Quantum Chemistry on Quantum Computers

#1 General Introduction

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*

Self introduction

Kenji Sugisaki

Special Appointment Lecturer, Osaka City University
&
JST PRESTO (Concurrent)
&
Visiting Associate Professor, CQuERE, TCG CREST, India

Office: D219, Science Bld. Osaka City Univ. (Sugimoto campus)

Molecular Physical Chemistry Lab (Sato Group)
Department of Chemistry and Molecular Materials Science,
Graduate School of Science,
Osaka City University

- Visiting Associate Professor, Centre for Quantum Engineering, Research and Education (CQuERE), TCG Centres for Research and Education in Science and Technology (TCG CREST), India (2020 Nov.–2021 Dec.)
- JST PRESTO (2019 Oct.–2023 Mar.)
- Special Appointment Lecturer, Osaka City University (2016–current)
- Special Appointment Assistant Professor, Osaka City University (2013–2016)
- Visiting Postdoctoral Researcher, Harvard University (2011 Feb.–2011 Apr.)
- Postdoctoral Researcher, Osaka City University (2008–2013)
- Research Associate, Osaka City University (2006–2008)
- DSci, Osaka City University (2006)
- MSc, Osaka City University (2004)
- BSc, Osaka City University (2003)

Schedule of this lecture series

#	Date Time in IST	Theme
1	10/28 (Thu) 10:00	**General introduction of quantum computers** History of quantum computers, qubits, quantum gates, quantum circuits, universal gate sets, NISQ devices, quantum error correction, etc.
2	11/11 (Thu) 10:00	**Quantum algorithms** Deutsch–Jozsa algorithm, quantum teleportation, quantum fingerprinting (SWAP test), etc.
3	11/17 (Wed) 10:00	**Quantum phase estimation algorithm** Hadamard test (1-qubit QPE), iterative QPE, Bayesian QPE, relationship between evolution time length and phase precisions, resource estimations, etc.
4	11/25 (Thu) 10:00	**Fermion–qubit transformation and quantum circuit constructions** Jordan–Wigner transformation, parity basis, Bravyi–Kitaev transformation, Trotter decomposition, etc.
5	12/2 (Thu) 10:00	**Variational quantum algorithms** Chemistry-inspired ansatzes, hardware-efficient ansatzes, error mitigations, excited states calculations, resource estimations, etc.
6	12/9 (Thu) 10:00	**Adiabatic quantum algorithms** Adiabatic theorem, quantum annealing, adiabatic state preparation, etc.
7	12/16 (Thu) 10:00	**Computational complexities** Computational complexity classes (in classical computing; P, NP, etc., and on quantum computing; BPP, BQP, QMA, etc)
8	12/23 (Thu) 10:00	**Techniques for resource (qubits/quantum gates) and error reductions** Symmetry adaptations, quantum circuit optimizations, Trotter decomposition error reductions, etc.

Quantum computers

R. P. Feynman, Simulating Physics with Computers. *Int. J. Theor. Phys.* **1982**, *21*, 467–488.

Photo taken from wikipedia

$\psi(x_1, x_2, \cdots, x_R, t)$ with large *R* cannot be simulated with a normal computer, because it has too many variables.

The problem is, how can we simulate the quantum mechanics?

> ***Let the computer itself be built of quantum mechanical elements which obey quantum mechanical laws.***

Quantum Turing machine

Photo taken from wikipedia

Proc. R. Soc. Lond. A **400**, 97–117 (1985)
Printed in Great Britain

Quantum theory, the Church–Turing principle and the universal quantum computer

BY D. DEUTSCH
Department of Astrophysics, South Parks Road, Oxford OX1 3RQ, U.K.

(*Communicated by R. Penrose, F.R.S. – Received* 13 *July* 1984)

ANNALS OF SCIENCE MAY 2, 2011 ISSUE

DREAM MACHINE

The mind-expanding world of quantum computing.

By Rivka Galchen
May 2, 2011

According to Deutsch, the insight for that paper came from a conversation in the early eighties with the physicist Charles Bennett, of I.B.M., about computational-complexity theory, at the time a sexy new field that investigated the difficulty of a computational task. Deutsch questioned whether computational complexity was a fundamental or a relative property. Mass, for instance, is a fundamental property, because it remains the same in any setting; weight is a relative property, because an object's weight depends on the strength of gravity acting on it. Identical baseballs on Earth and on the moon have equivalent masses, but different weights. If computational complexity was like mass—if it was a fundamental property—then complexity was quite profound; if not, then not.

https://www.newyorker.com/magazine/2011/05/02/dream-machine

Quantum computers

- ✓ Computers that operate according to **quantum mechanical principles**
- ✓ Use **quantum bits (qubits)** as the minimal unit of information
- ✓ Some problems those computational cost increase exponentially against the problem size on classical computer can be solved with polynomial costs

Nature **2019**, *574*, 505–510.

Article

Quantum supremacy using a programmable superconducting processor

Supercomputer “Summit”

53 qubit quantum computer “Sycamore”

Photo taken from website:
https://phys.org/news/2018-06-ornl-summit-supercomputer.html

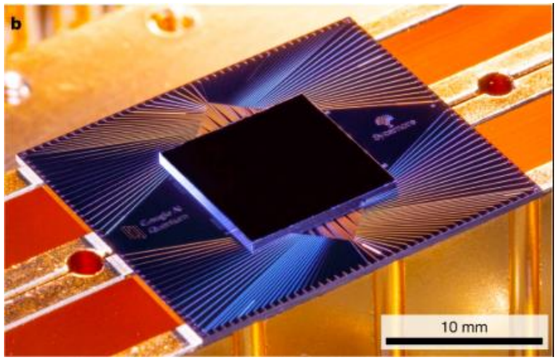


Photo taken from *Nature* **2019**, *574*, 505–510.

10,000 years → **200 seconds**

Misconceptions in quantum computing

Quantum computers can solve any problems faster than the classical computers.

Not any problems can be accelerated to solve by using quantum computers

Quantum computers can solve particular problems faster than the classical computers.

Still not exact.

Exponential speedup is guaranteed for some quantum algorithms (e.g., prime factorization and hidden subgroup problems). However, this states only for the **scaling of computational cost against the problem size**.

n: size of problem

Classical computer		Quantum computer
$O(a^n)$	$\xrightarrow{\textit{Exponential speedup}}$	$O(n^c)$
Exponential scaling		*Polynomial scaling*

Exponential improvement of computational cost scaling against the problem size n

Misconceptions in quantum computing

Exponential improvement of the computational cost scaling against the system size (number of electrons/basis sets) is possible by using quantum computers.

Depends on the algorithm being used.

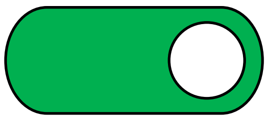
Quantum phase estimation (QPE): Obtain eigenfunction/eigenvalue with **polynomial cost**. On classical computer it needs exponential cost.

Variational quantum eigensolver (VQE): Obtain expectation value of approximated wave function with **(probably) polynomial cost**. On classical computer it can be solved polynomial cost, too.

