Variational Quantum Algorithms

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구성

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03 VQE / QAOA

04 Challenges for VQAs

Motivation

- **Why quantum algorithms?**
- Why VQAs? - NISQ Era

Motivation

Quantum Algorithms

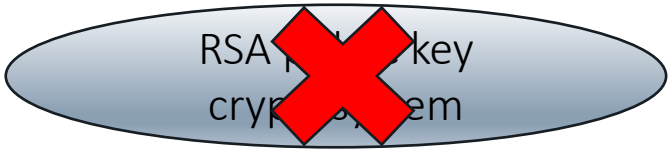
Why quantum algorithms?

- Quantum computer can theoretically solve some problems **much faster** than classical computers.

✓ Shor's factoring algorithm

✓ Grover's search algorithm

✓ Physics and chemistry simulations



[P. Shor, Polynomial-Time Algorithms for Prime Factorization and Discrete Logarithms on a Quantum Computer, SIAM J.Sci.Statist.Comput. 26 (1997)

Motivation

Quantum Algorithms

RSA Public key crypotsystem

- R.Rivest, A.Shamir, L.Adleman (1977)
- 국제표준 공개키 암호
- 소인수분해 문제 어려움에 기반

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Softforum Application Root Authority

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루트 인증 기관
사용 만료: 2035년 5월 2일 수요일 오후 4시 10분 35초 대한민국 표준시
이 인증서는 모든 사용자에 대해 신뢰된 것으로 표시됩니다

신뢰

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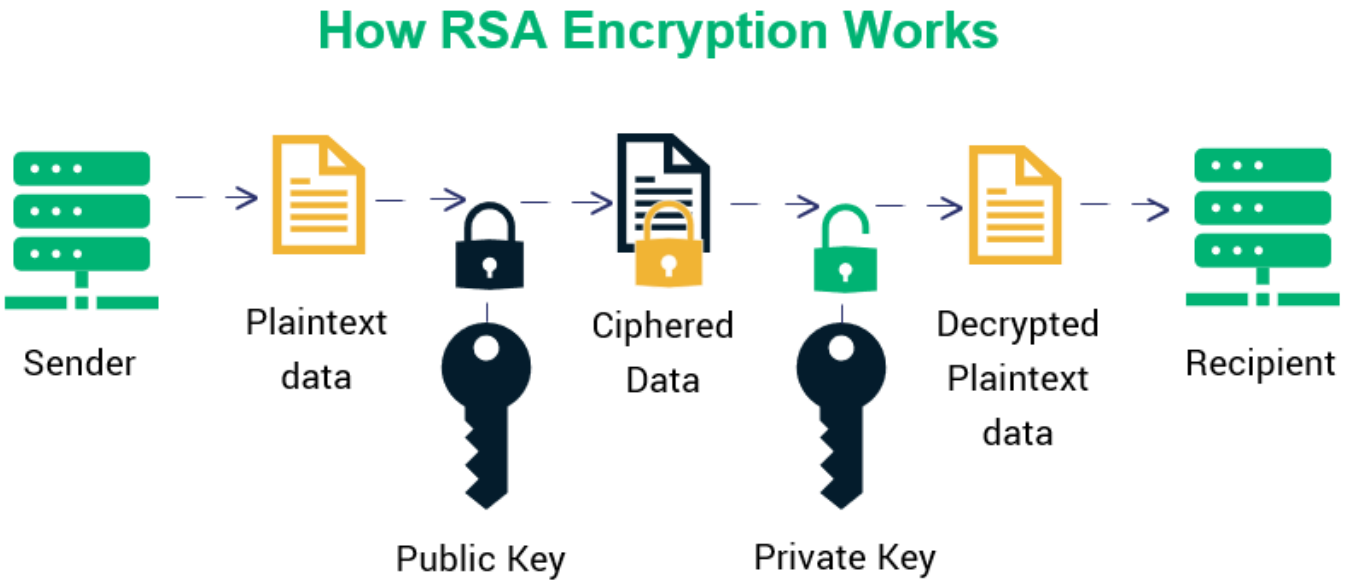
일련 번호	7
버전	3
서명 알고리즘	SHA-1(RSA 암호화)(1.2.840.113549.1.1.5)
매개변수	없음
다음 전에 유효하지 않음	2015년 5월 7일 목요일 오후 4시 10분 35초 대한민국 표준시
다음 후에 유효하지 않음	2035년 5월 2일 수요일 오후 4시 10분 35초 대한민국 표준시
공개 키 정보	
알고리즘	RSA 암호화(1.2.840.113549.1.1.1)
매개변수	없음
공개 키	256바이트 : 8F FB 64 1D 76 A5 D3 27 ...
지수	65537
키 크기	2,048비트
키 사용	확인

y crypotsystem

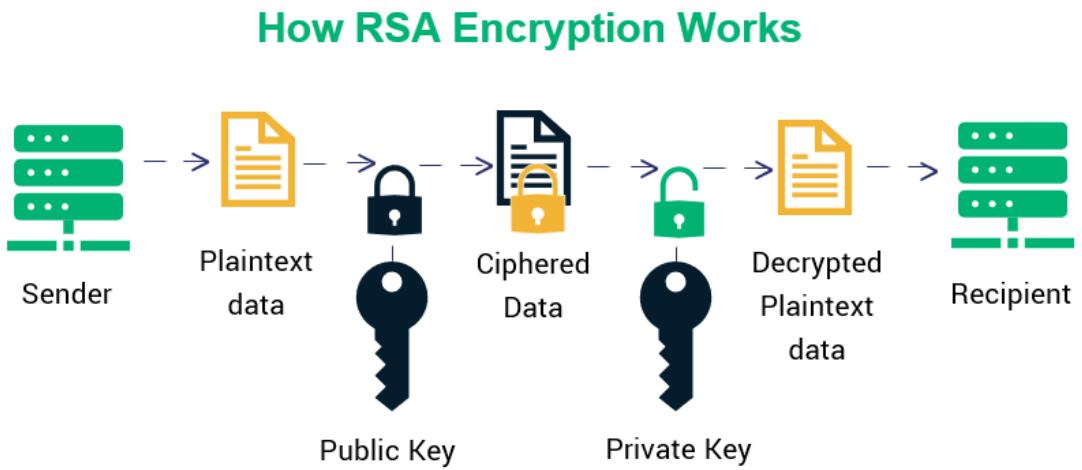
Motivation

Quantum Algorithms



Motivation

Quantum Algorithms



- 10848155538425511429005207944498062456168244306249886906809764553107935080834330292843201597849730250171094340013101876851402167330796759352537531560876539 = ??

  = 11139909967639021566931686256732036762547951767093648380471964452732067847263 7

  X 97380998319905235259677664165188969731382036683146715898427716312842129869847

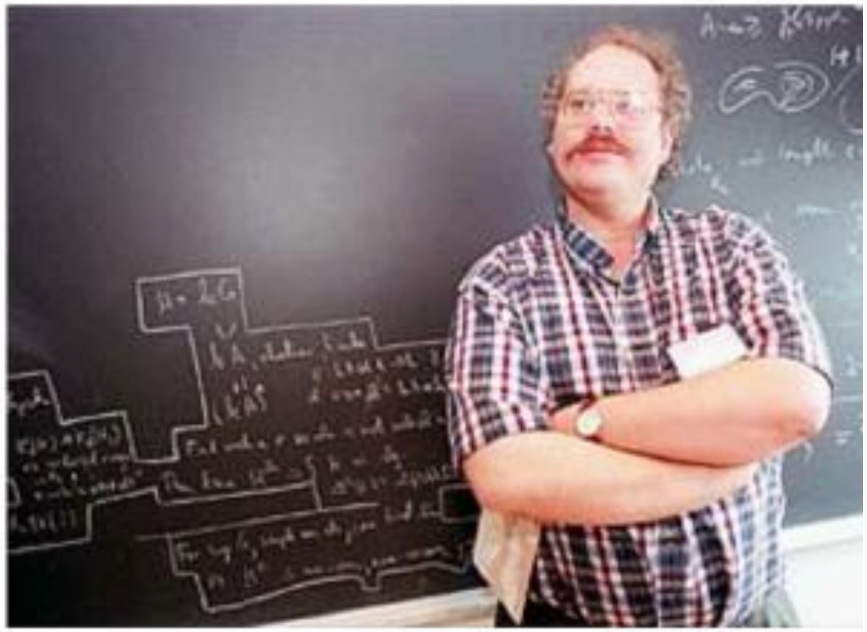
Motivation

Quantum Algorithms

Shor's factoring algorithm

- ✓ Peter Shor (1994)
- ✓ Quantum Algorithm to factor an integer N

- ✓ Classical: $O(e^{1.9(logN)^{1/3}(loglogN)^{2/3}})$
- ✓ Quantum: $O((logN)^2 loglogN)$



