting problems from atomic physics may be solved with between 50 and 100 quantum bits.

Quantum simulation

- 해밀토니안 바닥상태를 찾기 위한 양자 알고리즘

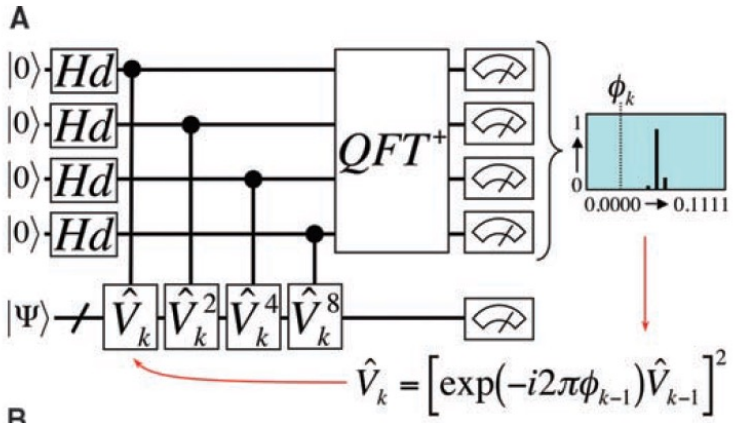
Science
AAAS

Simulated Quantum Computation of Molecular Energies
Alán Aspuru-Guzik *et al.*
Science **309**, 1704 (2005);
DOI: 10.1126/science.1113479

Simulated Quantum Computation of Molecular Energies

Alán Aspuru-Guzik,[1]*† Anthony D. Dutoi,[1]* Peter J. Love,[2] Martin Head-Gordon[1,3]

The calculation time for the energy of atoms and molecules scales exponentially with system size on a classical computer but polynomially using quantum algorithms. We demonstrate that such algorithms can be applied to problems of chemical interest using modest numbers of quantum bits. Calculations of the water and lithium hydride molecular ground-state energies have been carried out on a quantum computer simulator using a recursive phase-estimation algorithm. The recursive algorithm reduces the number of quantum bits required for the readout register from about 20 to 4. Mappings of the molecular wave function to the quantum bits are described. An adiabatic method for the preparation of a good approximate ground-state wave function is described and demonstrated for a stretched hydrogen molecule. The number of quantum bits required scales linearly with the number of basis functions, and the number of gates required grows polynomially with the number of quantum bits.



Quantum simulation

- **양자 컴퓨팅 / 양자 시뮬레이션**

파인만의 통찰:
효율적인 양자시스템 시뮬레이션을 위한 양자컴퓨터 필요성

1981

양자역학 기반의 범용컴퓨터 가능성 제시
(David Deutsch)

1985

쇼어 알고리즘:
소인수분해를 위한 양자 알고리즘 제시

1994

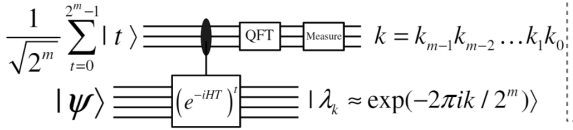
1996

Trotterization 기반 **양자 동역학 시뮬레이션**

Universal Quantum Simulators

Seth Lloyd

Feynman's 1982 conjecture, that quantum computers can be programmed to simulate any local quantum system, is shown to be correct.

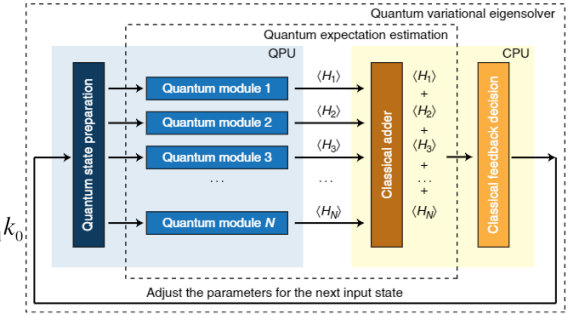


고유값 추정 양자 알고리즘:
양자 시뮬레이션 기반 고유값 추정 알고리즘

1999

2009

HHL 알고리즘:
양자 시뮬레이션 활용한 선형 방정식 공략 양자 알고리즘

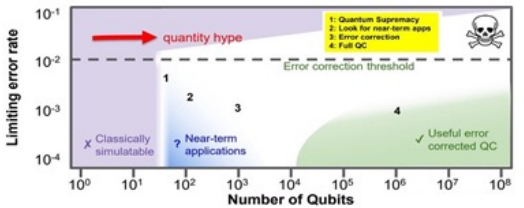


Variational Quantum Eigensolver (VQE): 바닥에너지 추정을 위한 하이브리드 양자 알고리즘

2014

2018

NISQ 개념 (Preskill):
Noisy Intermediate-Scale Quantum 알고리즘 개념 제안

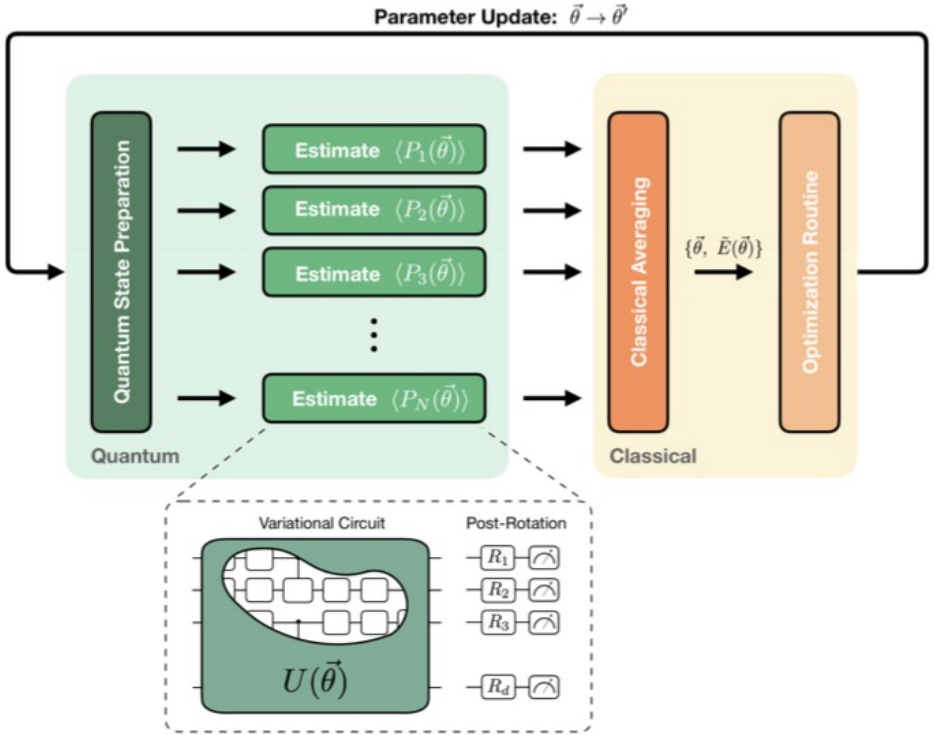


Variational Quantum Eigensolver(VQE)

Variational Quantum Eigensolver (VQE)

- Ground state of Hamiltonian

  - Finding ground state of system is the primary interest in the dynamics of large chemical systems such as finding the lowest-energy molecular crystal conformation or protein−ligand docking



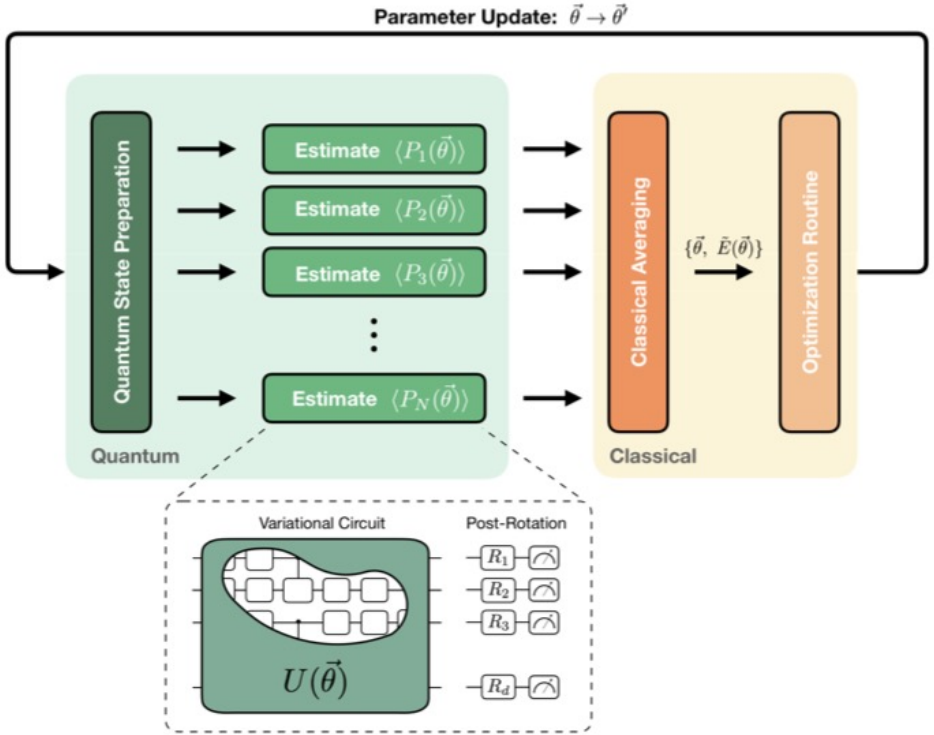
arXiv:1812.09976v2

Variational Quantum Eigensolver (VQE)