	Classical computer	Quantum computer
Full-CI calculation	Exponential	Polynomial using QPE
Approximated methods (e.g., CCSD)	Polynomial	Polynomial using VQE

Quantum bits (Qubits)

Bit: Either 1 or 0



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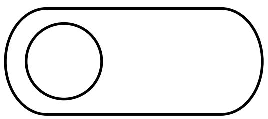

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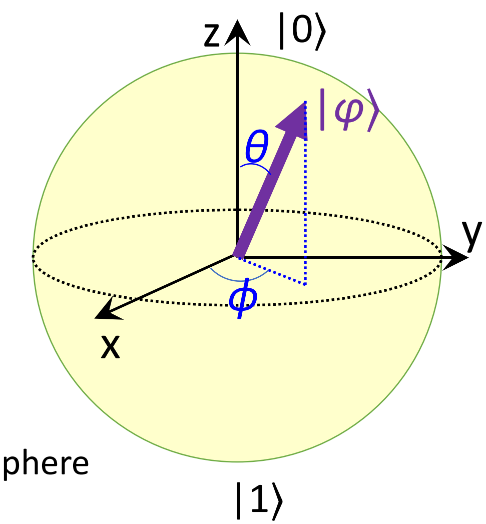
Qubit: Arbitrary superposition of $|0\rangle$ and $|1\rangle$ states

$$|\varphi\rangle = c_0|0\rangle + c_1|1\rangle$$

c_0 and c_1 are complex numbers satisfying
$|c_0|^2 + |c_1|^2 = 1$ (normalization condition)

$$|\varphi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$$



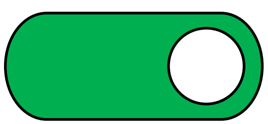
Bloch sphere

Quantum bits (Qubits)

$$|\varphi\rangle = 0.6|0\rangle + 0.8|1\rangle \xrightarrow{\text{Measurement}} \begin{cases} |\varphi\rangle = |0\rangle & \text{(36\% of probability)} \\ |\varphi\rangle = |1\rangle & \text{(64\% of probability)} \end{cases}$$

- When we measure qubit to readout the results, the quantum superposition is destroyed and projected to the eigenstate of the observable
- The probability to obtain $|0\rangle$ and $|1\rangle$ states in the measurement is proportional to the square of the coefficient

Bit: Either 1 or 0



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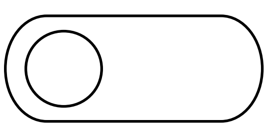

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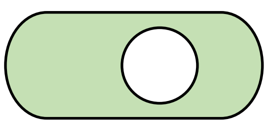


$$0.64 \neq 0.6|0\rangle + 0.8|1\rangle$$

Quantum bits (Qubits)

Quantum states can be entangled, in which measurement of one qubit affects the quantum state of other qubits

$$\frac{1}{2}(|00\rangle + |01\rangle + |10\rangle + |11\rangle)$$ (Unentangled state)

Measurement outcome of the 1st qubit	Measurement outcome of the 2nd qubit
$\lvert 0\rangle$	$\lvert 0\rangle$ or $\lvert 1\rangle$ with 50:50 probability
$\lvert 1\rangle$	$\lvert 0\rangle$ or $\lvert 1\rangle$ with 50:50 probability

$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$ (ENTANGLED state)

Measurement outcome of the 1st qubit	Measurement outcome of the 2nd qubit
$\lvert 0\rangle$	$\lvert 0\rangle$ with 100% probability
$\lvert 1\rangle$	$\lvert 1\rangle$ with 100% probability

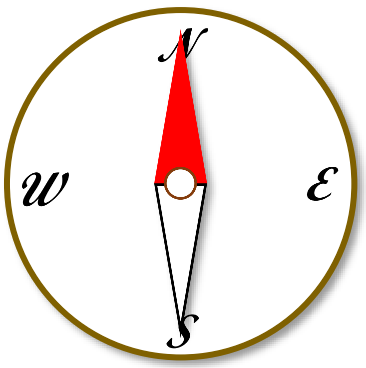
Examples of qubits

Figure taken from “The Economist”, 20th June, 2015.

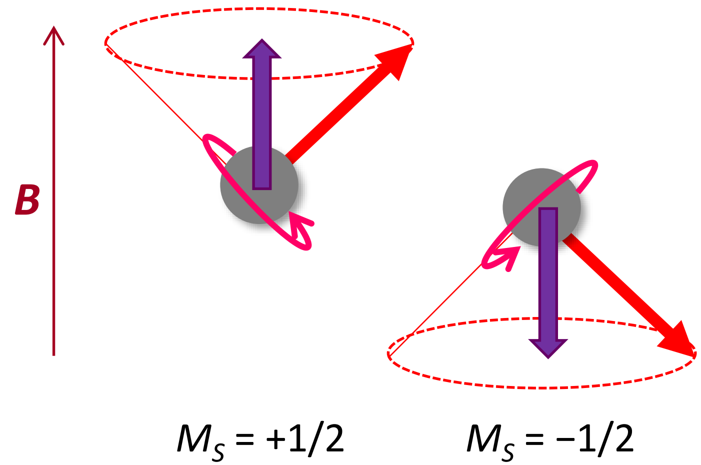
- **Superconducting circuits**
- **Photons (polarized light)**
- **Trapped ions**

