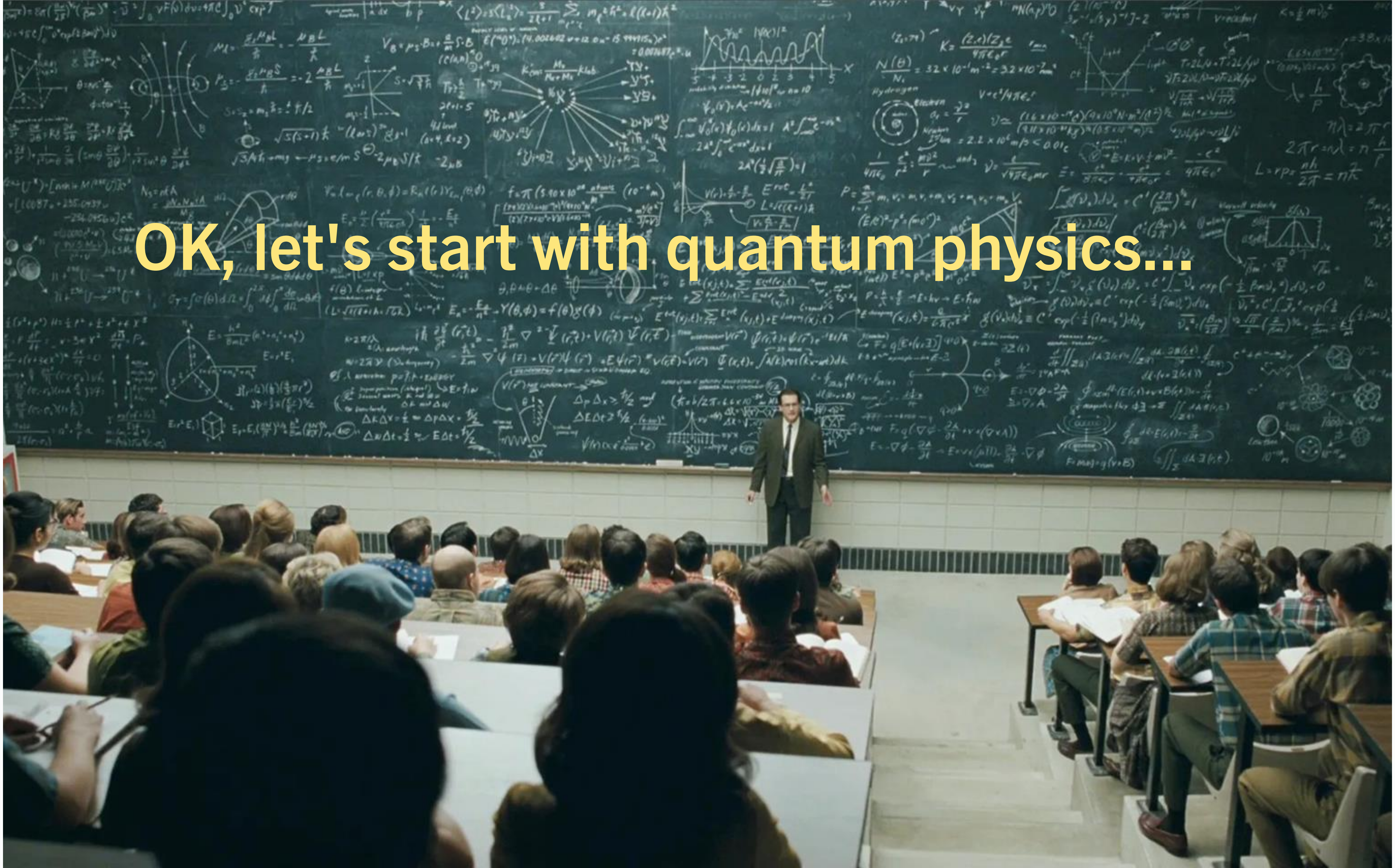
Photo by eberhard grossgasteiger on Unsplash

Introduction to Quantum Computing

Greg Byrd, NC State

Quantum Machine Learning Workshop

NC State, January 2023



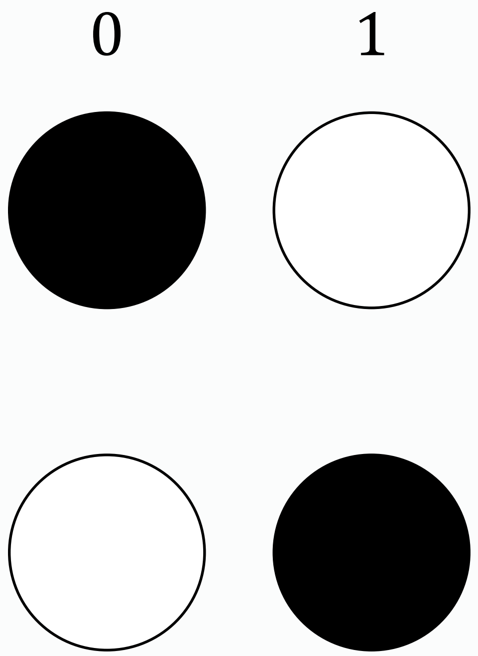
A Serious Man, Joel and Ethan Coen

1. Qubits, Gates, and Circuits
2. Quantum Computers

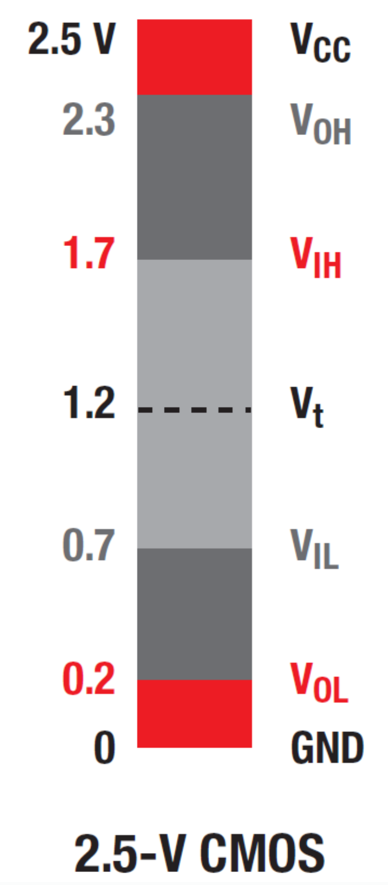
Break

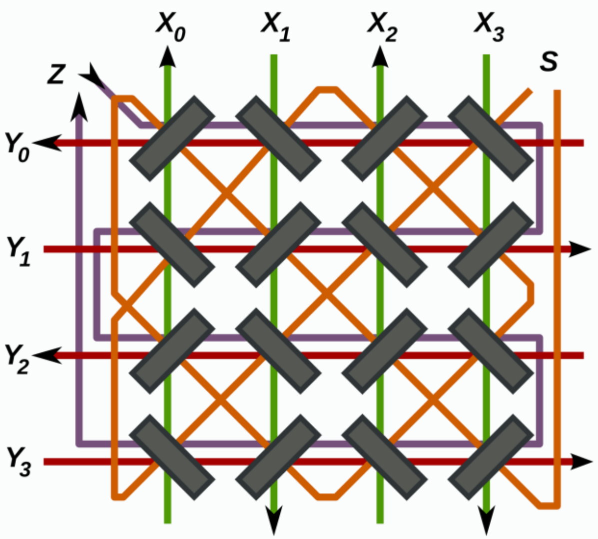
3. Introductory Algorithms
4. Variational Algorithms (VQA)

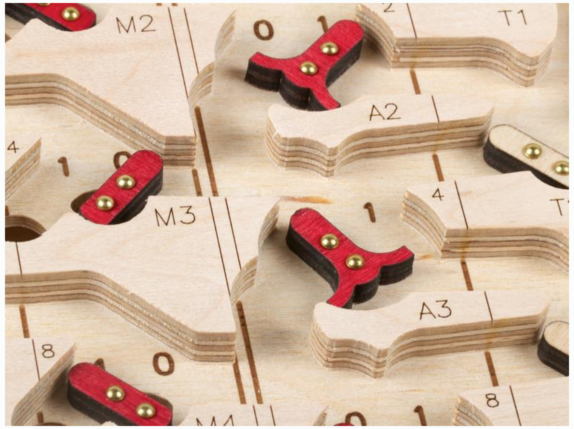
Classical Bit



Physical implementations





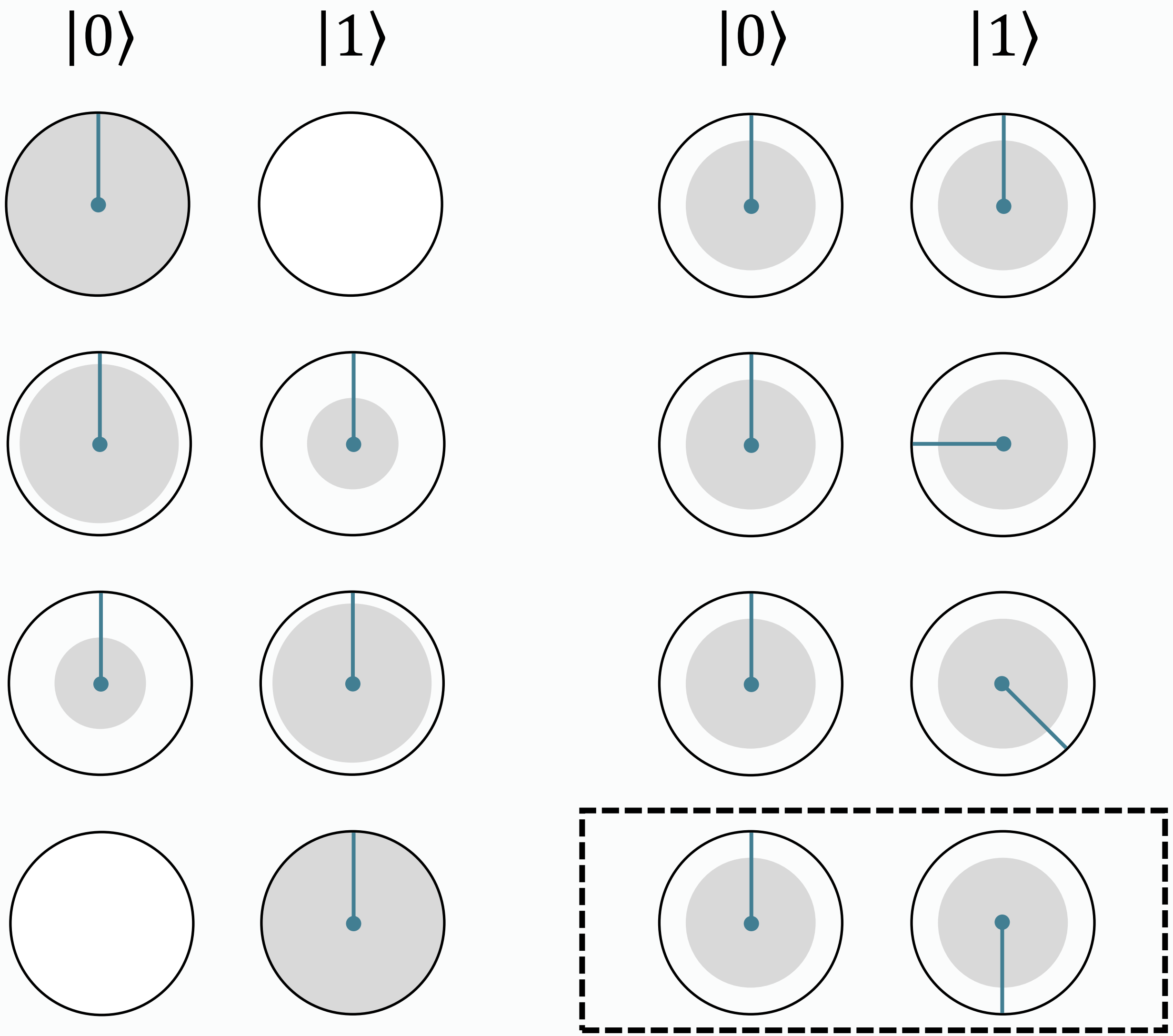


https://www.ti.com/lit/pdf/sdyu001

https://en.wikipedia.org/wiki/Magnetic-core_memory

https://shop.evilmadscientist.com/productsmenu/375

Quantum Bit (Qubit)



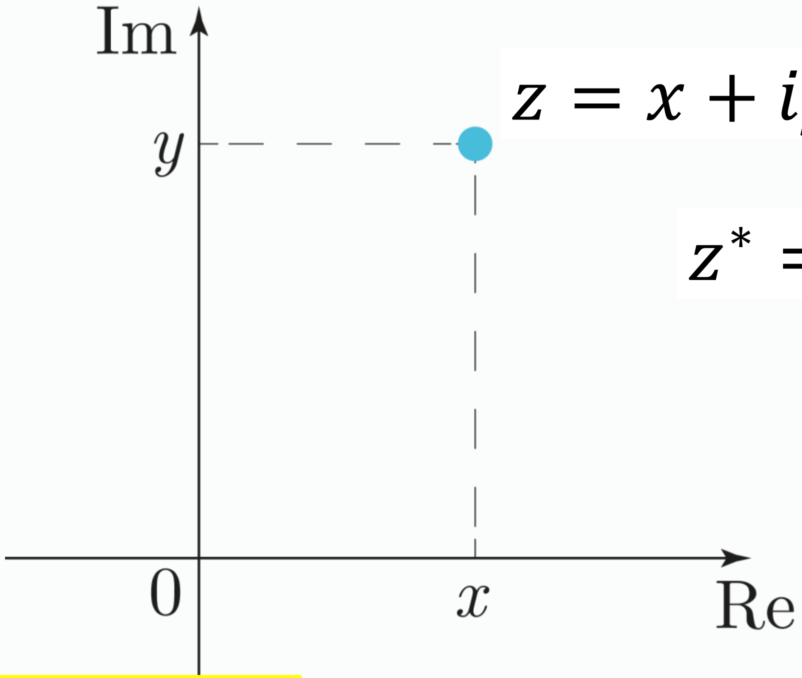
Superposition:
Linear combination of 0 and 1 states

$$\alpha|0\rangle + \beta|1\rangle$$

$$|\alpha|^2 + |\beta|^2 = 1$$

2 complex numbers

Complex Numbers

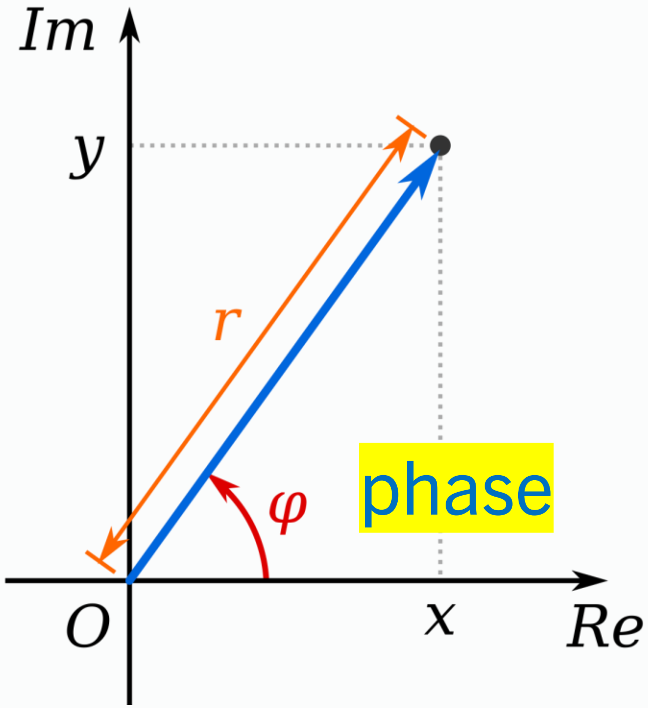


$z = x + iy$

$z^* = x - iy$

magnitude

$$|z| = \sqrt{x^2 + y^2} = \sqrt{zz^*}$$



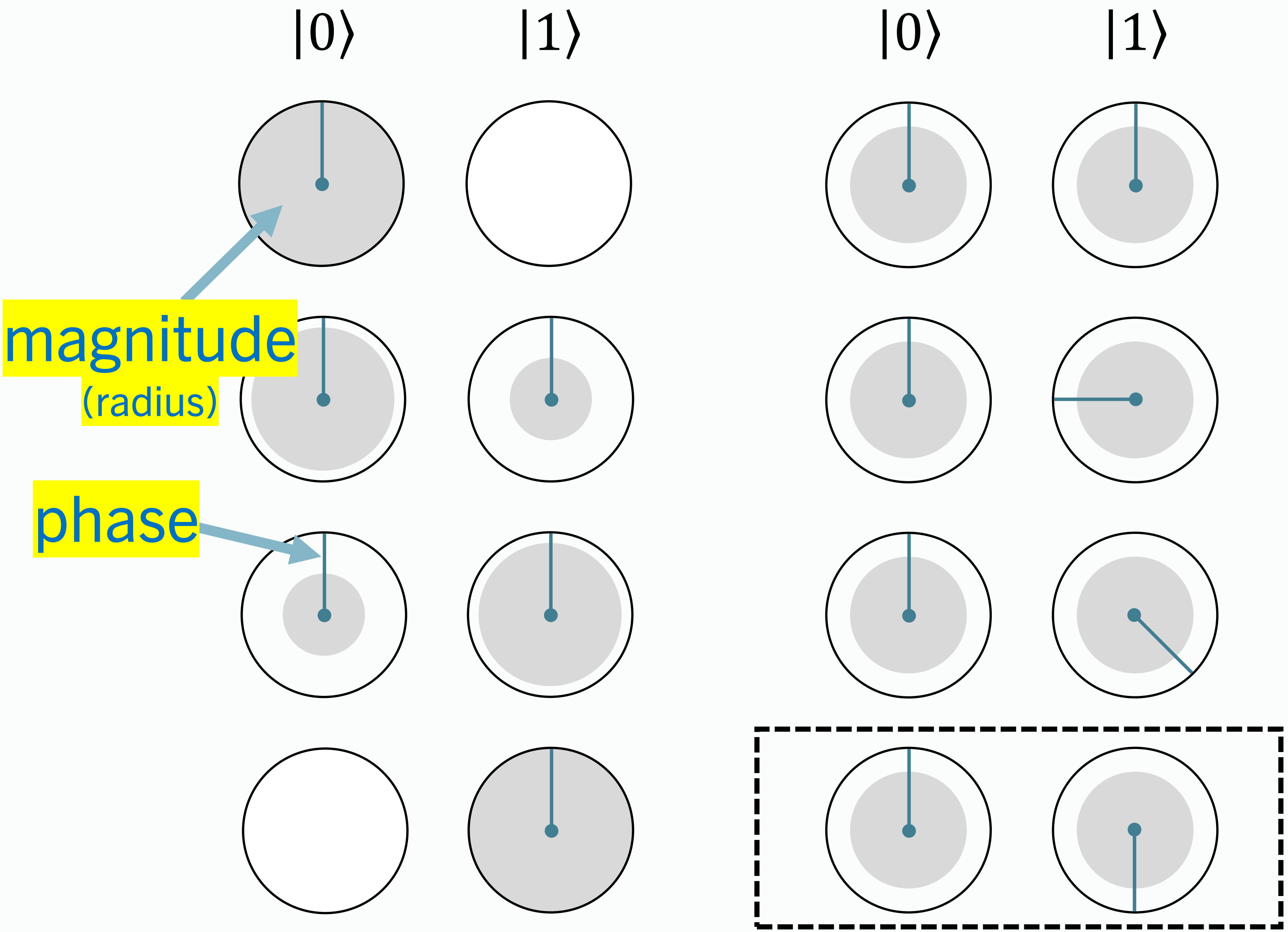
phase

$$z = re^{i\varphi} = r(\cos\varphi + i\sin\varphi)$$

$$e^{i\varphi} = \cos\varphi + i\sin\varphi$$

https://en.wikipedia.org/wiki/Complex_number

Quantum Bit (Qubit)



Superposition:
Linear combination of 0 and 1 states

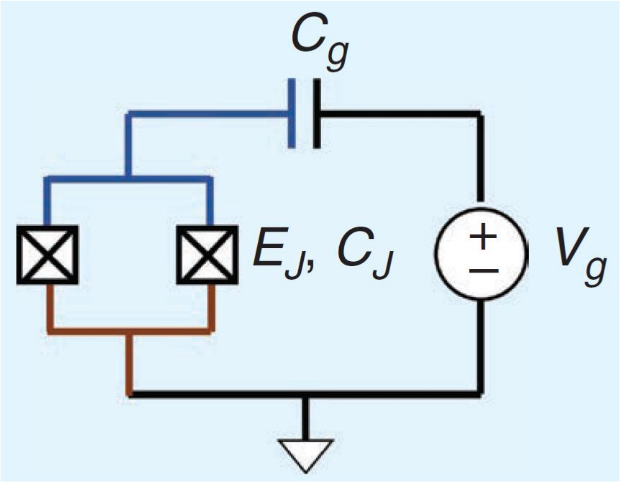
$$\alpha|0\rangle + \beta|1\rangle$$

$$|\alpha|^2 + |\beta|^2 = 1$$

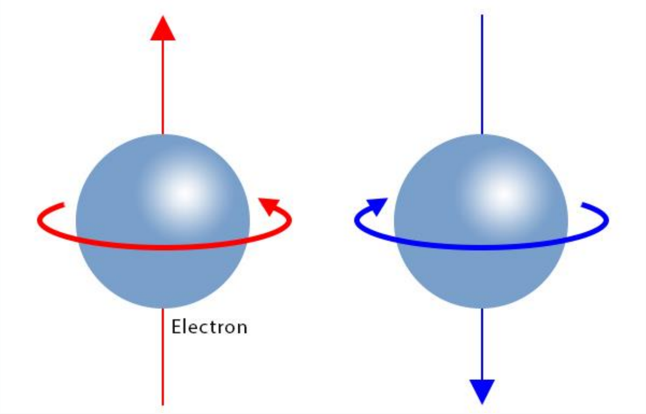
amplitude

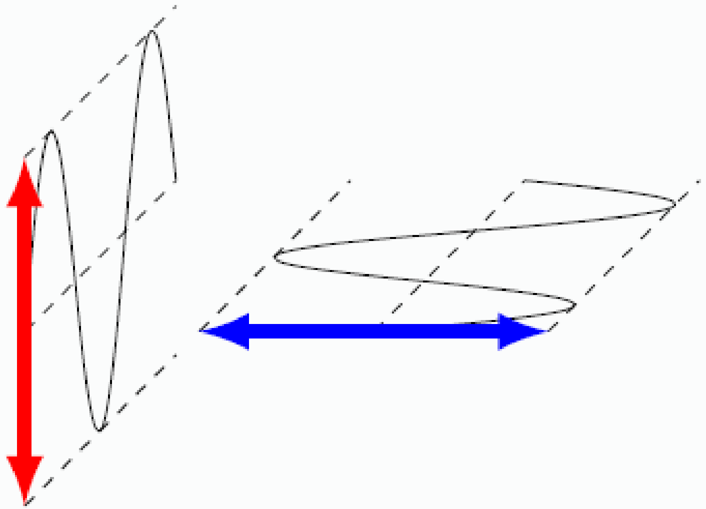
2 complex numbers

Physical Qubits

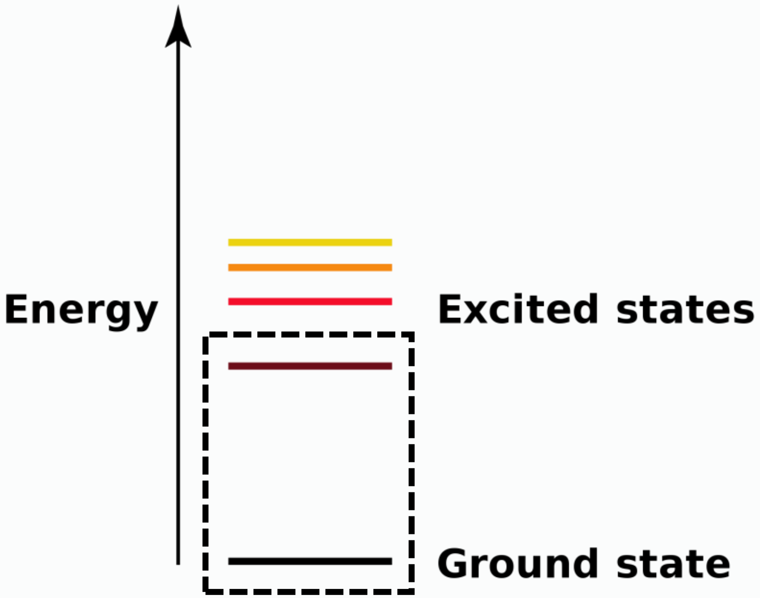


Roth, et al. IEEE Antennas & Prop. 2022





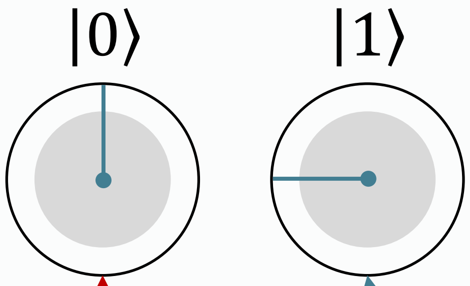
https://www.chemistrylearner.com/spin-quantum-number.html



https://en.wikipedia.org/wiki/Energy_level

https://medium.com/@lindat/how-quantum-computers-and-machine-learning-will-revolutionize-big-data-571d5594e9b8

Ket Notation, Vector Space



A qubit state is a unit-length ***vector.***

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$|\psi\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \alpha|0\rangle + \beta|1\rangle$$

$$|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\| |\psi\rangle \|_2 = \sqrt{|\alpha|^2 + |\beta|^2} = 1$$

ket

Any state can be expressed as a linear combination of $|0\rangle$ and $|1\rangle$.

Vector space (Hilbert space) with $|0\rangle$ and $|1\rangle$ as **basis vectors.**

Bra-Ket Notation

$$|\psi\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

A **ket** is a column vector.

$$\langle\psi| = |\psi\rangle^\dagger = [\alpha^* \quad \beta^*]$$

A **bra** is a row vector,
the conjugate transpose of a ket.

$$\langle\psi|\gamma\rangle$$

A **bra-ket** is an *inner product*.