- Variational method:

$$\langle\psi|H|\psi\rangle \geq E_0$$

해밀토니안의 평균값은 항상
바닥상태의 에너지보다 크다.

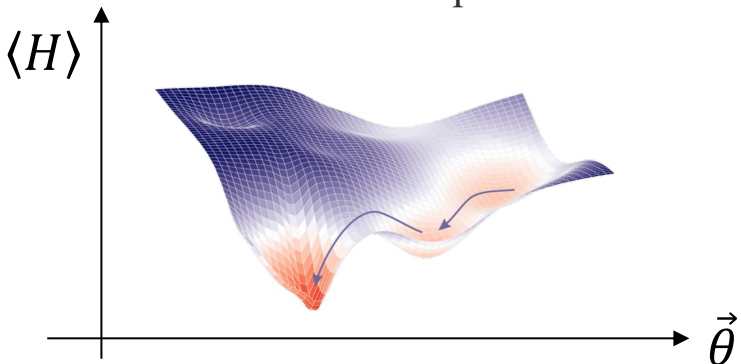


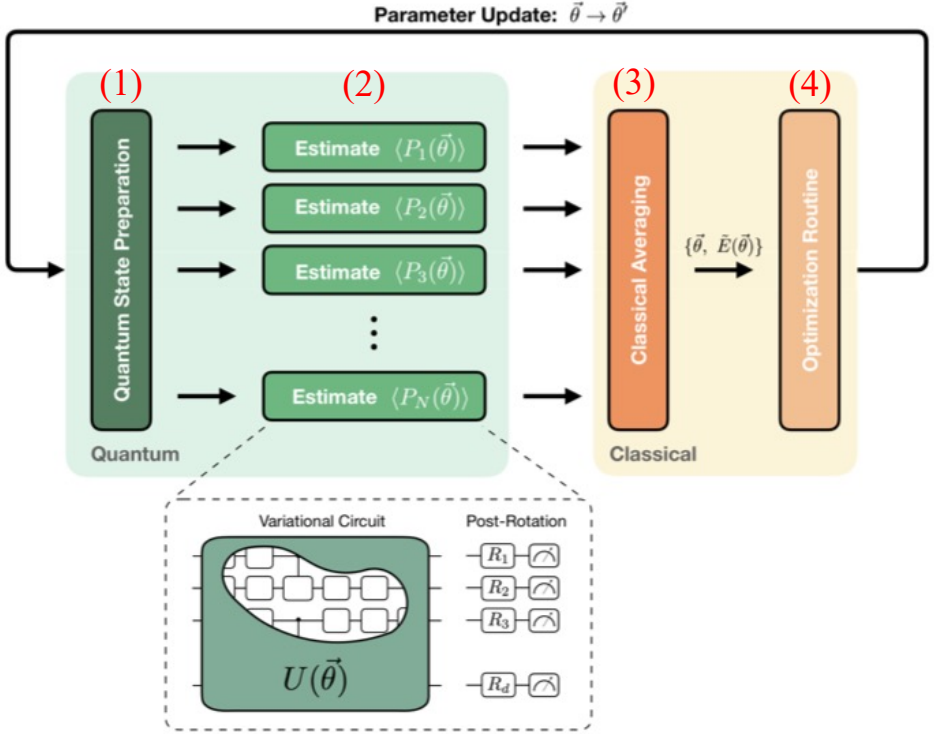
arXiv:1812.09976v2

Variational Quantum Eigensolver (VQE)

- Ground state energy estimation
  1. Prepare quantum states (Ansatz)
  2. Measure energy
  3. Classical averaging
  4. Optimization (Classical)

     → Parameter update





arXiv:1812.09976v2

Ex: Hydrogen model

- Hamiltonian

Coulomb interaction btw electrons and nuclei

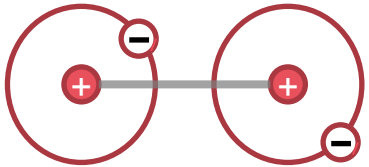
Coulomb interaction btw nuclei

$$H = -\sum_i \frac{\nabla_i^2}{2} - \sum_I \frac{\nabla_I^2}{2M_I'} - \sum_{i,I} \frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2}\sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{2}\sum_{I \neq J} \frac{Z_I Z_J}{|\mathbf{R}_I - \mathbf{R}_J|}.$$

Kinetic energy of nuclei

Kinetic energy of electrons

Coulomb interaction btw electrons



Hydrogen molecule

Rev. Mod. Phys., 92, 1, 015003 (2020)

Ex: Hydrogen model

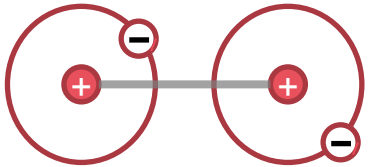
- Hamiltonian

Coulomb interaction
btw electrons and nuclei

$$H_{\mathrm{H}_2} = -\sum_i \frac{\nabla_i^2}{2} - \sum_{i,I} \frac{Z_I}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2}\sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}.$$

Kinetic energy
of electrons

Coulomb interaction
btw electrons



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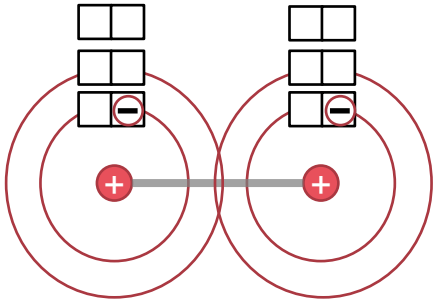


Hydrogen molecule

- Hamiltonian in the second quantized representation

$$H = \sum_{p,q} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

with

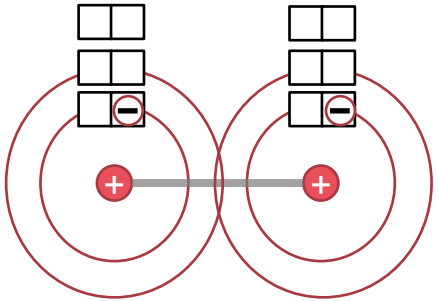
$$h_{pq} = \int d\mathbf{x} \phi_p^*(\mathbf{x}) \left(-\frac{\nabla^2}{2} - \sum_I \frac{Z_I}{|\mathbf{r} - \mathbf{R}_I|} \right) \phi_q(\mathbf{x}),$$

$$h_{pqrs} = \int d\mathbf{x}_1 d\mathbf{x}_2 \frac{\phi_p^*(\mathbf{x}_1) \phi_q^*(\mathbf{x}_2) \phi_r(\mathbf{x}_2) \phi_s(\mathbf{x}_1)}{|\mathbf{x}_1 - \mathbf{x}_2|},$$

for a specific basis set $\{\phi_s(x)\}$.