- Nuclear and electron spins
- Semiconductors
- Majorana fermions

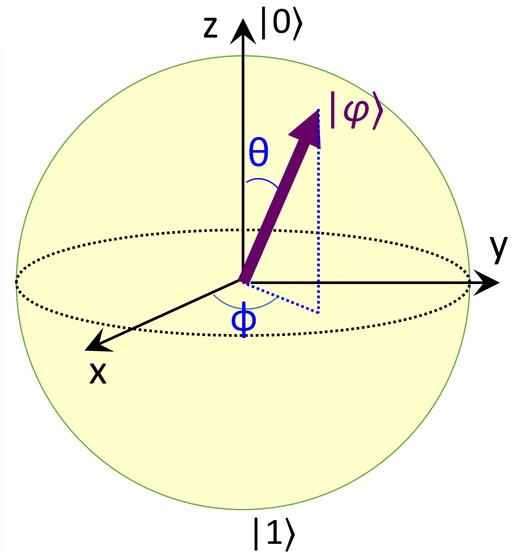
An example: Electron spin qubits



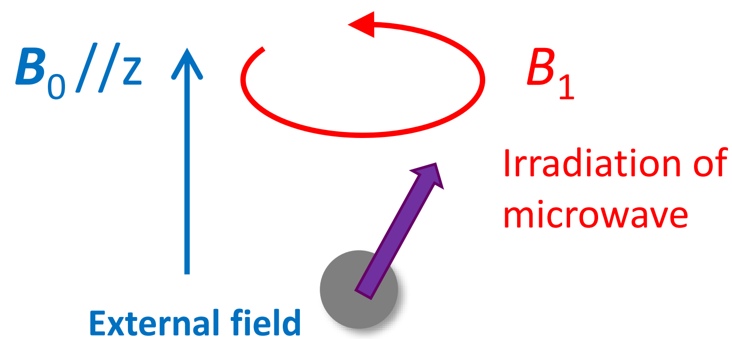
Classical magnets



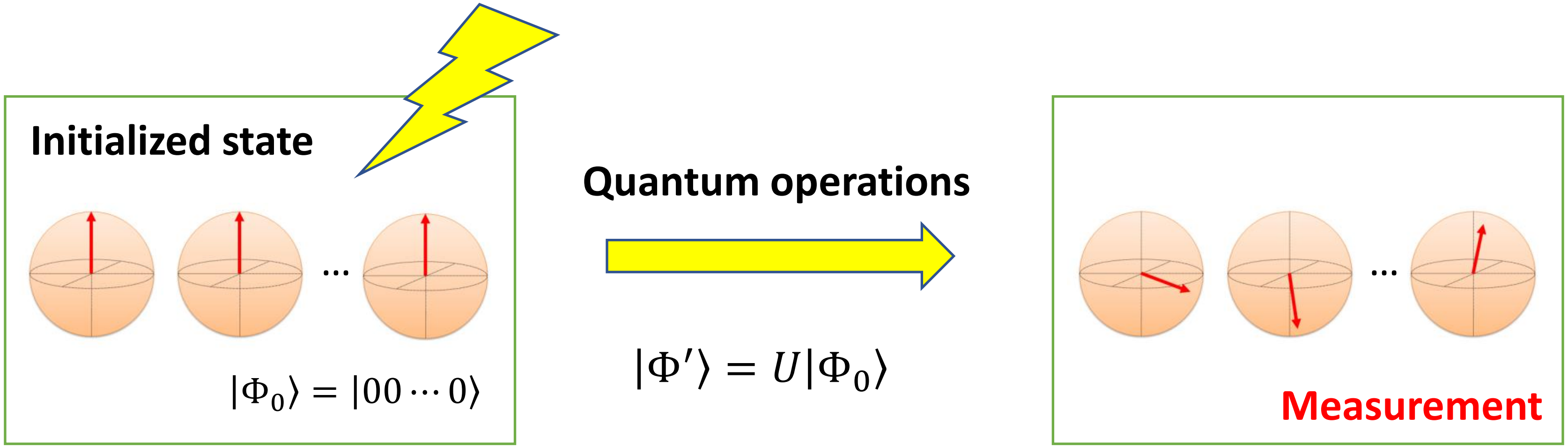
Electron spins: Quantum magnets

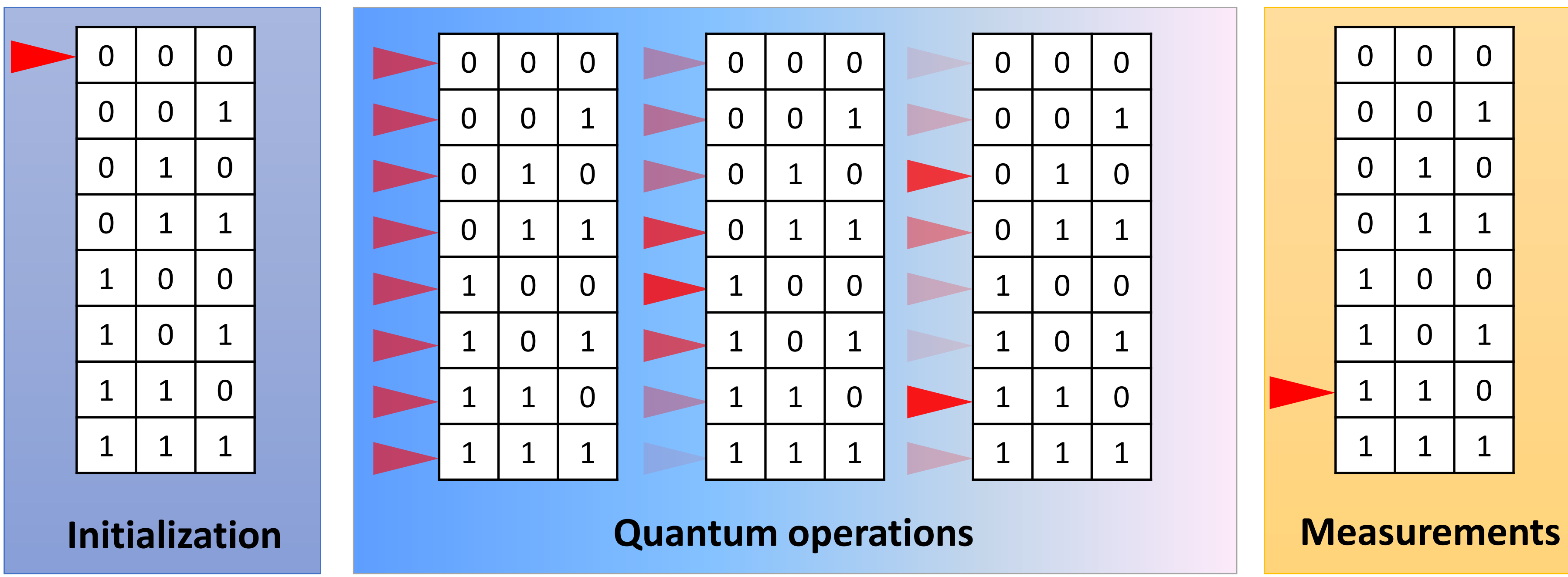


Pulsed ESR

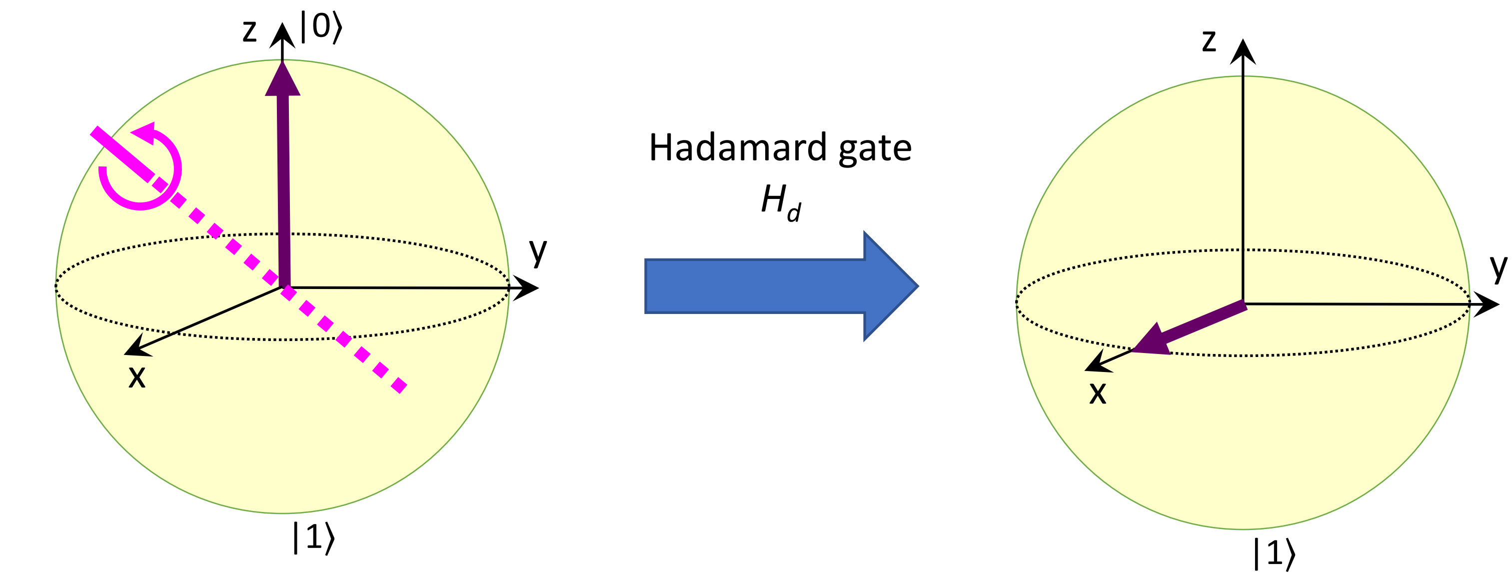


Quantum computing





An example of quantum operations



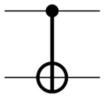
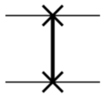
180° rotation along the axis
that bisects z and x axes

We can calculate the quantum state after quantum operations by matrix algebra

$$|\varphi\rangle = c_0|0\rangle + c_1|1\rangle = \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} \qquad H_d = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

$$H_d|\varphi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} c_0 + c_1 \\ c_0 - c_1 \end{pmatrix}$$