Inner Product

$$|\psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$$

$$|\gamma\rangle = \begin{bmatrix} c \\ d \end{bmatrix}$$

$$\langle\psi|\gamma\rangle = \begin{bmatrix} a^* & b^* \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix} = a^*c + b^*d$$

$$\langle\psi|\psi\rangle = 1$$

$$\langle 0|1\rangle = 0$$

$$|\langle\psi|\gamma\rangle| = \begin{cases} 0, \text{ if orthogonal} \\ 1, \qquad \text{if equal} \\ < 1, \text{ otherwise} \end{cases}$$

Outer Product

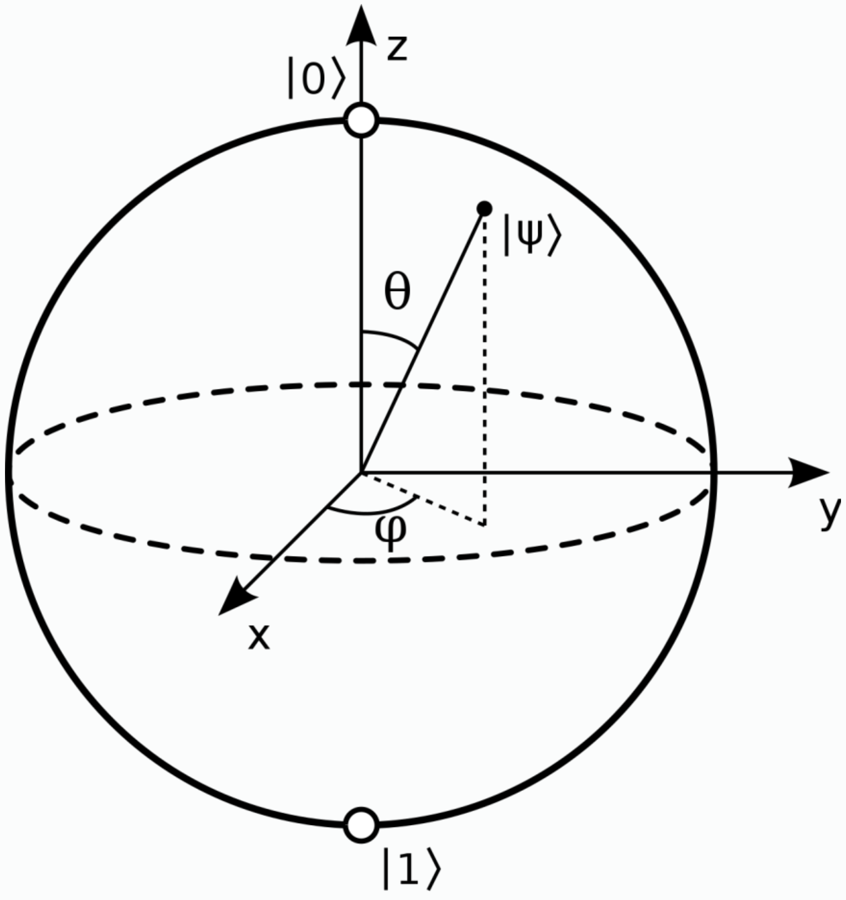
$$|\psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$$

$$|\gamma\rangle = \begin{bmatrix} c \\ d \end{bmatrix}$$

$$|\psi\rangle\langle\gamma| = \begin{bmatrix} a \\ b \end{bmatrix} \begin{bmatrix} c^* & d^* \end{bmatrix} = \begin{bmatrix} ac^* & ad^* \\ bc^* & bd^* \end{bmatrix}$$

Can be viewed as "a matrix that transforms state $|\gamma\rangle$ into state $|\psi\rangle$."

Bloch Sphere



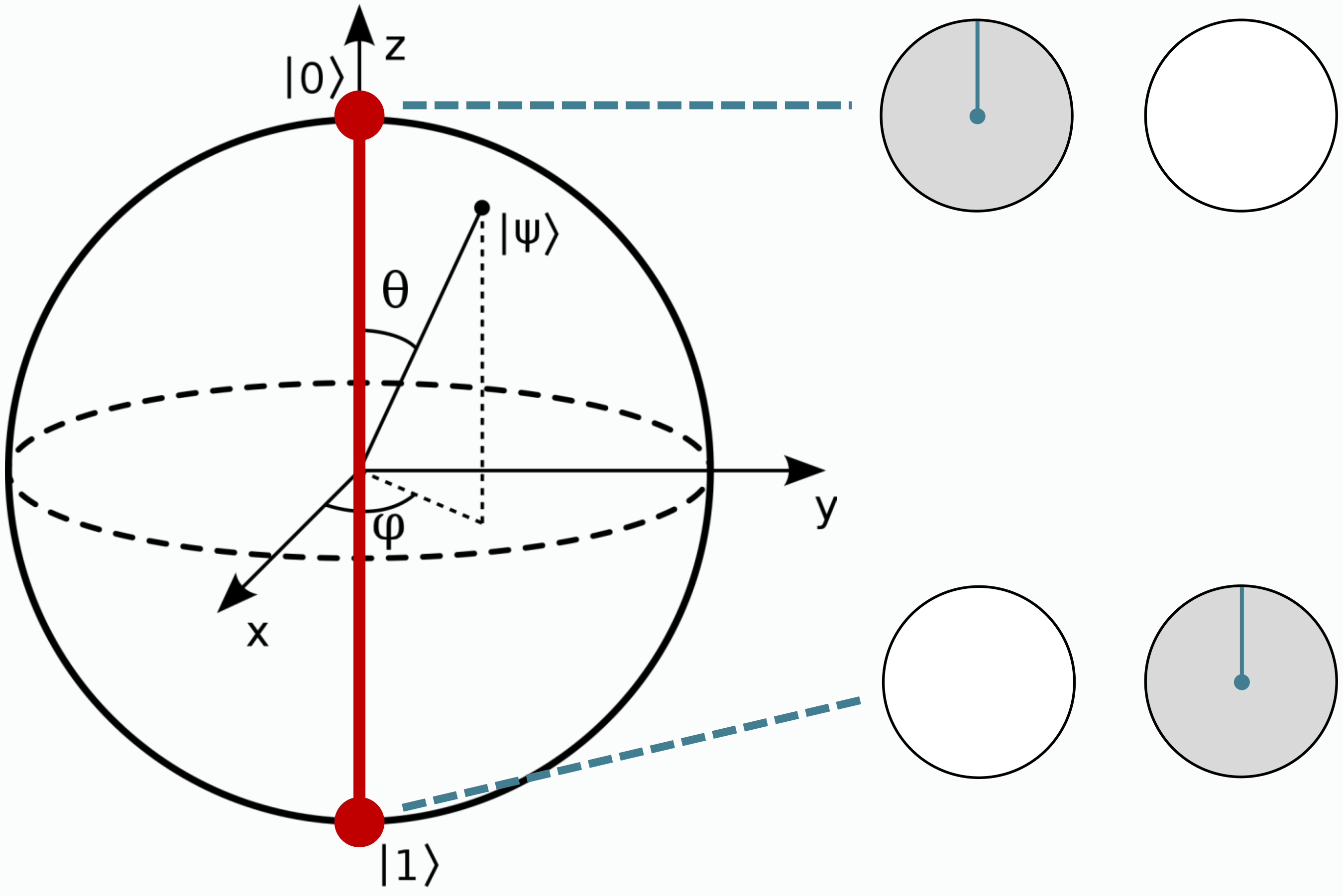
$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle$$

$$|\psi\rangle = \begin{bmatrix}\alpha \\ \beta\end{bmatrix} = \begin{bmatrix}\cos\frac{\theta}{2} \\ e^{i\varphi}\sin\frac{\theta}{2}\end{bmatrix}$$

Quantum state is a vector that ends on the **surface** (norm = 1).

https://en.wikipedia.org/wiki/Bloch_sphere

Bloch Sphere



$|0\rangle: \theta = 0, \varphi = 0$

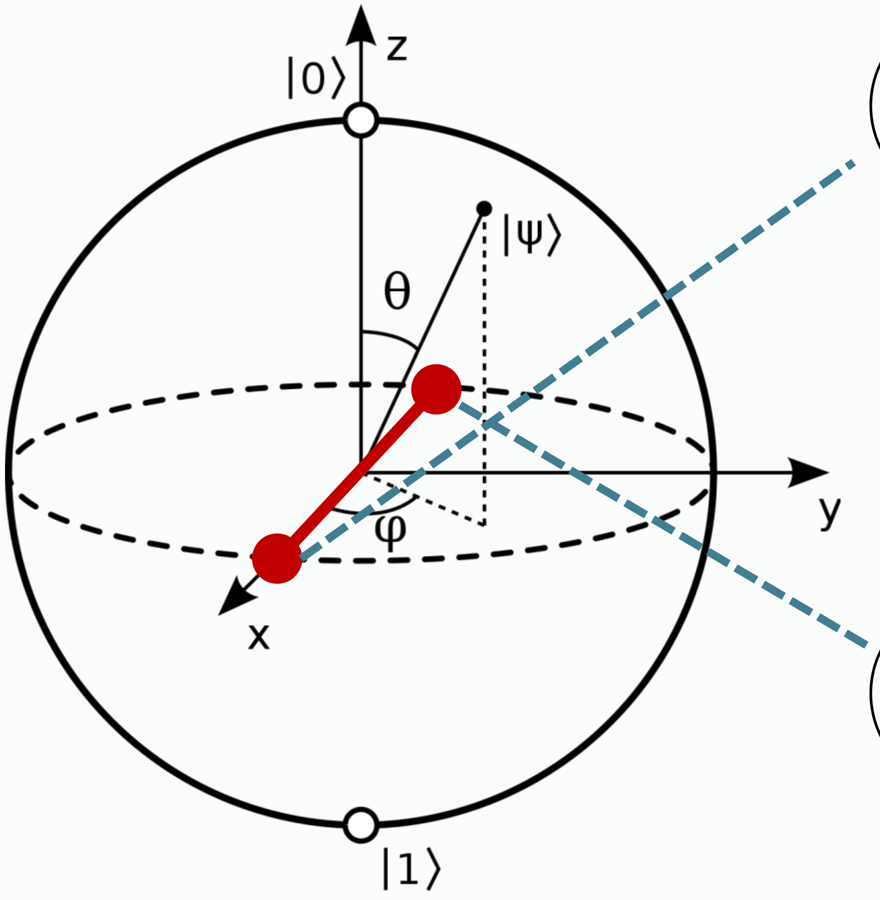
$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

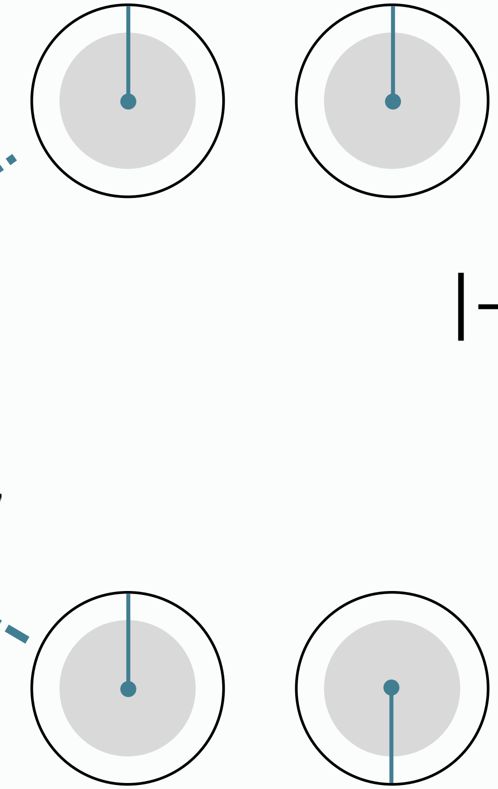
$|1\rangle: \theta = \pi, \varphi = 0$

$$|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

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

Bloch Sphere





$$|+\rangle: \theta = \frac{\pi}{2}, \varphi = 0$$

$$|+\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}$$

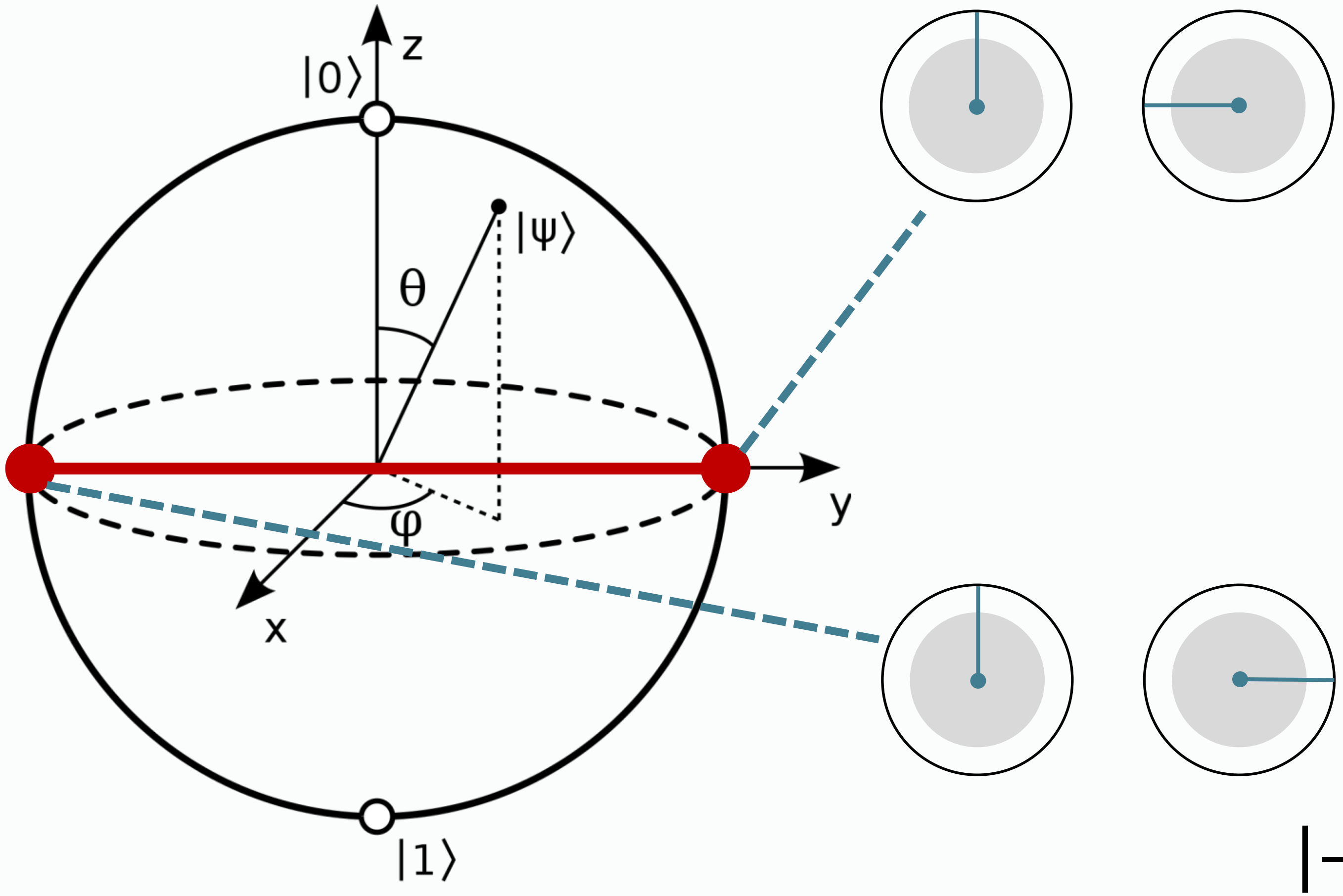
$$|-\rangle: \theta = \frac{\pi}{2}, \varphi = \pi$$

$$|-\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{\sqrt{2}}|1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}$$

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

$$e^{i\pi} = -1$$

Bloch Sphere



$$|i\rangle : \theta = \frac{\pi}{2}, \varphi = \frac{\pi}{2}$$

$$|i\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{i}{\sqrt{2}}|1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix}$$

$$e^{i\pi/2} = i$$

$$|-i\rangle : \theta = \frac{\pi}{2}, \varphi = \frac{3\pi}{2}$$

$$|-i\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{i}{\sqrt{2}}|1\rangle = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix}$$

$$e^{i3\pi/2} = -i$$

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

Density Matrix

$$|\psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$$ *pure state*

$$\mathrm{Tr}(\rho) = 1$$

$$\rho = |\psi\rangle\langle\psi| = \begin{bmatrix} a \\ b \end{bmatrix} \begin{bmatrix} a^* & b^* \end{bmatrix} = \begin{bmatrix} aa^* & ab^* \\ ba^* & bb^* \end{bmatrix}$$

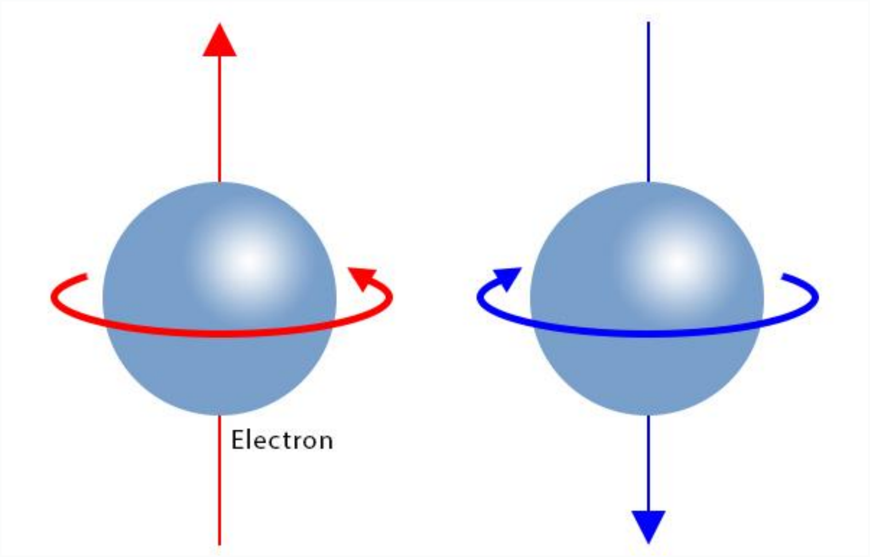
The density matrix ρ is a more general representation of a quantum state. States on the Bloch sphere surface are pure states. Can also represent mixed states, useful for other purposes.

A one-qubit quantum state is a two-dimensional vector in a Hilbert space.

$$|\psi\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \alpha \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \alpha|0\rangle + \beta|1\rangle$$

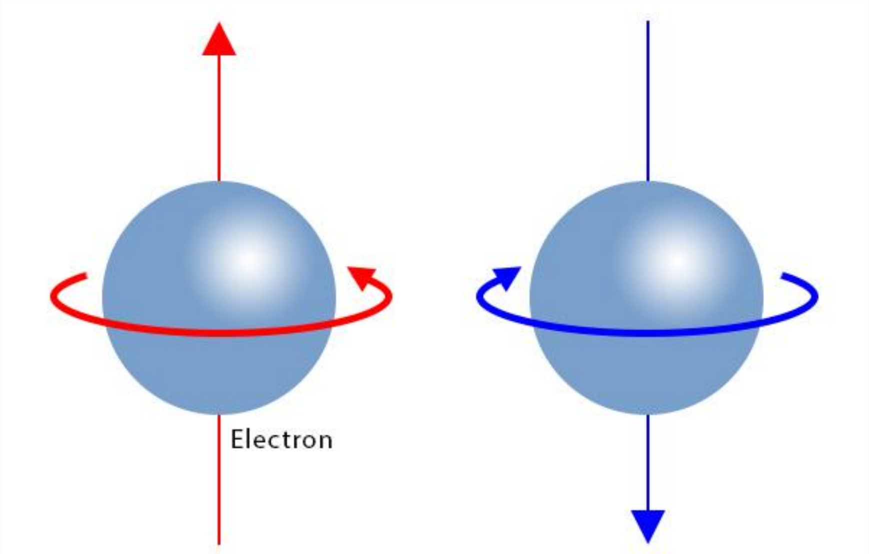
$$|\alpha|^2 + |\beta|^2 = 1$$

Photo by Immo Wegmann on Unsplash



To learn the state of a physical qubit,
we **measure** it.

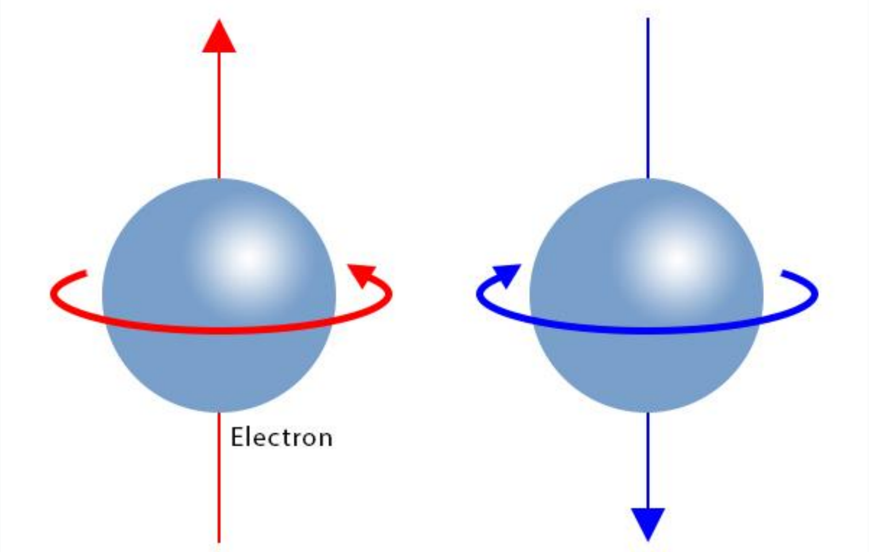
Measurement



When we measure the spin of
an electron, we get a binary result:

spin up
or
spin down

Measurement



When we measure the spin of an electron, we get a binary result:

spin up
or
spin down

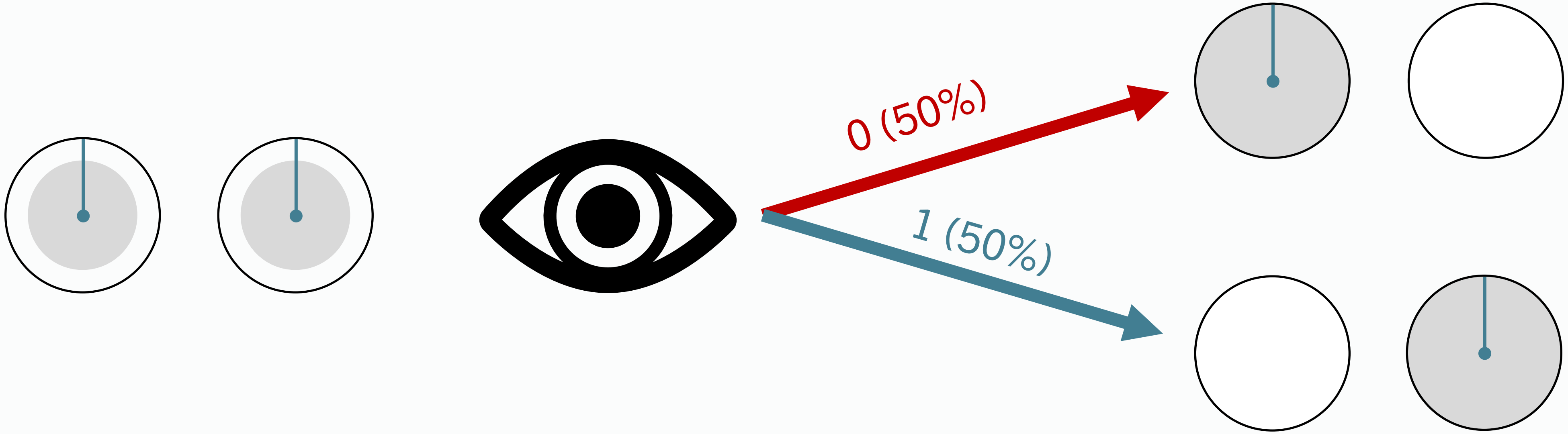
What if qubit is in superposition? $$|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$$

We get up with probability $|\alpha|^2$ and down with probability $|\beta|^2$.

Measurement is Destructive

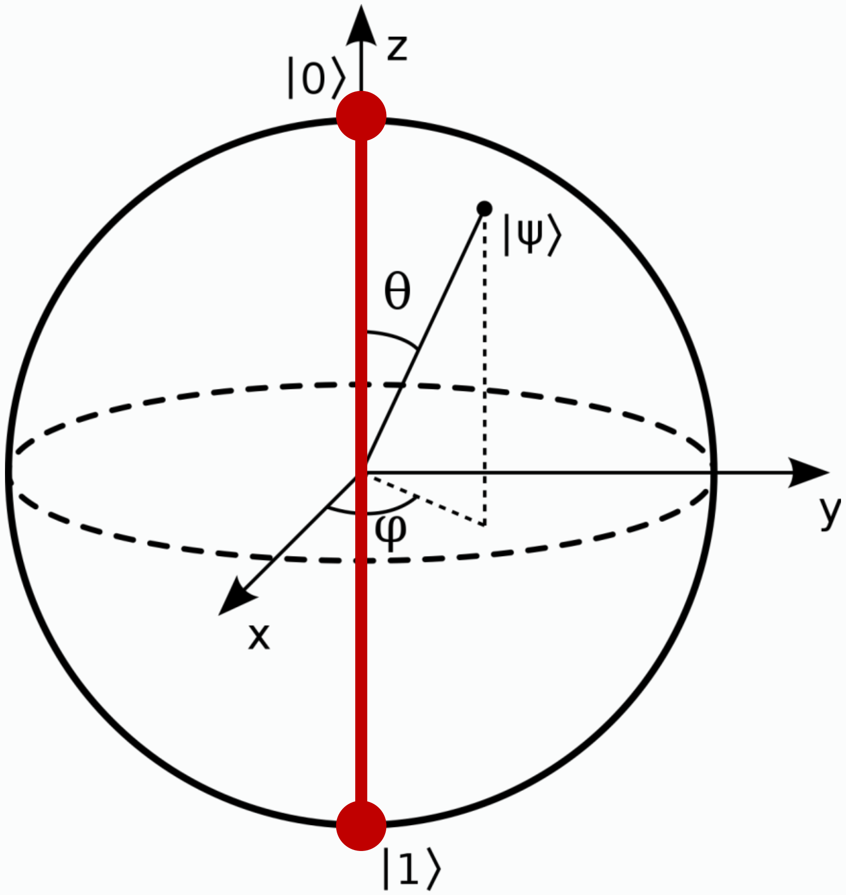
We get 0 with probability $|\alpha|^2$ and 1 with probability $|\beta|^2$.

In addition, the state of the qubit **changes** to match the result of the measurement.



Subsequent measurements will all be identical.

Z-Measurement



Measuring in the Z basis gives us information about magnitude (θ).

If θ is close to 0, more likely to measure $|0\rangle$.

$$\cos^2\frac{\theta}{2} \to 1\,, \sin^2\frac{\theta}{2} \to 0$$

If θ is close to π, more likely to measure $|1\rangle$.

$$\cos^2\frac{\theta}{2} \to 0\,, \sin^2\frac{\theta}{2} \to 1$$

Estimating Quantum State

We can't measure α and β. Can we estimate?

❌ Measure N times and calculate probability.

Measurement is destructive.

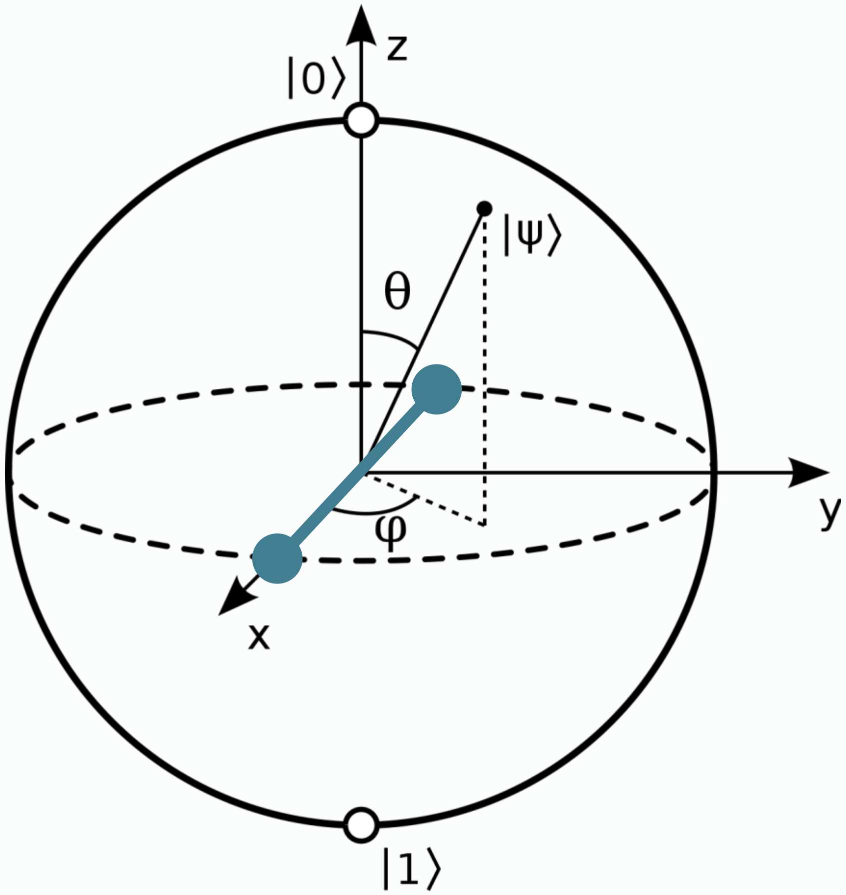
Get the same measurement N times...