Motivation

Quantum Algorithms

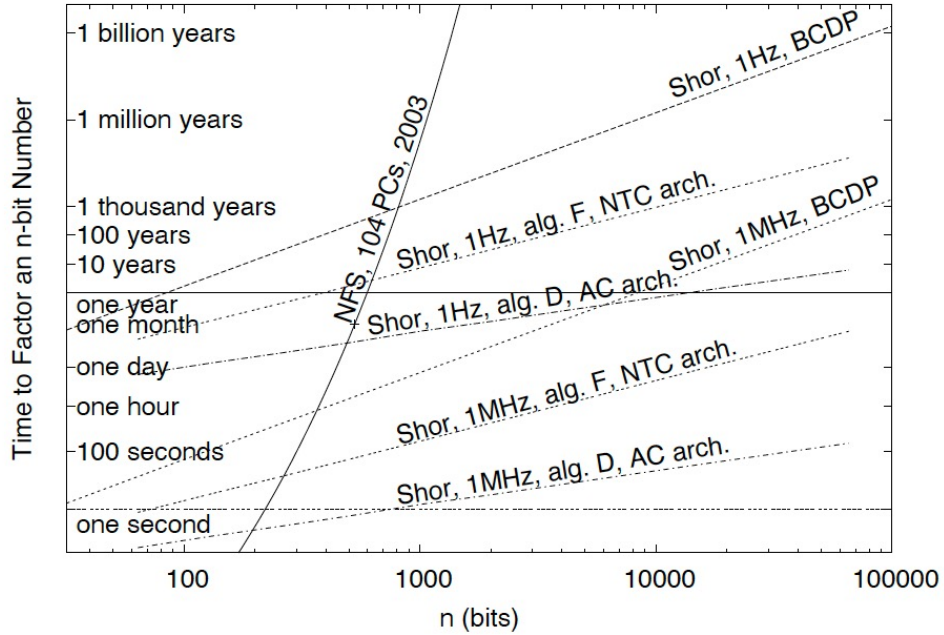


Figure 2. Scaling of number field sieve (NFS) and Shor's algorithms for factoring, using faster modular exponentiation algorithms.

[Van Meter et al., Architecture-Dependent Execution Time of Shor's Algorithm, Controllable Quantum States, pp.183-188 (2008)

Motivation

Quantum Algorithms

Shor's algorithm: complexity comparison

Very roughly (ignoring constant factors!):

Number of digits	Timesteps (quantum)	Timesteps (classical)
100	10^6	$\sim 4 \times 10^5$
1000	10^9	$\sim 5 \times 10^{15}$
10000	10^{12}	$\sim 1 \times 10^{41}$

Based on these figures, a 10000-digit number could be factorized by:

Motivation

Quantum Algorithms

Shor's algorithm: complexity comparison

- A quantum computer with a clock speed of 1MHz in 11 days.
- The fastest computer on the Top500 supercomputer list (~9.3 x 10^{16} operations per second) in ~3.4 x 10^{16} years.

(see e.g. [Van Meter et al '08] for a more detailed comparison)

[Van Meter et al., Architecture-Dependent Execution Time of Shor's Algorithm, Controllable Quantum States, pp.183-188 (2008)

When can this happen?

Motivation

Quantum Algorithms

Resources for Shor's factoring algorithm

- ✓ ≈ 5,000 qubits to factor cryptographically significant numbers (without error correction)
- ✓ ≈ 1,000,000 qubits with error correction
- ✓ ≈ 100,000,000 quantum gates

[C. Gidney and M. Ekerå, How to factor 2048 bit RSA integers in 8 hours using 20 million noisy qubits, Quantum 5, 433 (2021)

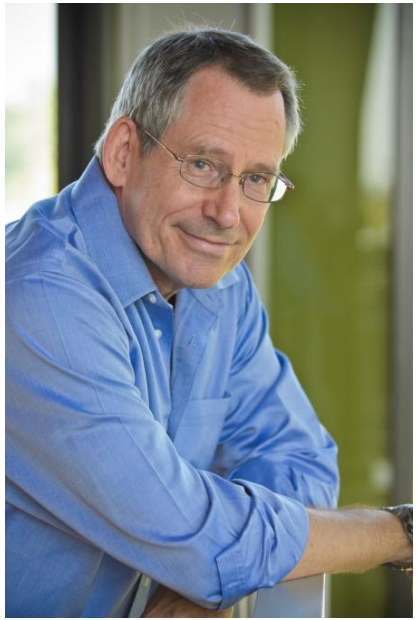
Motivation

- Why quantum algorithms?
- **Why VQAs? - NISQ Era**

Motivation

NISQ Era

NISQ (Noisy Intermediate-Scale Quantum) Era



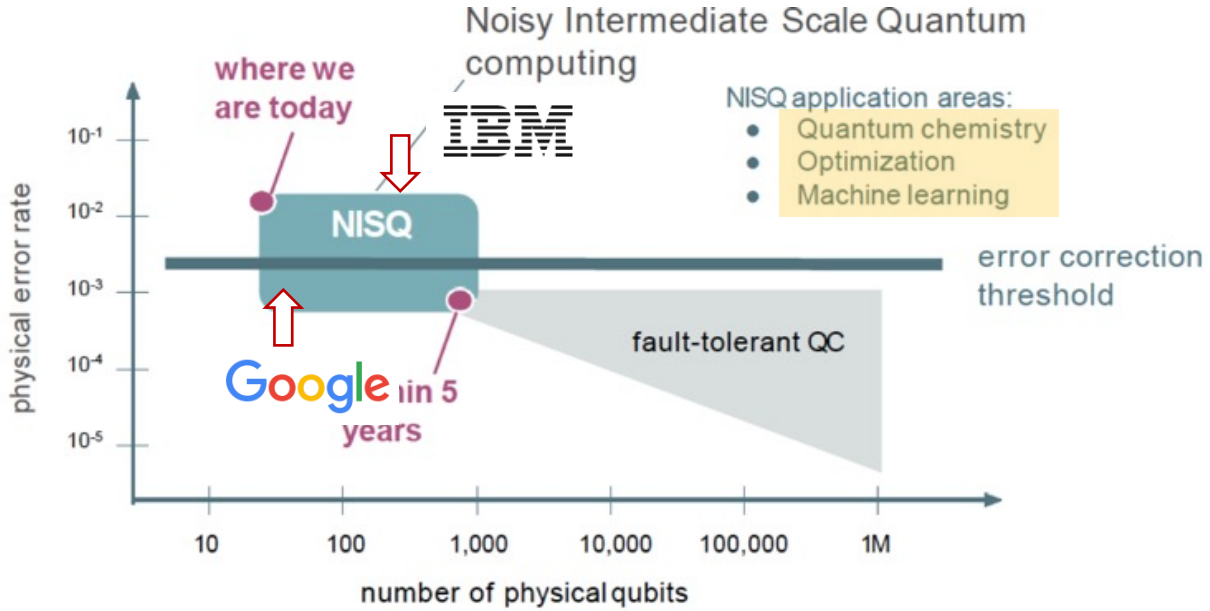
NISQ technology will be available in the near future. Quantum computers with **50-100** qubits may be able to perform tasks which surpass the capabilities of today's classical digital computers, but **noise in quantum gates** will limit the size of quantum circuits that can be executed reliably.

[J. Preskill, Quantum Computing in the NISQ era and beyond, Quantum 2, 79 (2018)]

Motivation

NISQ Era

NISQ (Noisy Intermediate-Scale Quantum) Era



[J. Preskill, Quantum Computing in the NISQ era and beyond, Quantum 2, 79 (2018)]

Motivation

Near-Term Quantum Algorithms

Near-Term Quantum Algorithms

- ✓ Algorithms run on small quantum computers
- ✓ Algorithms solve useful problems
- ✓ Low-depth, Robust to errors
- ✓ Efficient use of qubits
  - It needs enough qubits to store the problem

For example, VQE (Variational Quantum Eigensolver) or

QAOA (Quantum Approximate Optimization Algorithm)

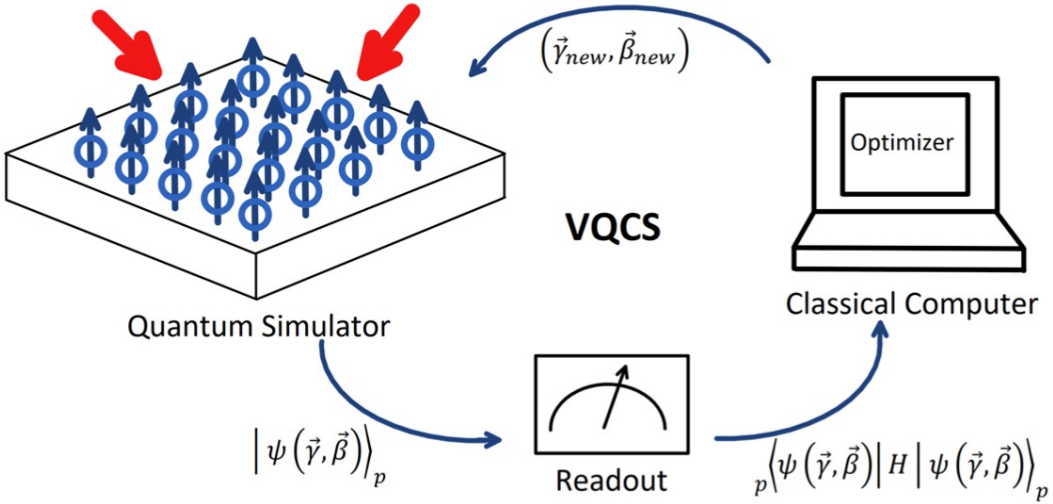
Variational Quantum Algorithms

- **What is VQAs?**
- VQE and QAOA

Variational Quantum Algorithms

What is VQAs?