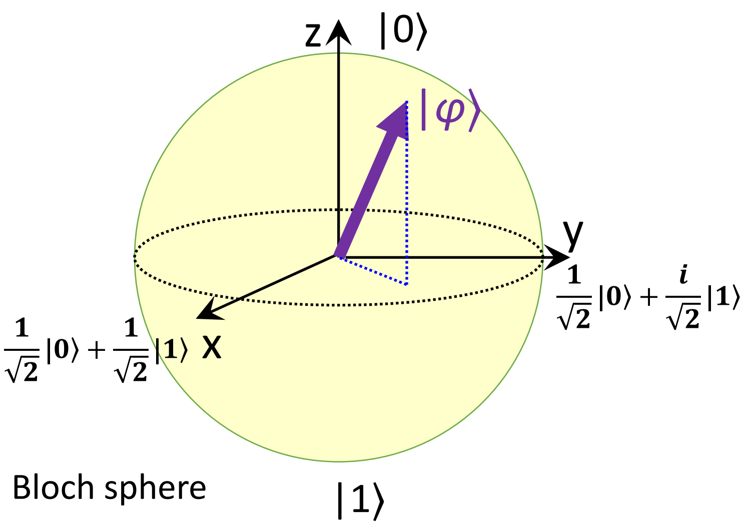
Quantum gates

Name	Circuit symbol	Matrix representation
Hadamard (H_d)	$\boxed{H_d}$	$\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$
Pauli-X	$\boxed{X}$	$\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$
Pauli-Y	$\boxed{Y}$	$\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$
Pauli-Z	$\boxed{Z}$	$\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$
$R_x(\theta)$	$\boxed{R_x(\theta)}$	$\begin{pmatrix}\cos\frac{\theta}{2} & -i\sin\frac{\theta}{2}\\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2}\end{pmatrix}$
$R_y(\theta)$	$\boxed{R_y(\theta)}$	$\begin{pmatrix}\cos\frac{\theta}{2} & -\sin\frac{\theta}{2}\\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2}\end{pmatrix}$
$R_z(\theta)$	$\boxed{R_z(\theta)}$	$\begin{pmatrix}e^{-i\theta/2} & 0\\ 0 & e^{i\theta/2}\end{pmatrix}$
$P(\theta)$	$\boxed{P(\theta)}$	$\begin{pmatrix}1 & 0\\ 0 & e^{i\theta}\end{pmatrix}$
CNOT		$\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & 1 & 0\end{pmatrix}$
SWAP		$\begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & 0 & 1\end{pmatrix}$

Pauli gates

Name	Circuit symbol	Matrix representation
Pauli-X	$\boxed{X}$	$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Pauli-Y	$\boxed{Y}$	$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
Pauli-Z	$\boxed{Z}$	$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

The quantum states on the *x*, *y*, and *z* axes are eigenfunction of the Pauli-*X*, *Y*, and *Z* operators, with the eigenvalues either 1 or −1.



Bloch sphere

$$X|+\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = |+\rangle$$

$$X|-\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} = \begin{pmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} = -|-\rangle$$

$$Y\left|+_y\right\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix} = \begin{pmatrix} -i^2/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix} = \left|+_y\right\rangle$$

$$Y\left|-_y\right\rangle = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1/\sqrt{2} \\ -i/\sqrt{2} \end{pmatrix} = \begin{pmatrix} i^2/\sqrt{2} \\ i/\sqrt{2} \end{pmatrix} = -\left|-_y\right\rangle$$

Rotational gates and phase shift gates

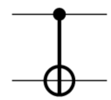
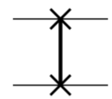
Name	Circuit symbol	Matrix representation
$R_x(\theta)$	$-\boxed{R_x(\theta)}-$	$\begin{pmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$
$R_y(\theta)$	$-\boxed{R_y(\theta)}-$	$\begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$
$R_z(\theta)$	$-\boxed{R_z(\theta)}-$	$\begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix}$
$P(\theta)$	$-\boxed{P(\theta)}-$	$\begin{pmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{pmatrix}$

R_x, R_y, and R_z gates are rotation gates along x, y, and z axes.
$P(\theta)$ is a phase shift gate.

The phase difference between the $|0\rangle$ and $|1\rangle$ states after the application of $R_z(\theta)$ and $P(\theta)$ gates are the same. Only global phase is different.

$P(\pi) = Z$, $P(\pi/2) = S$, $P(\pi/4) = T$

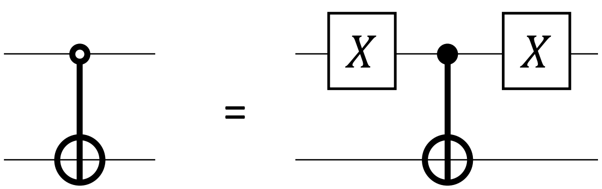
Two qubit gates

Name	Circuit symbol	Matrix representation
CNOT		$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$
SWAP		$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

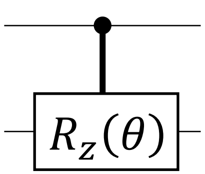
CNOT (controlled-NOT): Apply an NOT operation to the target qubit if and only if the control qubit is the $|1\rangle$ state.

SWAP exchanges quantum states of two qubits: $\mathrm{SWAP}[j,k]|q_j, q_k\rangle = |q_k, q_j\rangle$

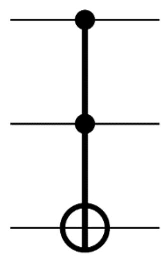
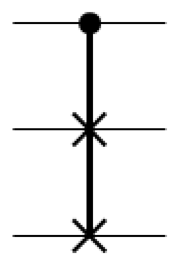
Open circle notation is also used when apply the quantum gate to the target qubit if and only if the control is the $|0\rangle$ state.



One can define a two qubit gate by adding a control qubit, like controlled-$R_z(\theta)$ gate,

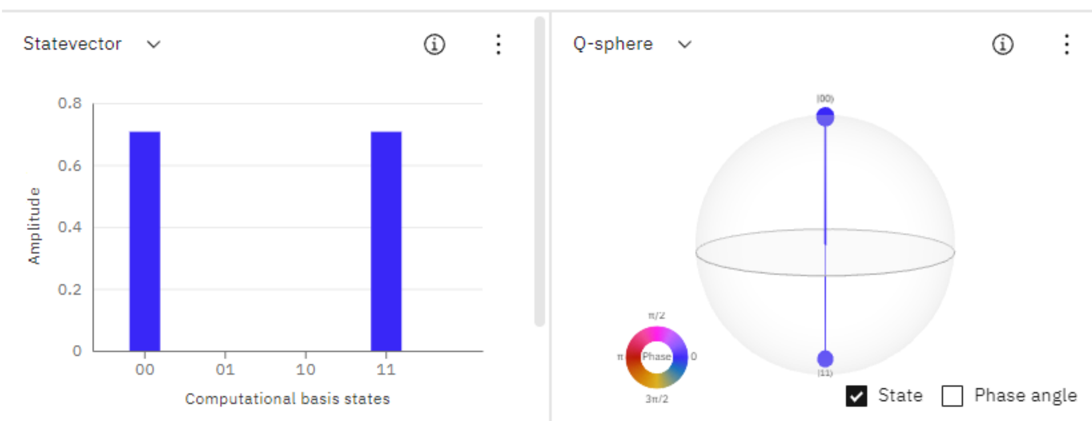


Three qubit gates

Name	Circuit symbol	Matrix representation
CCNOT (Toffoli)		$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$
C-Swap (Fredkin)		$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$
Deutsch's gate		$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & i\cos\theta & \sin\theta \\ 0 & 0 & 0 & 0 & 0 & 0 & \sin\theta & i\cos\theta \end{pmatrix}$

Bell states generations

Maximally entangled states in two-qubit system, known as <u>Bell states</u>, can be generated by combining Hadamard, Pauli-*X*, and CNOT gates.

