Variational Quantum Eigensolver

백경현
한국전자통신연구원
양자컴퓨팅실

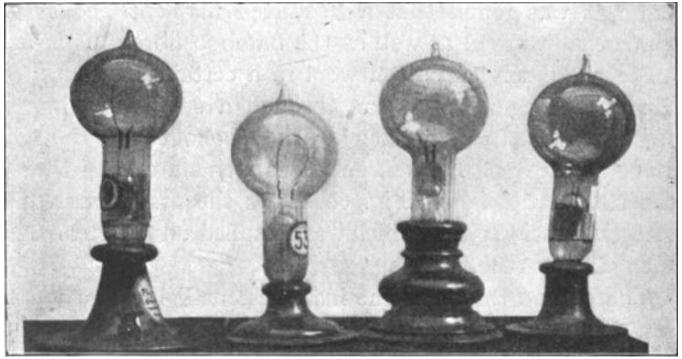
(2023.08.07 고려대학교)

개요

- 소개
  - Qubit (큐비트)
- 양자컴퓨팅
  - NISQ
  - 양자 우월성
- 양자컴퓨팅 활용
  - 양자 시뮬레이션
  - VQE

Introduction

- Quantum mechanics (양자역학)
  - Quantization (양자화)
    - Blackbody radiation(흑체 복사)



에디슨 탄소 필라멘트 램프, 1880년대 초

가우디 가스 램프
(Placa Reial Barcelona,1879)

Introduction

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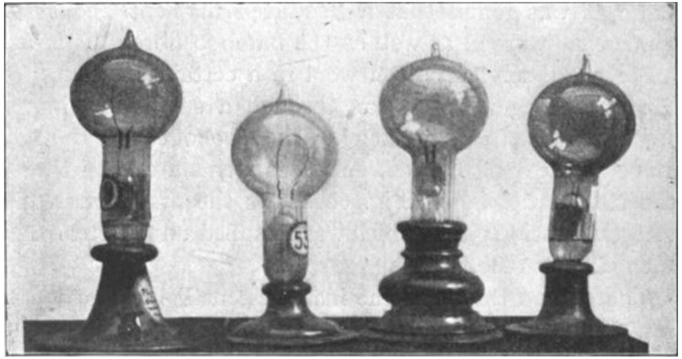
    - Quantization (양자화)
        - Blackbody radiation(흑체 복사)



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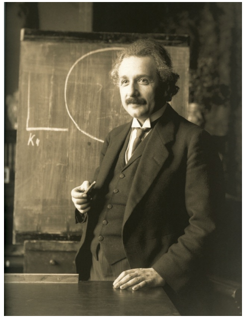
Quantum computer

- Concept of Quantum computer



Einstein
Photon eletric effect (1905)

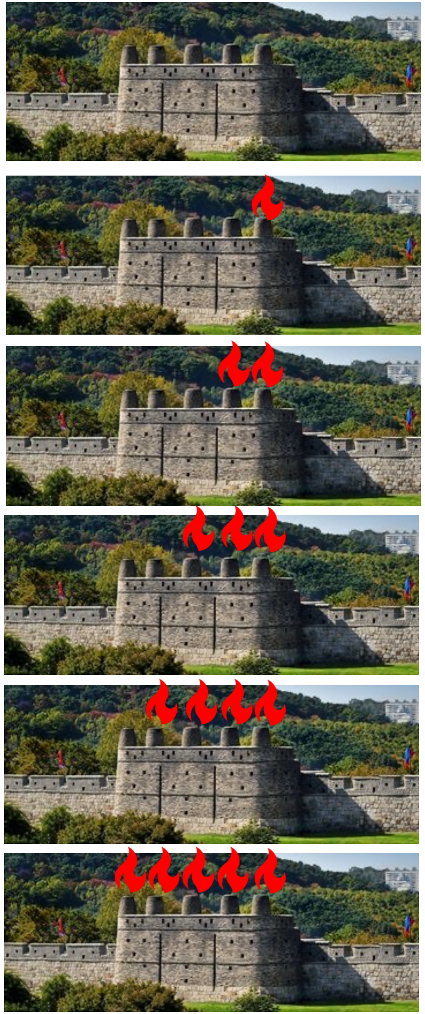
John S. Bell
Bell theorem (1964)

Richard Feynman
양자 컴퓨터 (1982)

David Deutsch
양자 알고리즘 (1985)