Rev. Mod. Phys., 92, 1, 015003 (2020)

Ex: Hydrogen model



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- Basis sets
  – STO-3G, STO-6G…
  - Slater-type orbital

$$R_n^{\mathrm{STO}}(r) \propto (\zeta r)^{n-1} e^{-\zeta r}$$

  - Gaussian-type orbital

$$R_{nl}^{\mathrm{GTO}}(r) \propto (\sqrt{\alpha_{nl}} r)^l e^{-\alpha_{nl} r^2}$$

Rev. Mod. Phys., 92, 1, 015003 (2020)

Ex: Hydrogen model

- Hamiltonian in the second quantized representation

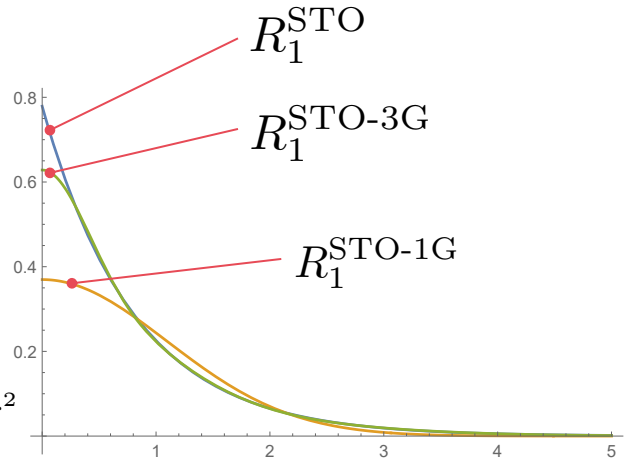
$$H = \sum_{p,q} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{p,q,r,s} h_{pqrs} a_p^\dagger a_q^\dagger a_r a_s$$

- Basis sets
  – STO-3G, STO-6G…

$$R_1^{STO}(r) = 0.779 e^{-1.24r}$$

$$R_1^{STO-1G}(r) = 0.3696 e^{-0.4166 r^2}$$

$$R_1^{\text{STO-3G}}(r) = 0.0835 e^{-0.1689 r^2} + 0.2678 e^{-0.6239 r^2} + 0.2769 e^{-3.4253 r^2}$$



Rev. Mod. Phys., 92, 1, 015003 (2020)

Ex: Hydrogen model

- Qubit Hamiltonian for Hydrogen molecule.

$$
\begin{aligned}
H = {} & h_0 I + h_1 Z_0 + h_2 Z_1 + h_3 Z_2 + h_4 Z_3 \\
& + h_5 Z_0 Z_1 + h_6 Z_0 Z_2 + h_7 Z_1 Z_2 + h_8 Z_0 Z_3 + h_9 Z_1 Z_3 \\
& + h_{10} Z_2 Z_3 + h_{11} Y_0 Y_1 X_2 X_3 + h_{12} X_0 Y_1 Y_2 X_3 \\
& + h_{13} Y_0 X_1 X_2 Y_3 + h_{14} X_0 X_1 Y_2 Y_3 .
\end{aligned}
$$

TABLE II. Example mappings of a fermionic Fock state and its fermionic operators onto the corresponding qubit state, and qubit operators. $\hat{n}_i$ is the fermionic number operator.

Fermion	Jordan-Wigner	Parity	Bravyi-Kitaev
$a\|0001\rangle + b\|0010\rangle$ $+c\|0100\rangle + d\|1000\rangle$	$a\|0001\rangle + b\|0010\rangle$ $+c\|0100\rangle + d\|1000\rangle$	$a\|1111\rangle + b\|1110\rangle$ $+c\|1100\rangle + d\|1000\rangle$	$a\|1011\rangle + b\|1010\rangle$ $+c\|1100\rangle + d\|1000\rangle$
a_0	Q_0	$X_3X_2X_1Q_0$	$X_3X_1Q_0$
a_1	Q_1Z_0	$X_3X_2(Q_1\|0\rangle\langle 0\|_0 - Q_1^\dagger\|1\rangle\langle 1\|_0)$	$X_3(Q_1\|0\rangle\langle 0\|_0 - Q_1^\dagger\|1\rangle\langle 1\|_0)$
a_2	$Q_2Z_1Z_0$	$X_3(Q_2\|0\rangle\langle 0\|_1 - Q_2^\dagger\|1\rangle\langle 1\|_1)$	$X_3Q_2Z_1$
a_3	$Q_3Z_2Z_1Z_0$	$Q_3\|0\rangle\langle 0\|_2 - Q_3^\dagger\|1\rangle\langle 1\|_2$	$1/2[Q_3(1+Z_2Z_1) - Q_3^\dagger(1-Z_2Z_1)]$
$\hat{n}_i = a_i^\dagger a_i$	$\|1\rangle\langle 1\|_i$	$\|1\rangle\langle 1\|_{i=0}$, $1/2(1-Z_iZ_{i-1})_{i=1,2,3}$	$\|1\rangle\langle 1\|_{i=0,2}$, $1/2(1-Z_1Z_0)_{i=1}$, $1/2(1-Z_3Z_2Z_1)_{i=3}$

Rev. Mod. Phys., 92, 1, 015003 (2020)

VQE ansatz

- Ansatz
  - Unitary coupled cluster (UCC) method

$$|\Psi_{CC}\rangle = e^{T-T^\dagger}|\Psi_{HF}\rangle$$

where $T = \sum_i T_i$,

$$T_1 = \sum_{i\in\text{virt},\alpha\in\text{occ}} t_{i\alpha} a_i^\dagger a_\alpha,$$

$$T_2 = \sum_{i,j\in\text{virt},\alpha,\beta\in\text{occ}} t_{ij\alpha\beta} a_i^\dagger a_j^\dagger a_\alpha a_\beta, \ldots$$

VQE ansatz

- Ansatz
  - Unitary coupled cluster (UCC) method

$$|\Psi_{CC}\rangle = e^{T-T^{\dagger}}|\Psi_{HF}\rangle$$

    - UCC is implementable in universal quantum computer via Hamiltonian simulation.
    - However, the implementation of UCCSD (single and double excitations) needs Trotterization.
    - The implementation of UCCSD requires $O(M^3N^2)$ gates when using the JW encoding, where M is the number of spin orbitals and N is the number of electrons. [Quantum Sci. Technol. 4, 014008 (2019)].

VQE ansatz

- Ansatz
  - Unitary coupled cluster (UCC) method for H_2.
    - Hartree-Fock state

$$|\Psi_{HF}^{H_2}\rangle = |0011\rangle$$

    - UCCSD operator

$$U = e^{t_{02}(a_2^\dagger a_0 - a_0^\dagger a_2) + t_{13}(a_3^\dagger a_1 - a_1^\dagger a_3) + t_{0123}(a_3^\dagger a_2^\dagger a_1 a_0 - a_0^\dagger a_1^\dagger a_2 a_3)}$$

$$\Rightarrow \quad U = e^{-i\theta X_3 X_2 X_1 Y_0}$$

- JW encoding
- Trotterization
- Specific technique for simplification

Variational Quantum Eigensolver (VQE)

nature COMMUNICATIONS

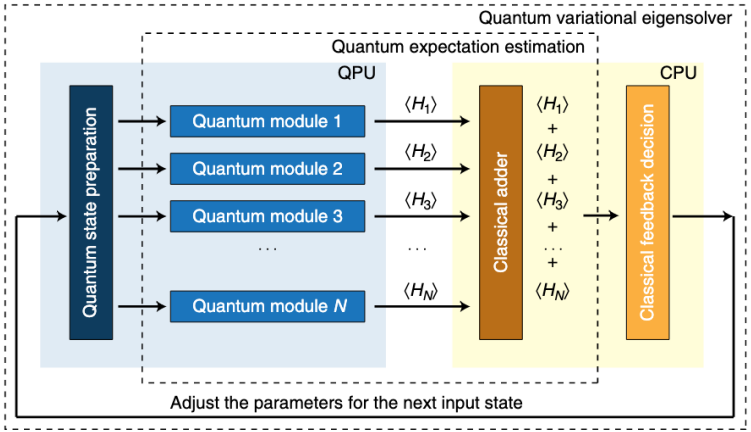
ARTICLE

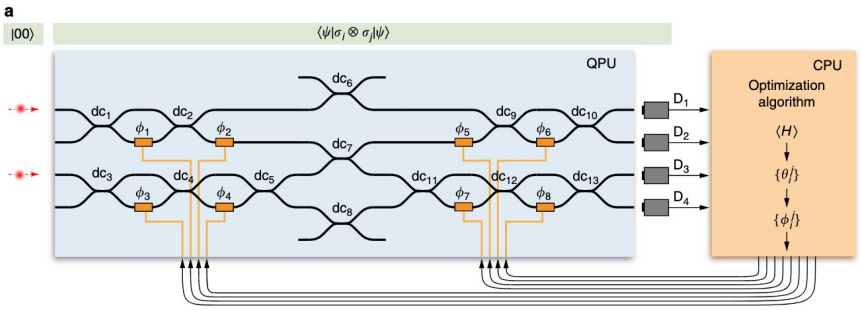
Received 9 Dec 2013 | Accepted 27 May 2014 | Published 23 Jul 2014