Variational Quantum-Classical Simulations

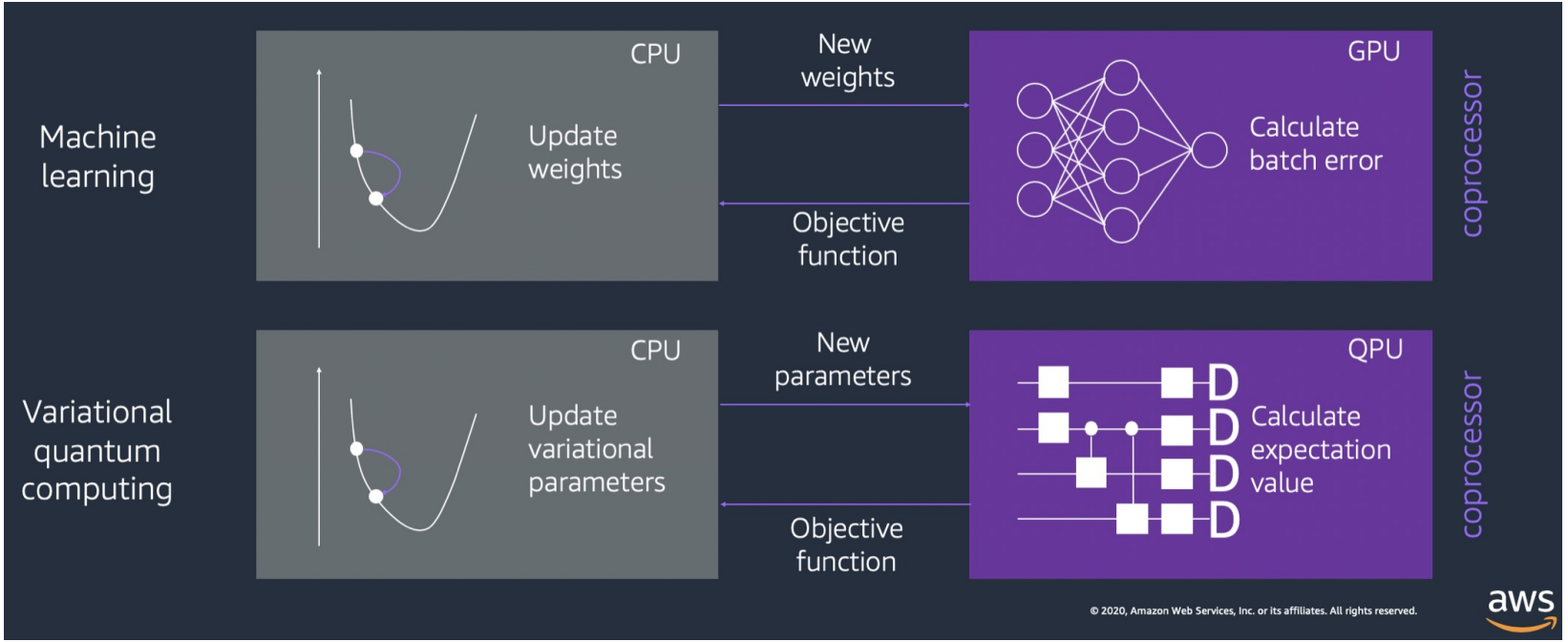


[W.W. Ho and T.H. Hsieh, Efficient variational simulation of non-trivial quantum states, SciPost Phys. 6, 029 (2019)]

Variational Quantum Algorithms

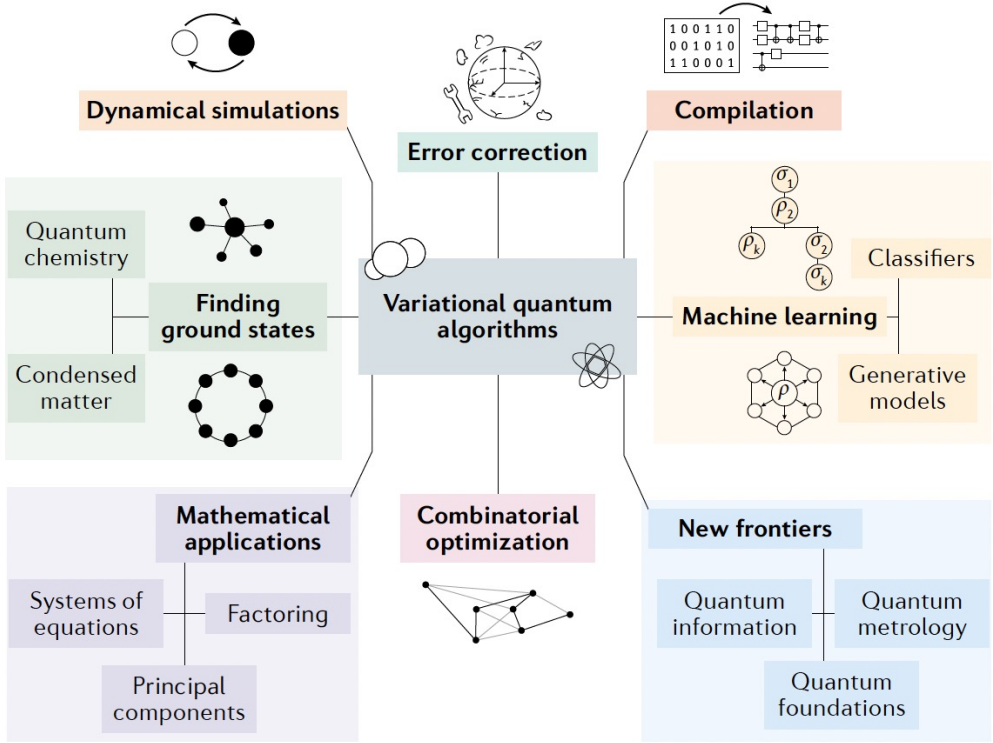
What is VQAs?

Variational Quantum-Classical Simulations



Variational Quantum Algorithms

What is VQAs?



[M. Cerezo et al., Variational quantum algorithms,, Nature Reviews Physics **3**, pages 625–644 (2021)]

Variational Quantum Algorithms

- What is VQAs?
- **VQE** and QAOA

Variational Quantum Eigensolver (VQE)

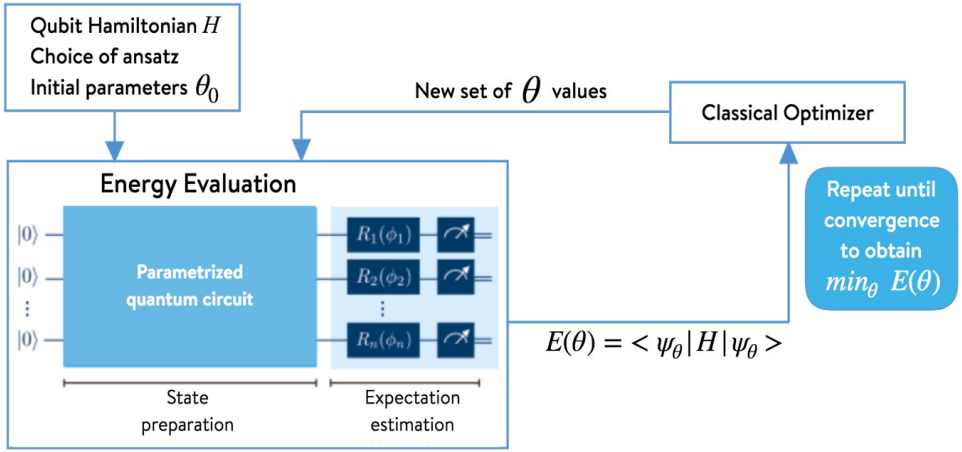
What is VQE?