✅ Prepare and measure N times and calculate probability.

But this still only gives us $|\alpha|^2$ and $|\beta|^2$.

No information about phase!

X-Measurement



Measuring in the X basis gives us information about phase (φ).

If φ is close to 0 or 2π,
more likely to measure $|+\rangle$.

If φ is close to π,
more likely to measure $|-\rangle$.

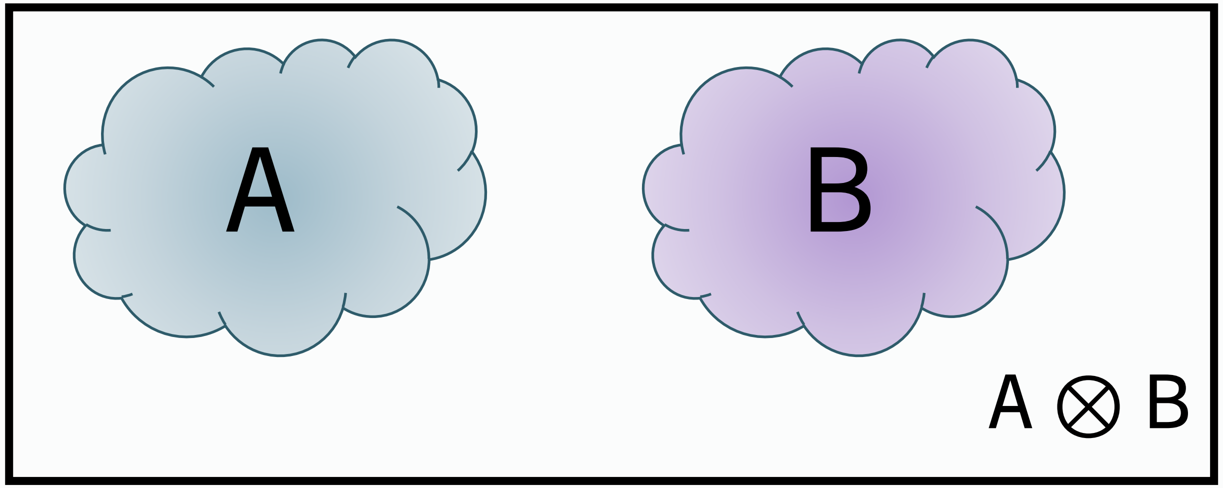
Can't do X-measurement and Z-measurement at the same time.

Measuring a qubit gives us one classical bit of information.

And it destroys any superposition.

Multiple Qubits

Suppose we have two quantum systems,
one in state A and the other in state B.



The state of the two systems combined is A ⊗ B,
where is ⊗ is the **tensor product**.

Tensor Product

$$|\psi\rangle = \begin{bmatrix} a \\ b \end{bmatrix}$$

$$|\gamma\rangle = \begin{bmatrix} c \\ d \end{bmatrix}$$

$$|\psi\rangle \otimes |\gamma\rangle = \begin{bmatrix} a \\ b \end{bmatrix} \otimes \begin{bmatrix} c \\ d \end{bmatrix} = \begin{bmatrix} a \begin{bmatrix} c \\ d \end{bmatrix} \\ b \begin{bmatrix} c \\ d \end{bmatrix} \end{bmatrix} = \begin{bmatrix} ac \\ ad \\ bc \\ bd \end{bmatrix}$$

$$|\psi\rangle \otimes |\gamma\rangle = |\psi\rangle|\gamma\rangle = |\psi, \gamma\rangle$$

Multi-Qubit State

$$|00\rangle = |0\rangle \otimes |0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

When we combine 2 qubits, we get a 4-element vector.

Multi-Qubit Vector Space

$$|00\rangle = \begin{bmatrix}1\\0\\0\\0\end{bmatrix} \quad |01\rangle = \begin{bmatrix}0\\1\\0\\0\end{bmatrix} \quad |10\rangle = \begin{bmatrix}0\\0\\1\\0\end{bmatrix} \quad |11\rangle = \begin{bmatrix}0\\0\\0\\1\end{bmatrix}$$

Superposition: *Two-qubit state is linear combination of **basis** vectors.*

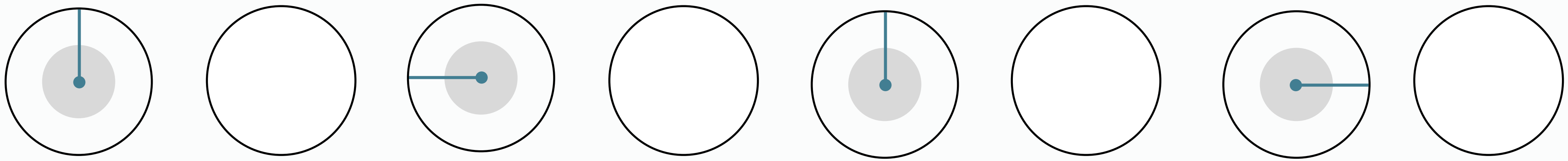
$$\begin{aligned}|\psi\rangle &= \alpha_0|00\rangle + \alpha_1|01\rangle + \alpha_2|10\rangle + \alpha_3|11\rangle \\ &= \alpha_0|0\rangle + \alpha_1|1\rangle + \alpha_2|2\rangle + \alpha_3|3\rangle\end{aligned}$$

Multi-Qubit Vector Space

An n-qubit space is a 2^n-dimensional vector space.
*Two-qubit state is linear combination of 2^n **basis** vectors.*

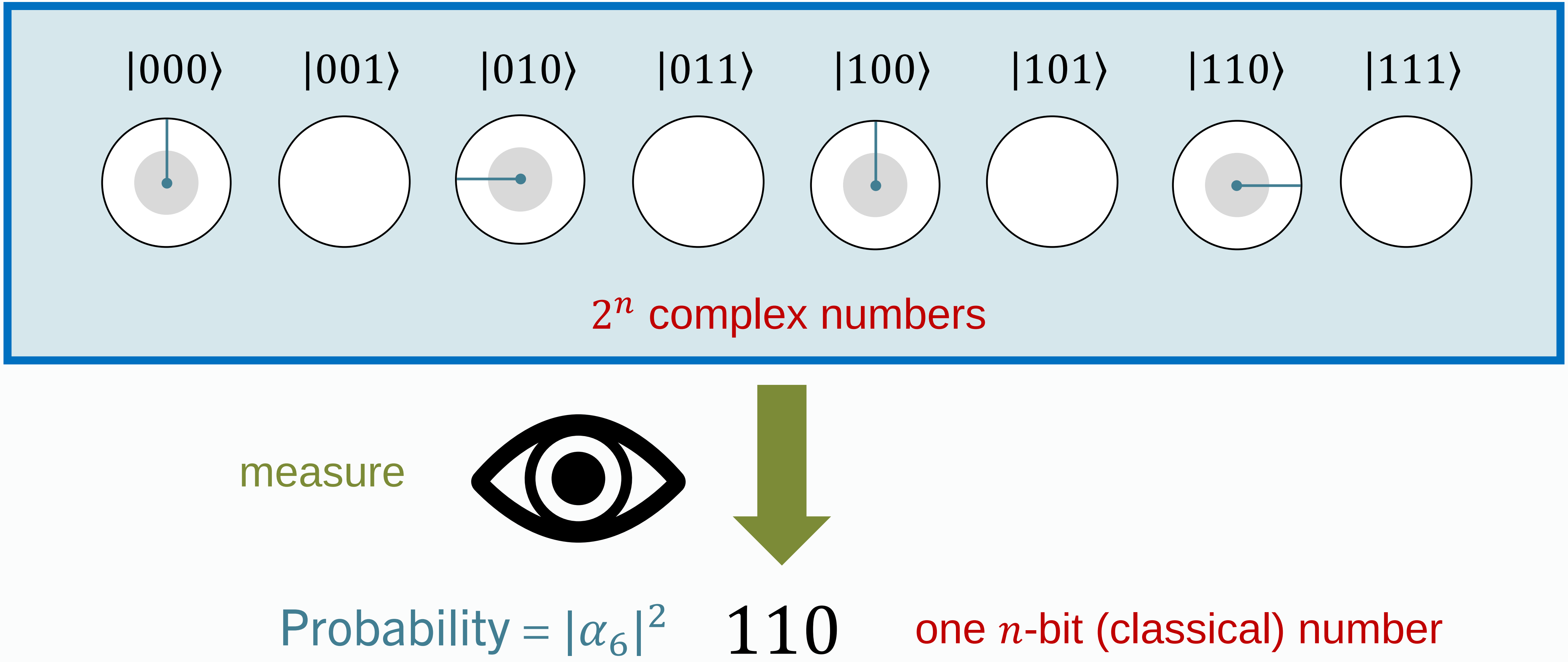
$$|\psi\rangle = \sum_i \alpha_i |i\rangle \qquad \sum |\alpha_i|^2 = 1$$

$|000\rangle$ $|001\rangle$ $|010\rangle$ $|011\rangle$ $|100\rangle$ $|101\rangle$ $|110\rangle$ $|111\rangle$

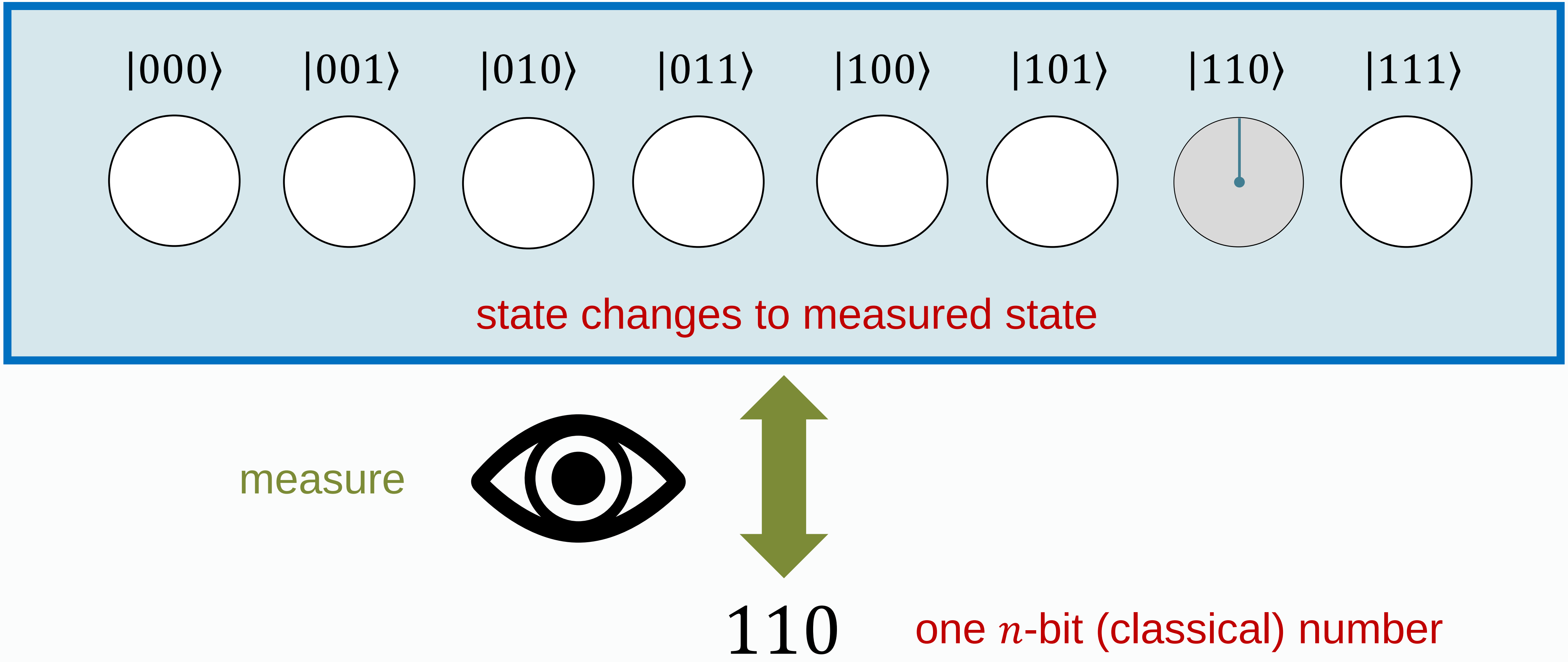


2^n complex numbers

Measurement

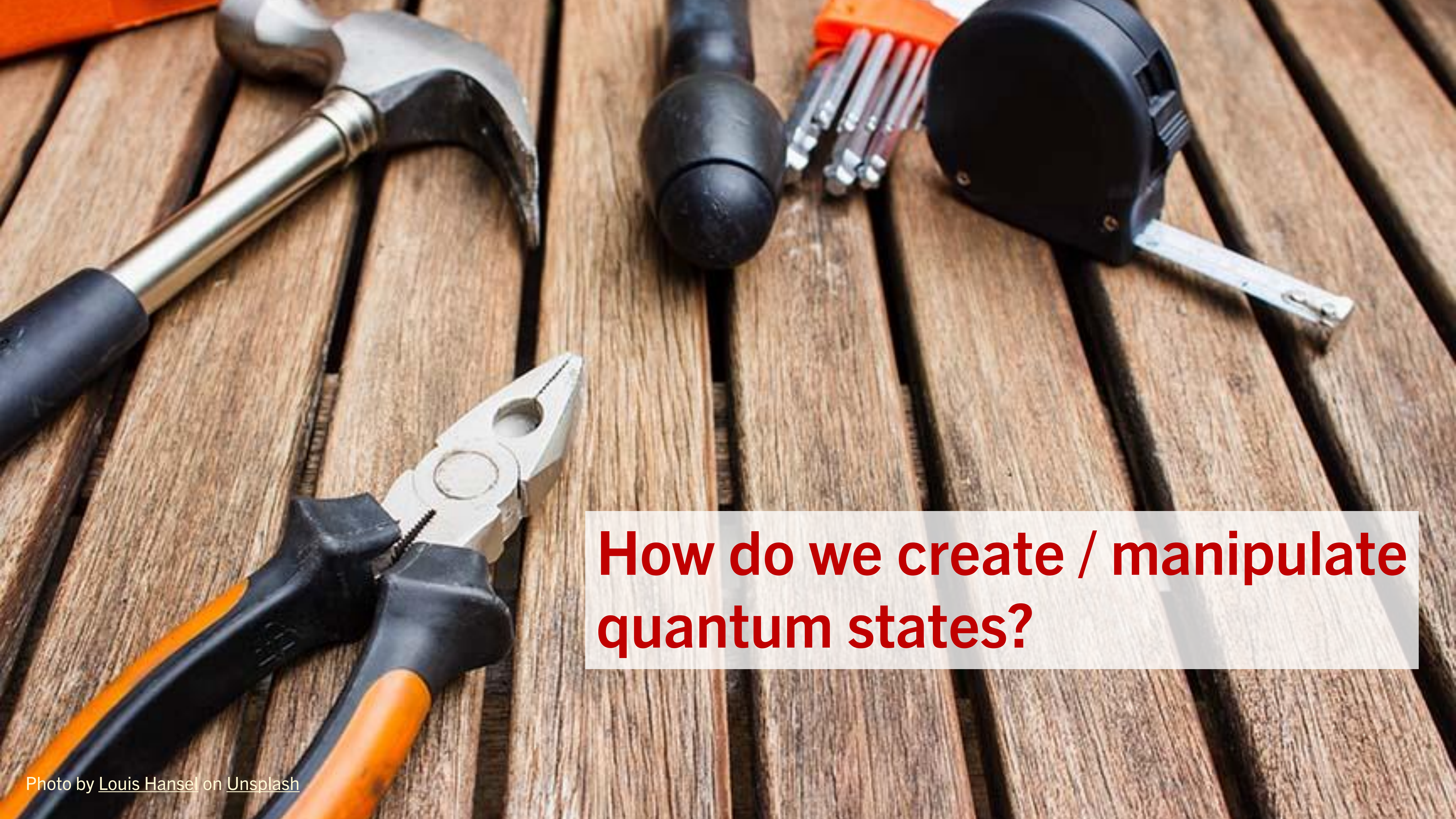


Measurement changes the state



An n-qubit quantum state is a 2^n-dimensional vector in a Hilbert space.

$$|\psi\rangle = \sum_i \alpha_i |i\rangle \qquad \sum |\alpha_i|^2 = 1$$



How do we create / manipulate quantum states?

Photo by Louis Hansel on Unsplash

Unitary Evolution

*The evolution of a **closed** quantum system is described by a **unitary** transformation.*

$$|\psi'\rangle = U|\psi\rangle$$

state at time t_2

state at time t_1

unitary matrix

(depends only on times t_1 and t_2)

Unitary:

$$U^\dagger U = I$$

The matrix does not change the length of the vector.

Always reversible.

Quantum Mechanics

The time evolution of a ***closed*** *quantum system is described by the Schrödinger equation.*

$$i\hbar \frac{d|\psi\rangle}{dt} = \mathcal{H}|\psi\rangle$$

$\mathcal{H}$ is a *Hermitian* matrix,
known as the **time-independent Hamiltonian**,
which describes the energy of a system.

$$\mathcal{H} = \mathcal{H}^\dagger$$

$$|\psi(t_2)\rangle = \exp\left[\frac{i\mathcal{H}(t_2 - t_1)}{\hbar}\right]|\psi(t_1)\rangle = U(t_2, t_1)|\psi(t_1)\rangle$$

This is unitary.

Quantum Gate

A quantum **gate** is a controlled evolution
of the qubit state to accomplish a specific transformation.

$$U|\psi\rangle = U(\alpha|0\rangle + \beta|1\rangle) = \alpha U|0\rangle + \beta U|1\rangle$$

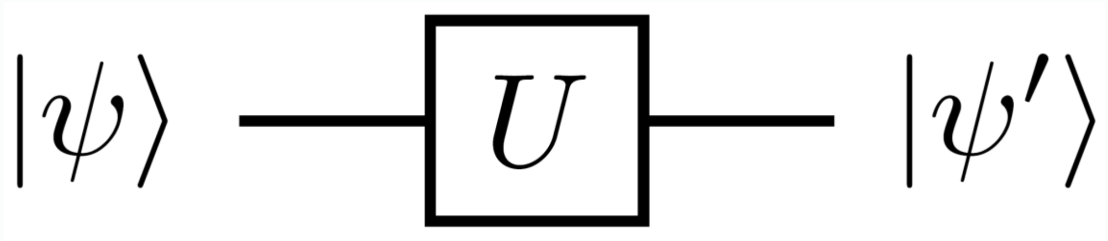
Matrix is **unitary.** It preserves the length (norm) of the vector.

Operation is **linear**, applied to each basis vector.

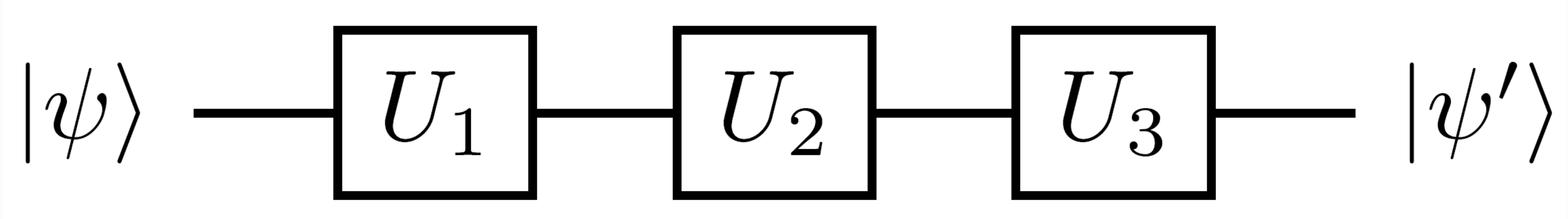
Matrix has an inverse $U^{-1} = U^{\dagger}$. Operation is **reversible.**

Quantum Circuit

A quantum **circuit** shows the **time evolution** of a qubit's state through a sequence of gates.

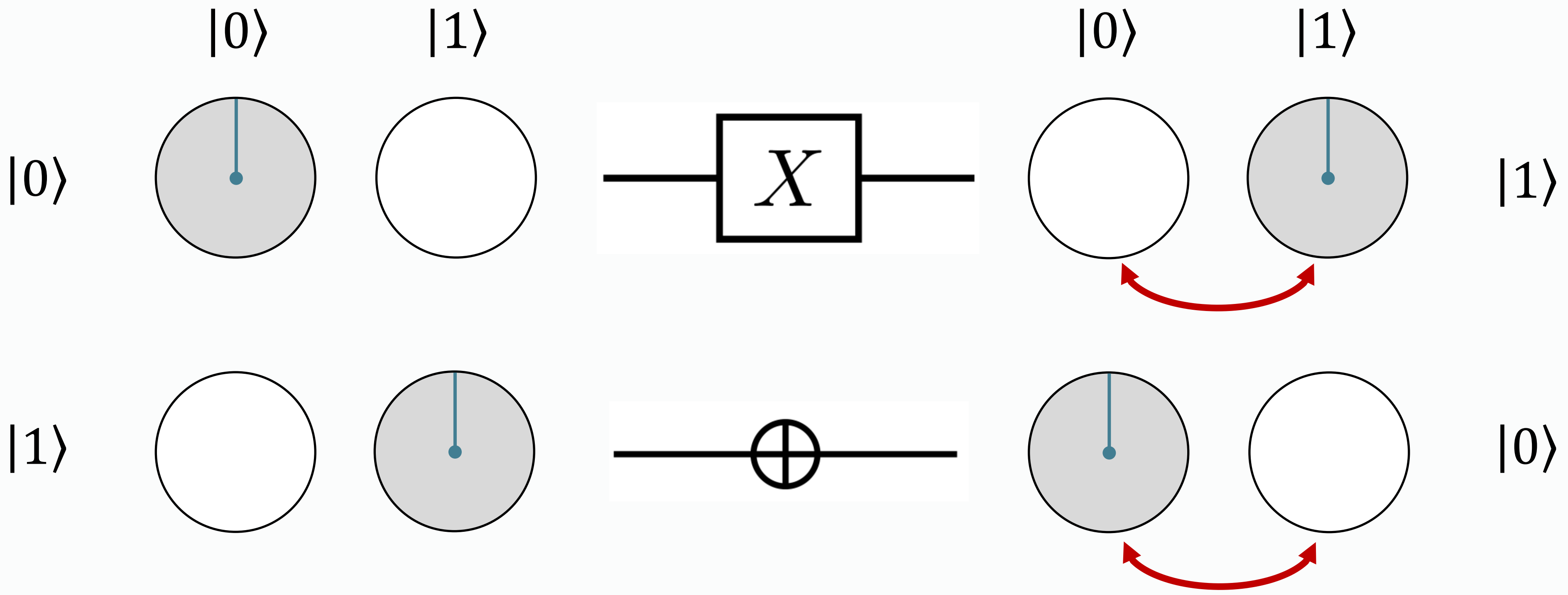


$$|\psi'\rangle = U|\psi\rangle$$



$$|\psi'\rangle = U_3 U_2 U_1 |\psi\rangle$$

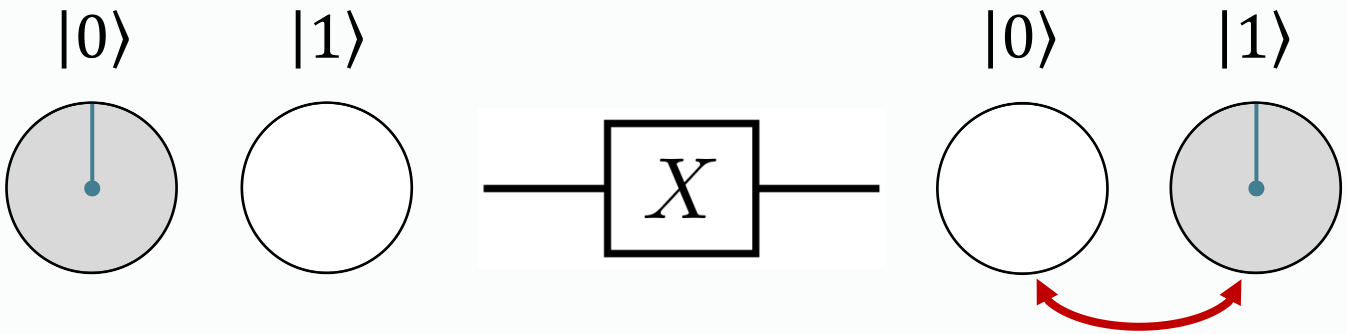
X Gate (NOT)



An X gate is analogous to a classical NOT gate.

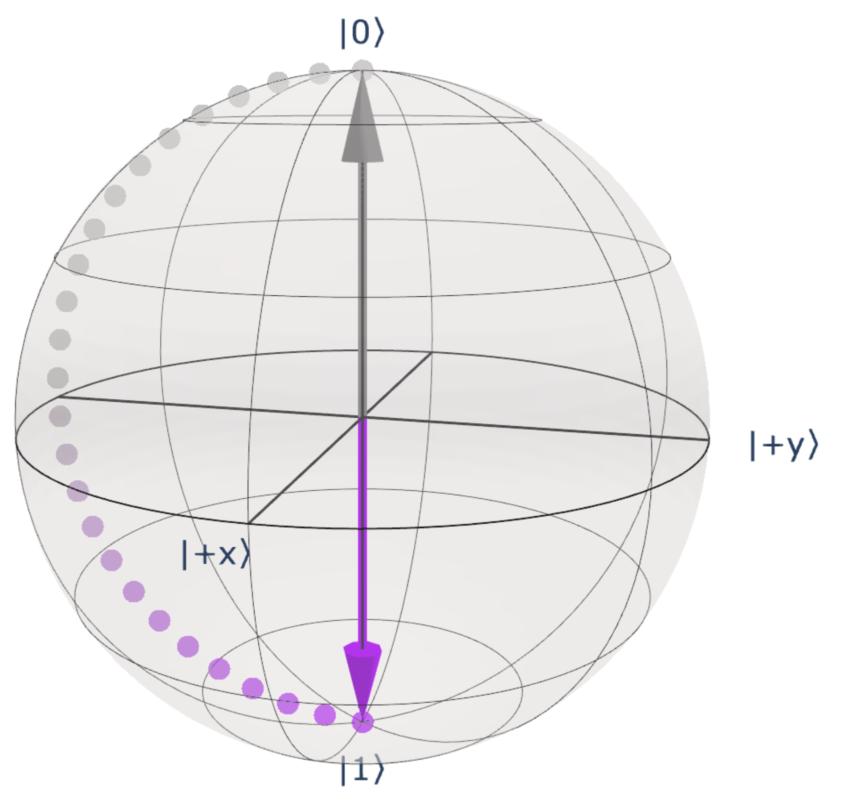
X Gate

$$X|\psi\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} \beta \\ \alpha \end{bmatrix} = \beta|0\rangle + \alpha|1\rangle$$



Gate = Rotation on Bloch Sphere

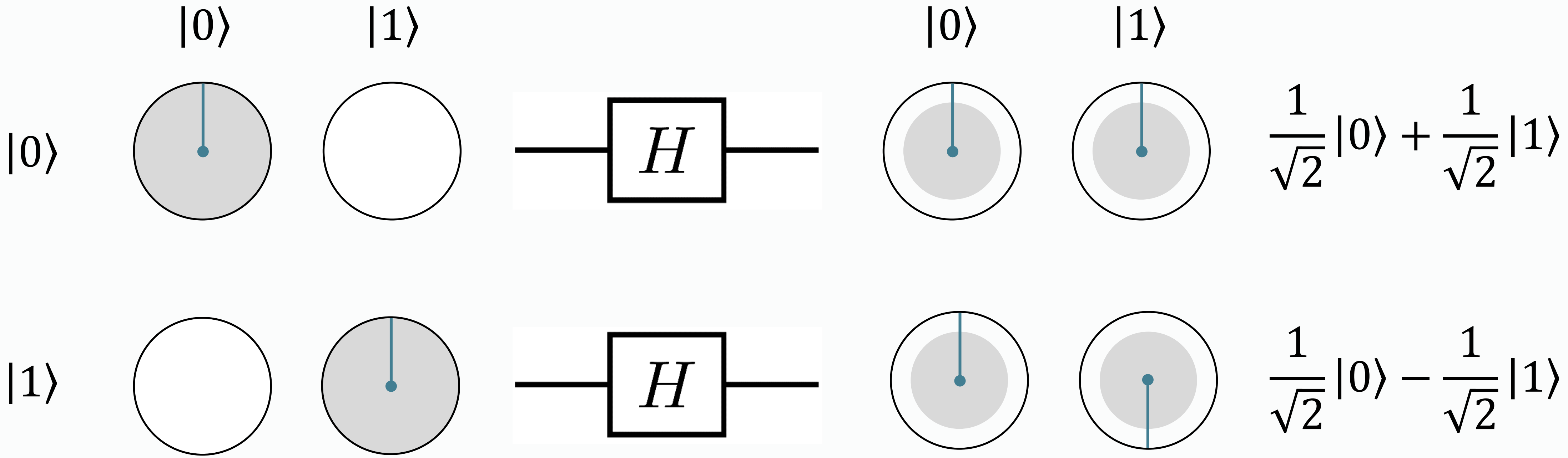
A quantum gate can be viewed as a **rotation** on the Bloch Sphere.
The X gate is a counter-clockwise rotation of π around the X axis.