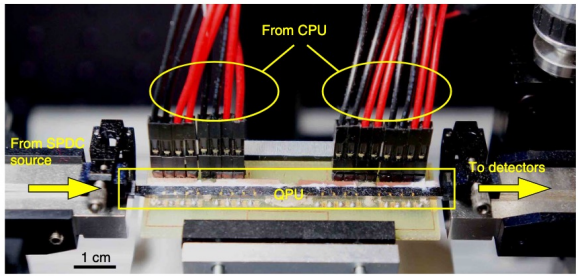
DOI: 10.1038/ncomms5213 OPEN

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. Lo
Alán Aspuru-Guzik[2] & Jeremy L. O'Brien[1]







Variational Quantum Eigensolver (VQE)

PHYSICAL REVIEW X **6,** 031007 (2016)

Scalable Quantum Simulation of Molecular Energies

P. J. J. O'Malley,[1,*] R. Babbush,[2,†] I. D. Kivlichan,[3] J. Romero,[3] J. R. McClean,[4] R. Barends,[5] J. Kelly,[5] P. Roushan,[5] A. Tranter,[6,7] N. Ding,[2] B. Campbell,[1] Y. Chen,[5] Z. Chen,[1] B. Chiaro,[1] A. Dunsworth,[1] A. G. Fowler,[5] E. Jeffrey,[5] E. Lucero,[5] A. Megrant,[5] J. Y. Mutus,[5] M. Neeley,[5] C. Neill,[1] C. Quintana,[1] D. Sank,[5] A. Vainsencher,[1] J. Wenner,[1] T. C. White,[5] P. V. Coveney,[7] P. J. Love,[6] H. Neven,[2] A. Aspuru-Guzik,[3] and J. M. Martinis[5,1,‡]

[1]*Department of Physics, University of California, Santa Barbara, California 93106, USA*
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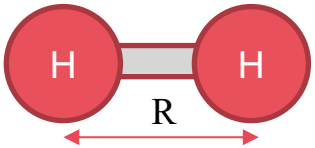
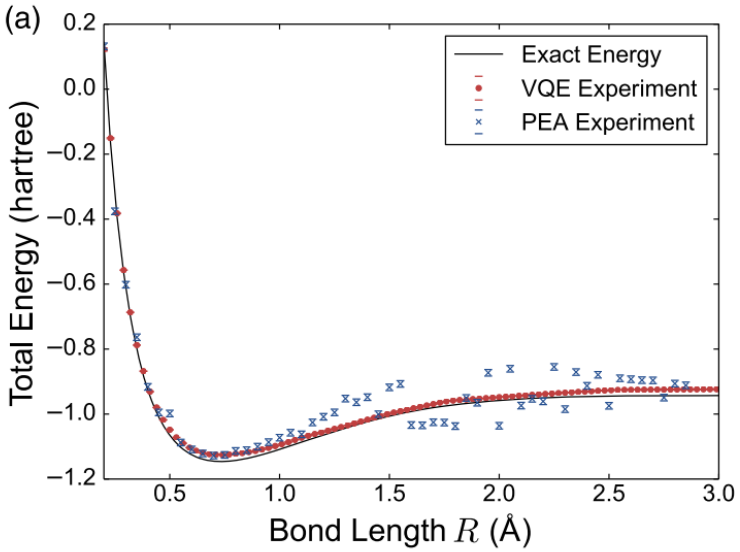
(Received 7 April 2016; published 18 July 2016)

We report the first electronic structure calculation performed on a quantum computer without exponentially costly precompilation. We use a programmable array of superconducting qubits to compute the energy surface of molecular hydrogen using two distinct quantum algorithms. First, we experimentally execute the unitary coupled cluster method using the variational quantum eigensolver. Our efficient implementation predicts the correct dissociation energy to within chemical accuracy of the numerically exact result. Second, we experimentally demonstrate the canonical quantum algorithm for chemistry, which consists of Trotterization and quantum phase estimation. We compare the experimental performance of these approaches to show clear evidence that the variational quantum eigensolver is robust to certain errors. This error tolerance inspires hope that variational quantum simulations of classically intractable molecules may be viable in the near future.





Hydrogen molecule

- Ansatz: Unitarily coupled cluster (UCC)
- We define the ansatz as

$$|\varphi(\theta)\rangle = e^{-i\theta X_0 Y_1}|01\rangle = \cos\theta|01\rangle - \sin\theta|10\rangle$$

where X_0 and Y_1 are Pauli operators on qubits 0 and 1, respectively, by following the reference presented on the right side.

- Thus, including the ancilla qubit, we have

$$|\psi(\theta)\rangle \equiv \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes (\cos\theta|01\rangle - \sin\theta|10\rangle)$$

PHYSICAL REVIEW X 6, 031007 (2016)

Scalable Quantum Simulation of Molecular Energies

P. J. J. O'Malley,[1,*] R. Babbush,[2,†] I. D. Kivlichan,[3] J. Romero,[3] J. R. McClean,[4] R. Barends,[5] J. Kelly,[5] P. Roushan,[5] A. Tranter,[6,7] N. Ding,[2] B. Campbell,[1] Y. Chen,[5] Z. Chen,[1] B. Chiaro,[1] A. Dunsworth,[1] A. G. Fowler,[5] E. Jeffrey,[5] E. Lucero,[5] A. Megrant,[5] J. Y. Mutus,[5] M. Neeley,[5] C. Neill,[1] C. Quintana,[1] D. Sank,[5] A. Vainsencher,[1] J. Wenner,[1] T. C. White,[5] P. V. Coveney,[7] P. J. Love,[6] H. Neven,[2] A. Aspuru-Guzik,[3] and J. M. Martinis[5,1,‡]

We can express the mapping $U(\vec{\theta})$ as a concatenation of parametrized quantum gates, $U_1(\theta_1)U_2(\theta_2)\ldots U_n(\theta_n)$. In this work, we parametrize our circuit according to unitary coupled cluster theory [20,22,23]. As described in Appendix D, unitary coupled cluster theory predicts that the ground state of Eq. (1) can be expressed as

$$|\varphi(\theta)\rangle = e^{-i\theta X_0 Y_1}|01\rangle, \qquad (3)$$

where $|\phi\rangle = |01\rangle$ is the Hartree-Fock (mean-field) state of molecular hydrogen in the representation of Eq. (1). As discussed in Appendix D, unitary coupled cluster theory is widely believed to be classically intractable and is known to be strictly more powerful than the "gold standard" of classical electronic structure theory, coupled cluster theory [43–46]. The gate model circuit that performs this unitary mapping is shown in the software section of Fig. 1.

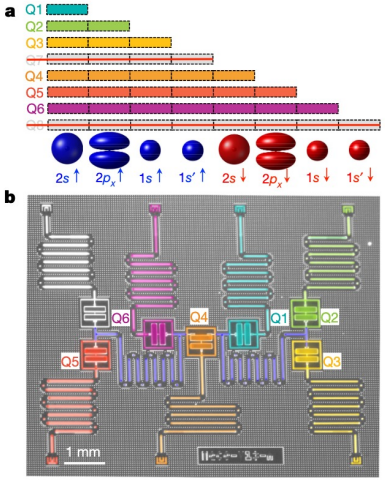
Variational Quantum Eigensolver (VQE)