- ✓ VQE is an approach to find the ground state of a quantum Hamiltonian H
- ✓ Based on the variational principle of quantum mechanics:

  For all state $|\psi\rangle$,

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

  where E_0 is the ground energy of H

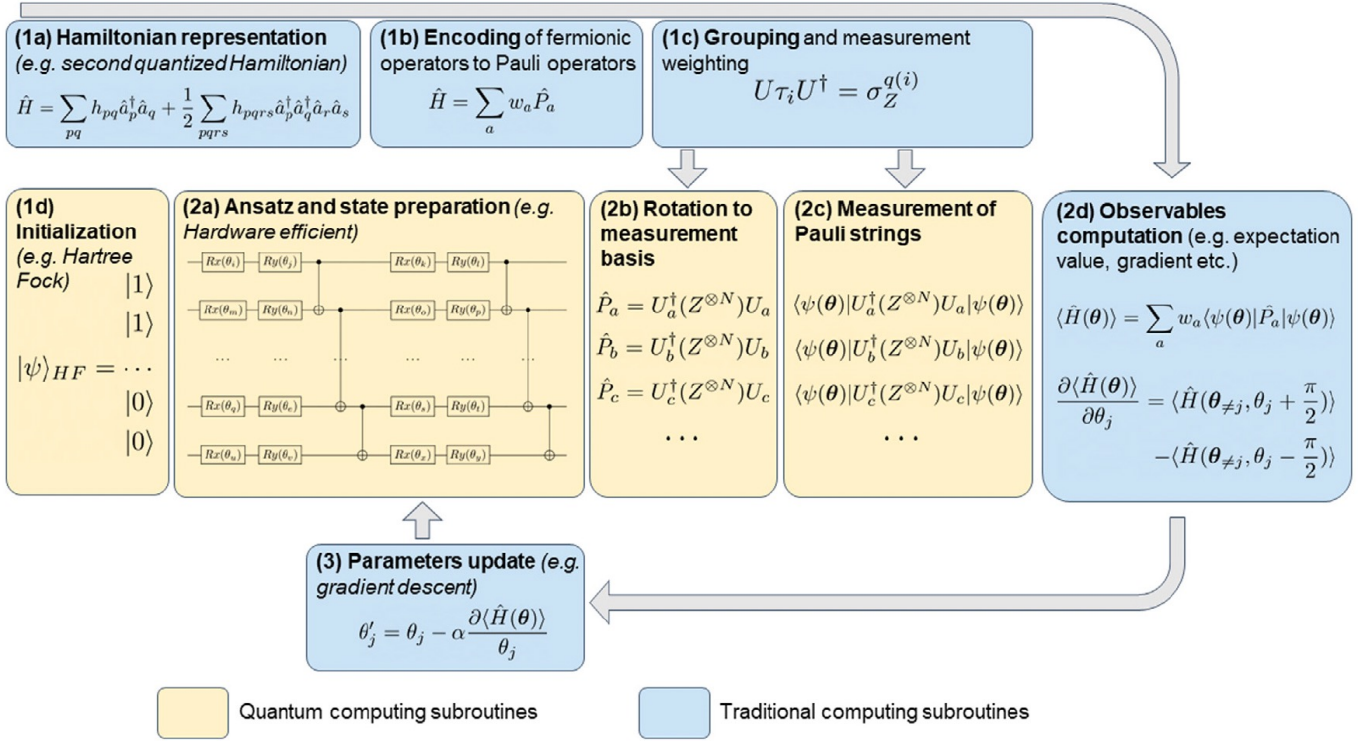


http://openqemist.1qbit.com/docs/_images/VQE_overview.png

[A. Peruzzo et al., A variational eigenvalue solver on a photonic quantum processor, Nature. Communications 5, (2014)]

Variational Quantum Eigensolver (VQE)

What is VQE?



[J. Tilly et al., The Variational Quantum Eigensolver: A review of methods and best practices, Physics Reports **986** 1–128 (2022)]

Variational Quantum Eigensolver (VQE)

VQE leaves a lot of questions open

- ✓ Good **family of circuits** to optimize
  - Variational ansatze (Hardware-efficient ansatze, UCC ansatze), QAOA ansatze, ⋯
- ✓ Efficient methods to **measure** the energy $\langle\psi|H|\psi\rangle$
  - Unitary partitioning approach, ⋯
- ✓ Good **optimization** over the variational ansatze
  - Gradient/Coordinate descent (Parameter shift rule), ⋯
- ✓ Best way to represent H on the quantum computer in the first place

Quantum Hamiltonians

Variational Quantum Eigensolver (VQE)

Various families of quantum Hamiltonians

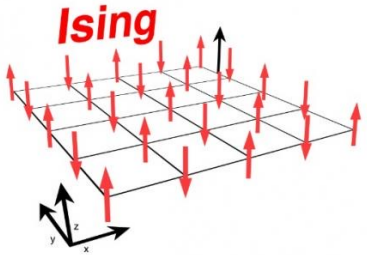
✓ **k-local Hamiltonians**: $H = \sum_i H_i$, and each H_i acts nontrivially on $\leq k$ qubits

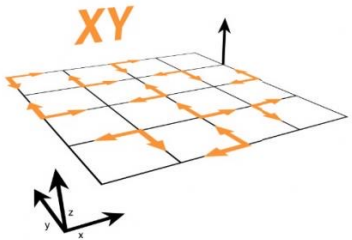
Eg) Ising model : $H = \sum_{\langle i,j \rangle} Z_i Z_j$,

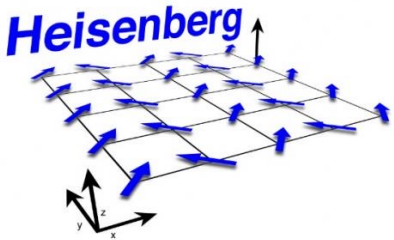
where $Z_i \equiv I \otimes \cdots \otimes Z \otimes \cdots \otimes I$ and $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

↑ i-th

Heisenberg model : $H = \sum_{\langle i,j \rangle} X_i X_j + Y_i Y_j + Z_i Z_j$

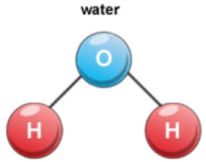


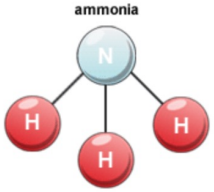


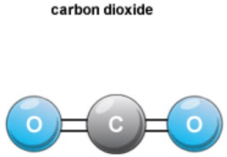


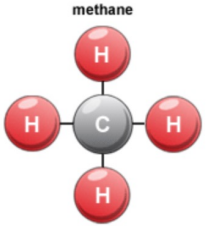
Variational Quantum Eigensolver (VQE)

Various families of quantum Hamiltonians







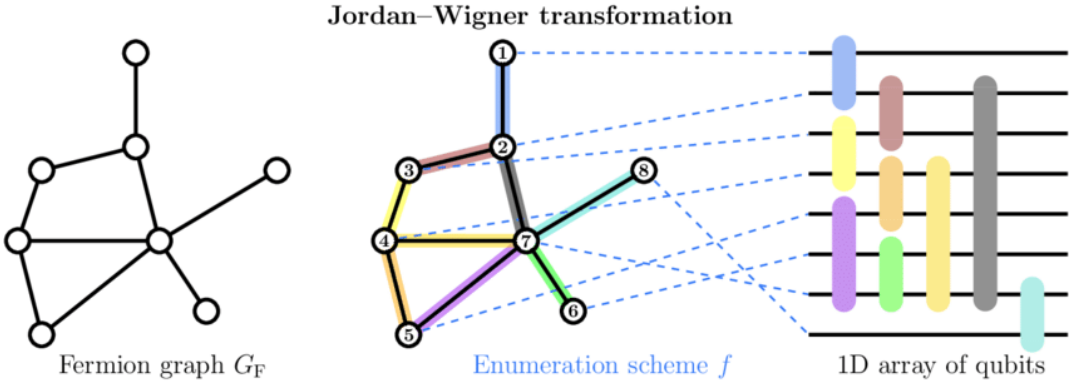


✓ **Fermionic Hamiltonians** (e.g. molecules):

$$H = \sum_{i,j} h_{ij} a_i^\dagger a_j + \sum_{i,j,k,l} h_{ijkl} a_i^\dagger a_j a_k^\dagger a_l$$

Here, $a_i^\dagger$ and a_i are fermionic creation and annihilation operators.