Similarly, π rotation around Z (Y) axis is known as Z (Y) gate.

X, Y, and Z are **Pauli gates**.

Hadamard Gate

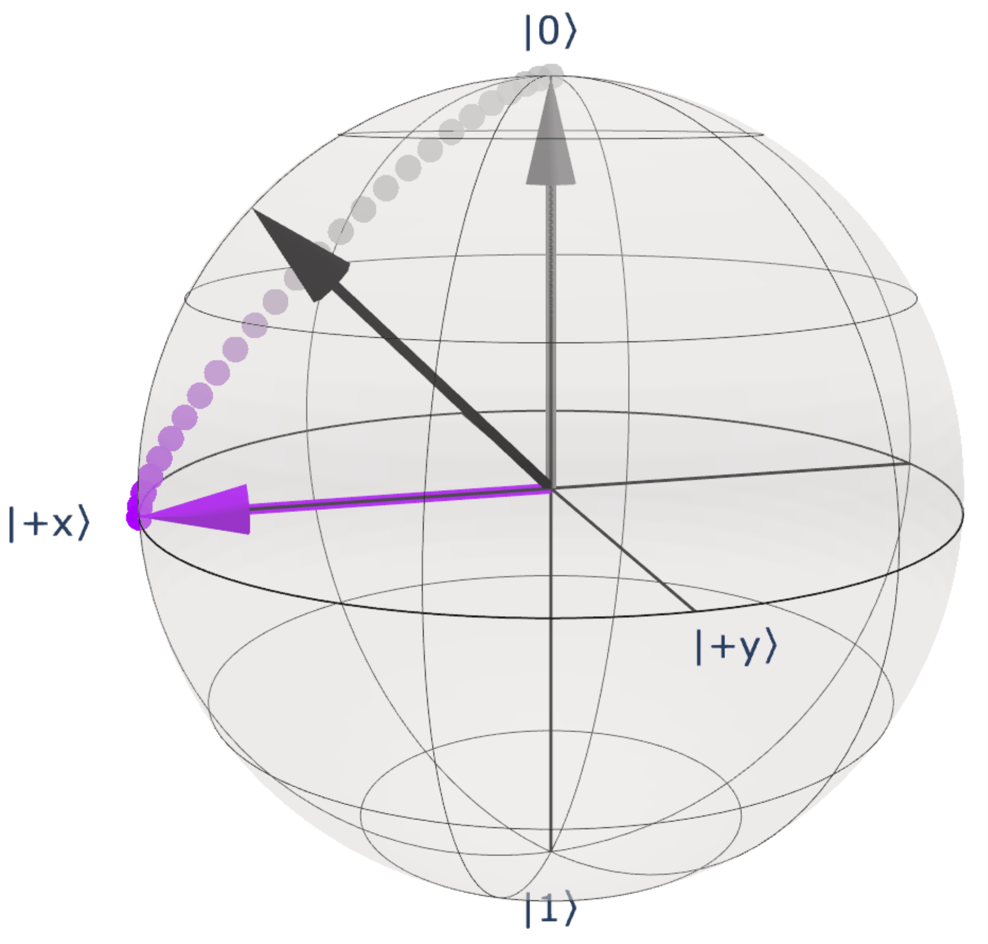


$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

NOTE: This is not the Hamiltonian $\mathcal{H}$ from a few slides back.

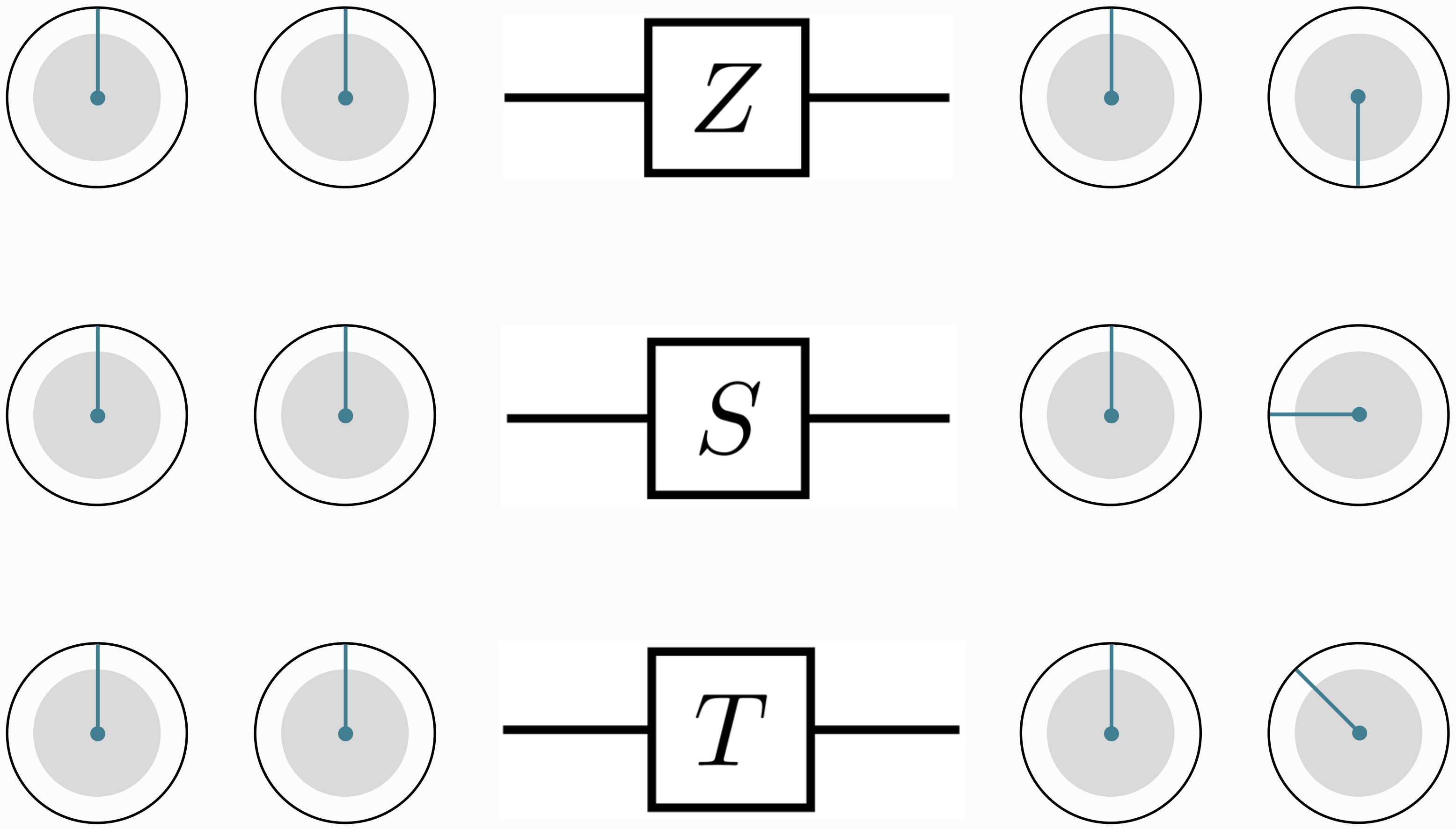
Hadamard Gate

$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$



The H gate is a CCW rotation of π around the X=Z axis.

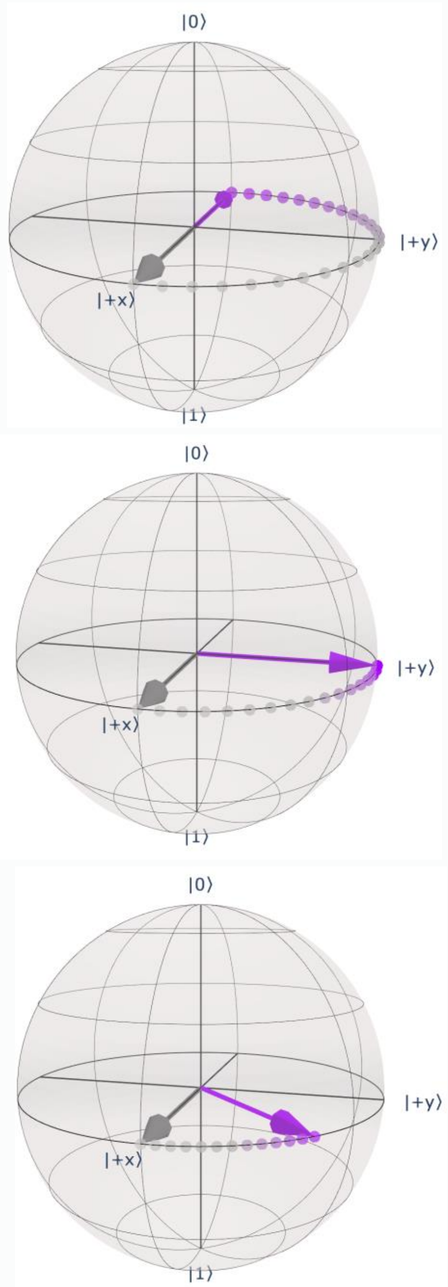
Phase Gates



π

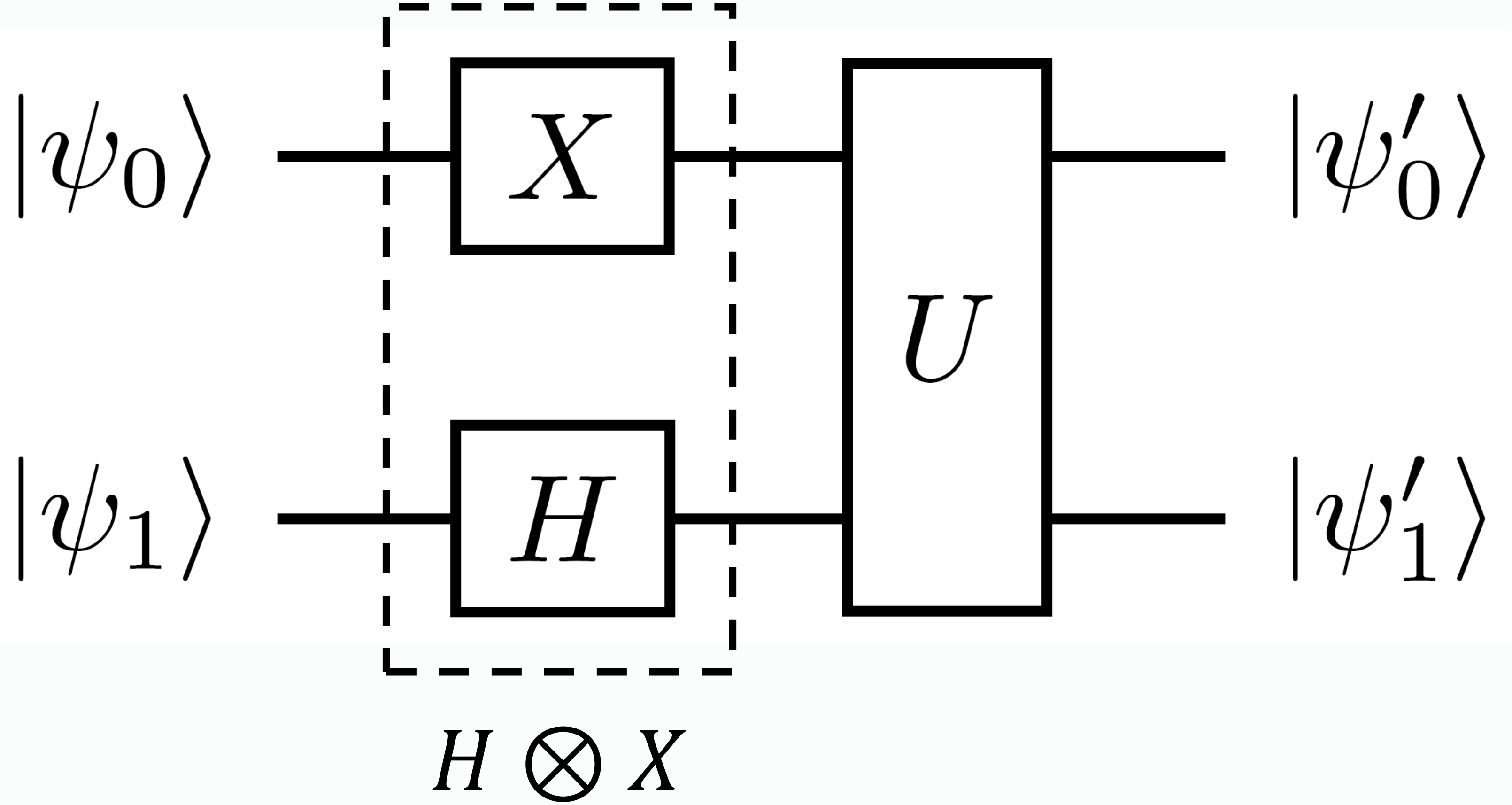
π/2

π/4



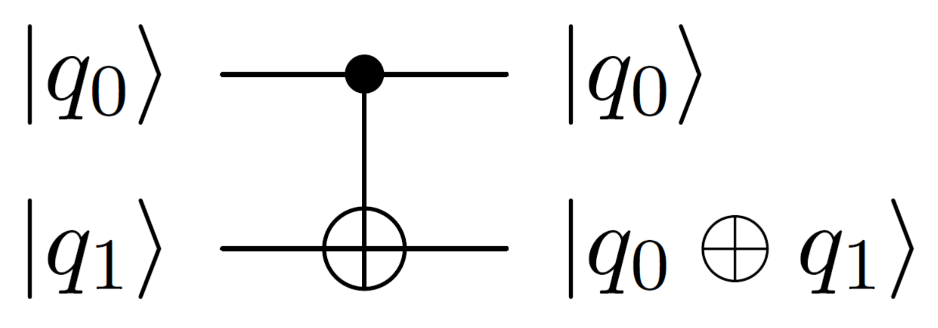
Multi-Qubit Gates

An n-qubit gate is described by a $2^n \times 2^n$ matrix.



CNOT Gate

CNOT = controlled-NOT



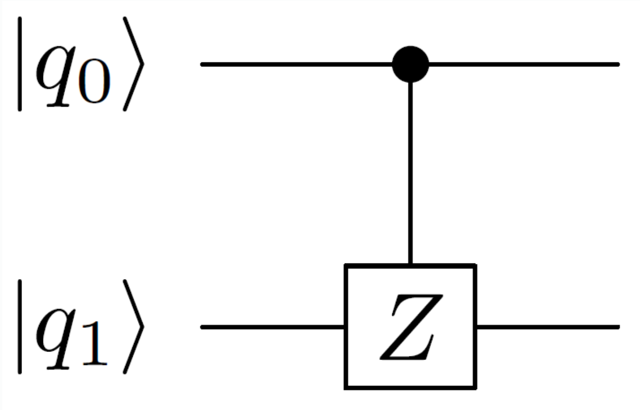
Qubit 0 is **control.**
Qubit 1 is **target.**

Start	End
$\|00\rangle$	$\|00\rangle$
$\|01\rangle$	$\|11\rangle$
$\|10\rangle$	$\|10\rangle$
$\|11\rangle$	$\|01\rangle$

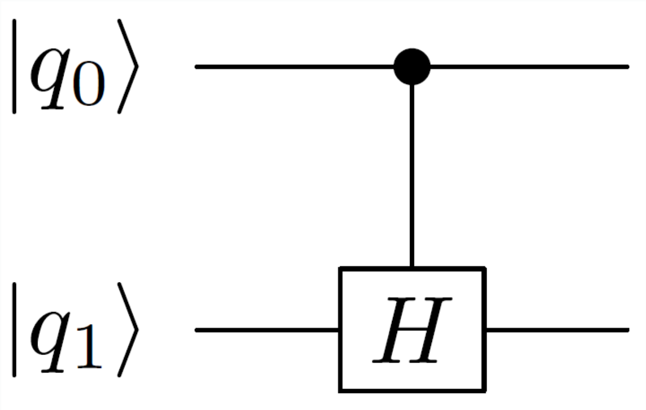
Flip the target bit
if the control bit is 1.

General Controlled Gates

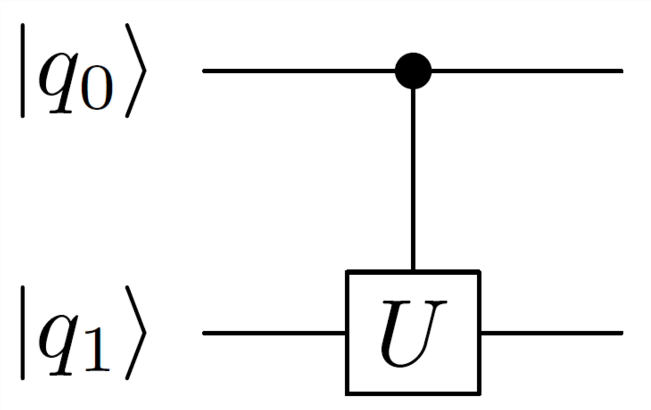
CZ = controlled-Z



CH = controlled-H

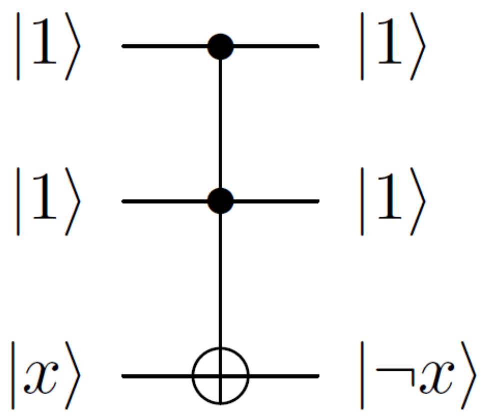


CU = controlled-U

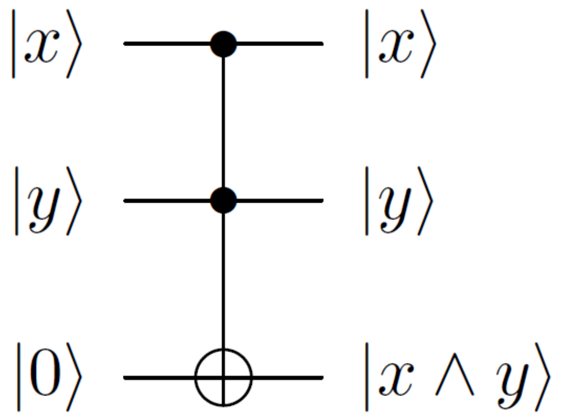


Gate is performed if the control bit is 1.

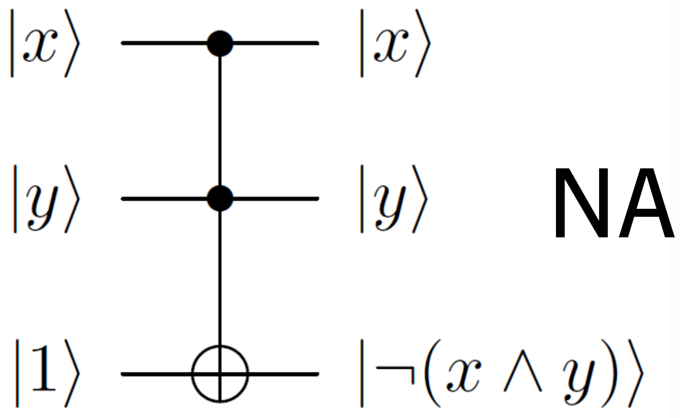
Toffoli: Reversible Classic Gates



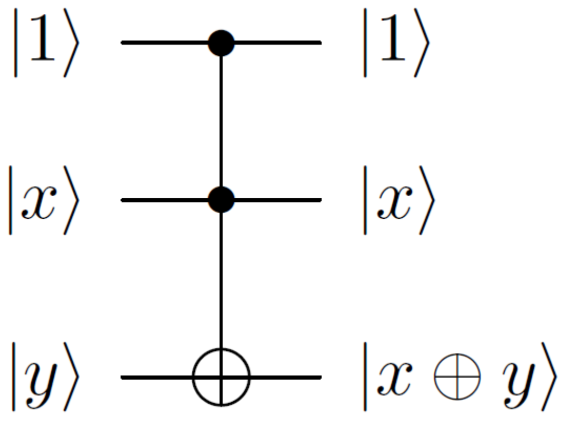
NOT



AND

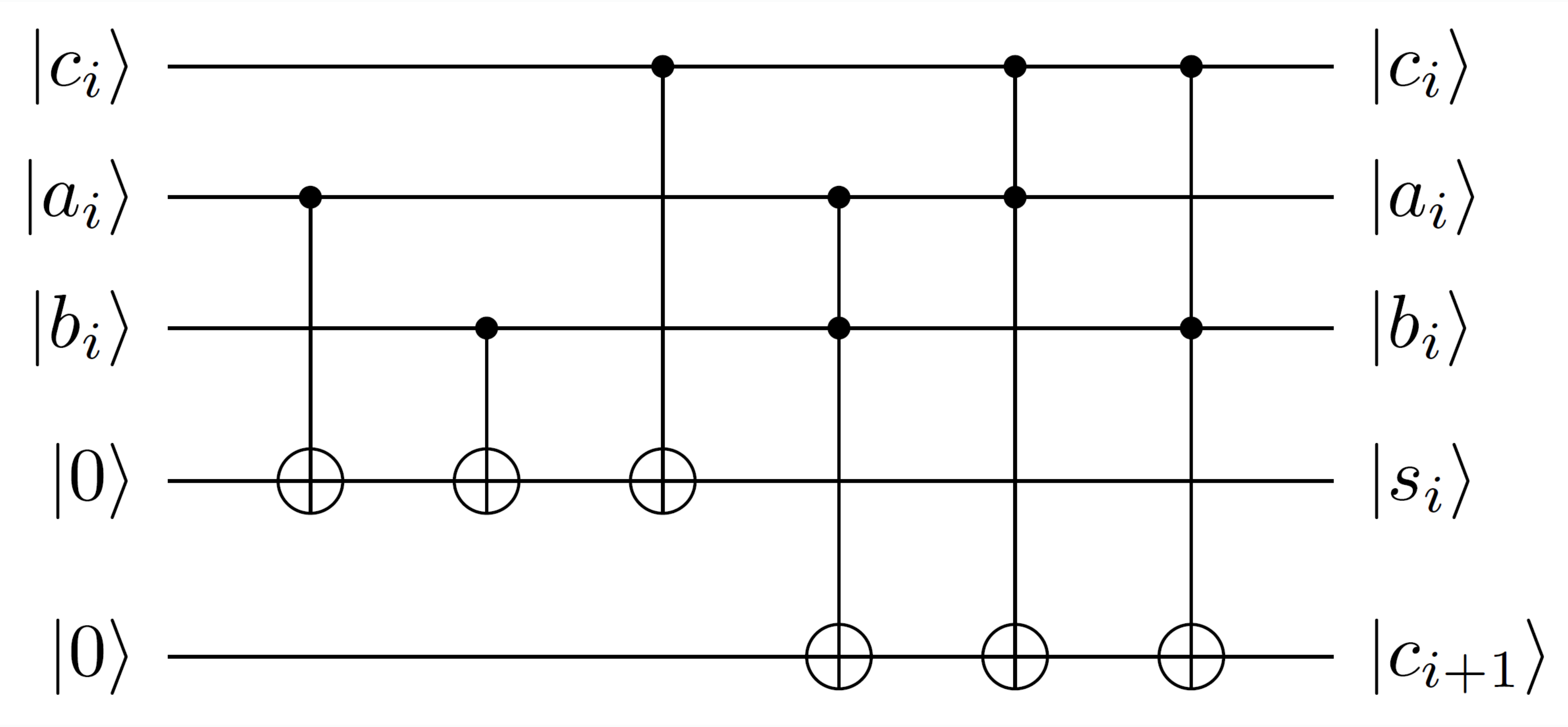


NAND



XOR

Circuit: 1-qubit adder



Any reversible classical computation can be done on a quantum computer.

Universal Quantum Computation

Any n-qubit circuit can be decomposed into 1- and 2-qubit gates.

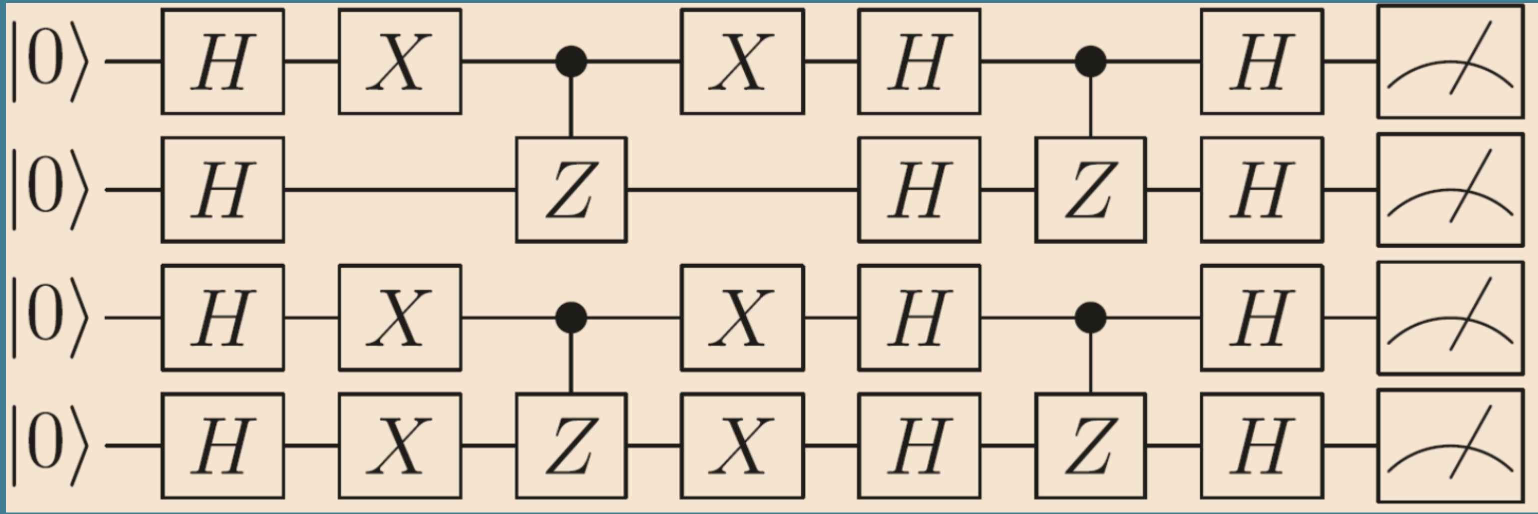
A **universal gate set** allows any unitary to be approximated within an error bounds ε.