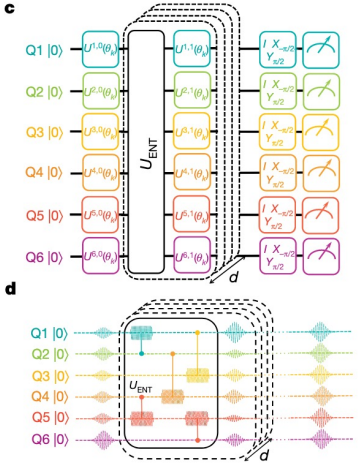
LETTER

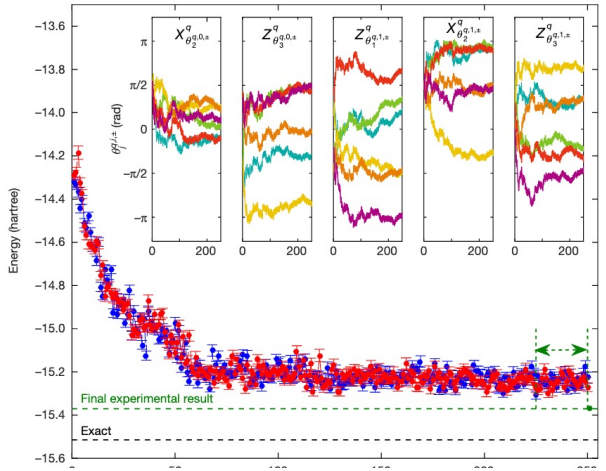
doi:10.1038/nature23879

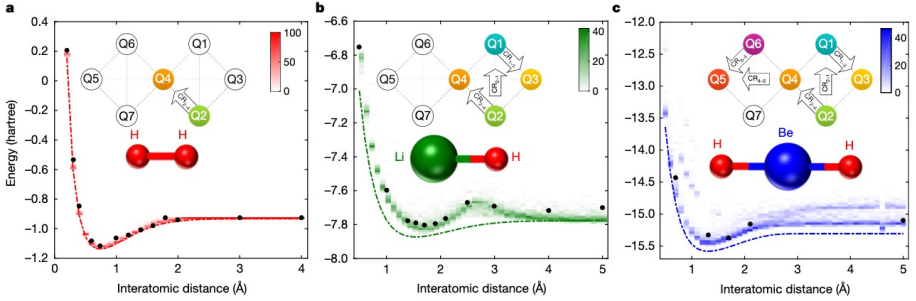
Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets

Abhinav Kandala[1]*, Antonio Mezzacapo[1]*, Kristan Temme[1], Maika Takita[1], Markus Brink[1], Jerry M. Chow[1] & Jay M. Gambetta[1]



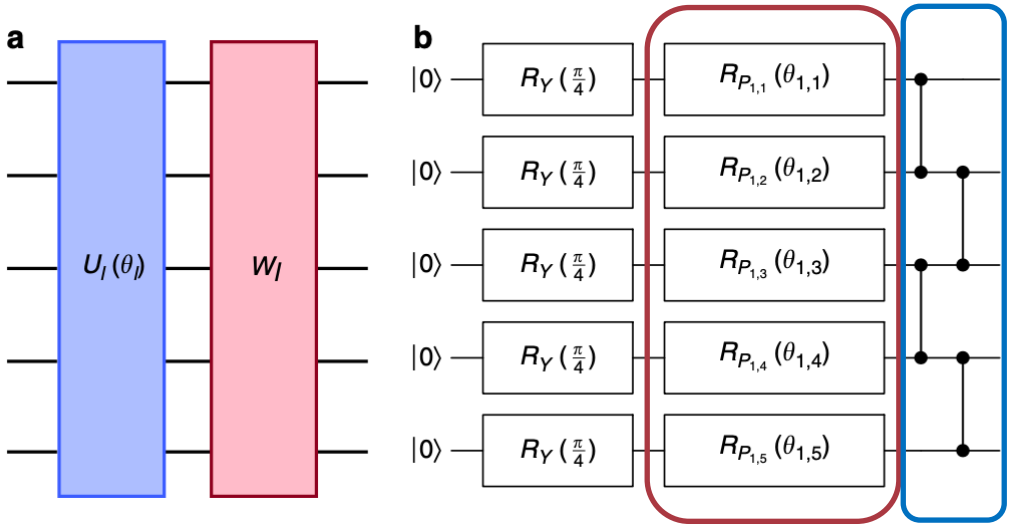






Variational Quantum Eigensolver (VQE)

- Ansatz
  - Hardware efficient

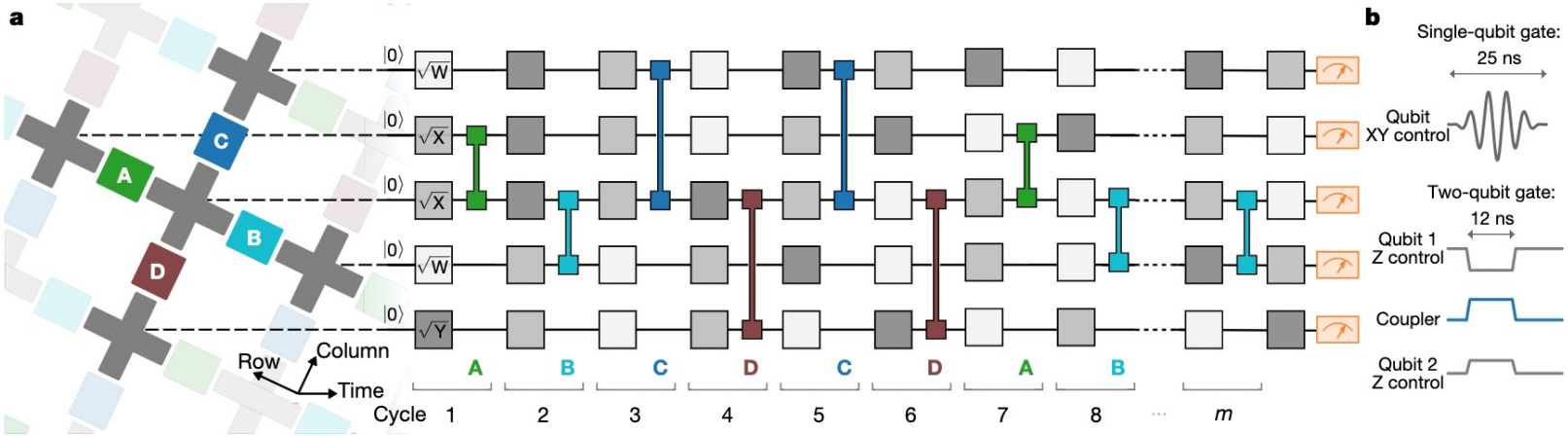


Randomly chosen Pauli rotations

1D ladder of Controlled Z gate

Variational Quantum Eigensolver (VQE)

- Ansatz
  - Hardware efficient



Variational Quantum Eigensolver (VQE)

Reference	Year	Max # qubits	Systems	Platform	Methods
Peruzzo et al.[20]	2013	2	HeH^+	Silicon Photonic	VQE-UCC
Shen et al.[29]	2015	2	HeH^+	Trapped ion	VQE-UCC
Google[21]	2015	2	H_2	Superconducting	VQE-UCC
Santagati et al.[30]	2016	2	H_2, H_3, H_3^+, H_4	Silicon photonic	IPEA, VQE-UCC
IBM[3]	2017	6	H_2, LiH, BeH_2, Heisenberg model	Superconducting	Hardware-efficient VQE
Berkeley[22]	2017	2	H_2 (excited states)	Superconducting	Hardware-specific VQE
Hempel et al.[31]	2018	3	H_2, LiH	Trapped-ion	VQE-UCC
IBM[32]	2018	4	Quantum magnetism H_2, LiH	Superconducting	Hardware-efficient VQE
OTI Lumionics[23]	2018	4	H_2, LiH	Superconducting	Qubit CC
Li et al.[33]	2019	2	H_2O	NMR	QPE
IonQ/JQI[34]	2019	4	H_2O	Trapped-ion	VQE-UCC
Oak Ridge[35]	2019	4	NaH, RbH, KH	Superconducting	Hardware-efficient VQE(-UCC)
Mitsubishi/IBM[36]	2019	2	Lithium superoxide dimer	Superconducting	VQE-UCC
Smart & Mazziotti[37]	2019	3	H_3	Superconducting	VQE-UCC
Google[19]	2020	12	H_6, H_8, H_{10}, H_{12} HNNH	Superconducting	VQE-HF
IBM[38]	2020	2	PSPCz, 2F-PSPCz, 4F-PSPCz	Superconducting	qEOM-VQE VQD

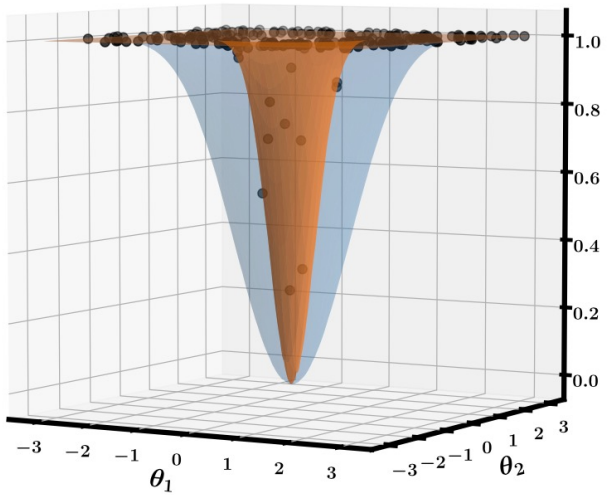
arXiv:2009.12472v1, V. E. Elfving et al

Barren plateaus

- Barren Plateaus
  - The magnitude of its partial derivatives is, on average, exponentially vanishing with the system size.

$$|\frac{\partial C(\theta)}{\partial \theta}| \sim O(e^{-d})$$

- ‘One needs an exponentially large precision to resolve against finite sampling noise and determine a cost-minimizing direction, with this being valid independently of using a gradient-based or gradient-free optimization method.’