$$a_i^\dagger \mapsto Z_1 \otimes \cdots \otimes Z_{i-1} \otimes |1\rangle\langle 0| \quad a_i \mapsto Z_1 \otimes \cdots \otimes Z_{i-1} \otimes |0\rangle\langle 1|$$



Variational Ansatze

Physics Reports 986 (2022) 1–128

Contents lists available at ScienceDirect

Physics Reports

journal homepage: www.elsevier.com/locate/physrep

The Variational Quantum Eigensolver: A review of methods and best practices

Jules Tilly [a,b,*], Hongxiang Chen [b,c], Shuxiang Cao [b,d], Dario Picozzi [a,b], Kanav Setia [e], Ying Li [f], Edward Grant [b,c], Leonard Wossnig [b,c], Ivan Rungger [g], George H. Booth [h], Jonathan Tennyson [a]

[a] University College London, Department of Physics and Astronomy, WC1E 6BT London, United Kingdom
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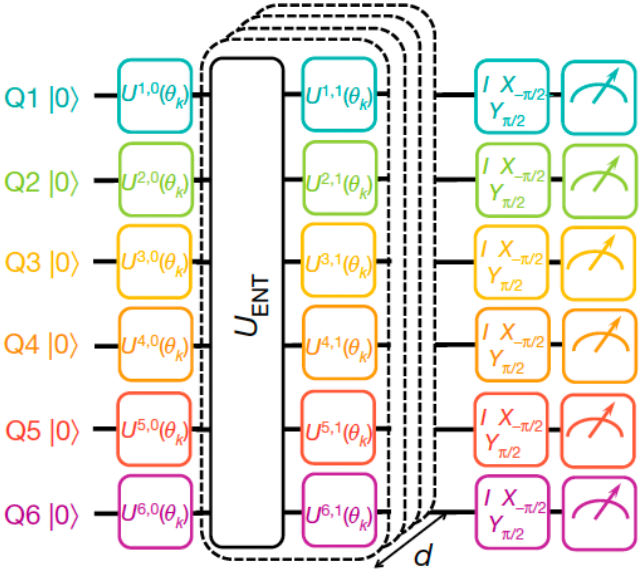
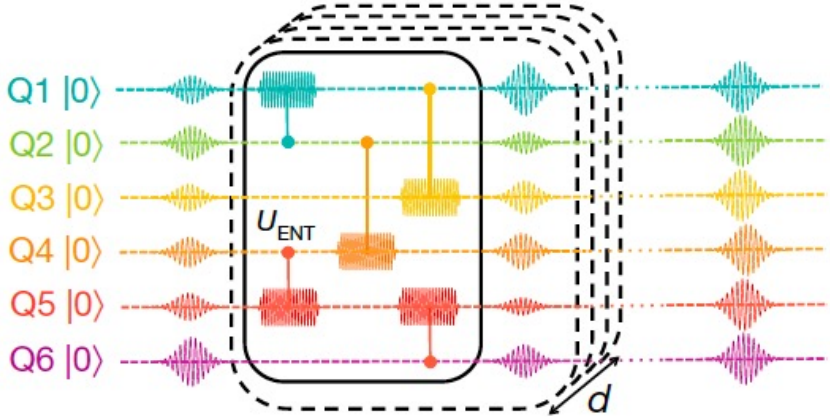
[e] qBraid, 5235, Harper Court, Chicago, IL, United States of America
[f] Graduate School of China Academy of Engineering Physics, Beijing 100193, China
[g] National Physical Laboratory, TW11 0LW Teddington, United Kingdom
[h] King's College London, Department of Physics, Strand, London, WC2R 2LS, United Kingdom

Variational Quantum Eigensolver (VQE)

What is a good family of circuits to optimize over?

✓ Hardware efficient ansatz:





[A. Kandala et al., Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets, Nature 549, pp 242–246 (2017)]

Variational Quantum Eigensolver (VQE)

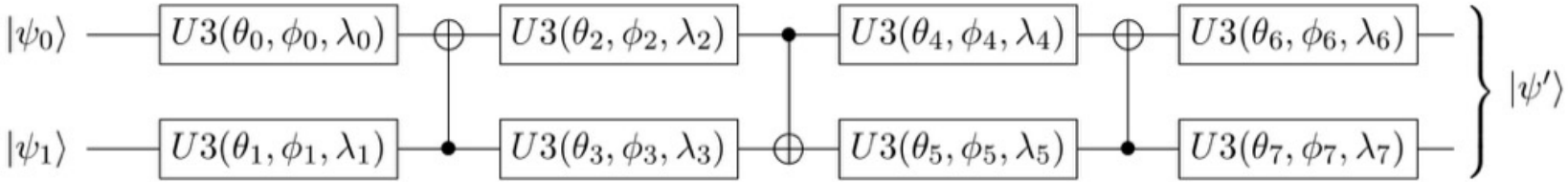
Hardware-efficient ansatze

- Single qubit transformation

$$U3(\theta,\phi,\lambda) = \begin{pmatrix} \cos(\frac{\theta}{2}) & -e^{i\lambda}\sin(\frac{\theta}{2}) \\ e^{i\phi}\sin(\frac{\theta}{2}) & e^{i\lambda+i\phi}\cos(\frac{\theta}{2}) \end{pmatrix}$$

$$|\psi\rangle \text{ —— } \boxed{U3(\theta,\phi,\lambda)} \text{ —— } U(\theta,\phi,\lambda)\,|\psi\rangle$$

- 2 qubit case

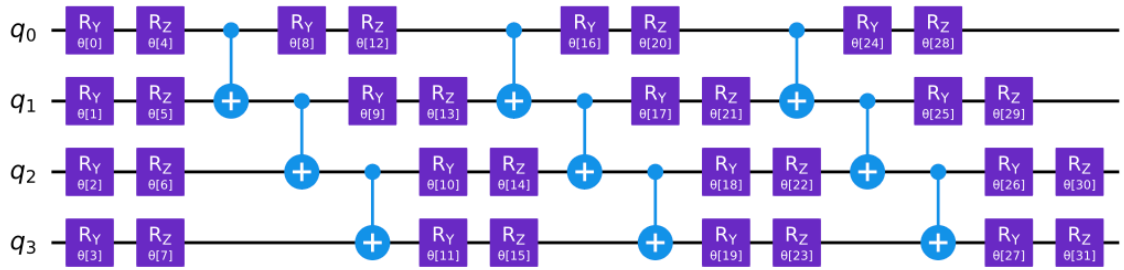


Variational Quantum Eigensolver (VQE)

Hardware-efficient ansatze

```
from qiskit.circuit.library import EfficientSU2
entanglements = ["linear", "full"]
for entanglement in entanglements:
    form = EfficientSU2(num_qubits=4, entanglement=entanglement)
    print(f"{entanglement} entanglement:")
    # We initialize all parameters to 0 for this demonstration
    display(form.decompose().draw(fold=-1))
```

Linear entanglement



Variational Quantum Eigensolver (VQE)