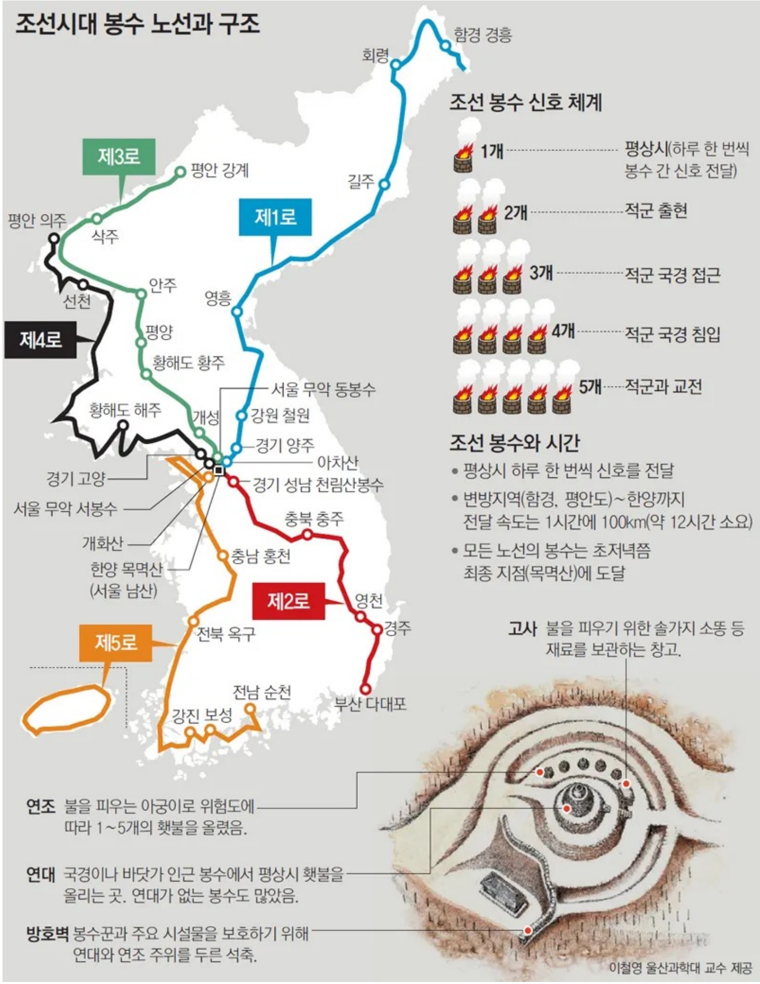
Qubit

- 정보 저장 및 전달
  - 봉화대



Qubit

- 정보 저장 및 전달



Qubit

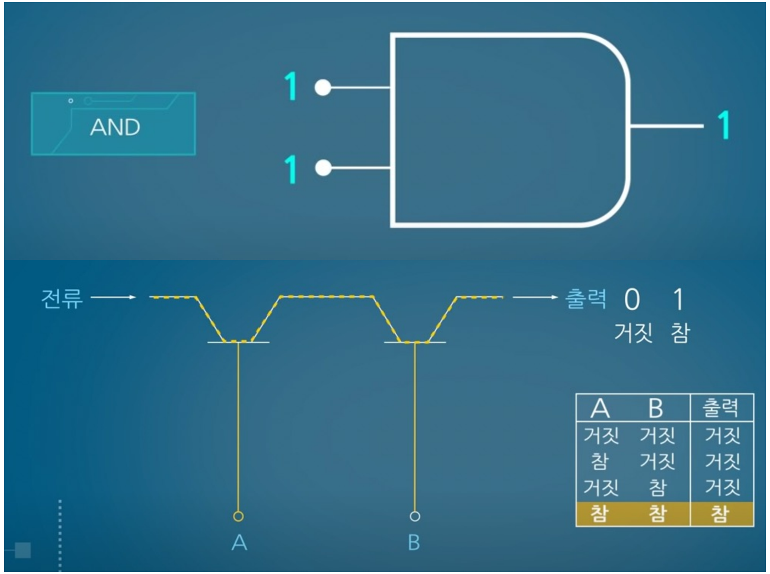
- Classical bit : 0 or 1

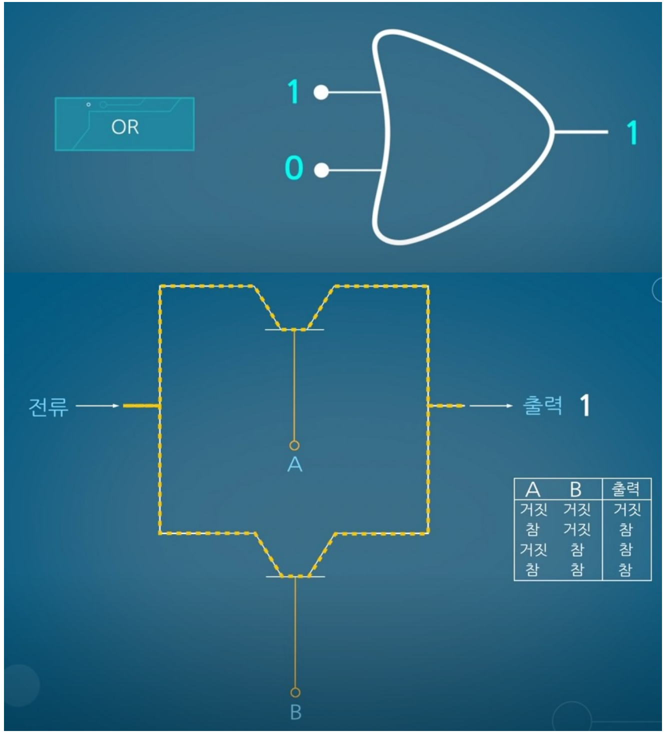
Off: 0

On: 1

Qubit

- Classical bit : 0 or 1

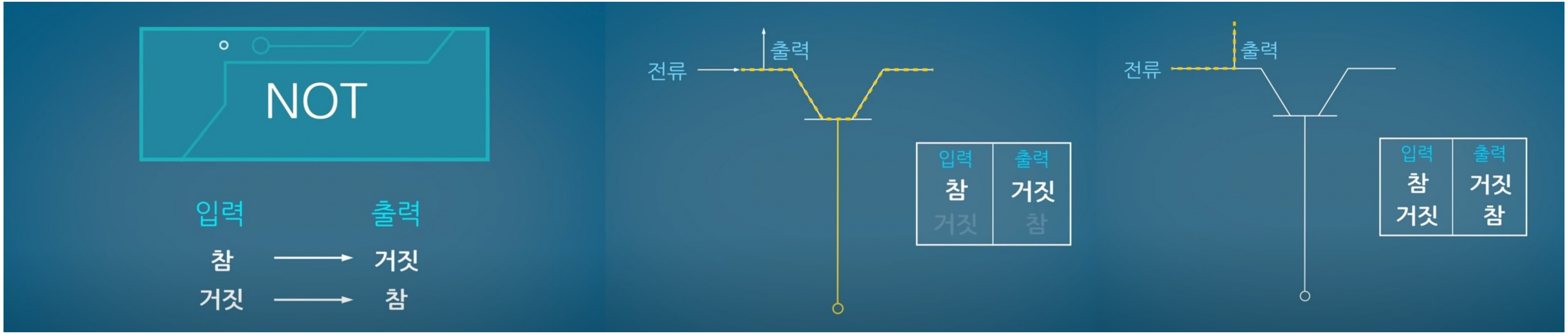




출처: https://www.youtube.com/watch?v=Fg00LN30Ezg&t=607s&ab_channel=bRd3D

Qubit

- Classical bit : 0 or 1