One such universal gate set is known as Clifford + T:
CNOT, H, S, T

IBM Qiskit tutorial on Sunday

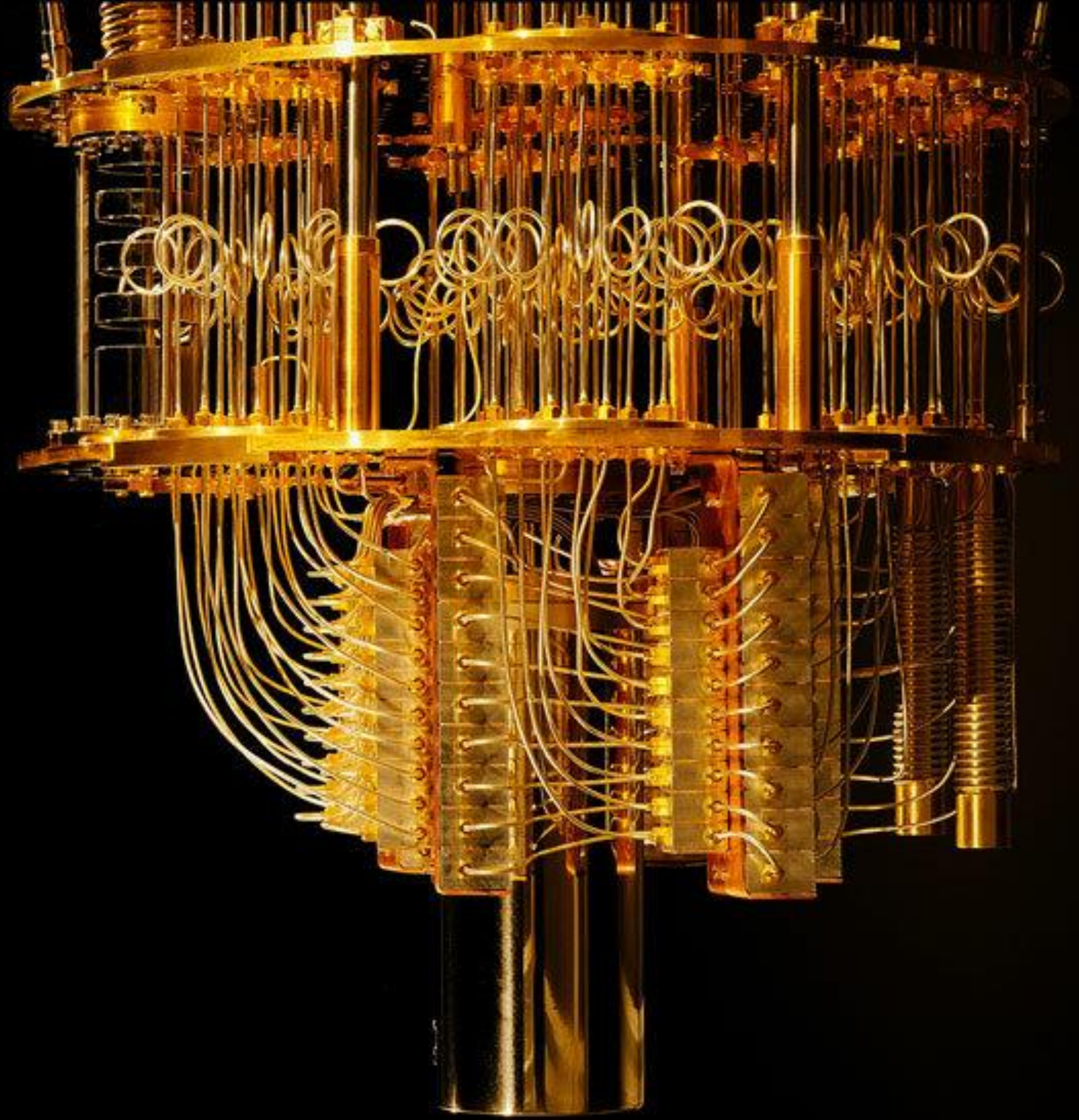
Quantum Circuit:

1. Prepare
2. Apply gates
3. Measure

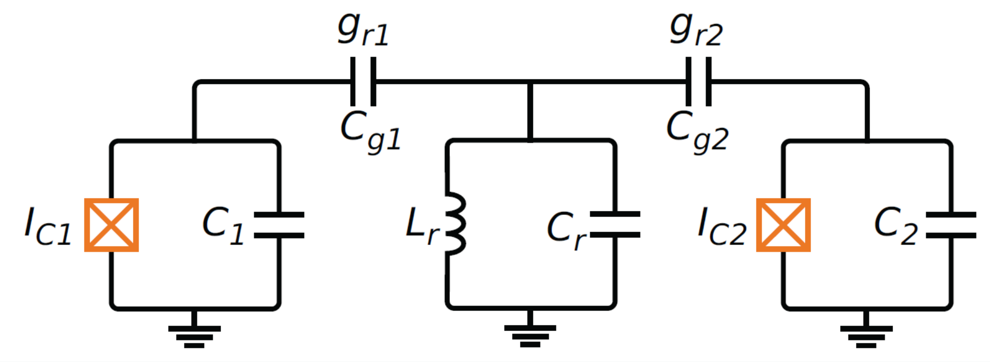


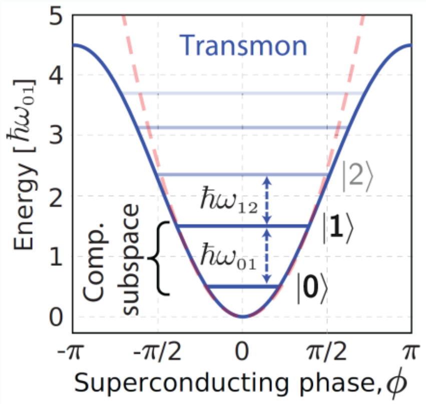
Example from Linke, et al. PNAS, 2017.

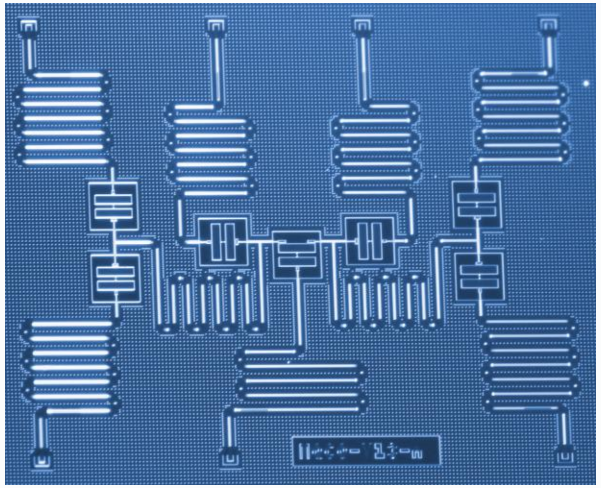
Quantum Computers



Example: Superconducting







Qubits: energy level of nonharmonic oscillator, physical coupling

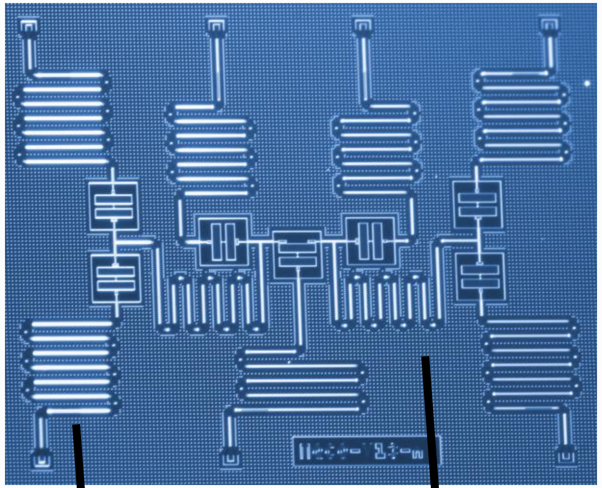
Control: microwave pulses

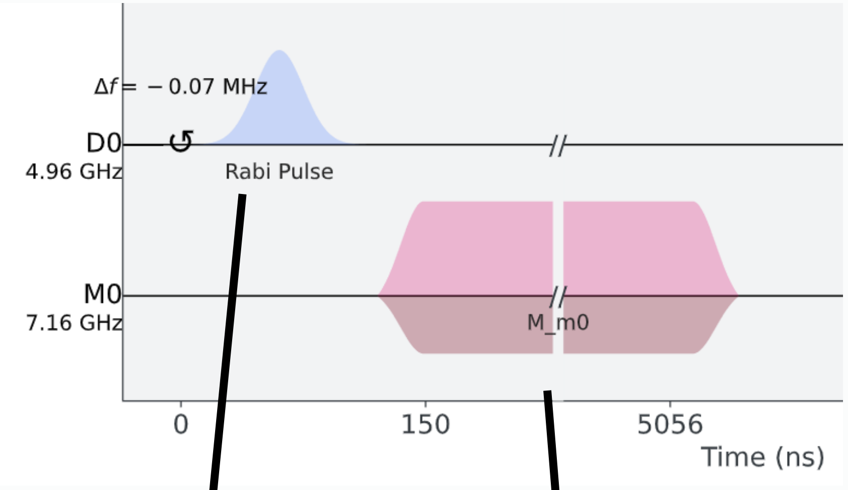
Current scale: 100s of qubits

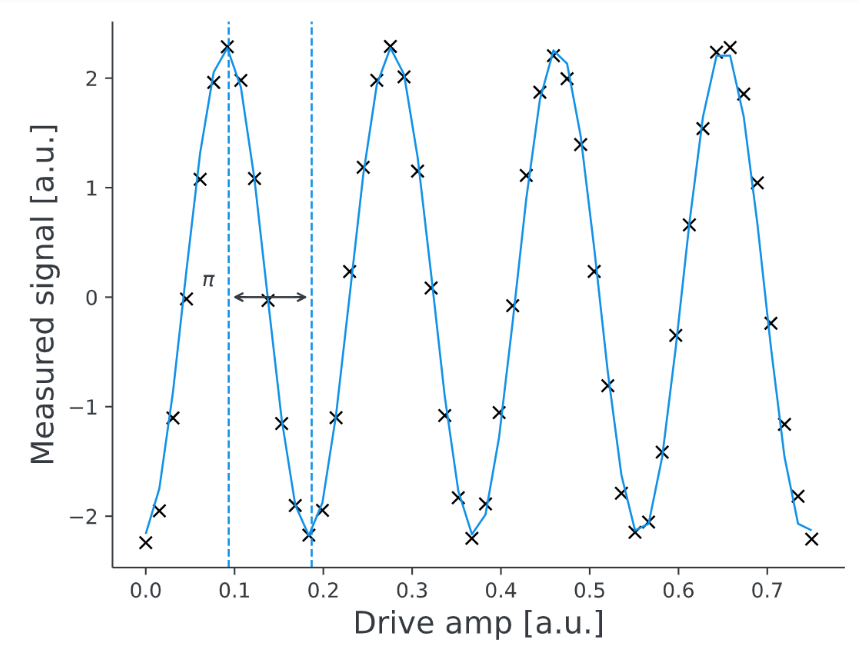
Advantages: fast gates, mature manufacturing

Vendors: IBM, Google, Rigetti

Pulses and Gates







Drive / Readout

Coupling

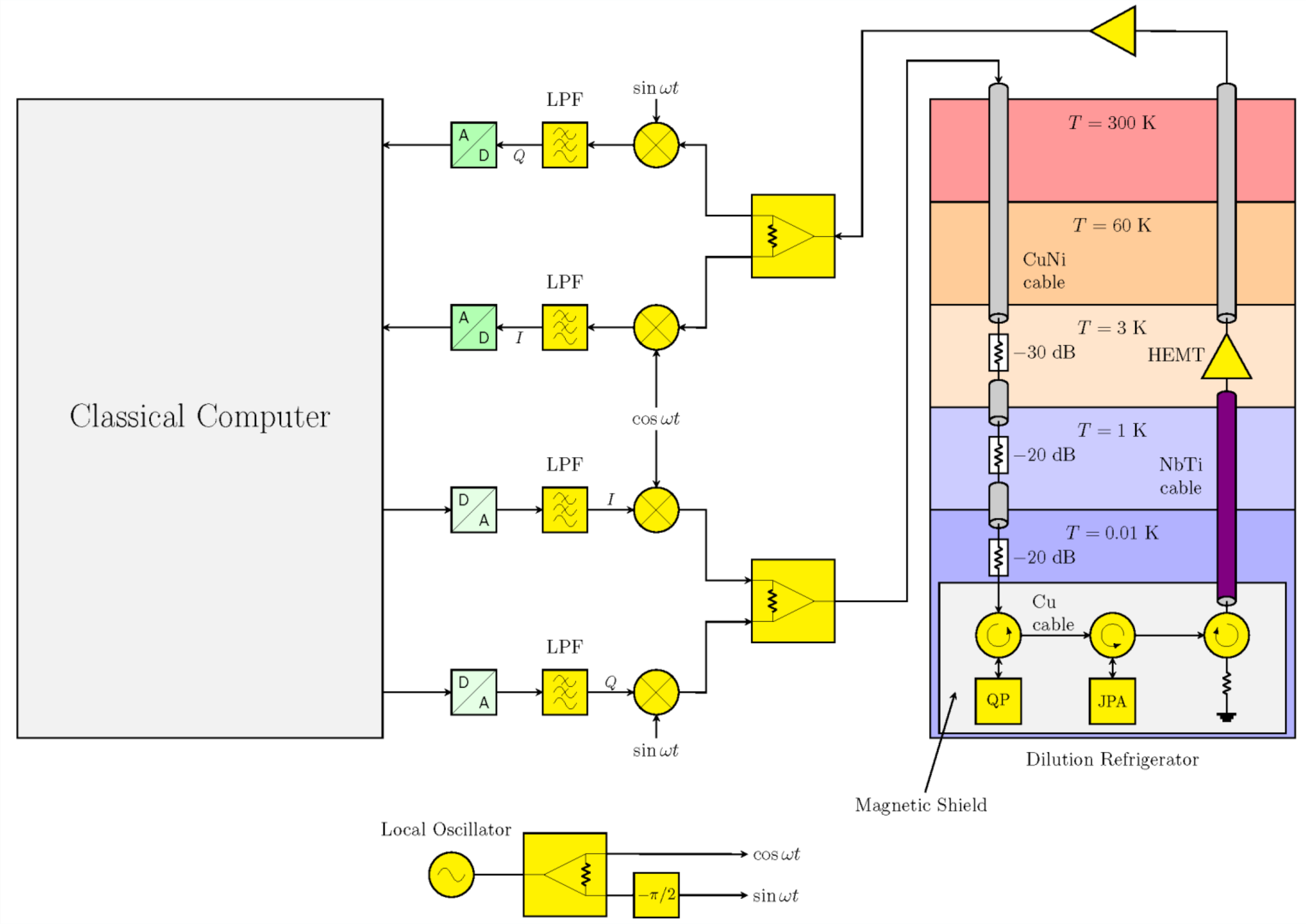
Drive Pulse
freq tuned to qubit

Measure Pulse

By varying the pulse amplitude (or duration), can control angle of rotation.

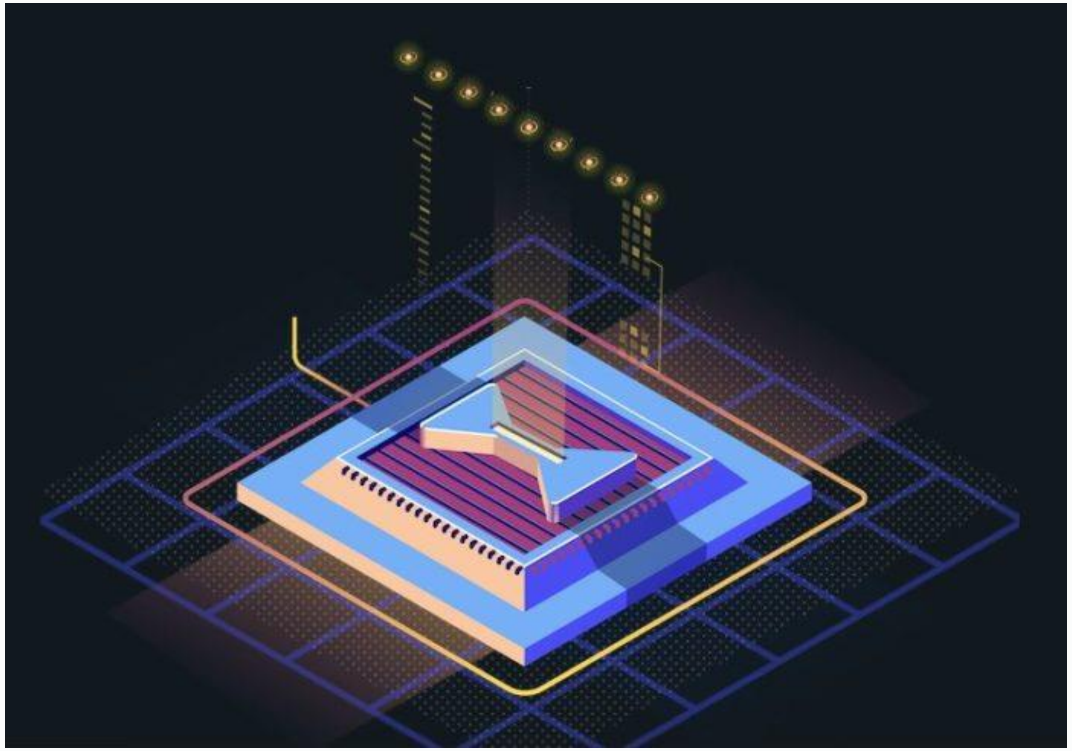
https://learn.qiskit.org/course/quantum-hardware-pulses/calibrating-qubits-using-qiskit-pulse

System


Classical Computer
LPF
LPF
LPF
LPF
A D
Q
I
D A
$\sin \omega t$
$\cos \omega t$
I
Q
$\sin \omega t$
$T = 300$ K
$T = 60$ K
CuNi cable
$T = 3$ K
−30 dB
HEMT
$T = 1$ K
−20 dB
NbTi cable
$T = 0.01$ K
−20 dB
Cu cable
QP
JPA
Dilution Refrigerator
Magnetic Shield
Local Oscillator
$\cos \omega t$
$-\pi/2$
$\sin \omega t$


IBM Q

Example: Ion Trap



Qubits: electron energy level of single ions

Control: lasers

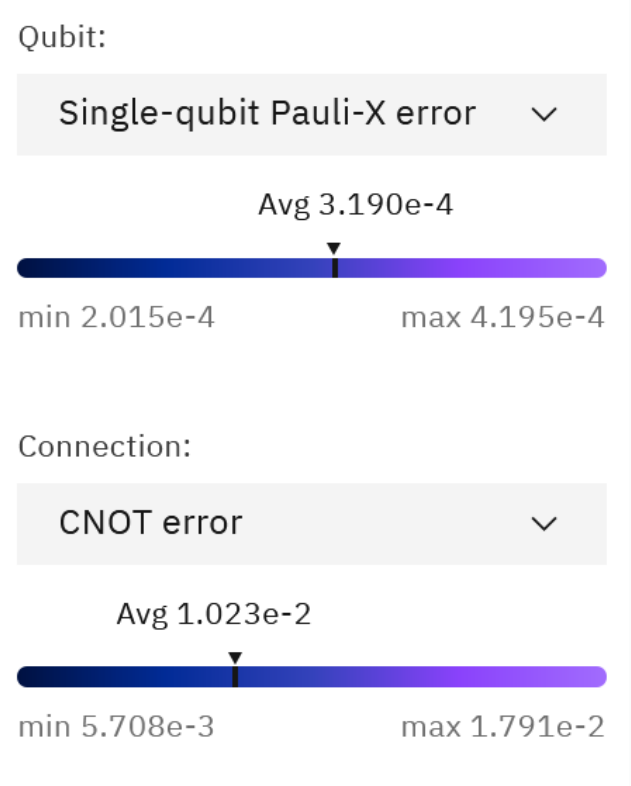
Current scale: 10s of qubits

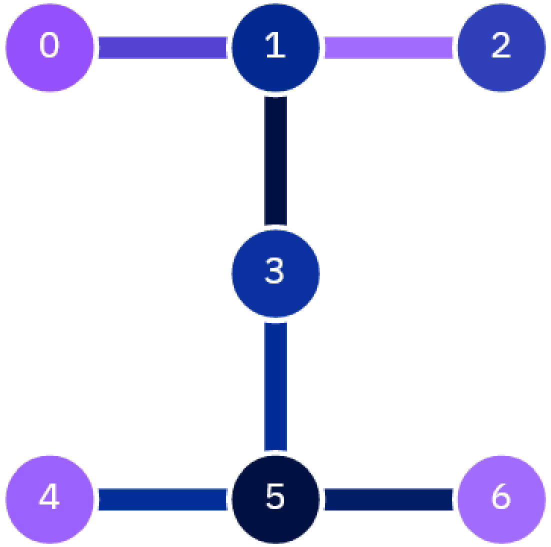
Advantages: lower error rates, high connectivity, identical qubits

Vendors: IonQ, Quantinuum

IonQ tutorial on Sunday

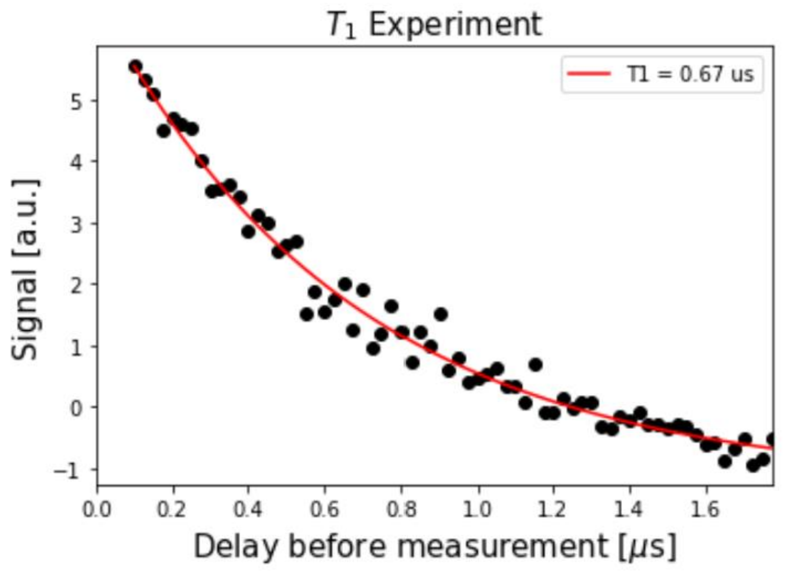
NISQ = Noise





Avg. CNOT Error:	1.023e-2
Avg. Readout Error:	2.189e-2
Avg. T1:	91.42 us
Avg. T2:	108.53 us

Decoherence: changing from 1 to 0 (T1)
Dephasing: changing from + to - (T2)
Measurement readout
Gate control
Crosstalk: interference from other qubits



ibmq_casablanca (03/22/2021)

Challenges

Noise / Errors

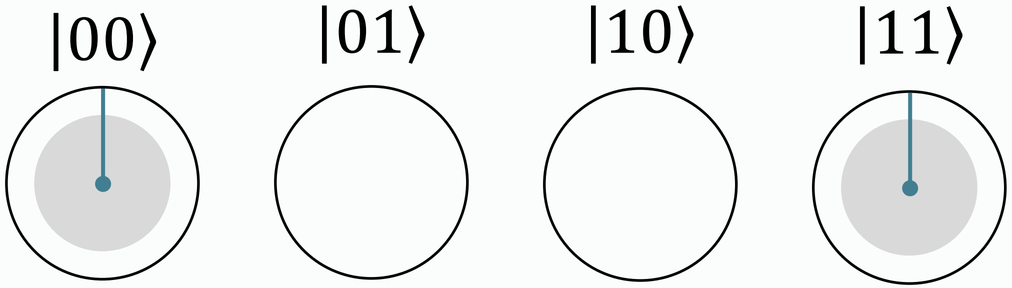
- Error mitigation: techniques to recover useful data from noisy circuits
  This is **current focus** for **near-term** devices.
  Can we get useful results from noisy systems?
  Can we achieve quantum advantage?

- Error correction: redundancy in physical qubits to detect and correct, may require 1000:1 overhead
  This is **requirement** for future large-scale devices.
  Long-lasting logical qubits, deep circuits.
  Known potential for quantum advantage.

Superposition and Entanglement

https://www.piqsels.com/en/public-domain-photo-ffsis/

Consider
this state.
Two qubits, A and B.

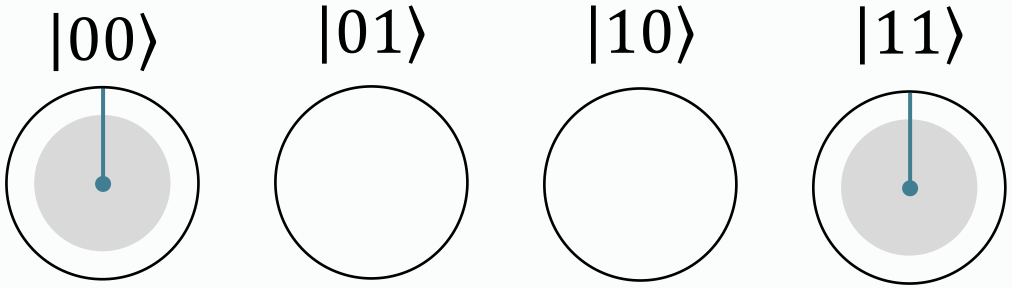


$$\frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

Both A and B have an equal chance of being 0 or 1, so is this $|+\rangle \otimes |+\rangle$? No.

$$|+\rangle \otimes |+\rangle = \frac{|00\rangle + |01\rangle + |10\rangle + |11\rangle}{2}$$

Consider this state.



$$\frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

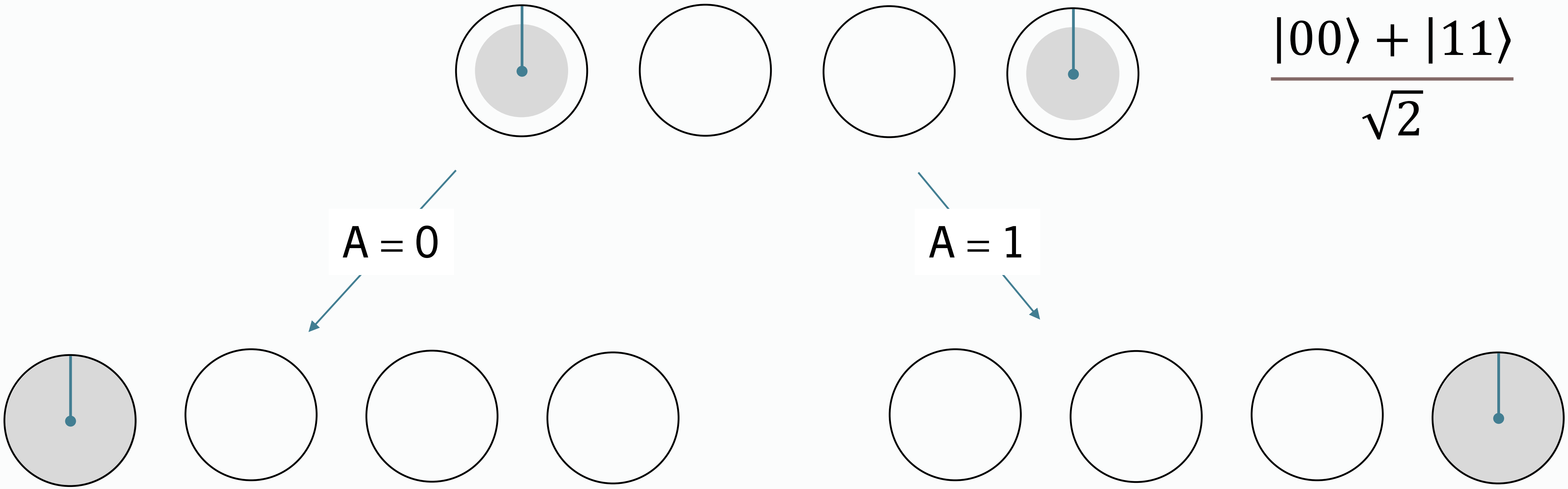
State is **entangled.**

It cannot be represented as the product of two single-qubit states.