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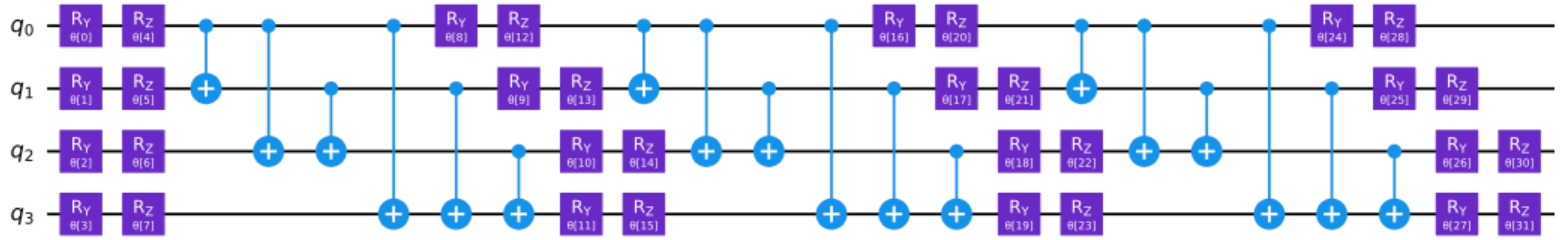
```

Full entanglement



Variational Quantum Eigensolver (VQE)

Unitary Coupled Cluster (UCC) ansatze

✓ UCC ansatz: More suitable for general larger-scale chemical problems

$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \cdots \hat{T}_\nu,$$

with for example the single and double excitation operators:

$$\hat{T}_1 = \sum_{ia} t_i^a \hat{a}_a^\dagger \hat{a}_i$$

$$\hat{T}_2 = \sum_{ijab} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i.$$

Using the Hartree–Fock state as reference state, the CC ansatz wave function is given by

$$|\psi\rangle = e^{\hat{T}} |\psi_{HF}\rangle. \longrightarrow |\psi\rangle = e^{\hat{T}-\hat{T}^\dagger} |\psi_{HF}\rangle.$$

Not a unitary Unitary

[J. Romero et al., Strategies for quantum computing molecular energies using the unitary coupled cluster ansatz, arXiv:1701.02691v2 (2017)]

Variational Quantum Eigensolver (VQE)

Some variational ansatze – targeted at quantum simulation

✓ Hamiltonian Variational ansatz:

- Assume that: we want to find the ground state of $H = \sum_i H_i$

  we can write $H = H_A + H_B$

  ↑ easy to prepare the ground state of H_A

- Then: prepare the ground state of H_A

  For each of L layers l, implement $\prod_k e^{it_{lk}H_k}$ for some times $t_{lk} \in \mathbb{R}$

- Intuition comes from the **quantum adiabatic theorem**:

  As $L \to \infty$, this ansatz provably can represent the ground state of H.

Table 10
Summary of circuit depth, parameters and entangling gates scaling across most fixed structure ansätze reviewed. The scaling in the number of entangling gates assumes full connectivity of the qubit lattice.

Method	Depth	Parameters	Entangling gates	Comments
Hardware Efficient Ansatz (HEA) [263]	$\mathcal{O}(L)$	$\mathcal{O}(NL)$	$\mathcal{O}((N-1)L)$	L is an arbitrary number of layers, its scaling for exact ground state is unknown, exponential in the worst case (i.e. if the entire Hilbert space needs to be spanned to find the ground state)
UCCSD [37,456]	$\mathcal{O}\left((N-m)^2 m\tau\right)$	$\mathcal{O}\left((N-m)^2 m^2\tau\right)$	$\mathcal{O}\left(2(\tilde{q}-1)N^4\tau\right)$	$\tilde{q}$ is the average Pauli weight across the operators used to build the ansatz. As an indication, maximum Pauli weight under Jordan–Wigner is N, and $log(N)$ under Bravyi–Kitaev. τ is the number of Trotter steps used
UCCGSD [37,80,82]	$\mathcal{O}\left(N^3\tau\right)$	$\mathcal{O}\left(N^4\tau\right)$	$\mathcal{O}\left(2(\tilde{q}-1)N^4\tau\right)$	As above
k-UpCCGSD [80]	$\mathcal{O}(kN\tau)$	$\mathcal{O}\left(k\tau N^2/4\right)$	$\mathcal{O}\left(k\tau(\tilde{q}-1)N^2/2\right)$	k is an arbitrary constant which determines the accuracy of the result. Scaling is unknown. Rest is as above.
OO-UCCD [457]	$\mathcal{O}\left((N-m)^2 m\tau\right)$	$\mathcal{O}\left((N-m)^2 m^2\tau\right)$	$\mathcal{O}\left(2(\tilde{q}-1)N^4\tau\right)$	Same as UCCSD. It is worth noting that OO-UCCD is a nested loop between orbital (one-body terms) optimization, done on a conventional machine, and two-body terms optimization done on the quantum computer.
Symmetry preserving [148]	$\mathcal{O}((N-1)L)$	$\mathcal{O}(2(N-1)L)$	$\mathcal{O}(3(N-1)L)$	This ansatz spans a wider range of the Hilbert space than the EPS. It is therefore likely it requires more circuit resources and as such we suspect that L grows exponentially in N for exact resolution of the ground state. This logic also applies to HEA.
Efficient Symmetry Preserving (EPS) ansatz [218]	$\mathcal{O}\left(2\binom{N-1}{m}\right)$	$\mathcal{O}\left(2\binom{N}{m}-2\right)$	$\mathcal{O}\left(3\binom{N}{m}\right)$	Scaling range from linear when $m=1$, or $m=N-1$, to exponential if $m{\sim}N/2$
Hamiltonian Variational Ansatz [82,150]	$\mathcal{O}\left(\tilde{C}L\right)$	$\mathcal{O}\left(\tilde{C}L\right)$	$\mathcal{O}\left(2(\tilde{q}-1)CL\right)$	L represents the number of repetition of the ansatz required to achieve the desired accuracy. C is the number of terms in the Hamiltonian, and $\tilde{C}$ the number of commutative groups among these terms.

Energy Measurements

Variational Quantum Eigensolver (VQE)

Energy measurements

- We need to measure energies $E_\psi = \langle\psi|H|\psi\rangle$
- Assume that: we want to find the ground state of $H = \sum_i H_i$, where H_i are simple terms
- $\langle\psi|H_i|\psi\rangle \pm \varepsilon$ can be computed by using $O(1/\varepsilon^2)$ measurements
- More works on optimizing measurements
  - [Gokhale et al '19, Crawford et al '21, ⋯]

Algorithm 1: Variational Quantum Eigensolver (VQE).

Result: Approximate ground state energy, $\min_{\vec{\theta}} \langle H \rangle_{\psi(\vec{\theta})}$

$\vec{\theta_1} \leftarrow$ random angles or initial guess;
$i \leftarrow 1$;
while *(not classical optimizer termination condition)* **do**
  for $j \in [O(N^4)]$ **do**
    for $O(1/\epsilon^2)$ *repetitions* **do**
      Prepare $\psi(\vec{\theta_i})$;
      Measure $\langle H_j \rangle_{\psi(\vec{\theta_i})}$;
    end
  end
  $\langle H \rangle_{\psi(\vec{\theta_i})} \leftarrow \sum_j \langle H_j \rangle_{\psi(\vec{\theta_i})}$;
  Record $(\theta_i, \langle H \rangle_{\psi(\vec{\theta_i})})$;
  i++;