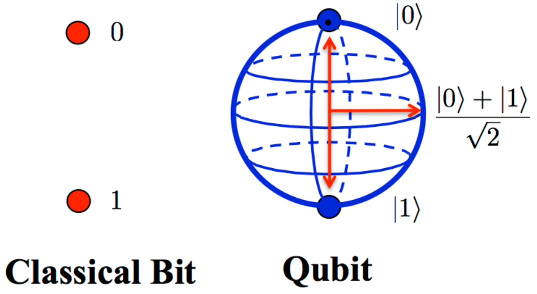
출처: https://www.youtube.com/watch?v=Fg00LN30Ezg&t=607s&ab_channel=bRd3D

Qubit

- Classical bit : 0 or 1

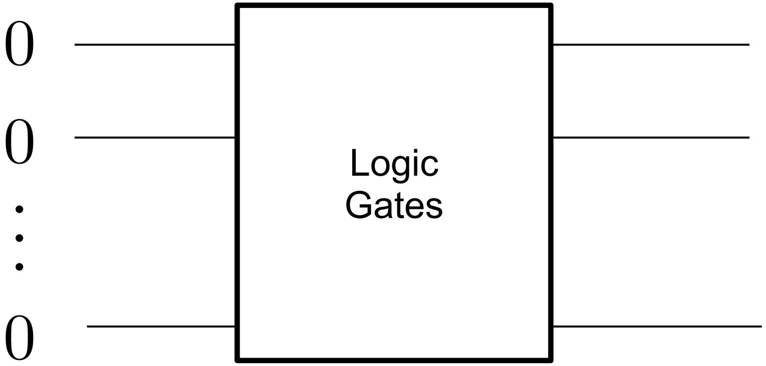
- Qubit (Quantum bit, 큐비트)

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\varphi}\sin\left(\frac{\theta}{2}\right)|1\rangle$$



Quantum computer

- Universal quantum computing
  - Classical logic circuit (논리 회로)