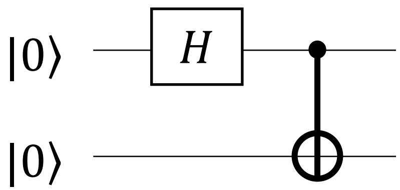


$$|00\rangle \xrightarrow{H\otimes I} \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle)$$

$$\xrightarrow{\mathrm{CNOT}[0,1]} \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

Bell states generations

Maximally entangled states in two-qubit system, known as <u>Bell states</u>, can be generated by combining Hadamard, Pauli-*X*, and CNOT gates.



$$|00\rangle \xrightarrow{H\otimes I} \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle) \xrightarrow{\mathrm{CNOT}[0,1]} \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

[Question]

How to construct quantum circuits to generate other three Bell states

$\boldsymbol{\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)}$, $\boldsymbol{\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)}$, **and** $\boldsymbol{\frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)}$

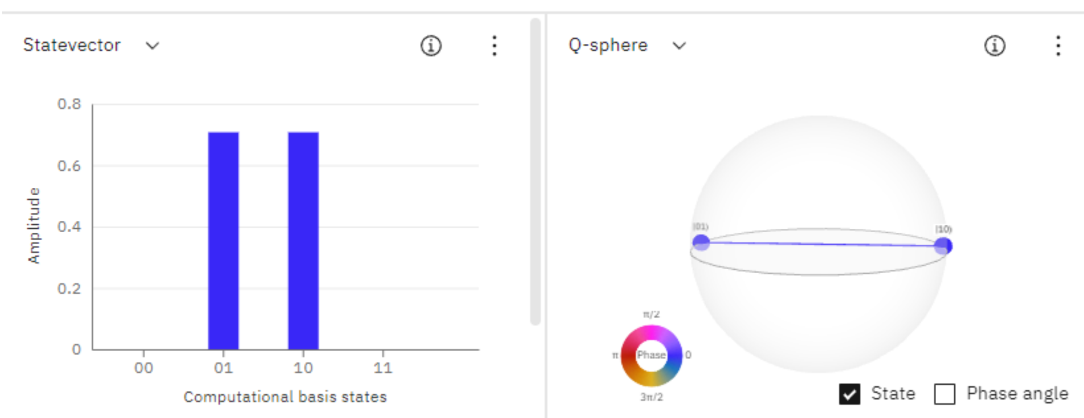
from the quantum state initialized to the $|00\rangle$ state using Hadamard, Pauli-X, and CNOT gates?

$$\begin{cases} H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \\ H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \end{cases} \quad \begin{cases} X|0\rangle = |1\rangle \\ X|1\rangle = |0\rangle \end{cases} \quad \begin{cases} \mathrm{CNOT}|00\rangle = |00\rangle \\ \mathrm{CNOT}|01\rangle = |01\rangle \\ \mathrm{CNOT}|10\rangle = |11\rangle \\ \mathrm{CNOT}|11\rangle = |10\rangle \end{cases}$$

Bell states generations

[Answer]

Generation of $\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$



$$|00\rangle \xrightarrow{H\otimes I} \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle)$$

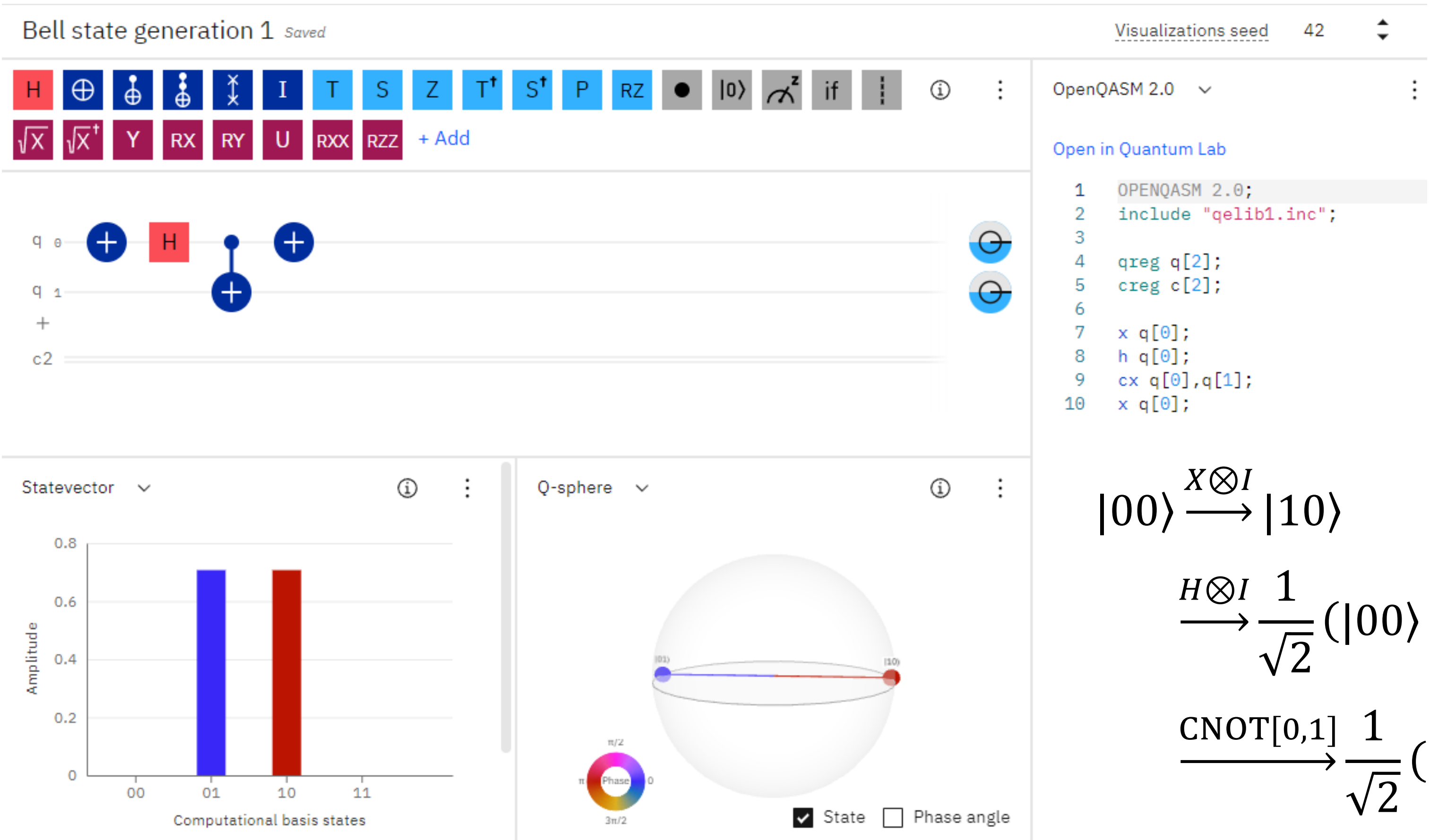
$$\xrightarrow{\text{CNOT}[0,1]} \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

$$\xrightarrow{X\otimes I} \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle)$$

Bell states generations

[Answer]