  Pick new θ_i via classical optimizer;
end

Classical Optimizer

Variational Quantum Eigensolver (VQE)

Classical Optimizers – A key ingredient in VQE

✓ Stochastic approximation methods

- Finite Difference (FD) SA, Simultaneous Perturbation (SP) SA

✓ Analytical gradient calculation

- Direct analytical gradient measurement

$$\frac{\partial \langle \hat{O}_k(\boldsymbol{\theta}) \rangle}{\partial \theta_j} = 2\,\mathrm{Im}(\langle \phi_0 | V_k^{j\dagger}(\boldsymbol{\theta}) \hat{M}_k U(\boldsymbol{\theta}) | \phi_0 \rangle),$$

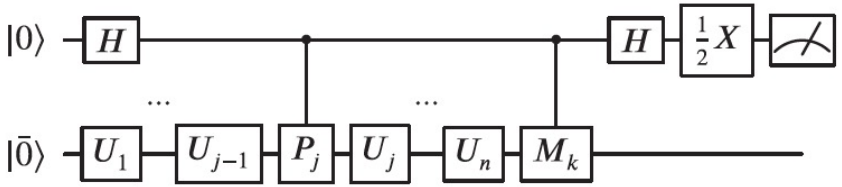


Fig. 13. Quantum circuit that evaluates $\mathrm{Im}(\langle \phi_0 | V_k^{j\dagger}(\boldsymbol{\theta}) \hat{M}_k U(\boldsymbol{\theta}) | \phi_0 \rangle)$.

- Indirect (Parameter shift rule)

$$\frac{\partial \langle \hat{O}_k(\boldsymbol{\theta}) \rangle}{\partial \theta_j} = \langle \hat{O}_k(\boldsymbol{\theta} + \frac{\pi}{2}\mathbf{e}_j) \rangle - \langle \hat{O}_k(\boldsymbol{\theta} - \frac{\pi}{2}\mathbf{e}_j) \rangle$$

[J. Tilly et al., The Variational Quantum Eigensolver: A review of methods and best practices, Physics Reports 986, pp 1–128 (2022)]

Variational Quantum Eigensolver (VQE)

Classical Optimizers – A key ingredient in VQE

✓ Gradient-based searching strategy

- First order optimizers (Simple gradient descent, Adam optimizer)
- Second order optimizers (BFGS algorithm, Quantum natural gradient)

✓ Gradient-free searching strategy

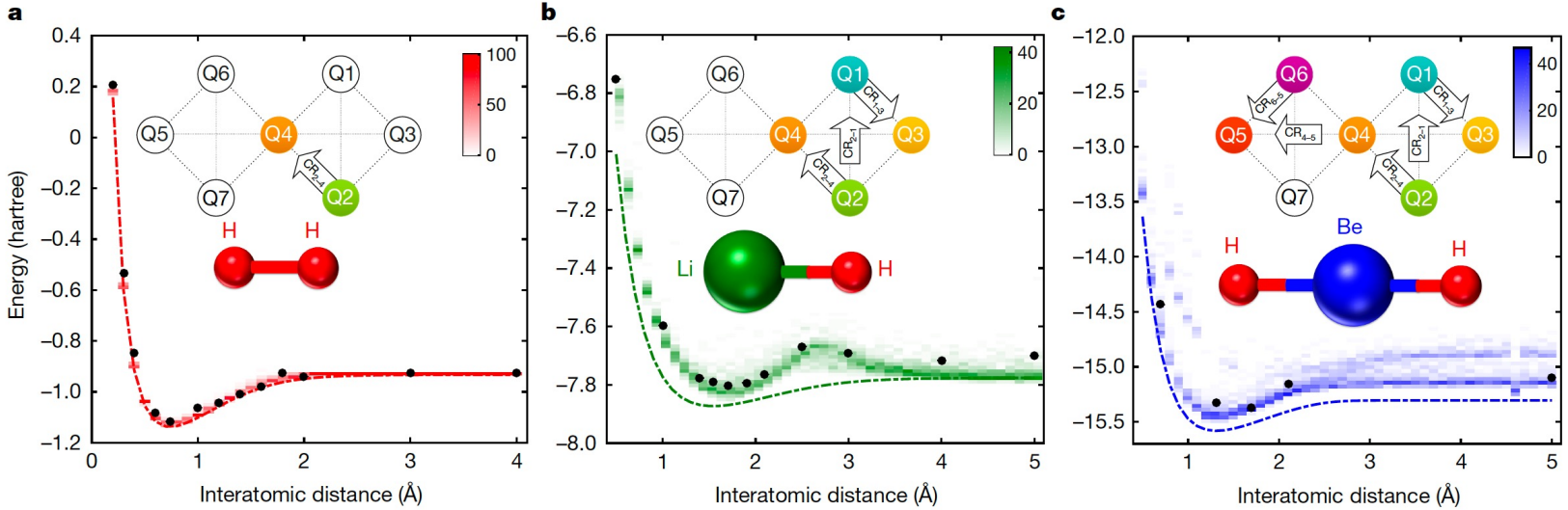
- Nelder-Mead algorithm (based on a simplex)
- Sequential optimization

Applications of VQE

Variational Quantum Eigensolver (VQE)

Applications of VQE

✓ Application to Quantum Chemistry



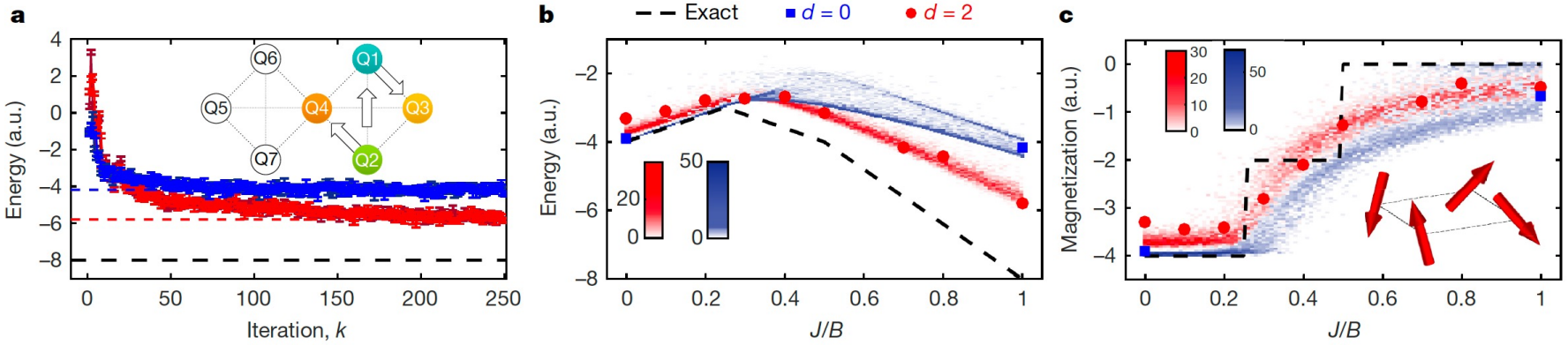
[A. Kandala et al., Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets, Nature 549, pp 242–246 (2017)]

Variational Quantum Eigensolver (VQE)

Applications of VQE

✓ Application to Quantum Magnetism

$$H = J \sum_{\langle i,j \rangle} (X_i X_j + Y_i Y_j + Z_i Z_j) + B \sum_i Z_i$$



The optimization of a four-qubit Heisenberg model on a square lattice, in an external magnetic field

[A. Kandala et al., Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets, Nature 549, pp 242–246 (2017)]

Variational Quantum Algorithms

- What is VQAs?
- VQE and **QAOA**

Quantum Approximate Optimization Algorithm

What is QAOA?

QAOA

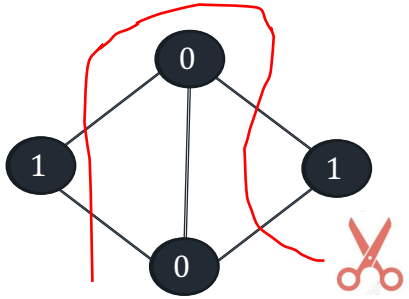
MAX-CUT Problem

- ✓ QAOA was introduced by Farhi *et al.* (2014)
- ✓ Apply VQE framework to solve classical optimization problem by setting

$$H = \sum_{x \in \{0,1\}^n} C(x)|x\rangle\langle x|$$

where $C(x)$ is a cost function.

- ✓ The ground state of H = the lowest-cost x



Cut = 4

[E. Farhi et al., A Quantum Approximate Optimization Algorithm, arXiv:1411.4028 (2014)]

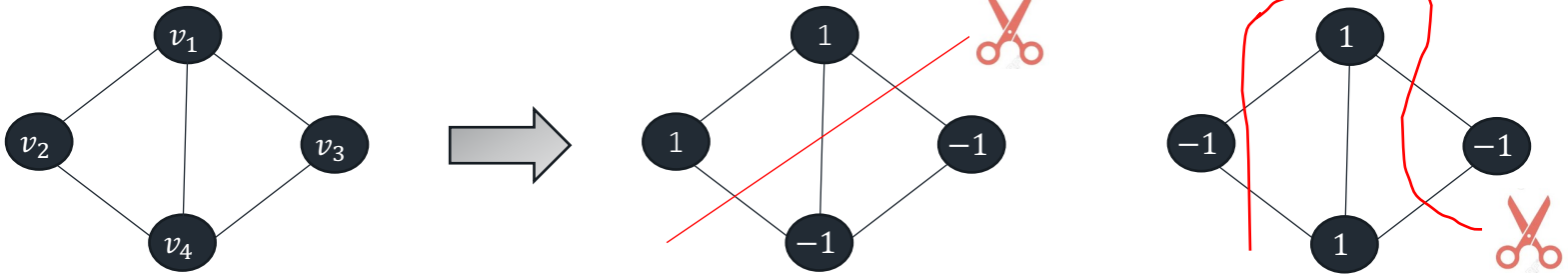
MAX-CUT problem

Quantum Approximate Optimization Algorithm

What is MAX-CUT problem?

MAX-CUT Problem

✓ **Goal**: Split the set of vertices V of a graph G into two disjoint parts such that the number of edges spanning two parts is maximized



Cut = 3

Cut = 4

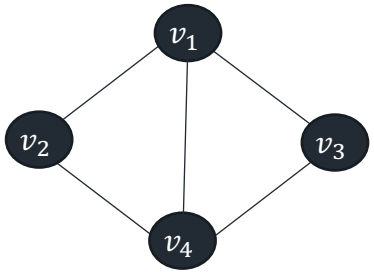
Quantum Approximate Optimization Algorithm

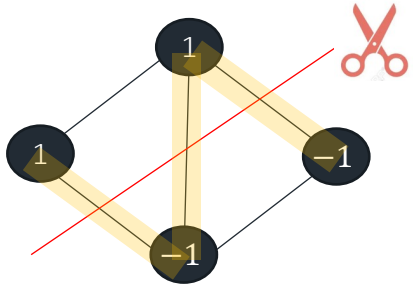
What is MAX-CUT problem?

MAX-CUT Problem

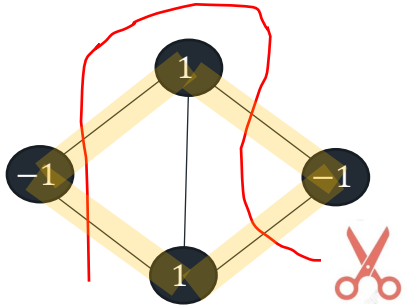
✓ Formulated as an optimization problem : for $z = (z_1, \cdots, z_N)$, $z_i \in \{-1,1\}$ $\forall i$

$$\max_z C(z) = \max \frac{1}{2} \sum_{\{i,j\} \in E} (1 - z_i z_j)$$





$$C(s) = \frac{1}{2}(2 + 2 + 2) = 3$$



$$C(s) = \frac{1}{2}(2 + 2 + 2 + 2) = 4$$

Quantum Approximate Optimization Algorithm

QAOA for MAX-CUT Problem

QAOA for MAX-CUT Problem

- ✓ MAX-CUT Hamiltonian:

$$H_C = \frac{1}{2}\sum_{\{i,j\}\in E}(1 - Z_i Z_j)$$

- ✓ Note that $Z_i \equiv I \otimes \cdots \otimes Z \otimes \cdots \otimes I$ and $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

↑ i-th

- ✓ $H_C|x\rangle = C(x)|x\rangle \quad \forall\, x \in \{0,1\}^N$

- ✓ $\max_x C(x) = \max_x \frac{1}{2}\sum_{\{i,j\}\in E}(1 - (-1)^{x_i}(-1)^{x_j}) = \max_z C(z)$

Quantum Approximate Optimization Algorithm

What is QAOA?

Level p-QAOA

1. Initialize the quantum processor in $|+\rangle^{\otimes N}$
2. Generate a variational wavefunction

$$|\psi_p(\vec{\gamma},\vec{\beta})\rangle = e^{-i\beta_p H_B} e^{-i\gamma_p H_C} \cdots e^{-i\beta_1 H_B} e^{-i\gamma_1 H_C} |+\rangle^{\otimes N}$$

by applying the problem Hamiltonian H_C and a mixing Hamiltonian $H_B = \sum_{j=1}^{N} X_j$

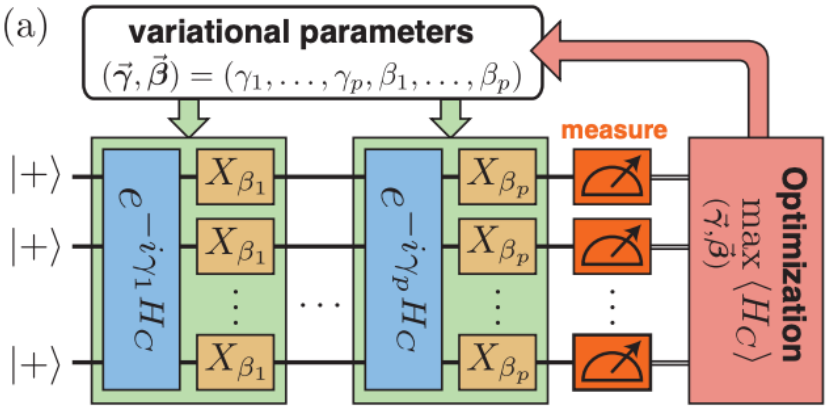
3. Determine the expectation value

$$F_p(\vec{\gamma},\vec{\beta}) = \langle \psi_p(\vec{\gamma},\vec{\beta}) | H_C | \psi_p(\vec{\gamma},\vec{\beta}) \rangle$$

4. Search for the optimal parameters

$$(\vec{\gamma}^*,\vec{\beta}^*) = \arg\max_{\vec{\gamma},\vec{\beta}} F_p(\vec{\gamma},\vec{\beta})$$

by a classical computer

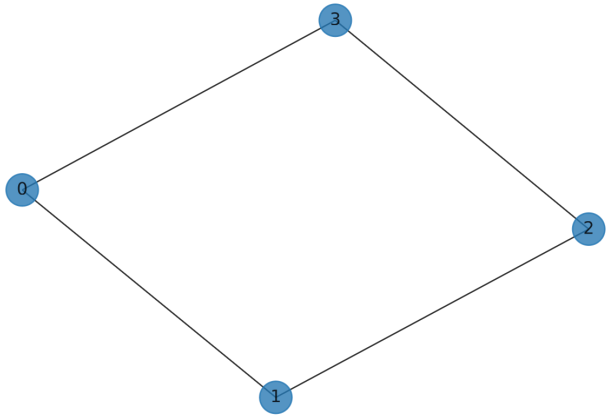


[L. Zhou et al., Quantum Approximate Optimization Algorithm: Performance, Mechanism, and Implementation on Near-Term Devices, Phys. Rev. X 10, 021067, 2020]

Approximation ratio $r = \dfrac{F_p(\vec{\gamma}^*,\vec{\beta}^*)}{C_{\max}}$

Implementing QAOA

The circuits of H_C and H_B



$$H_B = \sum_{j=1}^{N} X_j \qquad U(\beta) = e^{-i\beta H_B}$$

The Mixing Unitary