Q = **A** NOR **B**

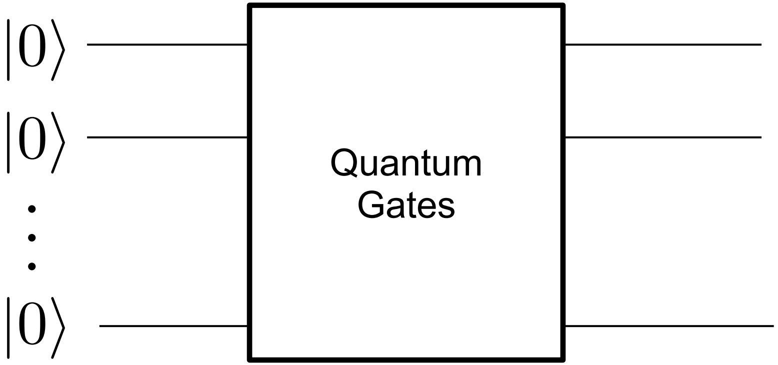
Truth Table

Input A	Input B	Output Q
0	0	1
0	1	0
1	0	0
1	1	0

Any gates (NOT, AND, XOR…) can be represented by NOR gate.

Quantum computer

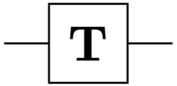
- Universal quantum computing
  - Quantum circuit (양자 회로)



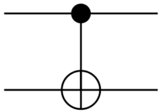
- Hadamard gate

- Phase gate

- T gate

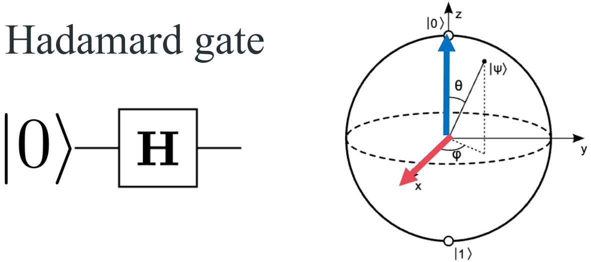


- CNOT gate

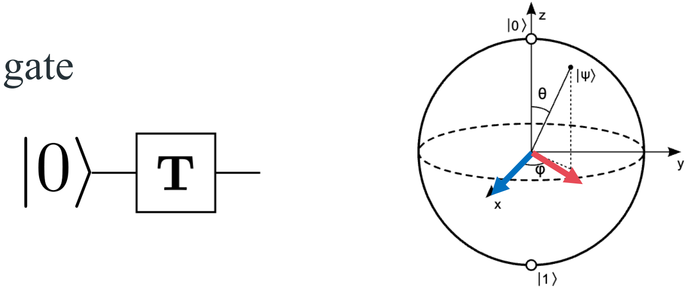


Quantum computer

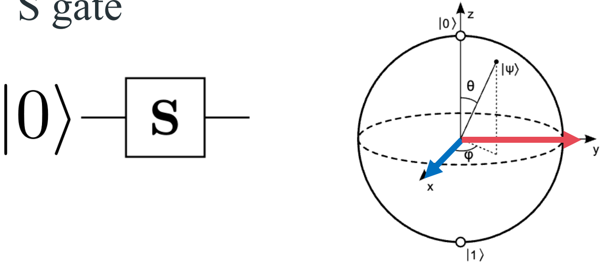
- Universal quantum computing
  - Hadamard gate