[arXiv:2001.00550]

Barren plateaus (불모의 고원)

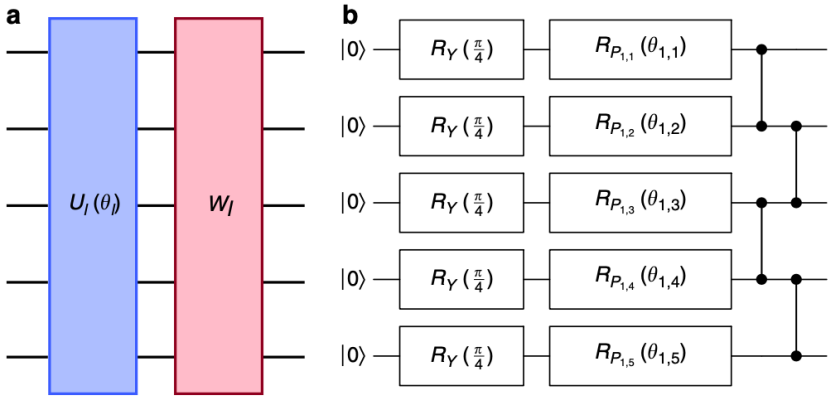
nature COMMUNICATIONS

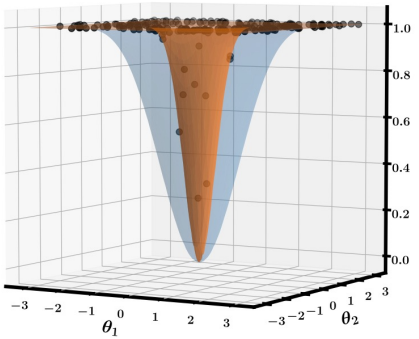
ARTICLE

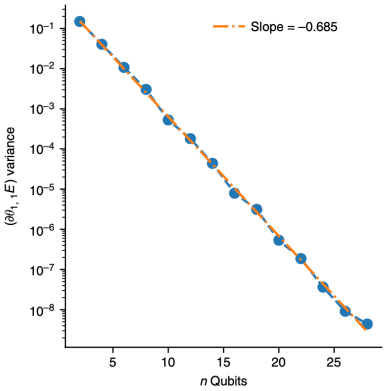
DOI: 10.1038/s41467-018-07090-4 OPEN

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]







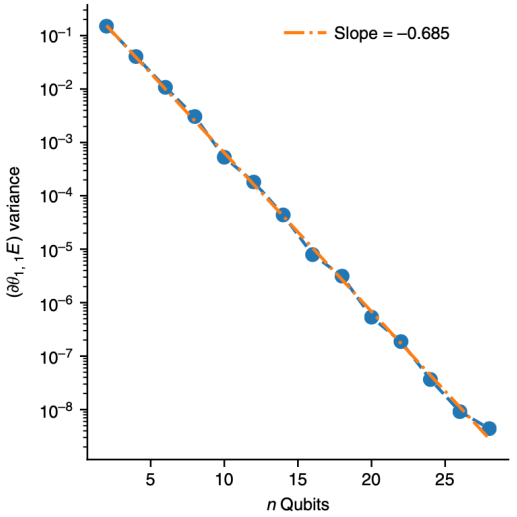
Barren plateaus

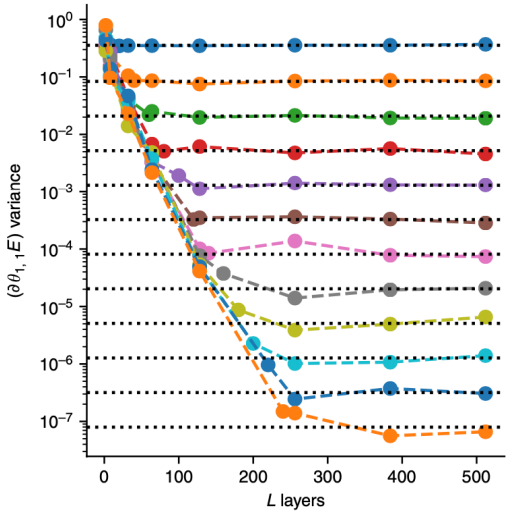
- Exponential decay of variance
  - The objective operator (e.g. Hamiltonian)

$$H = Z_1 Z_2$$

- ‘As complex objectives can be written as sums of these operators, the results for large objectives can be inferred from these numbers.’

- ‘Moreover, it is clear that for any polynomial sum of these operators, the exponential decay of the signal in the gradient will not be circumvented.’





Barren plateaus (불모의 고원)

nature COMMUNICATIONS

Noise-induced barren plateaus in variational quantum algorithms

Samson Wang[1,2✉], Enrico Fontana[1,3,4], M. Cerezo[1,5✉], Kunal Sharma[1,6,7], Akira Sone[1,5,8], Lukasz Cincio[1] & Patrick J. Coles[1✉]

Variational Quantum Algorithms (VQAs) may be a path to quantum advantage on Noisy Intermediate-Scale Quantum (NISQ) computers. A natural question is whether noise on NISQ devices places fundamental limitations on VQA performance. We rigorously prove a serious limitation for noisy VQAs, in that the noise causes the training landscape to have a barren plateau (i.e., vanishing gradient). Specifically, for the local Pauli noise considered, we prove that the gradient vanishes exponentially in the number of qubits n if the depth of the ansatz grows linearly with n. These noise-induced barren plateaus (NIBPs) are conceptually different from noise-free barren plateaus, which are linked to random parameter initialization. Our result is formulated for a generic ansatz that includes as special cases the Quantum Alternating Operator Ansatz and the Unitary Coupled Cluster Ansatz, among others. For the former, our numerical heuristics demonstrate the NIBP phenomenon for a realistic hardware noise model.

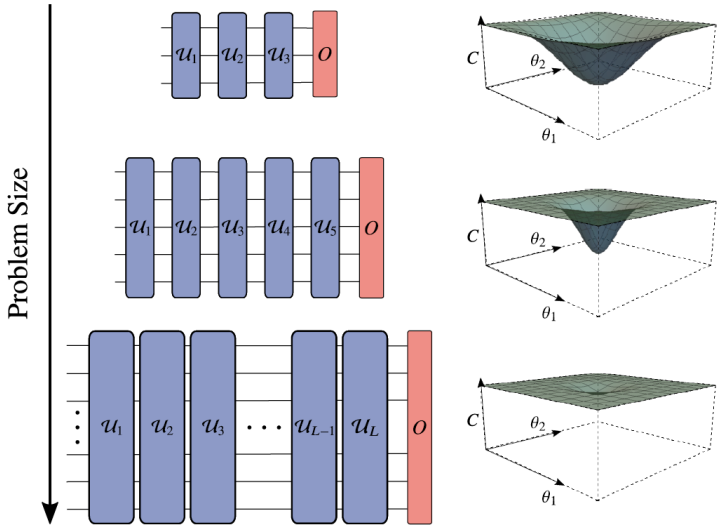


FIG. 1. **Schematic diagram of the Noise-Induced Barren Plateau (NIBP) phenomenon.** For various appli-

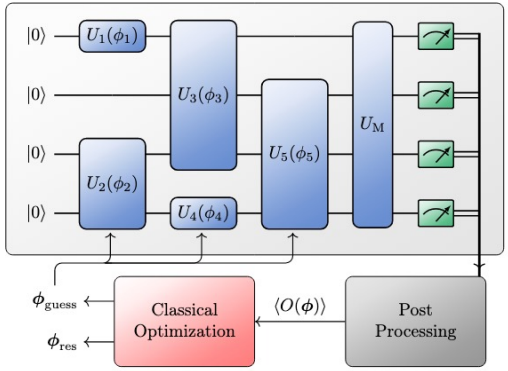
Barren plateaus (불모의 고원)

Editors' Suggestion

PHYSICAL REVIEW LETTERS **127,** 120502 (2021)