If we measure both qubits, we will get either $|00\rangle$ or $|11\rangle$.

What happens if we measure only A?

$$\frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

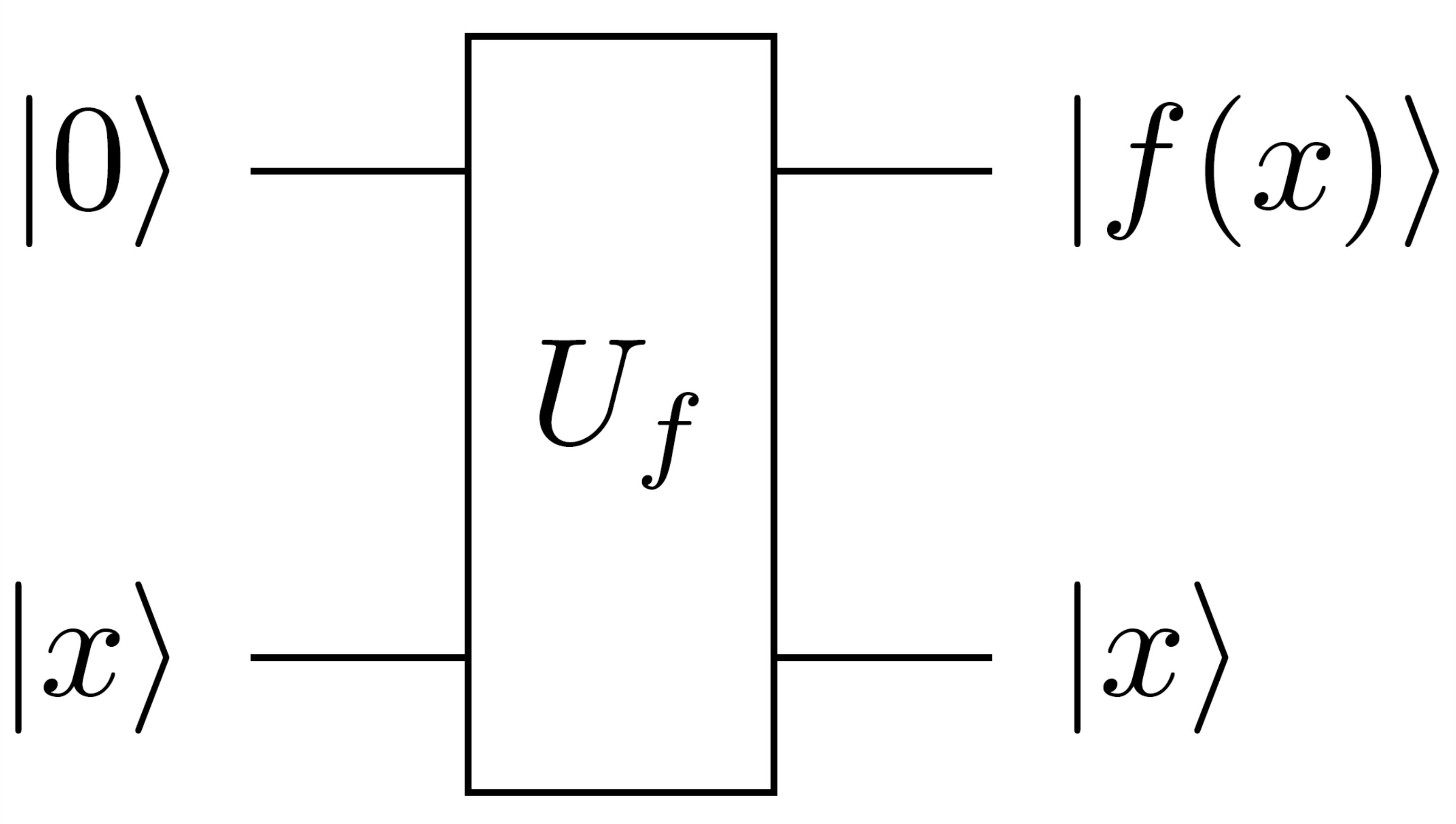


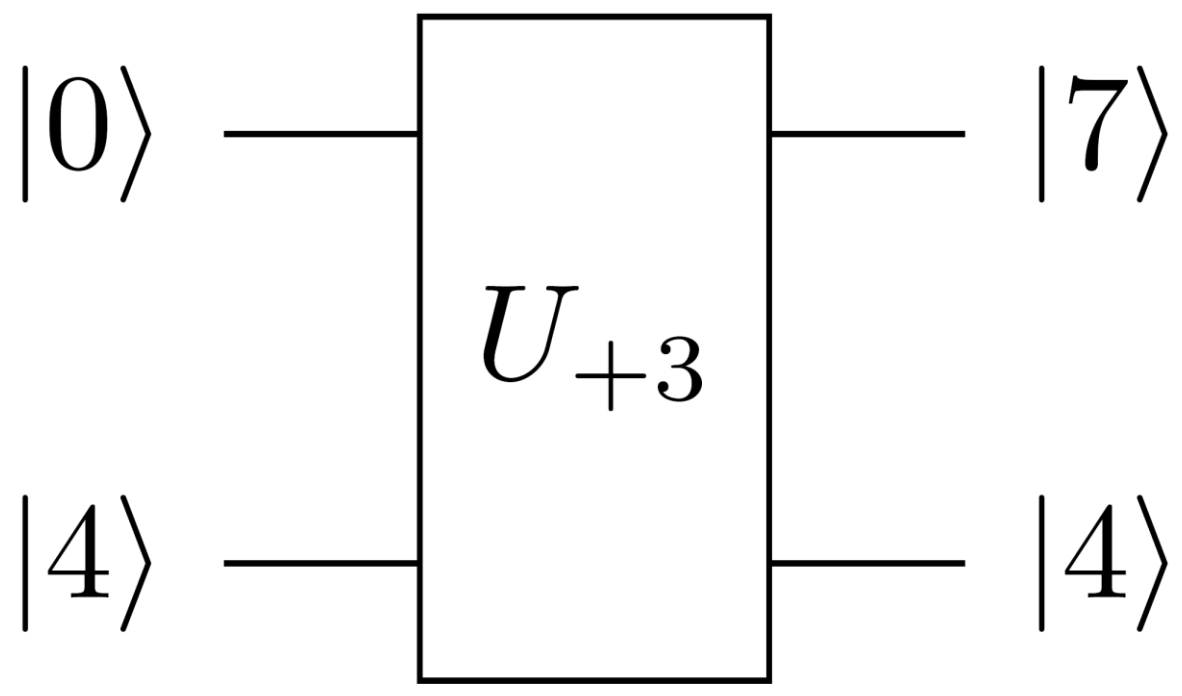
$$|00\rangle = \underbrace{|0\rangle}_{A} \otimes \underbrace{|0\rangle}_{B}$$

$$|11\rangle = \underbrace{|1\rangle}_{A} \otimes \underbrace{|1\rangle}_{B}$$

Measurements of A and B are correlated.

Quantum Functional Block

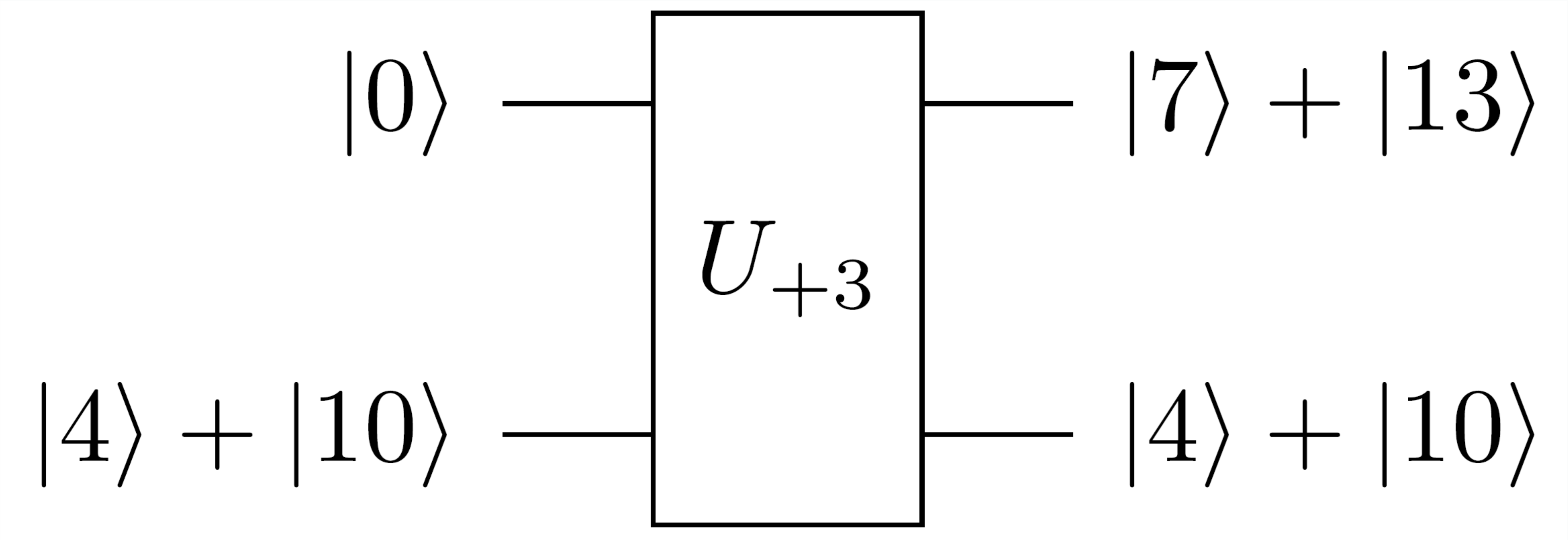




Example:

$f(x) = x + 3$

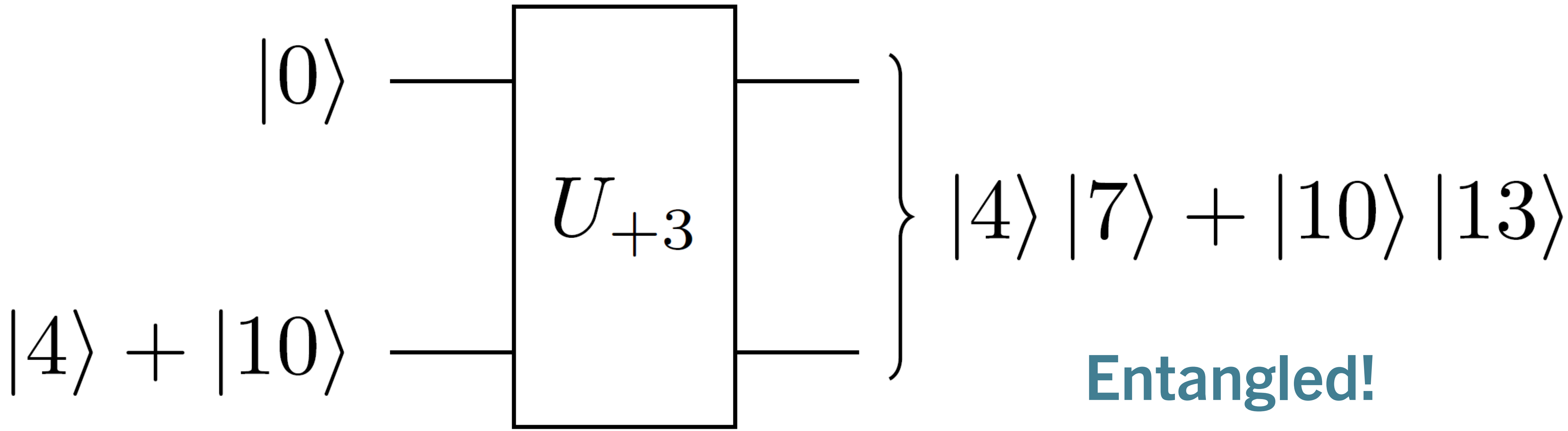
What happens if input is a superposition?



?

Note: Leaving off normalizing coefficient for convenience.

Not exactly...

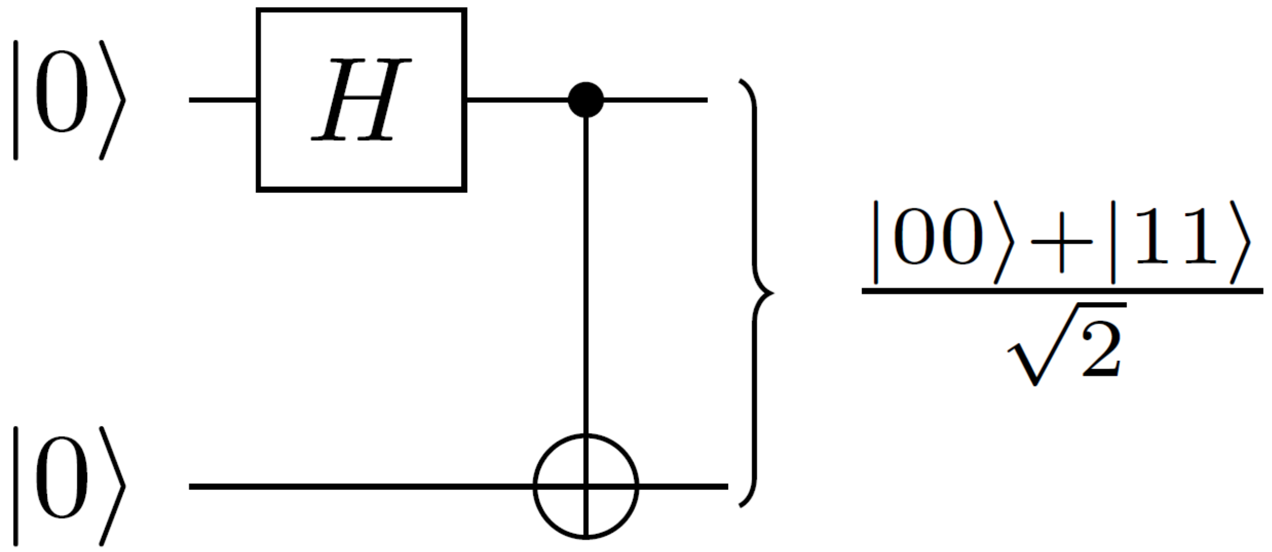


Entangled!

If we measure x = 4,
must measure f(x) = 7.

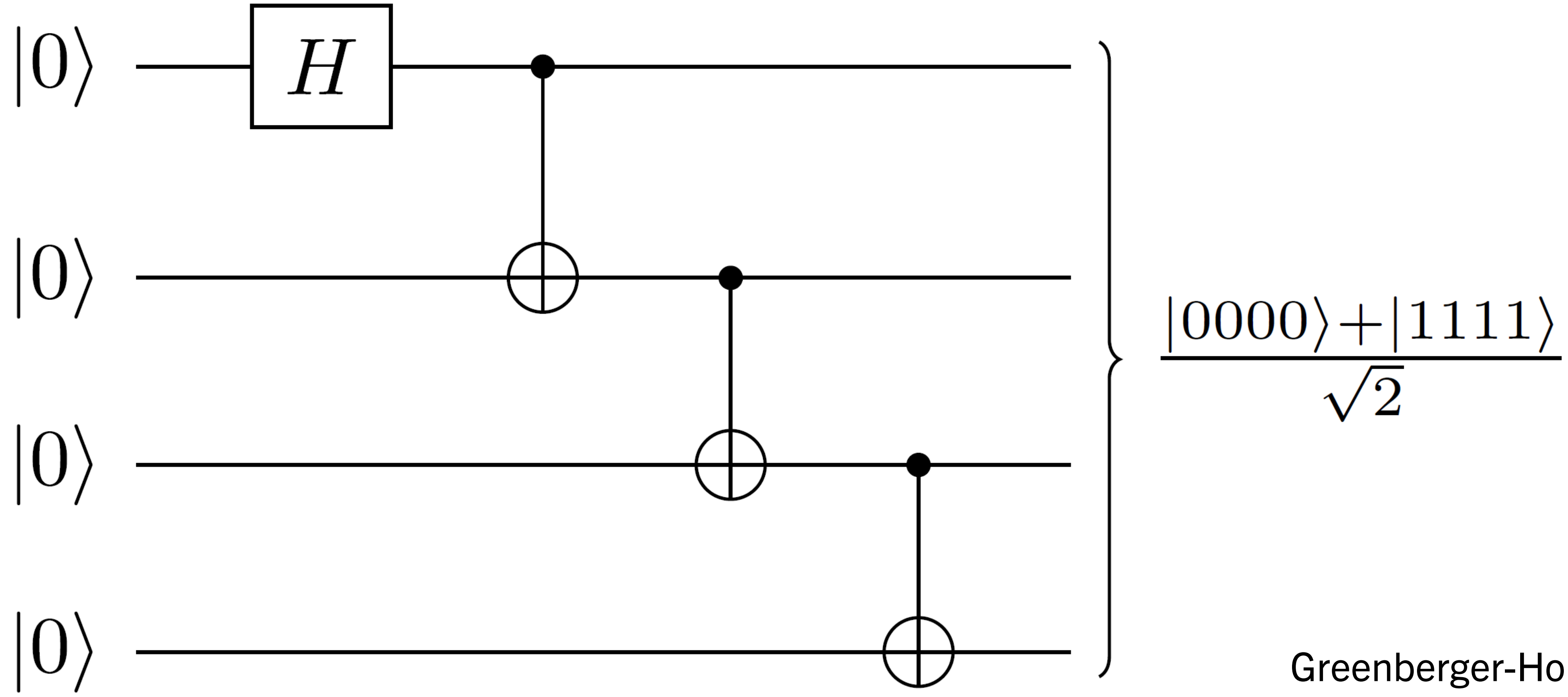
Bell State (EPR Pair)

It's easy to create an entangled state.



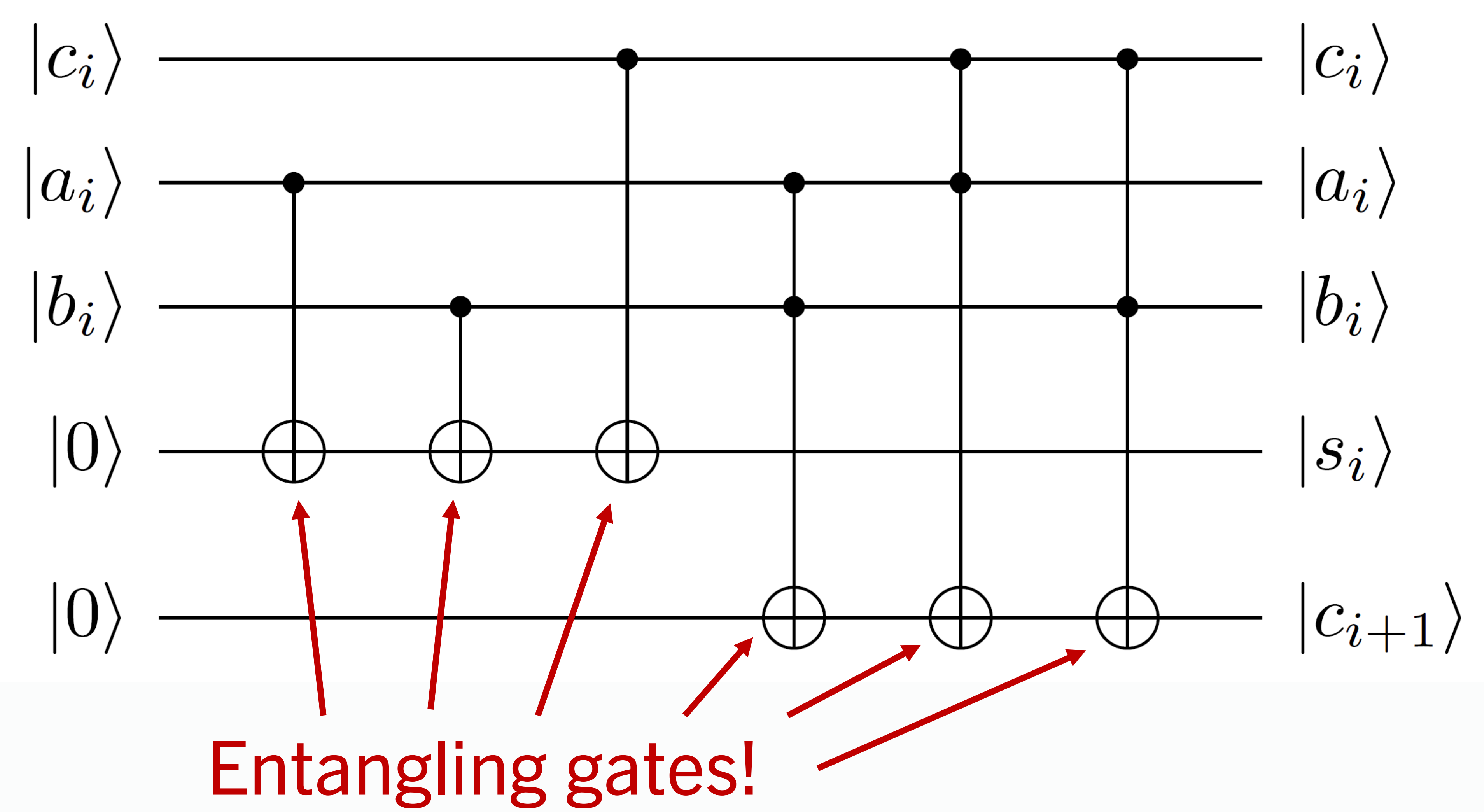
GHZ State

Entanglement is not limited to two qubits...

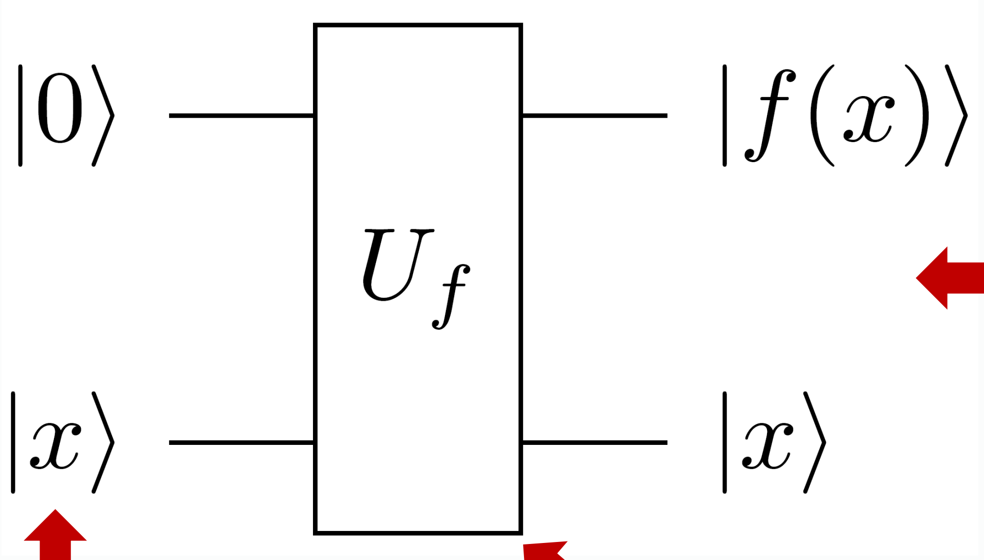


Greenberger-Horne-Zeilinger

Adder Revisited



Quantum Logic: Summary



Output is usually **entangled**.

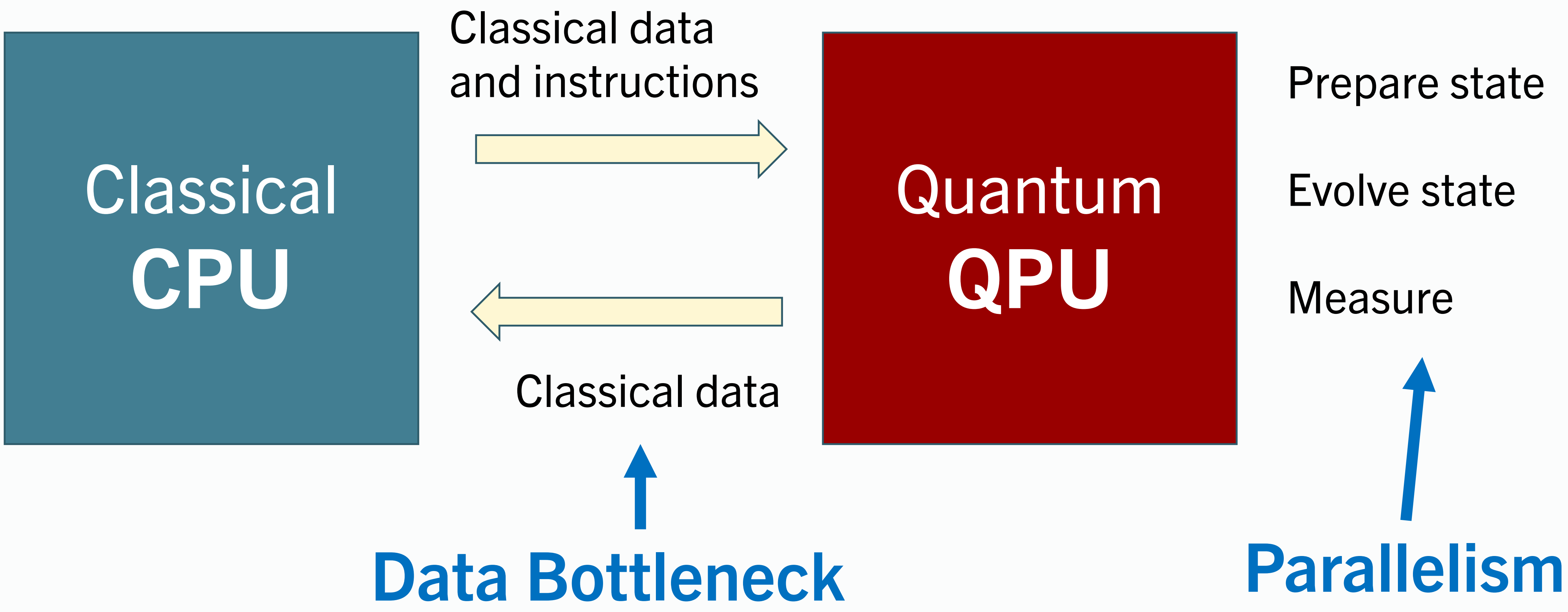
Function is applied to all basis states.
Quantum parallelism!