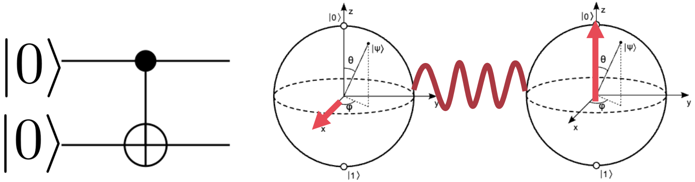
  - T gate



  - S gate



  - CNOT gate

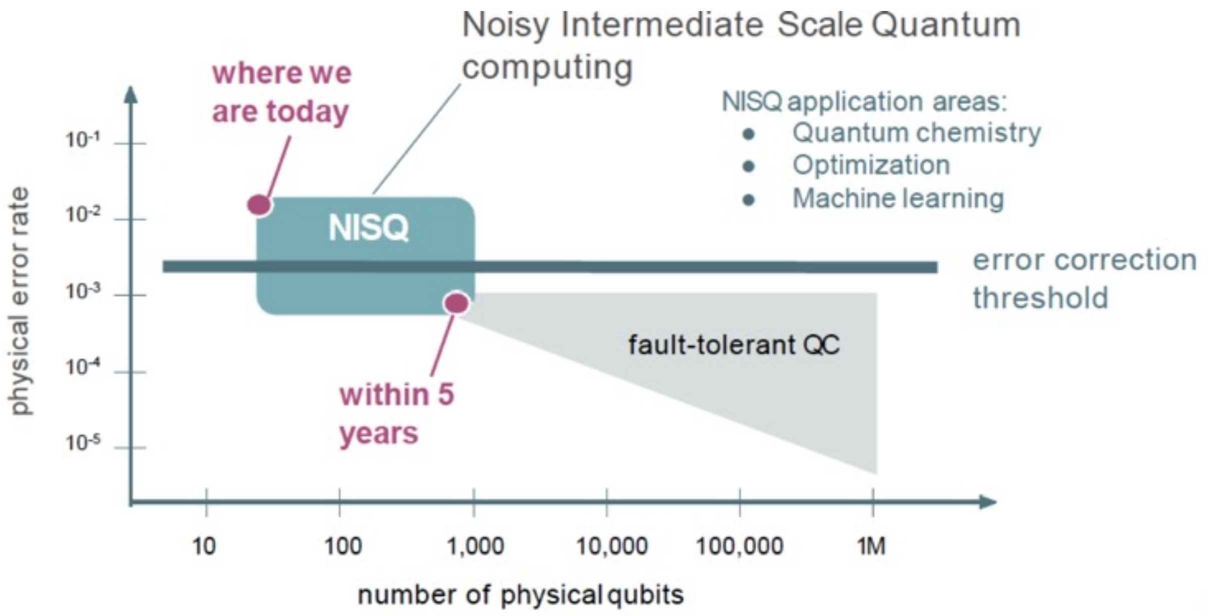


에러 보정
Error correction

Fault tolerant quantum computing

- 이상적인 양자컴퓨터는 유망한가?
  - 풀어야 할 많은 문제들이 남아있다.
  - Decoherence or Quantum noise
    - Error correction
      - 효과적으로 에러를 발견하고 보정하는 수학적인 연구가 필요.
        e.g.) Hamming code in classical computing
    - Quantum threshold
      - 에러 보정을 위해서는 99%의 정확성이 필요
    - Redundant qubits
      - 1개의 큐비트를 보호하기 위해 약 1000~10000개의 큐비트 필요

NISQ (Noisy Intermediate-Scale Quantum)



"Quantum computing in the NISQ era and beyond" Preskill, 2018 https://arxiv.org/abs/1801.00862

NISQ (Noisy Intermediate-Scale Quantum)

Quantum Computing in the NISQ era and beyond

John Preskill

Institute for Quantum Information and Matter and Walter Burke Institute for Theoretical Physics,
California Institute of Technology, Pasadena CA 91125, USA
30 July 2018

Noisy Intermediate-Scale Quantum (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. NISQ devices will be useful tools for exploring many-body quantum physics, and may have other useful applications, but the 100-qubit quantum computer will not change the world right away — we should regard it as a significant step toward the more powerful quantum technologies of the future. Quantum technologists should continue to strive for more accurate quantum gates and, eventually, fully fault-tolerant quantum computing.

- 어느 정도의 오류를 허용하고(Noisy) 중간 정도의 스케일의 (Intermediate-Scale) 양자 기술을 이용해보자.(Quantum)

- How can we make something cool by using a few leg pieces.

Photo by Dr. Bang

양자 우월성
Quantum supremacy

Quantum supremacy (양자 우월성)

- 특정 작업(task) 이 고전 알고리즘으로 시행하기 어렵다는 것을 일반적으로 보여야 한다.
  - Good theoretical hardness evidence from complexity theory.
  - Also cannot be solved in a “comparable” amount of time by classical supercomputer.

- 이 작업을 양자 컴퓨터로 효과적으로 할 수 있는 방법이 있어야 한다.

- 실험이 가능해야 한다. (Experimental feasibility)

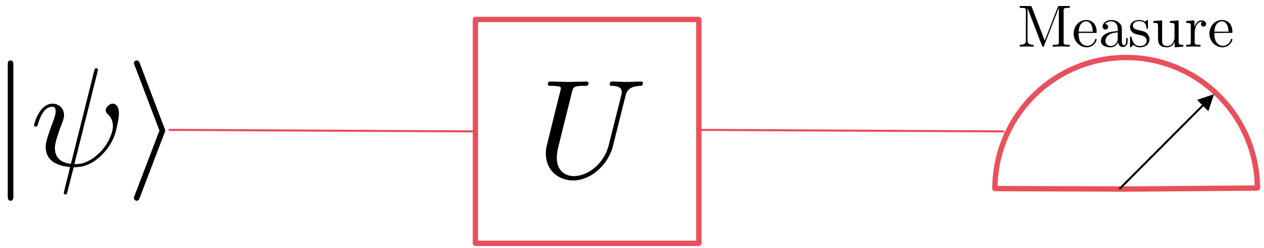
- 실험 데이터가 작업을 잘 수행하였다는 것을 보일 수 있는 기준이 있어야 한다. (Verification)

Quantum supremacy (양자 우월성)