Generation of $\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$



$$|00\rangle \xrightarrow{X\otimes I} |10\rangle$$

$$\xrightarrow{H\otimes I} \frac{1}{\sqrt{2}}(|00\rangle - |10\rangle)$$

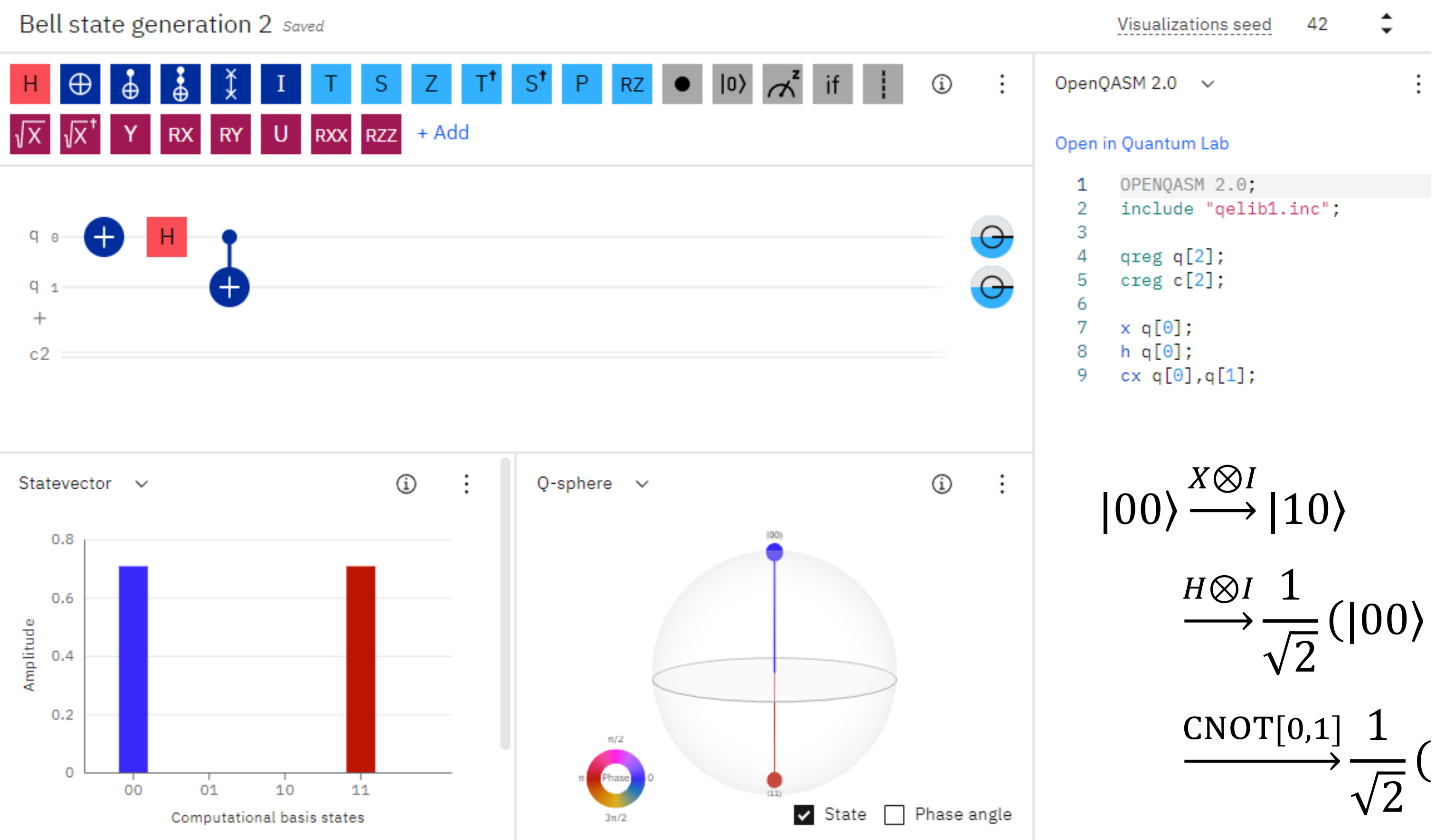
$$\xrightarrow{\mathrm{CNOT}[0,1]} \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$$

$$\xrightarrow{X\otimes I} \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle)$$

Bell states generations

[Answer]

Generation of $\frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$



$$|00\rangle \xrightarrow{X \otimes I} |10\rangle$$

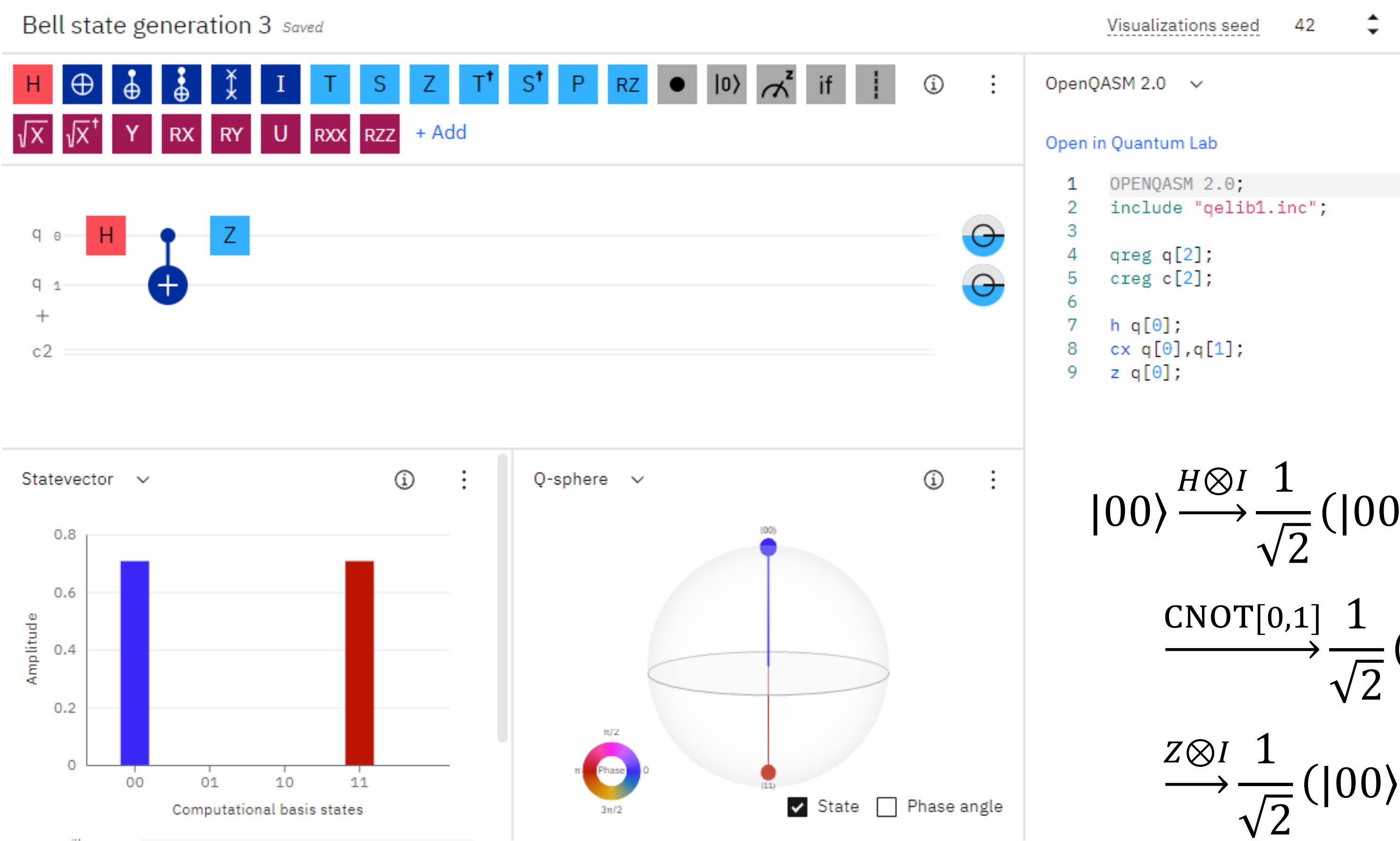
$$\xrightarrow{H \otimes I} \frac{1}{\sqrt{2}}(|00\rangle - |10\rangle)$$

$$\xrightarrow{\text{CNOT}[0,1]} \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$$

* There are many other quantum circuits to generate the same Bell state.

Bell states generations

Generation of $\frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$



$$|00\rangle \xrightarrow{H\otimes I} \frac{1}{\sqrt{2}}(|00\rangle + |10\rangle)$$

$$\xrightarrow{\text{CNOT}[0,1]} \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$$

$$\xrightarrow{Z\otimes I} \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$$

Universal quantum gate sets

Any unitary operation in the Hilbert space of *n*-qubits can be decomposed by using universal quantum gate sets.