If superposition…

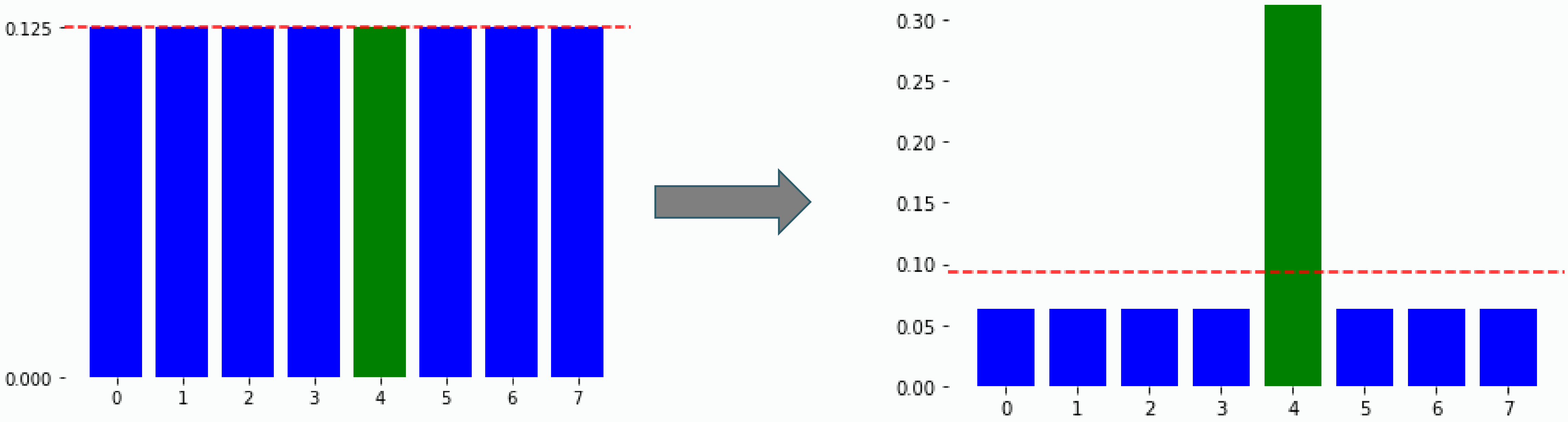
Introductory Algorithms

Photo by Conny Schneider on Unsplash

Quantum Processor as Accelerator



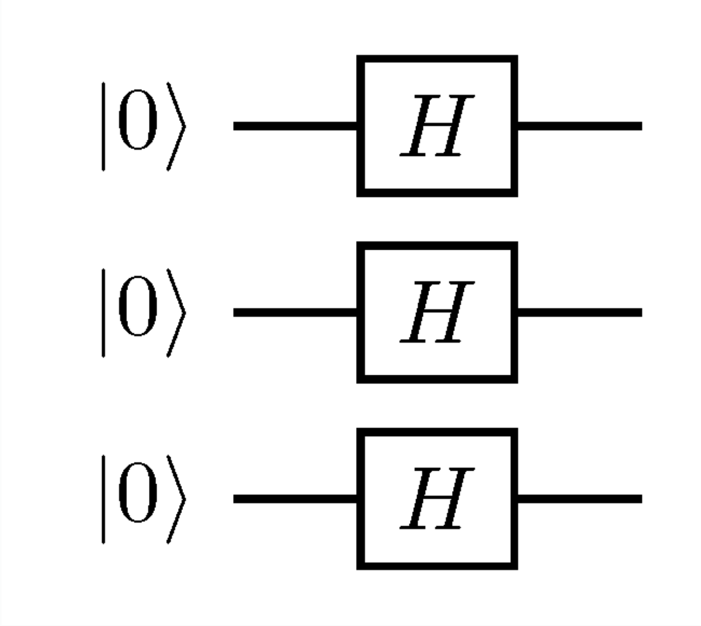
Main Idea



Superposition allows computation on many states at once.

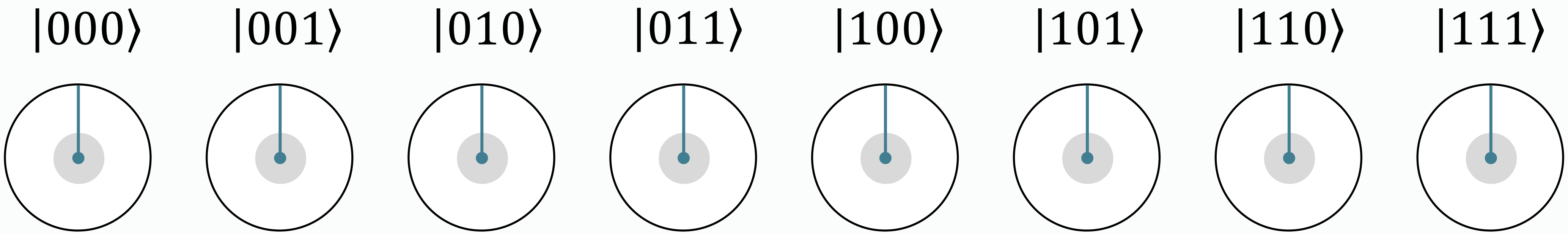
Use **entanglement** and **phase** (interference) to amplify "good" states and suppress "bad" states.

Walsh-Hadamard Transform

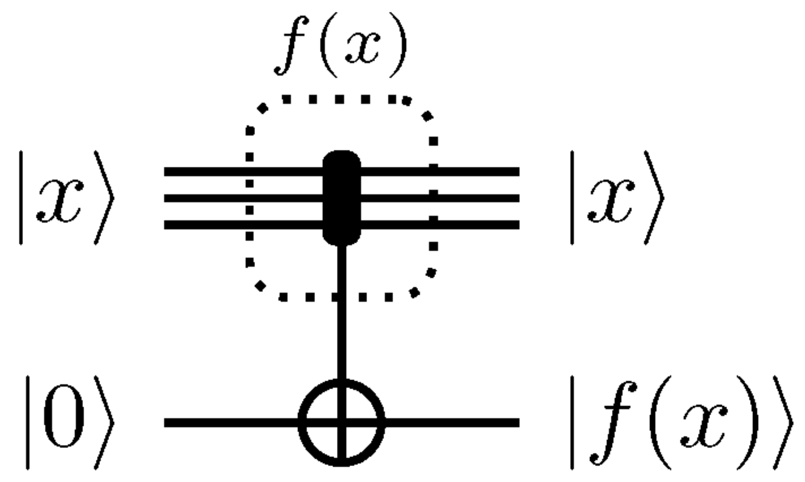


Create an equal superposition of all binary values.

$$H^{\otimes n}|0\rangle = \frac{1}{\sqrt{2^n}} \sum_{i=0}^{2^n-1} |i\rangle$$



Logic Oracle

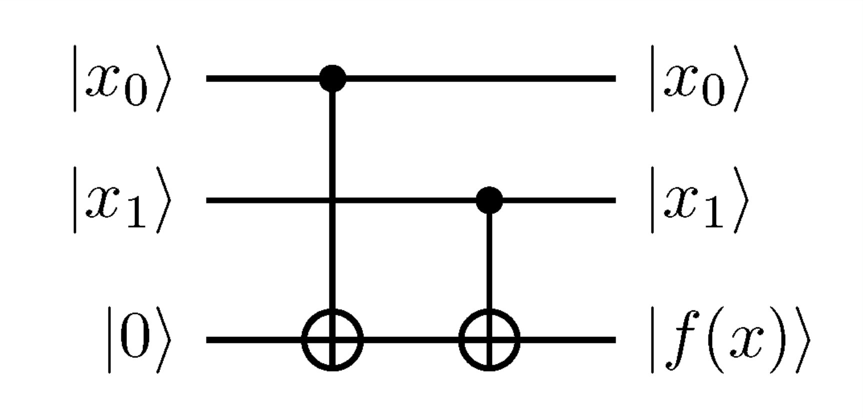


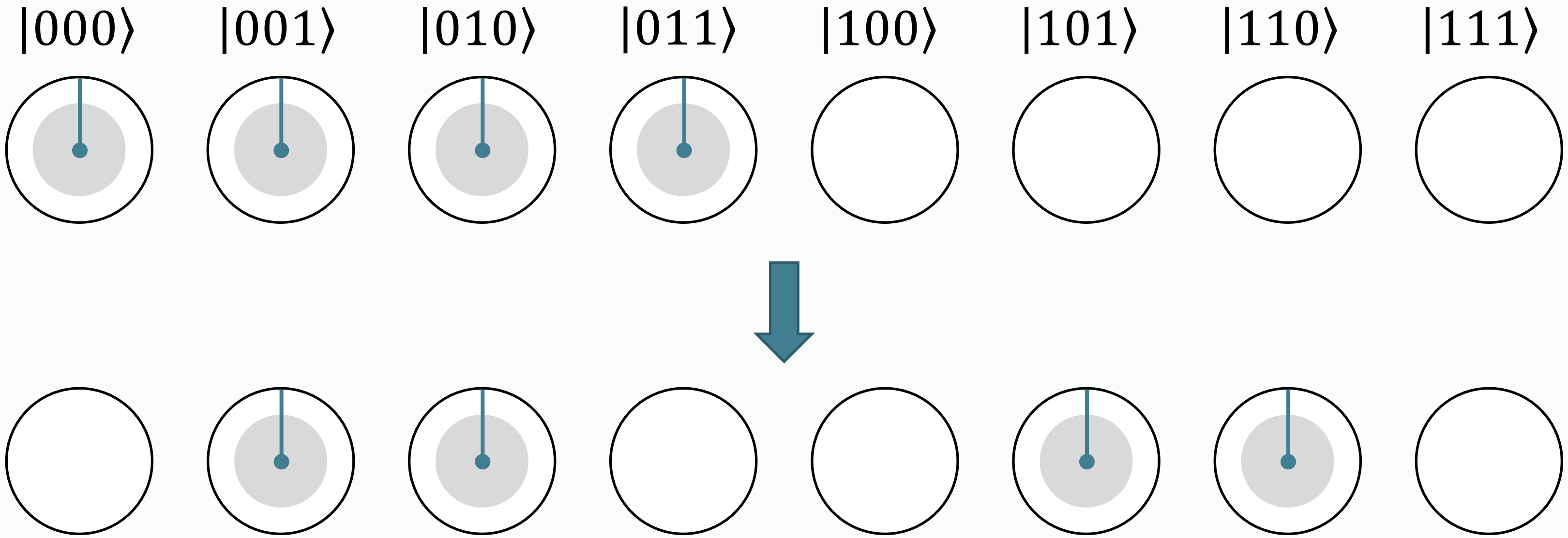
Control bits are set whenever $f(x)$ is true.

Output bit is 1 whenever $f(x)$ is true.

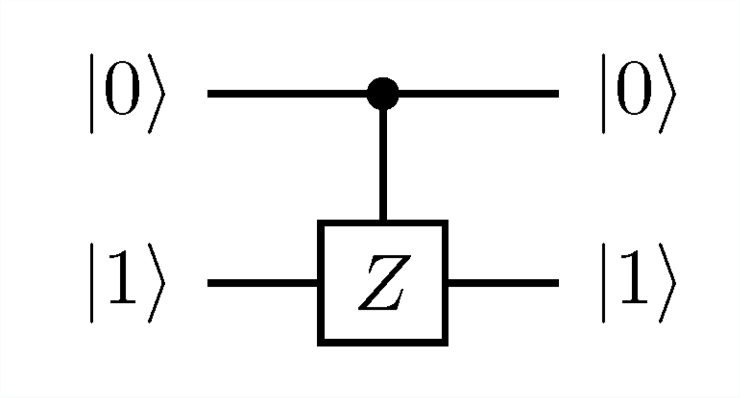
Logic Oracle

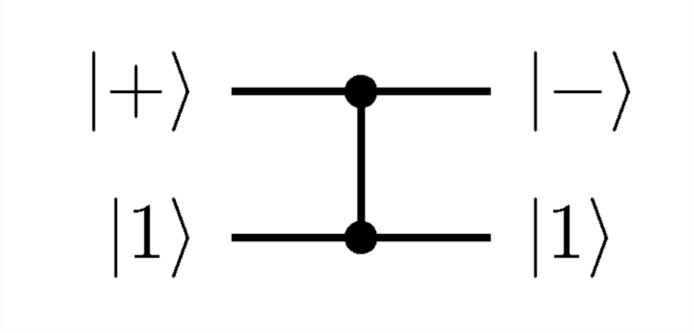
Example: $f(x)$ is true when the two input qubits are not equal.

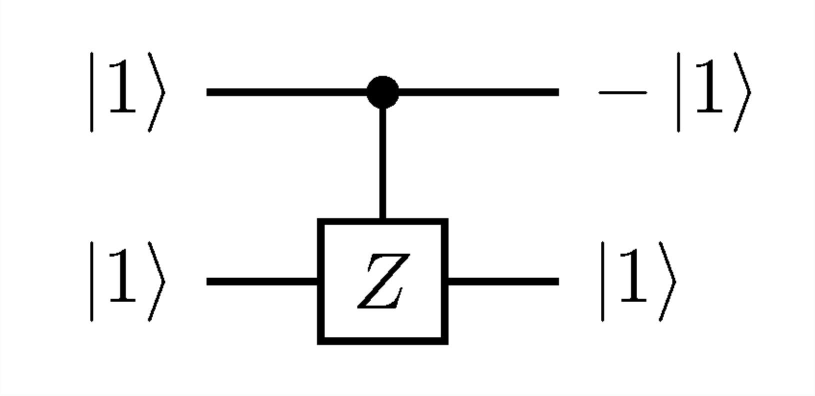




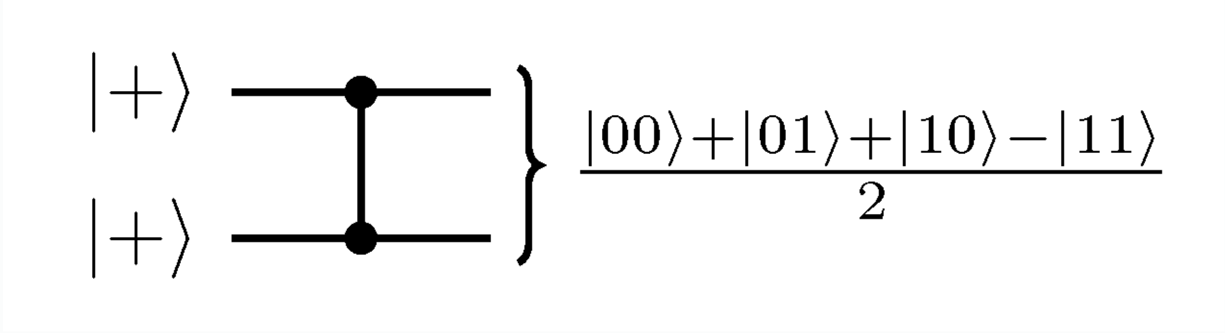
Control-Z Gate





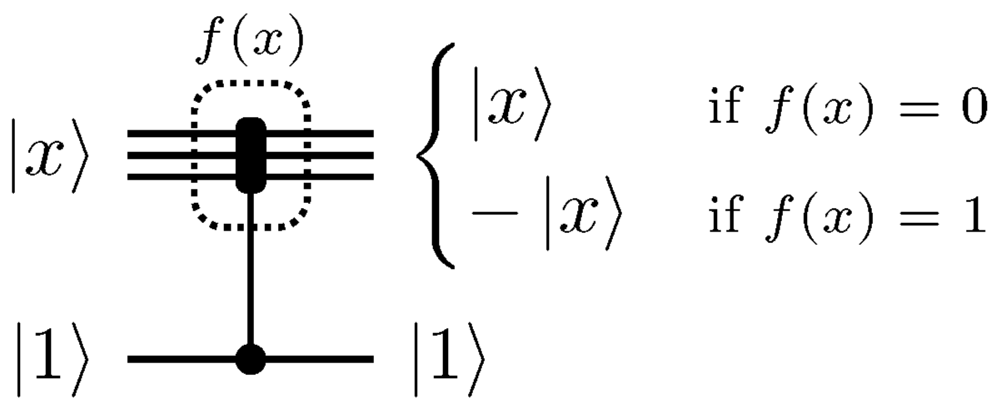


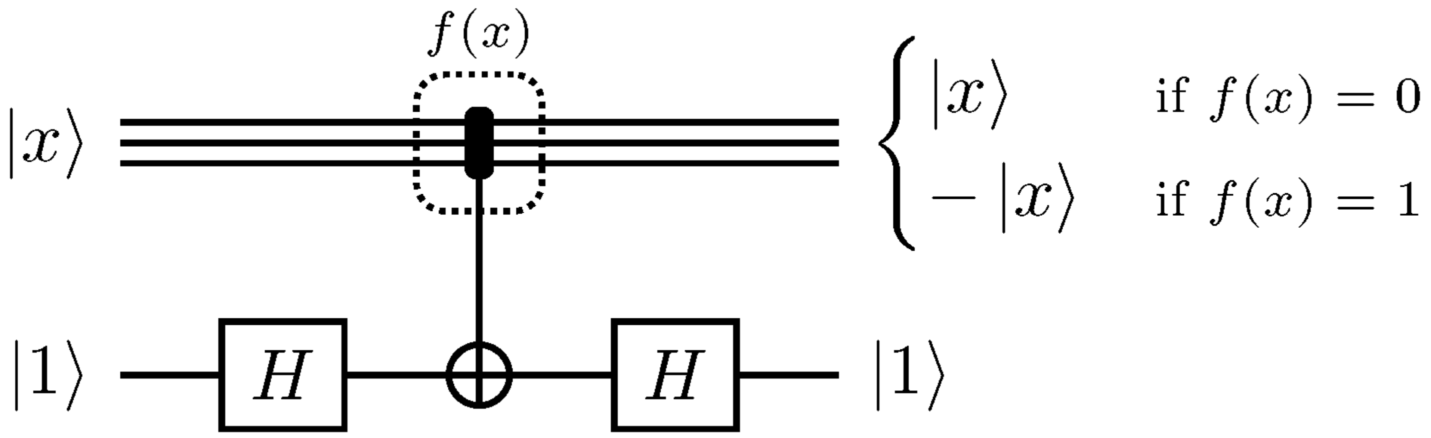
$$-|11\rangle = -|1\rangle \otimes |1\rangle = |1\rangle \otimes -|1\rangle$$



Phase changes when both inputs = 1.

Phase Oracle



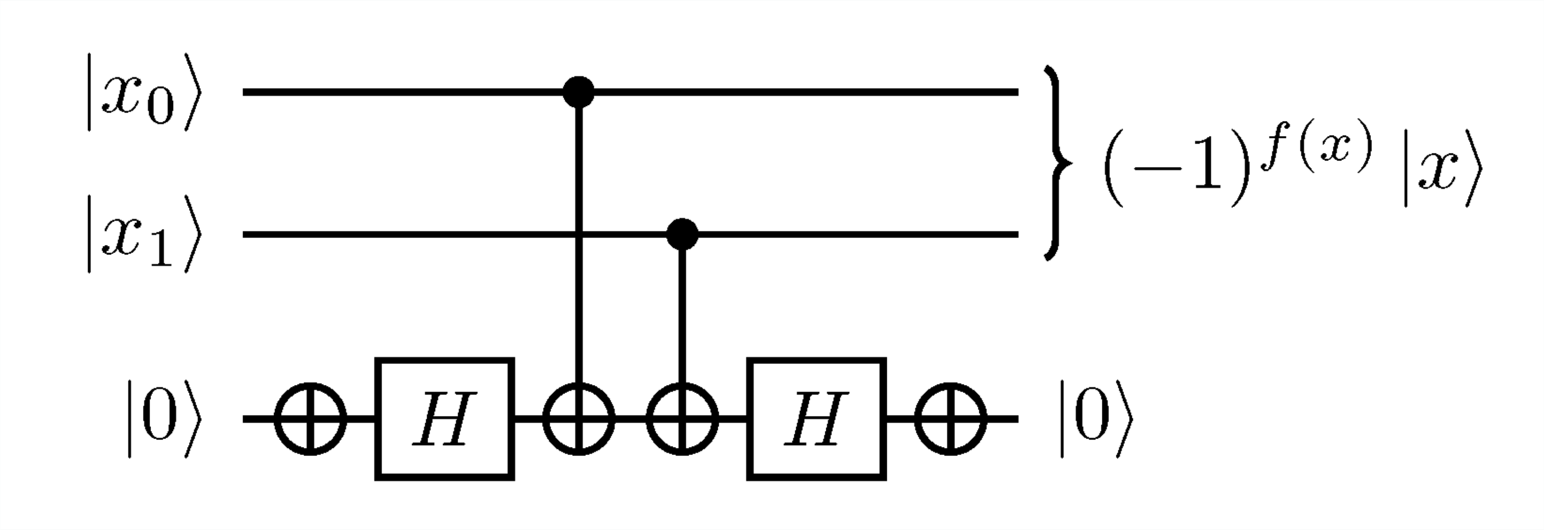


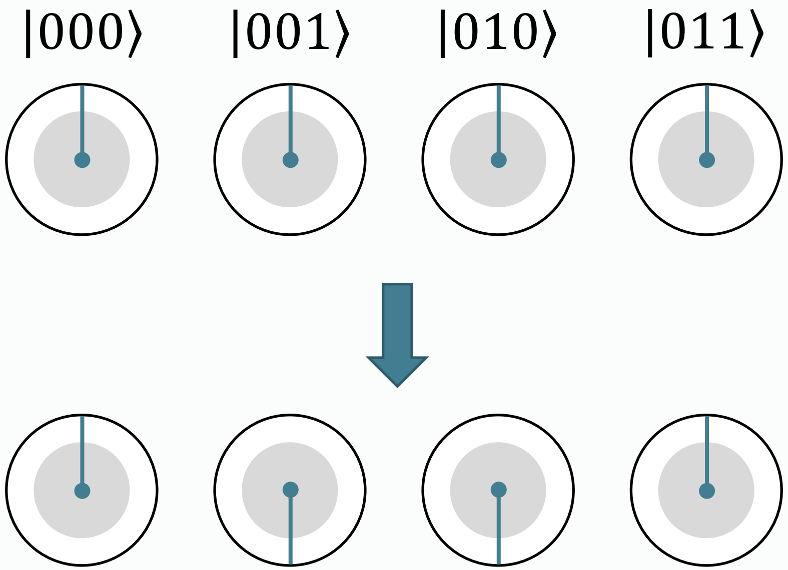
$$HXH = Z$$

Also known as "phase kickback"

Phase Oracle

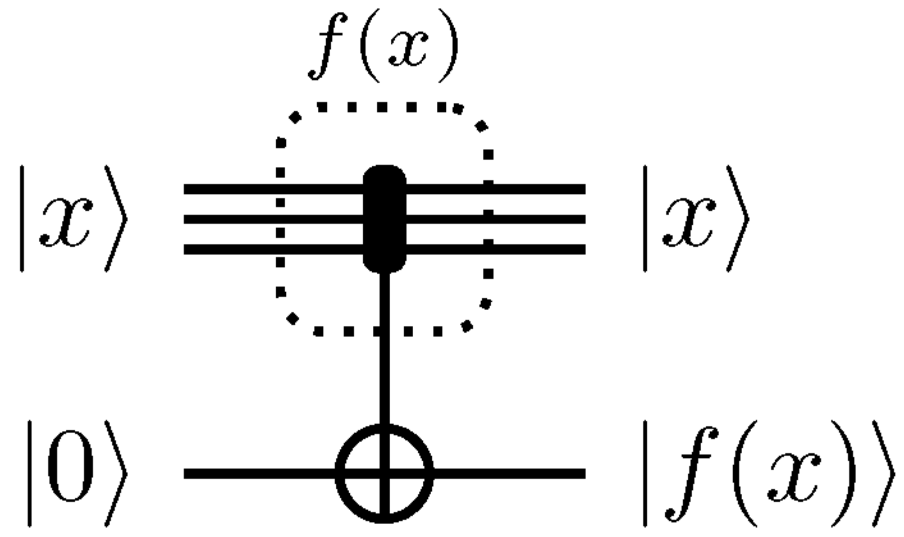
Example: $f(x)$ is true when the two input qubits are not equal.



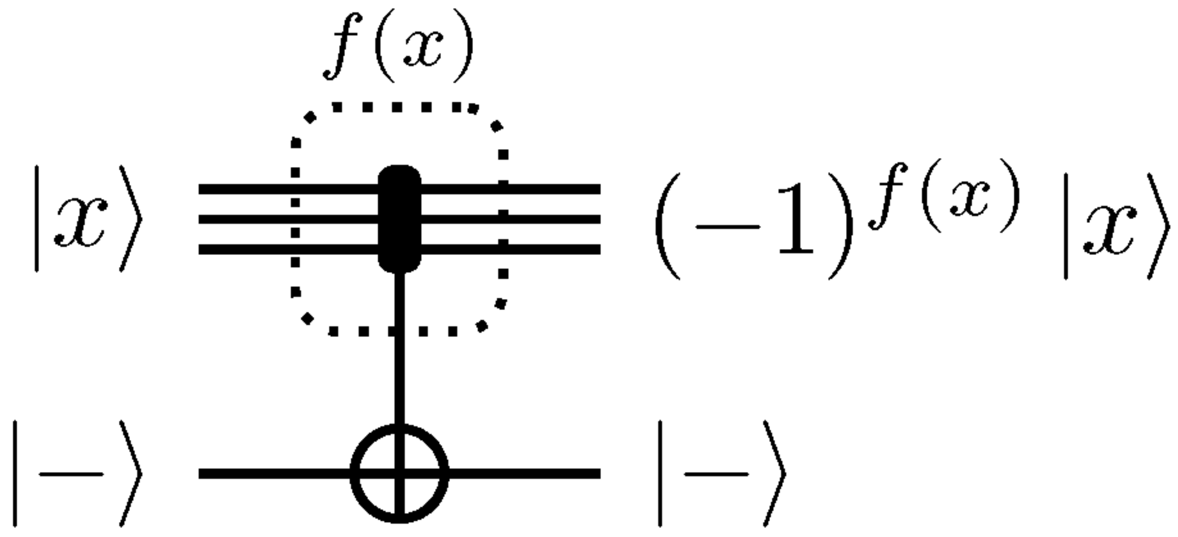


If phase isn't measured, what good is a phase oracle?

Summary: Oracles



Oracle



Phase Oracle

Photo by NICO BHLR on Unsplash

Grover's Search Algorithm

Grover's Algorithm

1996

Problem: Given $f(x)$: $\{0,1\}^n \rightarrow \{0,1\}$, where $f(w) = 1$ for one input w, and $f(x) = 0$ for all other inputs, find w.