Training Variational Quantum Algorithms Is NP-Hard

Variational quantum algorithms are proposed to solve relevant computational problems on near term quantum devices. Popular versions are variational quantum eigensolvers and quantum approximate optimization algorithms that solve ground state problems from quantum chemistry and binary optimization problems, respectively. They are based on the idea of using a classical computer to train a parametrized quantum circuit. We show that the corresponding classical optimization problems are NP-hard. Moreover,



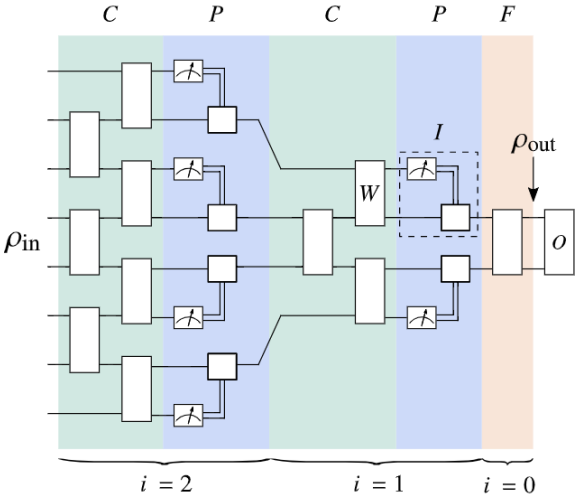
Barren plateaus (불모의 고원)

PHYSICAL REVIEW X **11,** 041011 (2021)

Absence of Barren Plateaus in Quantum Convolutional Neural Networks

Arthur Pesah,[1,2] M. Cerezo,[1,3] Samson Wang,[1,4] Tyler Volkoff,[1] Andrew T. Sornborger,[5] and Patrick J. Coles[1]

Quantum neural networks (QNNs) have generated excitement around the possibility of efficiently analyzing quantum data. But this excitement has been tempered by the existence of exponentially vanishing gradients, known as barren plateau landscapes, for many QNN architectures. Recently, quantum convolutional neural networks (QCNNs) have been proposed, involving a sequence of convolutional and pooling layers that reduce the number of qubits while preserving information about relevant data features. In this work, we rigorously analyze the gradient scaling for the parameters in the QCNN architecture. We find that the variance of the gradient vanishes no faster than polynomially, implying that QCNNs do not exhibit barren plateaus. This result provides an analytical guarantee for the trainability of randomly initialized QCNNs, which highlights QCNNs as being trainable under random initialization unlike many other QNN architectures. To derive our results, we introduce a novel graph-based method to analyze expectation values over Haar-distributed unitaries, which will likely be useful in other contexts. Finally, we perform numerical simulations to verify our analytical results.



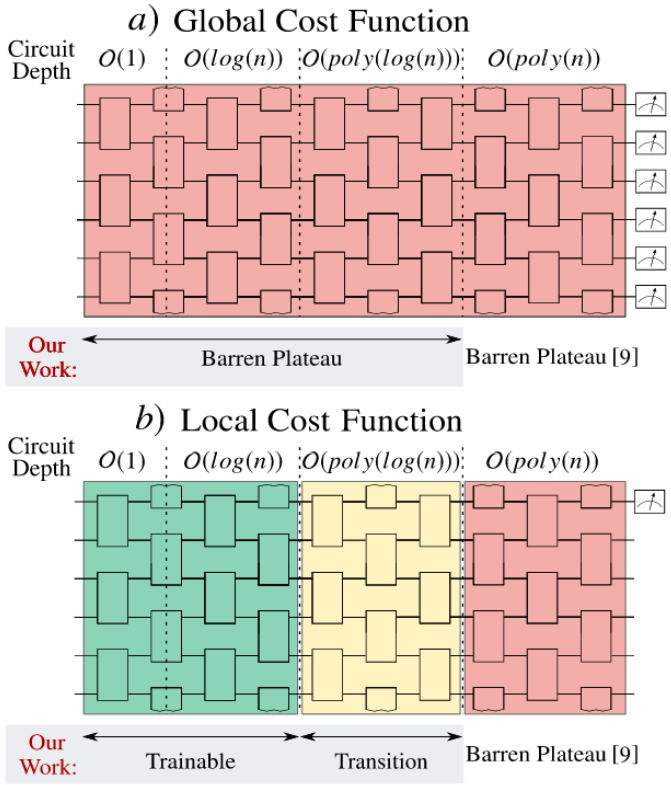
Barren plateaus (불모의 고원)

nature COMMUNICATIONS

Cost function dependent barren plateaus in shallow parametrized quantum circuits

M. Cerezo[1,2✉], Akira Sone[1,2], Tyler Volkoff[1], Lukasz Cincio[1] & Patrick J. Coles[1✉]

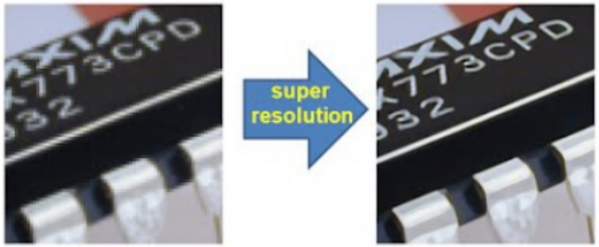
layered ansatz composed of blocks forming local 2-designs. Our first result states that defining C in terms of global observables leads to exponentially vanishing gradients (i.e., barren plateaus) even when $V(\boldsymbol{\theta})$ is shallow. Hence, several VQAs in the literature must revise their proposed costs. On the other hand, our second result states that defining C with local observables leads to at worst a polynomially vanishing gradient, so long as the depth of $V(\boldsymbol{\theta})$ is $\mathcal{O}(\log n)$. Our results establish a connection between locality and trainability.