- 샘플링

  - 통계의 목적으로 전체 분포의 특성을 파악하기 위해 모집단에서 표본을 골라내는 일

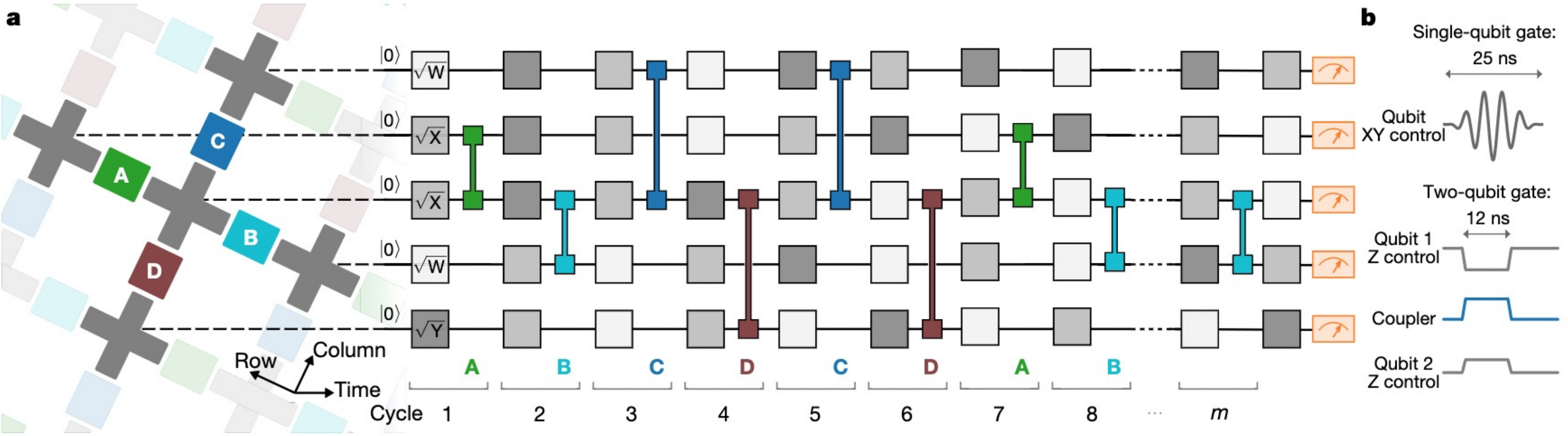
  - 양자 측정이 갖는 통계의 무작위성은 양자 역학이 갖는 가장 근본적 특성 중 하나이다.



Quantum supremacy (양자 우월성)

- Sampling

 - In statistics, sampling is the selection of a subset (a statistical sample) of individuals from within a statistical population to estimate characteristics of the whole population.



Quantum supremacy (양자 우월성)

- Random Circuit Sampling (RCS)

  - The task is to take an (efficient) quantum circuit of a specific form, in which each gate is chosen randomly, and generate samples from its output distribution.

	Worst-case hardness	Average-case hardness	Anti-Concentration	Experimentally Feasible
RCS	OK	OK (Nature physics, 2019)	OK	OK (Nature physics, 2018)

  - Average-case hardness: showing that a distribution D is uniformly difficult to sample from corresponds to showing that for most outputs x, it is hard to compute D(x).
  - Anti-concentration states that the output distribution of random quantum circuit is ‘spread out'.

Random circuit sampling

Article

Quantum supremacy using a programmable superconducting processor

https://doi.org/10.1038/s41586-019-1666-5

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Frank Arute[1], Kunal Arya[1], Ryan Babbush[1], Dave Bacon[1], Joseph C. Bardin[1,2], Rami Barends[1], Rupak Biswas[3], Sergio Boixo[1], Fernando G. S. L. Brandao[1,4], David A. Buell[1], Brian Burkett[1], Yu Chen[1], Zijun Chen[1], Ben Chiaro[5], Roberto Collins[1], William Courtney[1], Andrew Dunsworth[1], Edward Farhi[1], Brooks Foxen[1,5], Austin Fowler[1], Craig Gidney[1], Marissa Giustina[1], Rob Graff[1], Keith Guerin[1], Steve Habegger[1], Matthew P. Harrigan[1], Michael J. Hartmann[1,6], Alan Ho[1], Markus Hoffmann[1], Trent Huang[1], Travis S. Humble[7], Sergei V. Isakov[1], Evan Jeffrey[1], Zhang Jiang[1], Dvir Kafri[1], Kostyantyn Kechedzhi[1], Julian Kelly[1], Paul V. Klimov[1], Sergey Knysh[1], Alexander Korotkov[1,8], Fedor Kostritsa[1], David Landhuis[1], Mike Lindmark[1], Erik Lucero[1], Dmitry Lyakh[9], Salvatore Mandrà[3,10], Jarrod R. McClean[1], Matthew McEwen[5], Anthony Megrant[1], Xiao Mi[1], Kristel Michielsen[11,12], Masoud Mohseni[1], Josh Mutus[1], Ofer Naaman[1], Matthew Neeley[1], Charles Neill[1], Murphy Yuezhen Niu[1], Eric Ostby[1], Andre Petukhov[1], John C. Platt[1], Chris Quintana[1], Eleanor G. Rieffel[3], Pedram Roushan[1], Nicholas C. Rubin[1], Daniel Sank[1], Kevin J. Satzinger[1], Vadim Smelyanskiy[1], Kevin J. Sung[1,13], Matthew D. Trevithick[1], Amit Vainsencher[1], Benjamin Villalonga[1,14], Theodore White[1], Z. Jamie Yao[1], Ping Yeh[1], Adam Zalcman[1], Hartmut Neven[1] & John M. Martinis[1,5]*