```
from qiskit import QuantumCircuit, ClassicalRegister, QuantumRegister
from qiskit import Aer, execute
from qiskit.circuit import Parameter

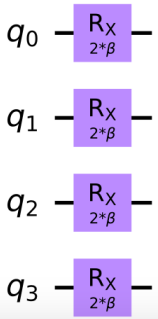
# Adjacency is essentially a matrix which tells you which nodes are
# connected. This matrix is given as a sparse matrix, so we need to
# convert it to a dense matrix
adjacency = nx.adjacency_matrix(G).todense()

nqubits = 4

beta = Parameter("$\\beta$")
qc_mix = QuantumCircuit(nqubits)
for i in range(0, nqubits):
    qc_mix.rx(2 * beta, i)

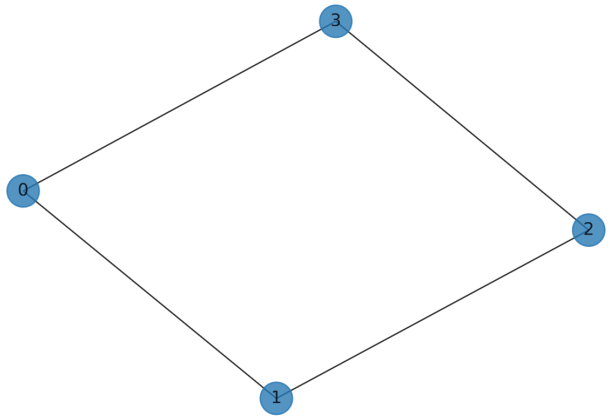
qc_mix.draw()
```

try



Implementing QAOA

The circuits of H_C and H_B



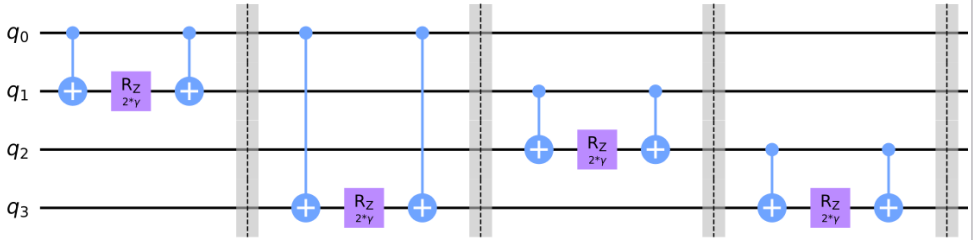
$$H_C = \frac{1}{2} \sum_{\{i,j\} \in E} (1 - Z_i Z_j) \qquad U(\gamma) = e^{-i\gamma H_C}$$

The Problem Unitary

```
gamma = Parameter("$\\gamma$")
qc_p = QuantumCircuit(nqubits)
for pair in list(G.edges()):  # pairs of nodes
    qc_p.rzz(2 * gamma, pair[0], pair[1])
    qc_p.barrier()

qc_p.decompose().draw()
```

try



Challenges for VQAs

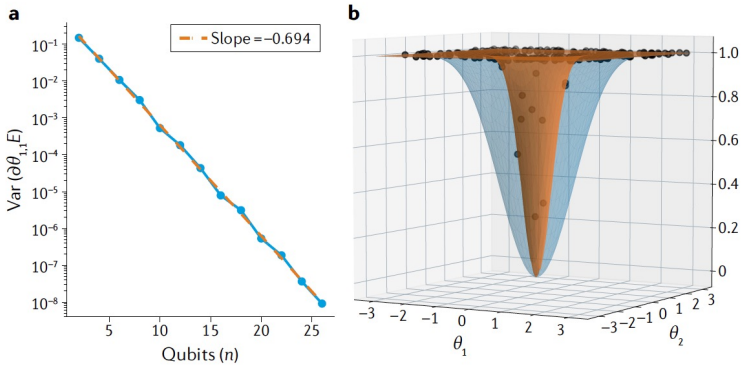
Challenges for VQAs

✓ Shortage of theoretical justification for performance

✓ Hard to train

- Finding optimal parameters for VQE is QCMA-hard [Bittel and Kliesch '21]
- VQE iterations on real hardware can be slow
- Barren plateaus

✓ Not easy to find a good variational ansatze.



Thank you!

—

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