1) Arbitrary one qubit rotation gates and CNOT gate
2) Hadamard + phase (S) + CNOT + π/8 (T) gates
3) Deutsch's gate

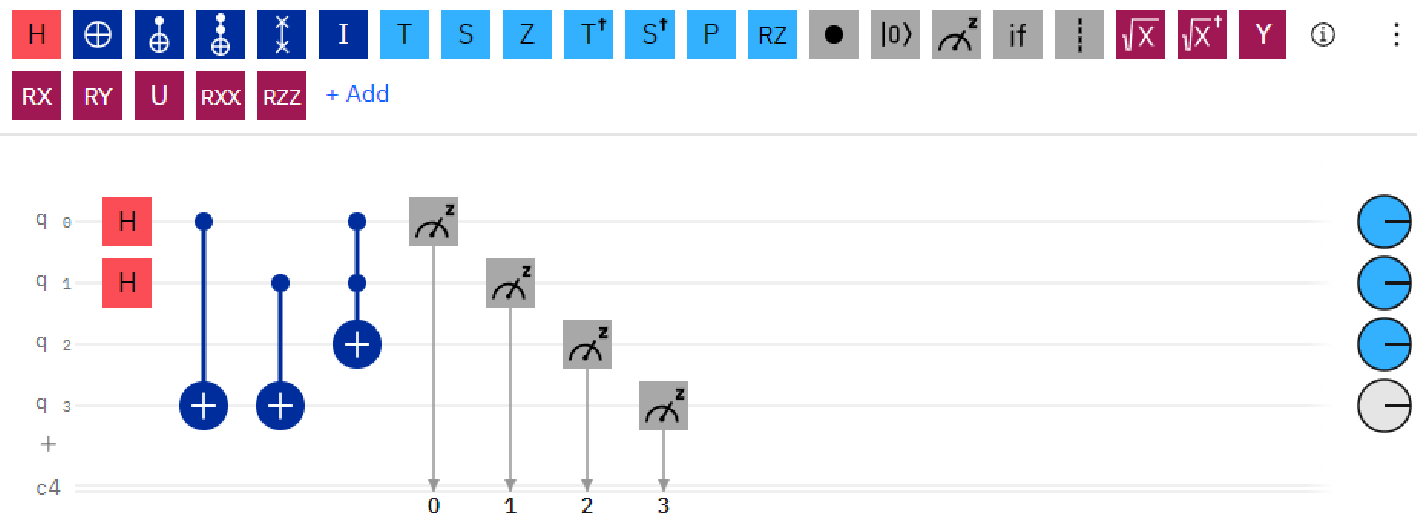
☆ **Gottesman–Knill theorem**

Stabilizer circuits can be efficiently simulated on classical computers.

Preparation of qubits in computational basis states.
Quantum gates from the Clifford group (H_d, S, $S^\dagger$, CNOT, and Pauli-X, Y, and Z)
Measurement in computational basis

D. Gottesman, The Heisenberg representation of quantum computers. arXiv:quant-ph/9807006.

Quantum circuits



OpenQASM 2.0

Open in Quantum Lab

```
OPENQASM 2.0;
include "qelib1.inc";

qreg q[4];
creg c[4];

h q[0];
h q[1];
cx q[0],q[3];
cx q[1],q[3];
ccx q[0],q[1],q[2];
measure q[0] -> c[0];
measure q[1] -> c[1];
measure q[2] -> c[2];
measure q[3] -> c[3];
```

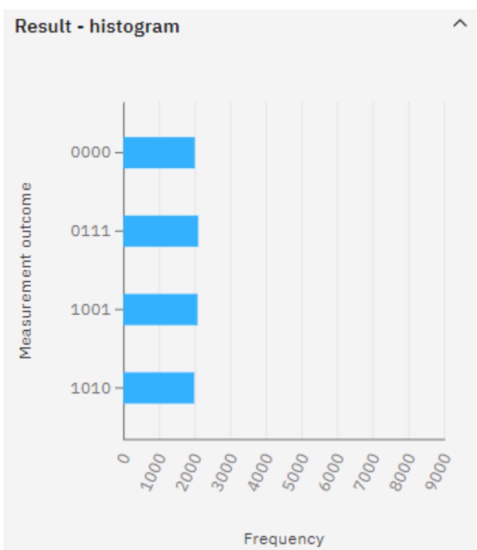
$$|0000\rangle \xrightarrow{H\otimes I\otimes I\otimes I} \frac{1}{\sqrt{2}}(|0000\rangle + |1000\rangle)$$

$$\xrightarrow{I\otimes H\otimes I\otimes I} \frac{1}{2}(|0000\rangle + |0100\rangle + |1000\rangle + |1100\rangle)$$

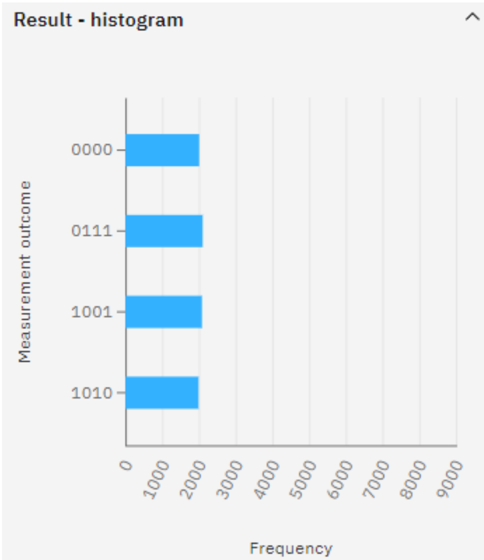
$$\xrightarrow{\mathrm{CNOT}[0,3]} \frac{1}{2}(|0000\rangle + |0100\rangle + |1001\rangle + |1101\rangle)$$

$$\xrightarrow{\mathrm{CNOT}[1,3]} \frac{1}{2}(|0000\rangle + |0101\rangle + |1001\rangle + |1100\rangle)$$

$$\xrightarrow{\mathrm{CCNOT}[0,1,2]} \frac{1}{2}(|0000\rangle + |0101\rangle + |1001\rangle + |1110\rangle)$$

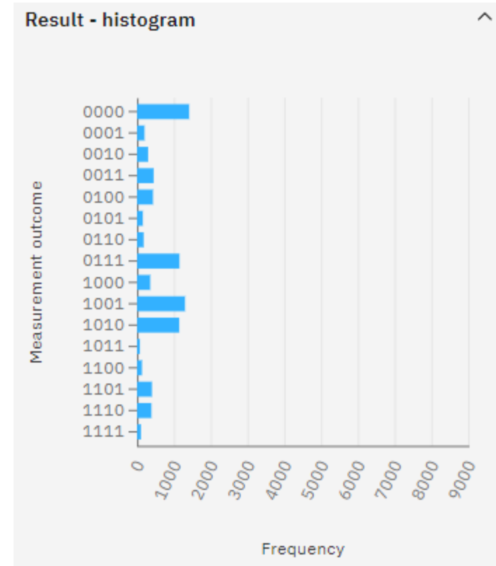


Quantum circuits

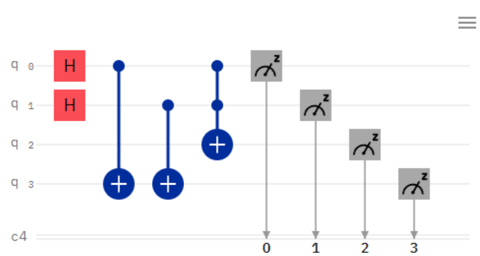


Ideal results

Results from real quantum computer (ibmq_manila)

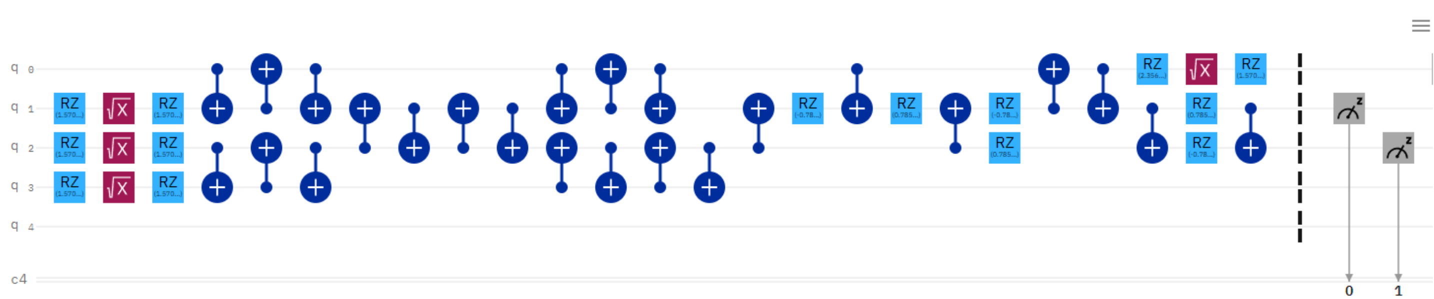


Original circuit



5 quantum gates –(transpilation)→ 42 quantum gates

Transpiled circuit



Quantum devices

ibmq_manila

Details

5
Qubits

32
Quantum Volume

Status:	Online
Total pending jobs:	73 jobs
Processor type ⓘ:	Falcon r5.11L
Version:	1.0.10
Basis gates:	CX, ID, RZ, SX, X
Your usage:	66 jobs