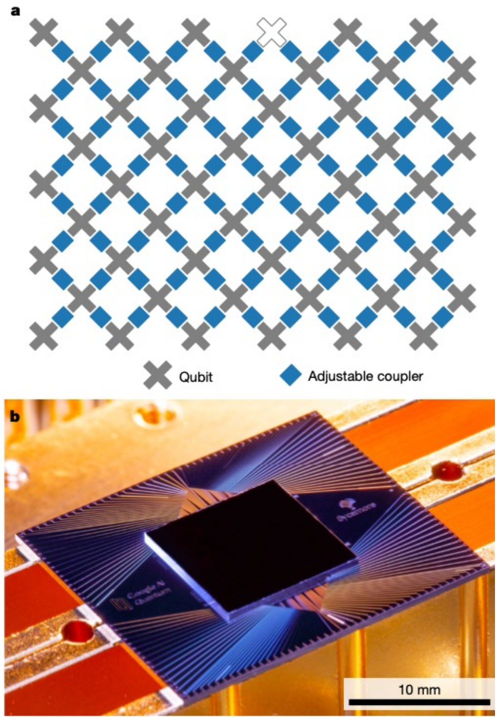

Fig. 1 | The Sycamore processor. a, Layout of processor, showing a rectangular array of 54 qubits (grey), each connected to its four nearest neighbours with couplers (blue). The inoperable qubit is outlined. **b**, Photograph of the Sycamore chip.

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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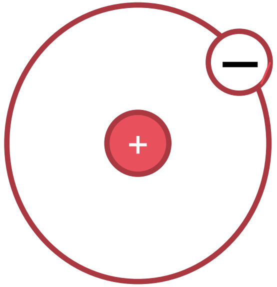
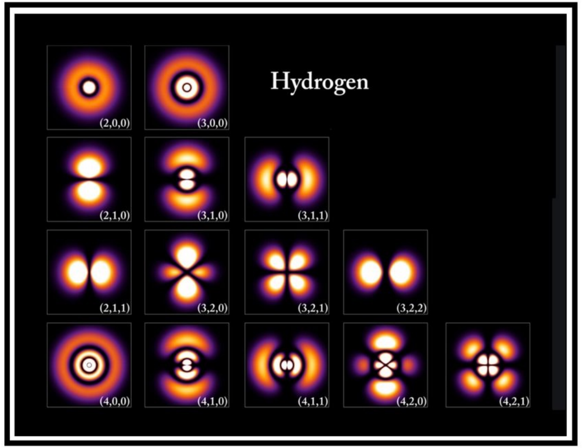


Hydrogen atom



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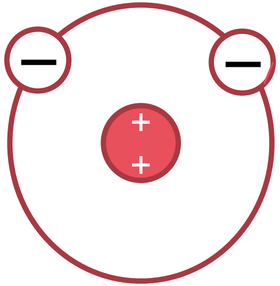
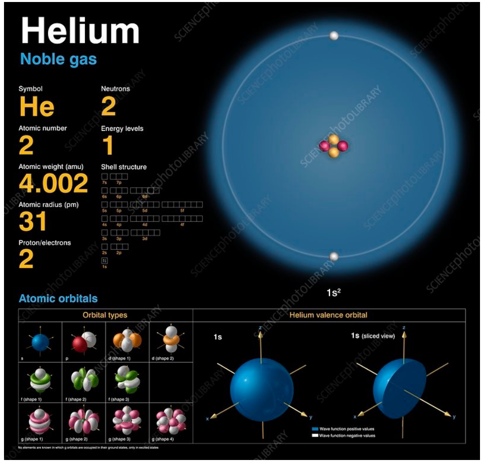


Helium atom



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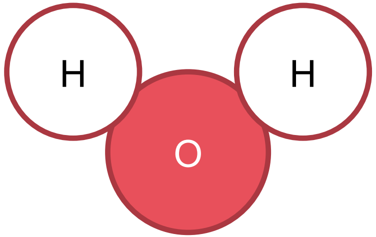