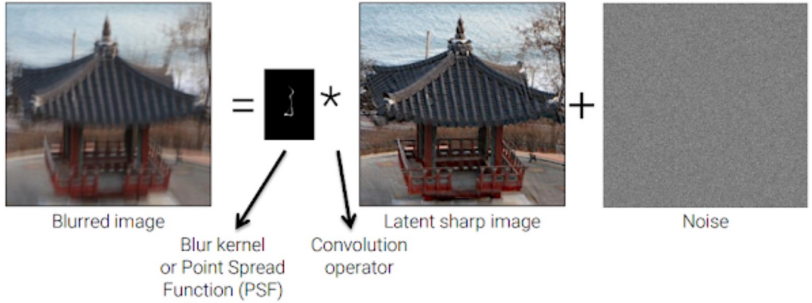
Error mitigation

Error mitigation

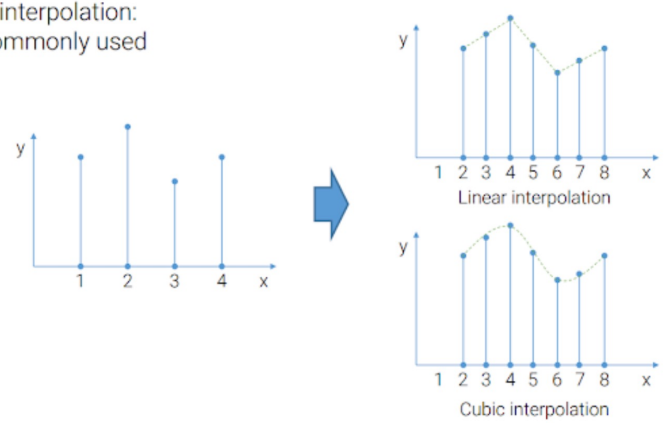
- **Super-resolution**



- **Deblurring**

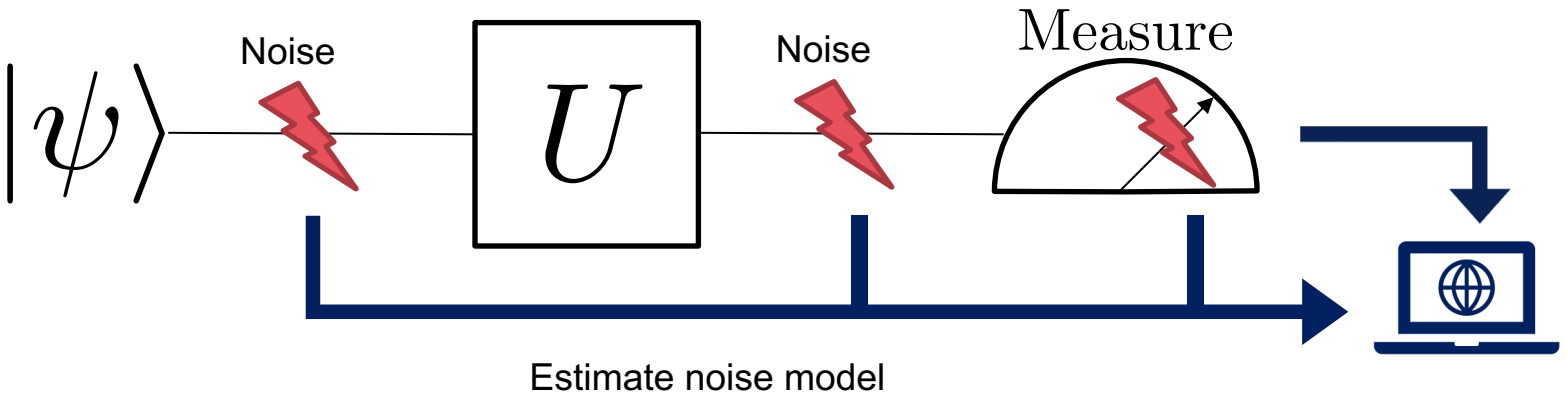


Bicubic interpolation:
most commonly used

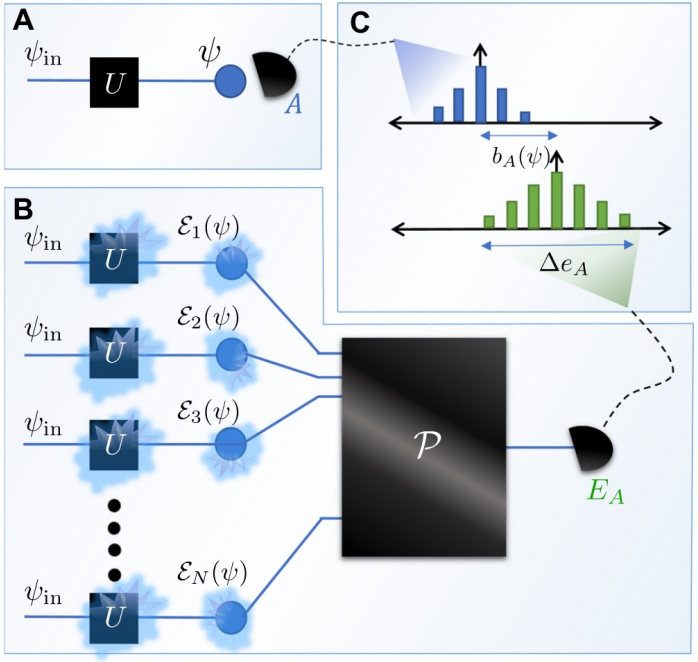


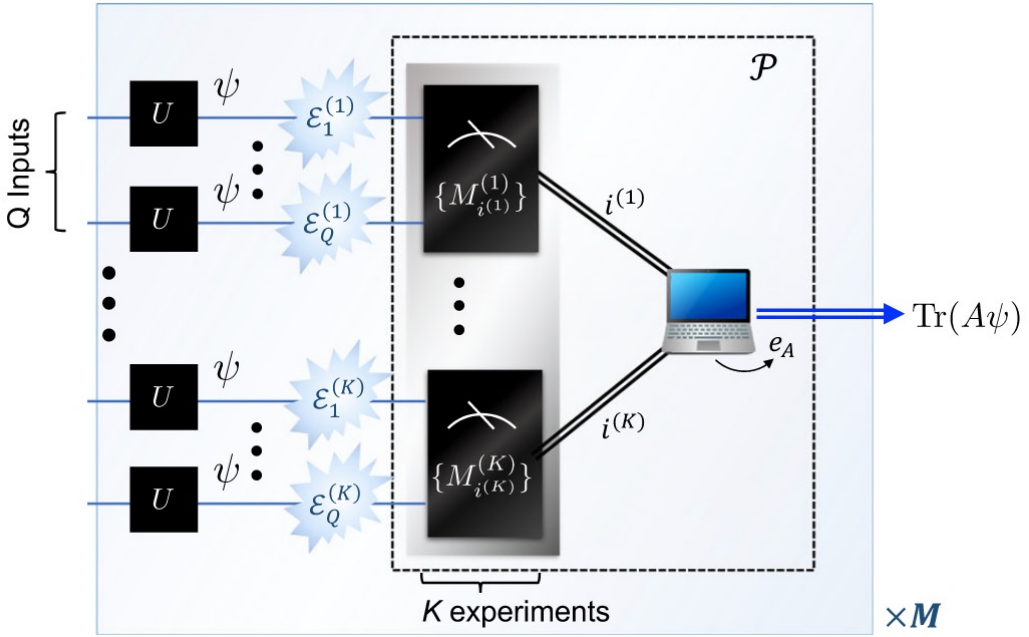
Error mitigation

- **Error mitigation algorithms** suppress errors by **sampling available noisy devices many times** and **classically post-processing these measurement outcomes**. Such techniques generally have drastically reduced technological requirements, providing potential near-term solutions for suppressing errors in other NISQ algorithms (e.g., variational algorithms for estimating the ground state energy in quantum chemistry).



Error mitigation





Takagi, R., Endo, S., Minagawa, S. & Gu, M. Fundamental limits of quantum error mitigation. *Npj Quantum Information* **8**, 114 (2022).

Error mitigation

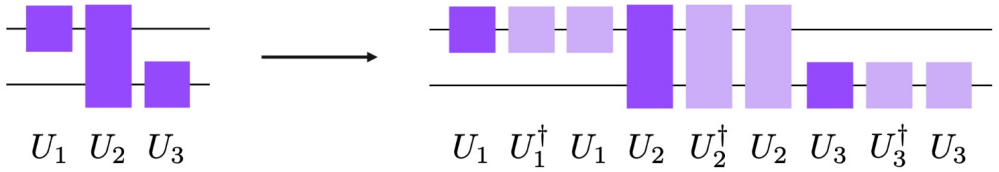
Goal: Mitigate the effects of **gate errors** in expectation value computations

Steps:

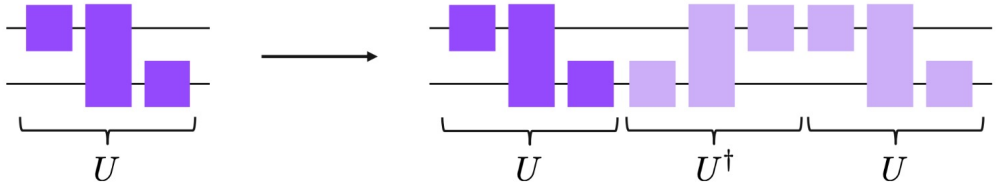
1. Amplify the noise introduced by the gates of the circuit

2. Extrapolate the noisy expectation values to the zero-noise limit

Local folding – repeatedly folding the **gates** inside the circuit



Global folding – repeatedly folding the whole **circuit**



Error mitigation

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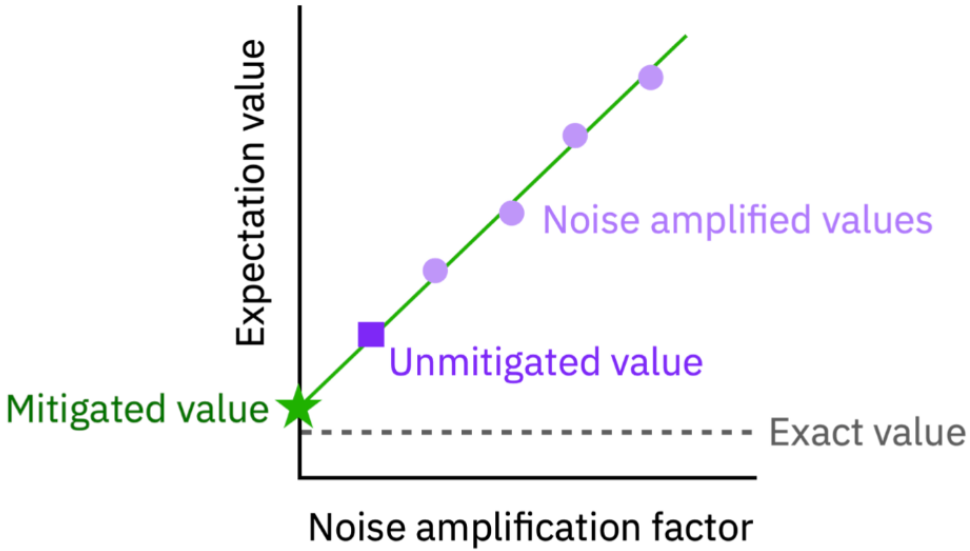

감사합니다.