Avg. CNOT Error:	8.525e-3
Avg. Readout Error:	2.218e-2
Avg. T1:	135.26 us
Avg. T2:	71.21 us
Providers with access:	2 Providers ↓
Supports Qiskit Runtime:	Yes

Your upcoming reservations 0

Calibration data

Last calibrated: 25 minutes ago

Map view | Graph view | Table view

Qubit:
Frequency (GHz)
Avg 4.971
min 4.838 max 5.066

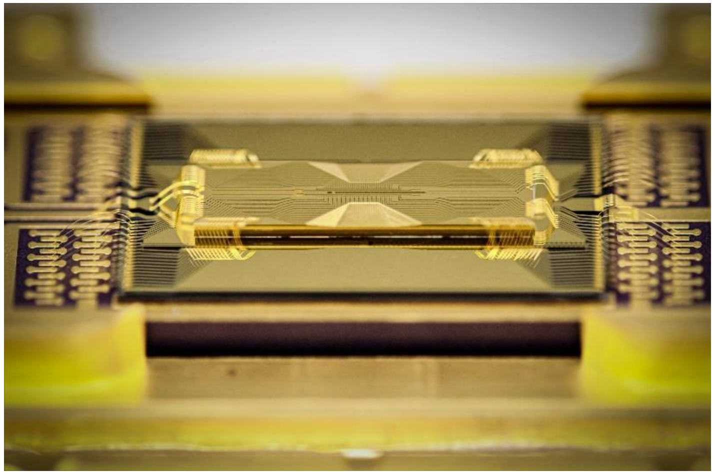
Connection:
CNOT error
Avg 8.525e-3
min 6.823e-3 max 1.017e-2

NISQ devices

Noisy Intermediate-Scale Quantum devices

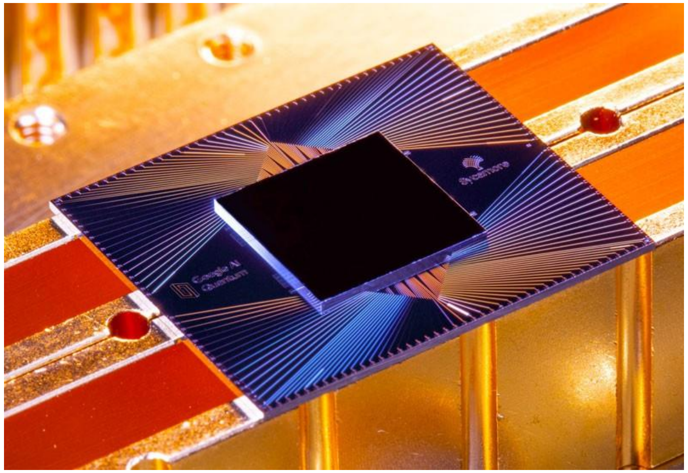
J. Preskill, *Quantum* **2018**, *2*, 79.

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



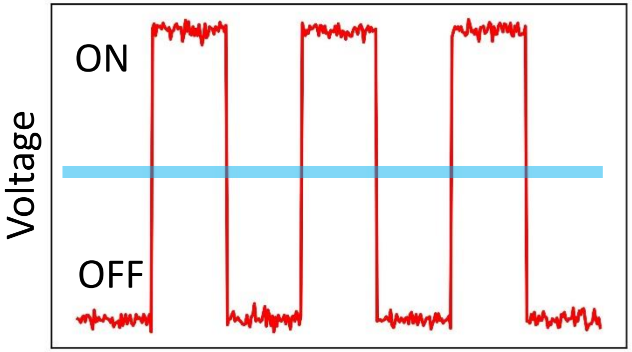
IonQ's EGT Series Ion Trap Chip
Photo taken from IonQ's website

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



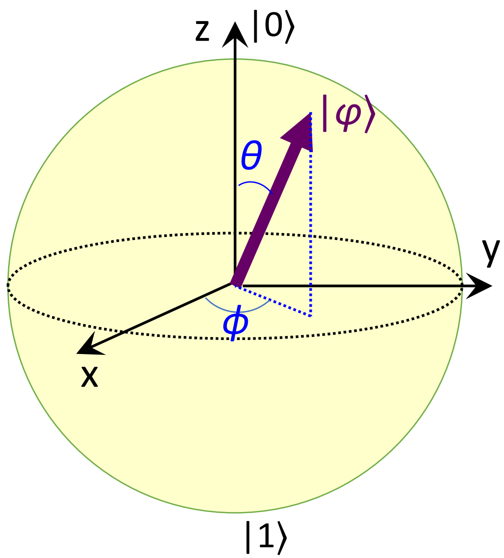
Google's 54-qubit quantum chip "Sycamore"
Photo taken from *Nature* **2019**, *574*, 461–462.

Quantum error correction



Classical bit is robust against noise

- "On" if the voltage is higher than the threshold, otherwise "Off".
- Noises and errors will reset every time the operation proceeds.



Quantum bit is very fragile against noise

- Different θ and ϕ means different quantum states
- The error accumulates by proceeding operations.
- Quantum superposition can be broken by system-environment interactions (decoherence)

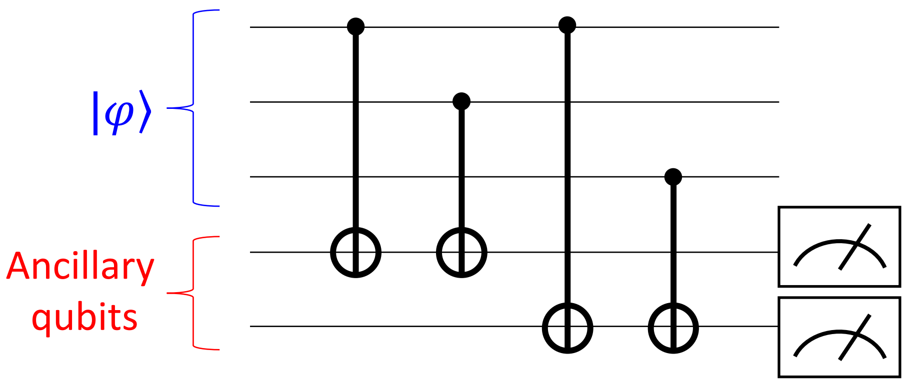
Use multiple physical qubits to retain information of one logical qubit!

The three-qubit bit-flip code

- Use three physical qubits for one logical qubits.
- Need two ancillary qubits to detect/correct single bit-flip error.

$$|0\rangle \rightarrow |0_L\rangle \equiv |000\rangle \qquad |1\rangle \rightarrow |1_L\rangle \equiv |111\rangle$$

$$|\varphi\rangle = c_0|0_L\rangle + c_1|1_L\rangle \equiv c_0|000\rangle + c_1|111\rangle$$



Situation	Quantum state before error correction	Quantum state after measurement	Measurement outcome
No bit-flip error	$(c_0|000\rangle + c_1|111\rangle) \otimes |00\rangle$	$(c_0|000\rangle + c_1|111\rangle) \otimes |00\rangle$	00
1st qubit flip	$(c_0|100\rangle + c_1|011\rangle) \otimes |00\rangle$	$(c_0|100\rangle + c_1|011\rangle) \otimes |11\rangle$	**11**
2nd qubit flip	$(c_0|010\rangle + c_1|101\rangle) \otimes |00\rangle$	$(c_0|010\rangle + c_1|101\rangle) \otimes |10\rangle$	10
3rd qubit flip	$(c_0|001\rangle + c_1|110\rangle) \otimes |00\rangle$	$(c_0|001\rangle + c_1|110\rangle) \otimes |01\rangle$	01