Water molecule

Quantum simulation

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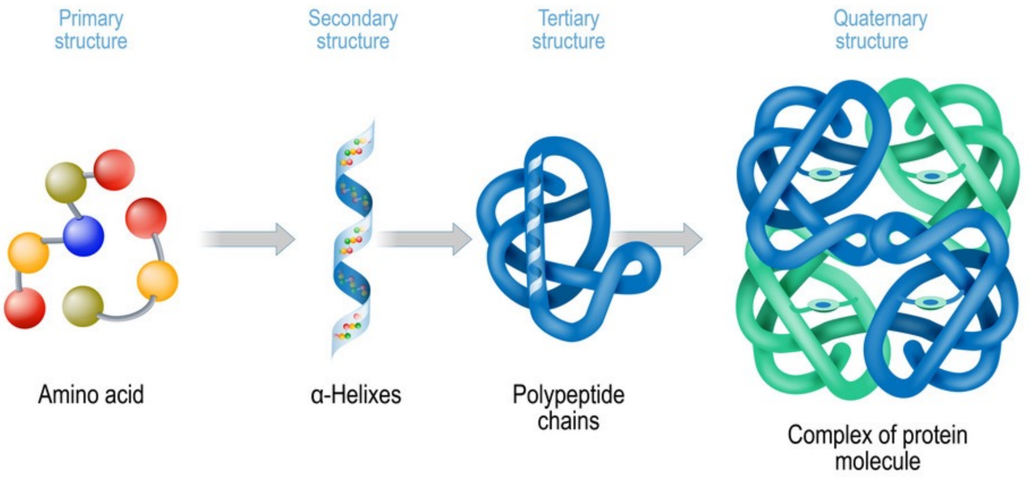


Quantum simulation

- 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

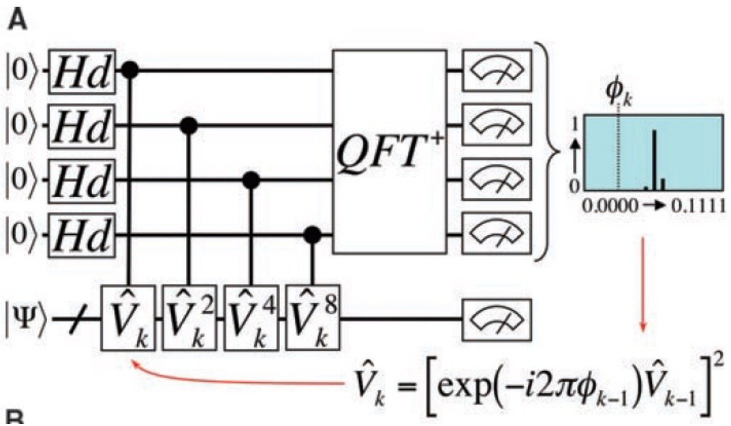
- 해밀토니안 바닥상태를 찾기 위한 양자 알고리즘

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

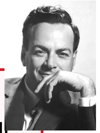
Alán Aspuru-Guzik,[1*†] Anthony D. Dutoi,[1*] Peter J. Love,[2] Martin Head-Gordon[1,3]

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

1985

양자역학 기반의
범용컴퓨터 가능성 제시
(David Deutsch)

쇼어 알고리즘:
소인수분해를 위한
양자 알고리즘 제시

1994

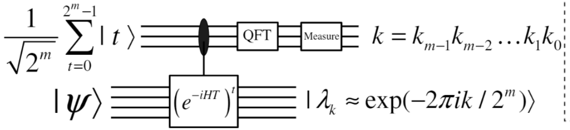
1996

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.

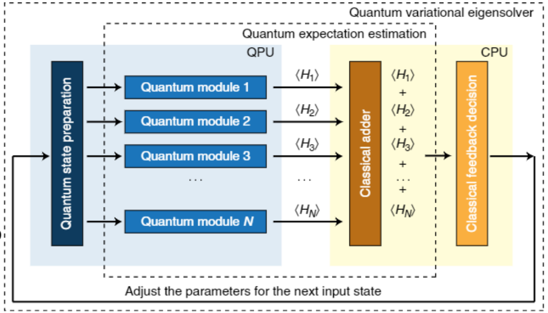


고유값 추정 양자 알고리즘:
양자 시뮬레이션 기반 고유값
추정 알고리즘

1999

2009

HHL 알고리즘:
양자 시뮬레이션
활용한 선형
방정식 공략 양자
알고리즘

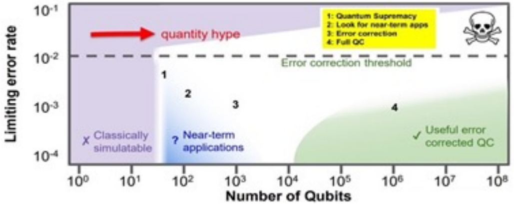


Variational Quantum Eigensolver (VQE): 바닥에너지 추정을 위한
하이브리드 양자 알고리즘

2014

2018

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



감사합니다.