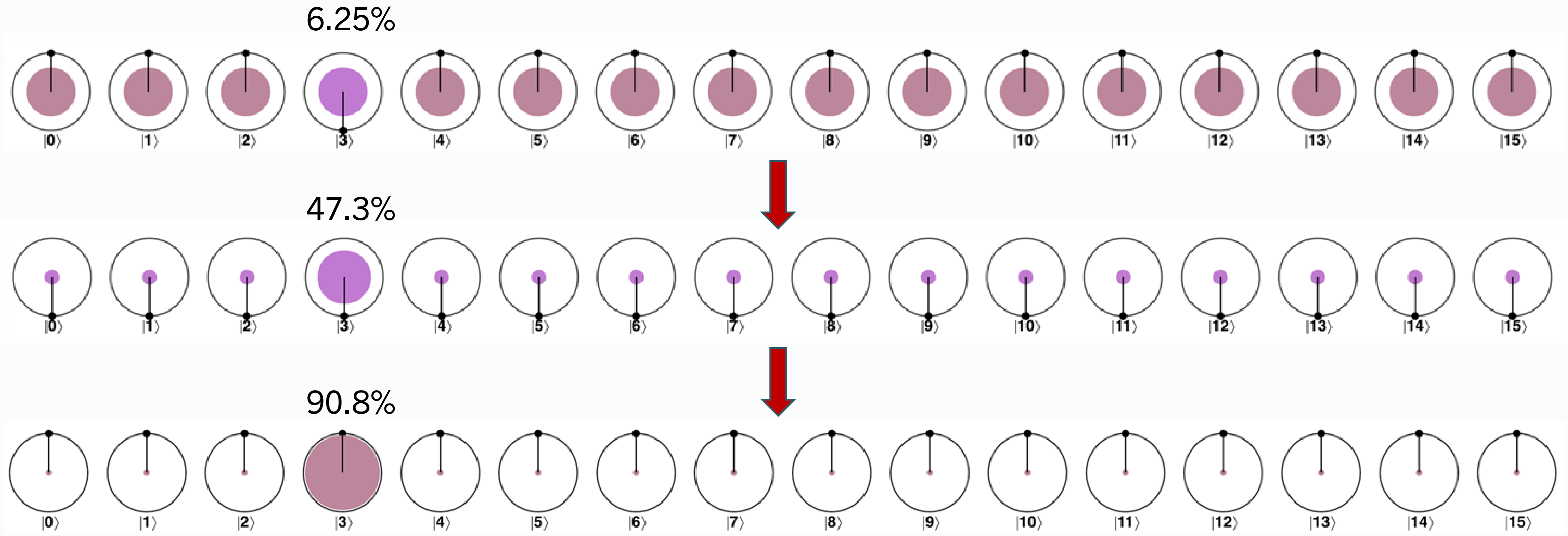
Classical Solution: Requires $2^{n-1} = N/2$ **queries**, on average.
With no additional information, have to try every input until we find the solution.

Quantum Solution:
Requires $O(2^{n/2}) = O(\sqrt{N})$ **queries**, to find solution with high probability.

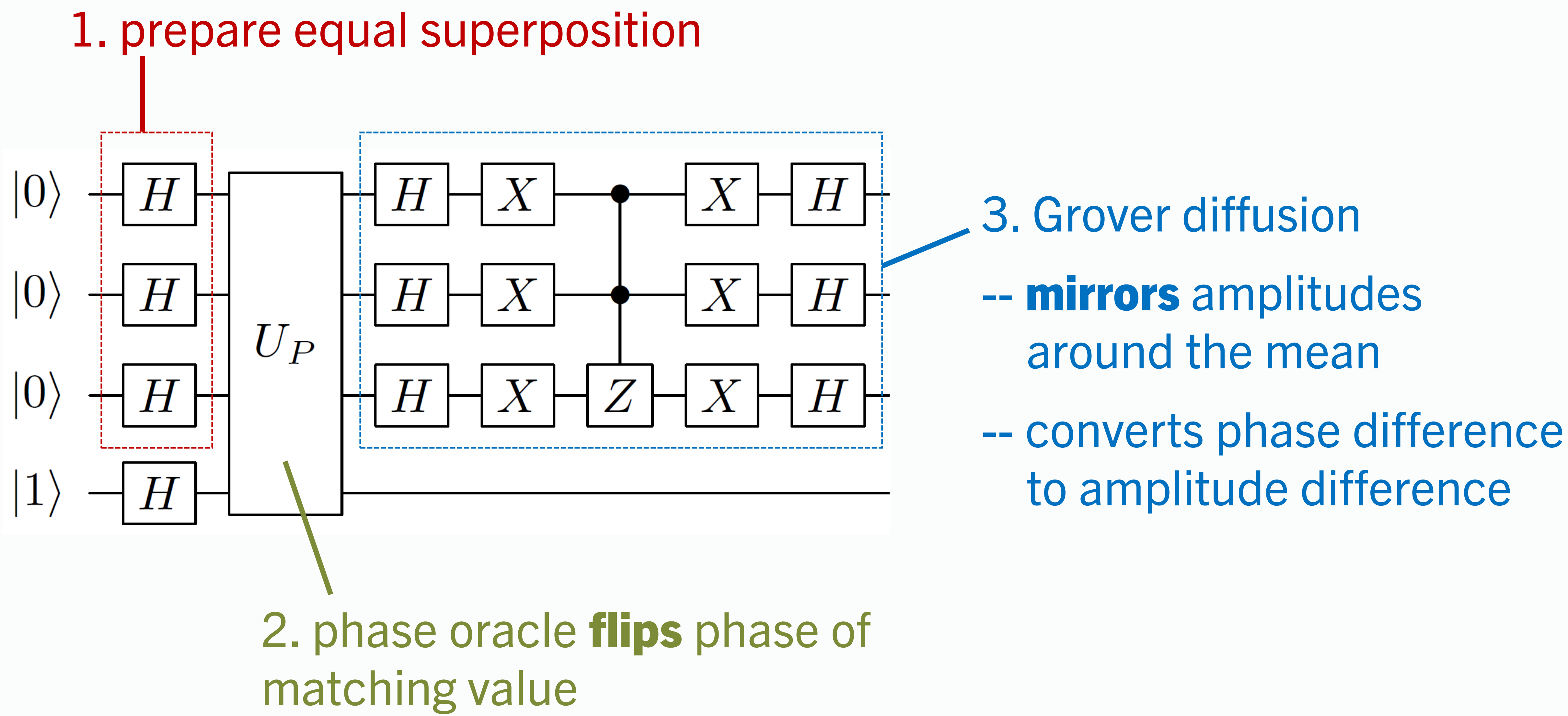
Quadratic advantage

Amplitude Amplification

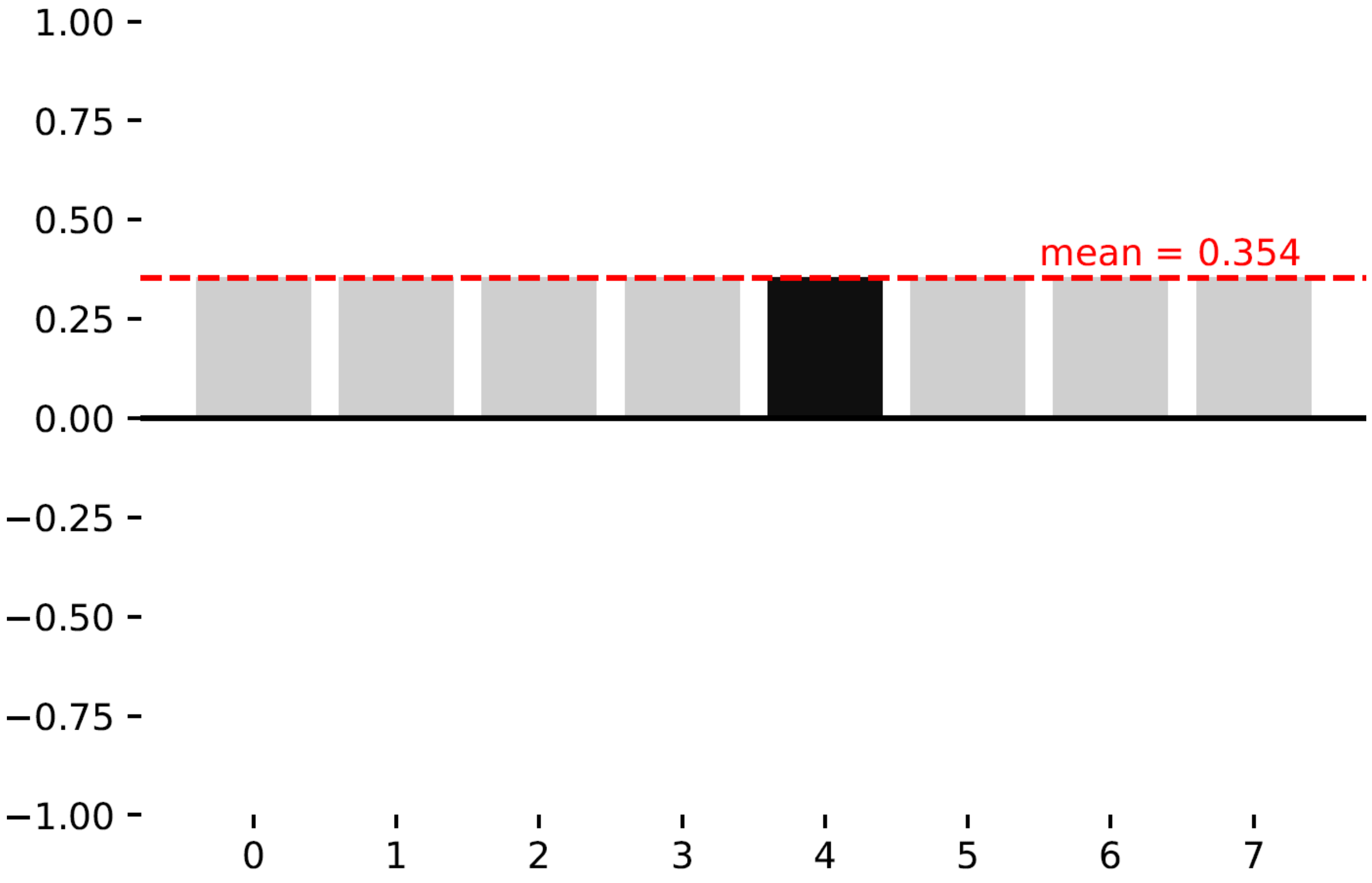
Converts a phase difference into a magnitude difference.



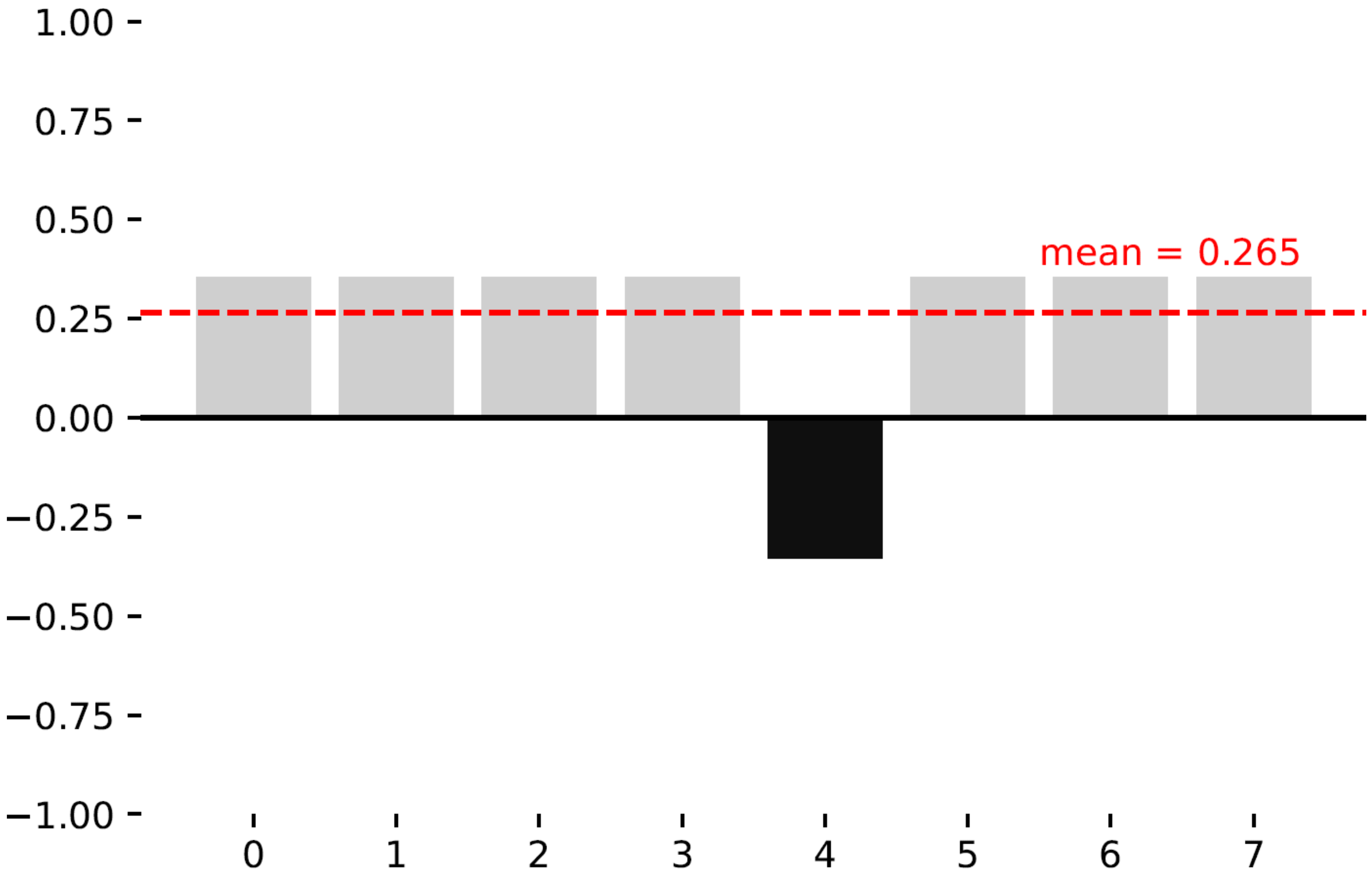
Johnston, et al. Programming Quantum Computers, 2019.


1. prepare equal superposition
|0⟩
|0⟩
|0⟩
|1⟩
H
U_P
X
Z
2. phase oracle **flips** phase of matching value
3. Grover diffusion
-- **mirrors** amplitudes around the mean
-- converts phase difference to amplitude difference

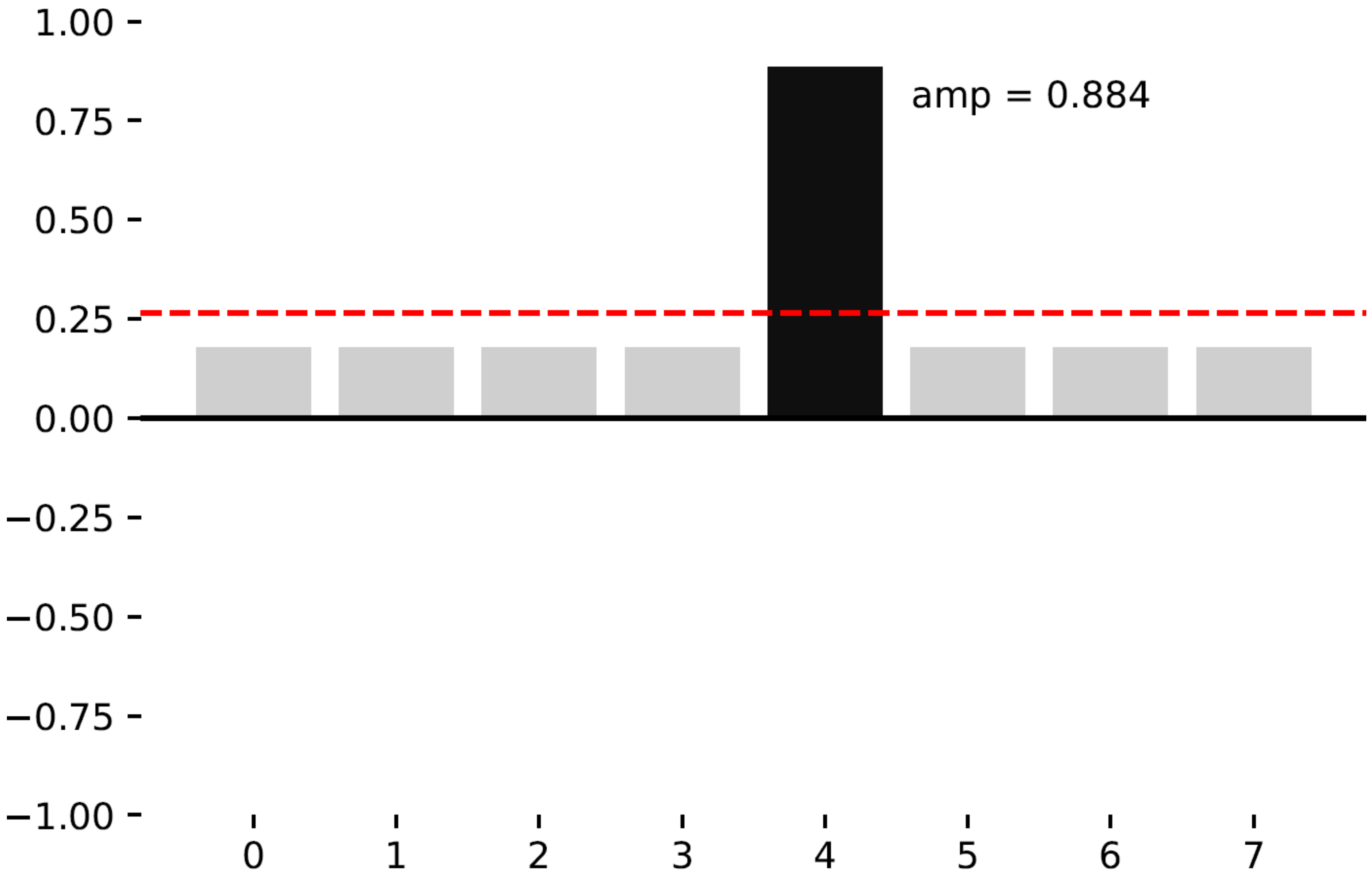
Initial State

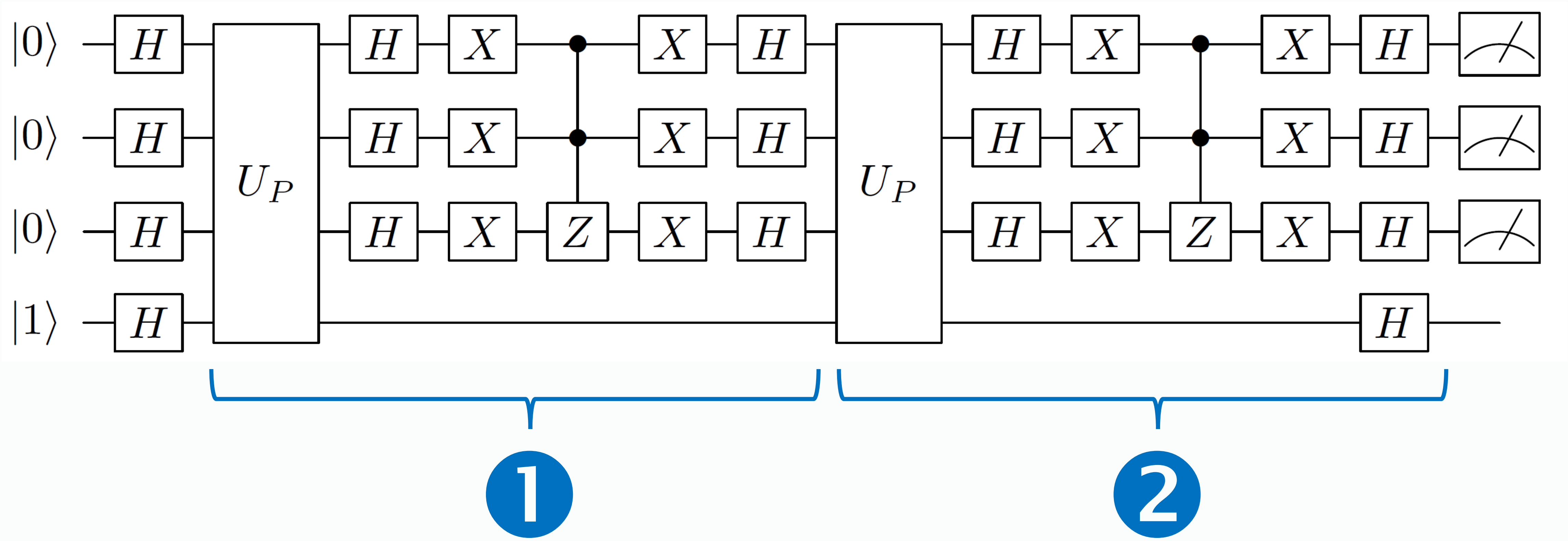


After Flip



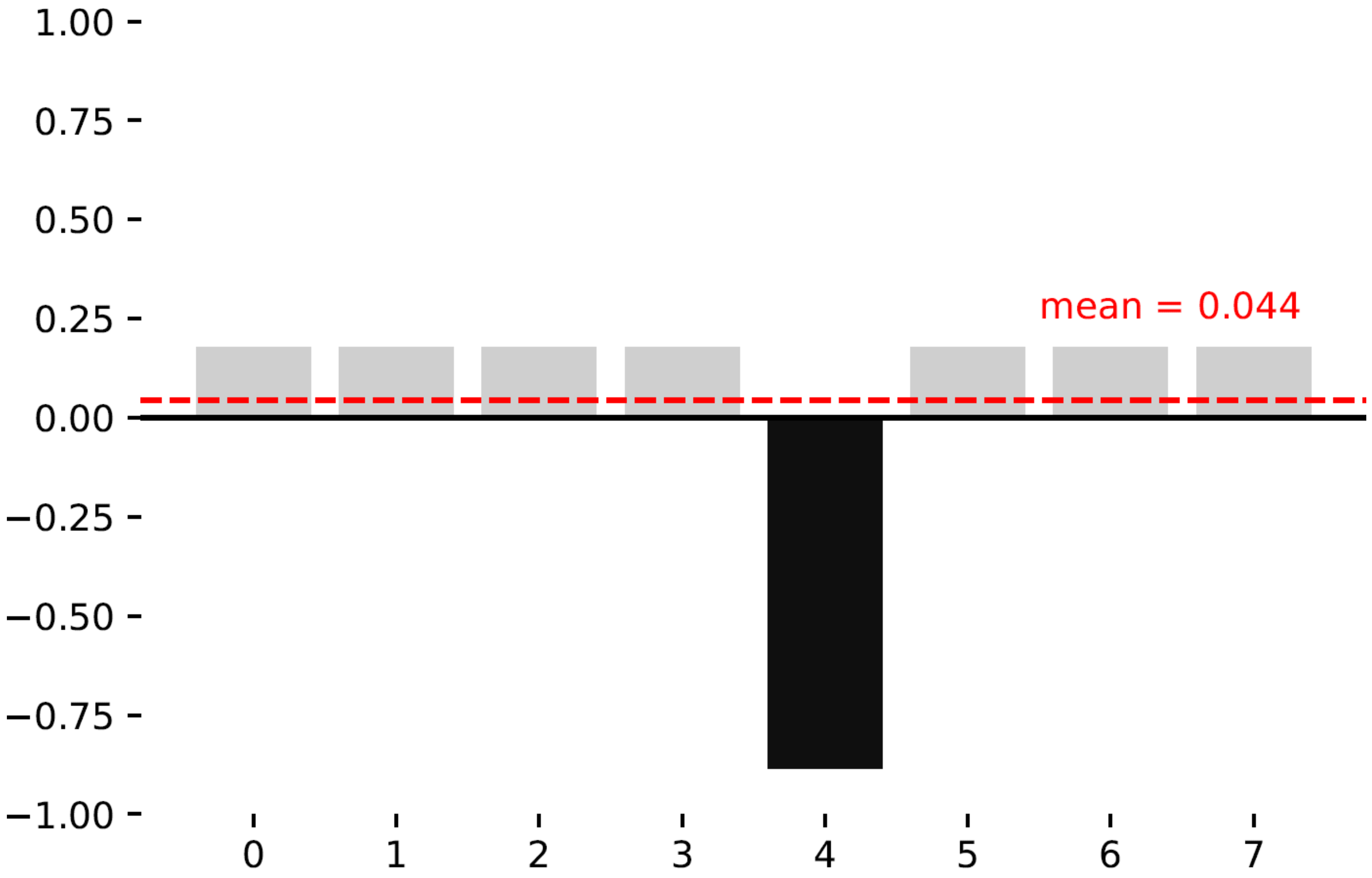
Mirror: reflect around the mean



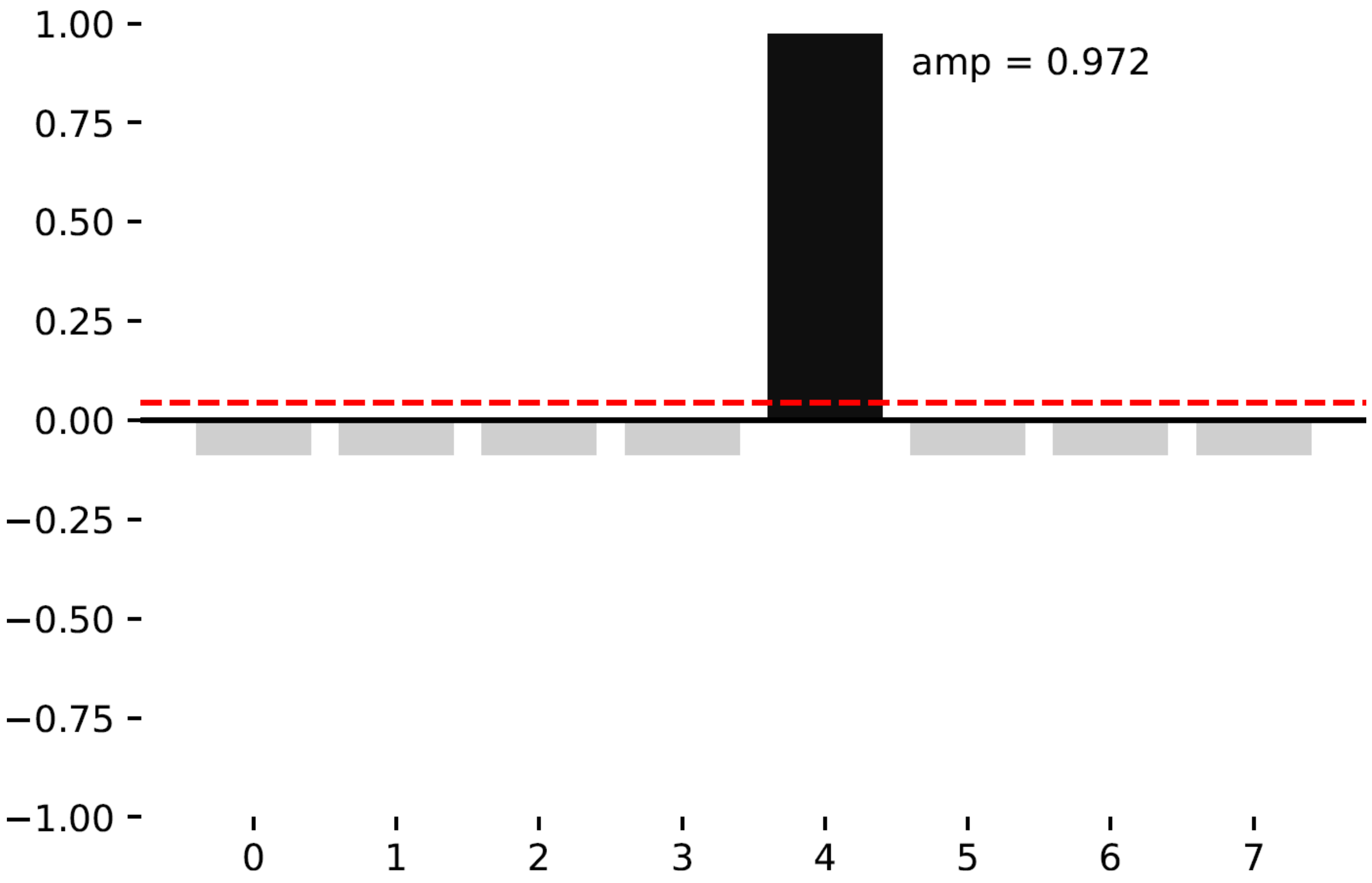


How many iterations?

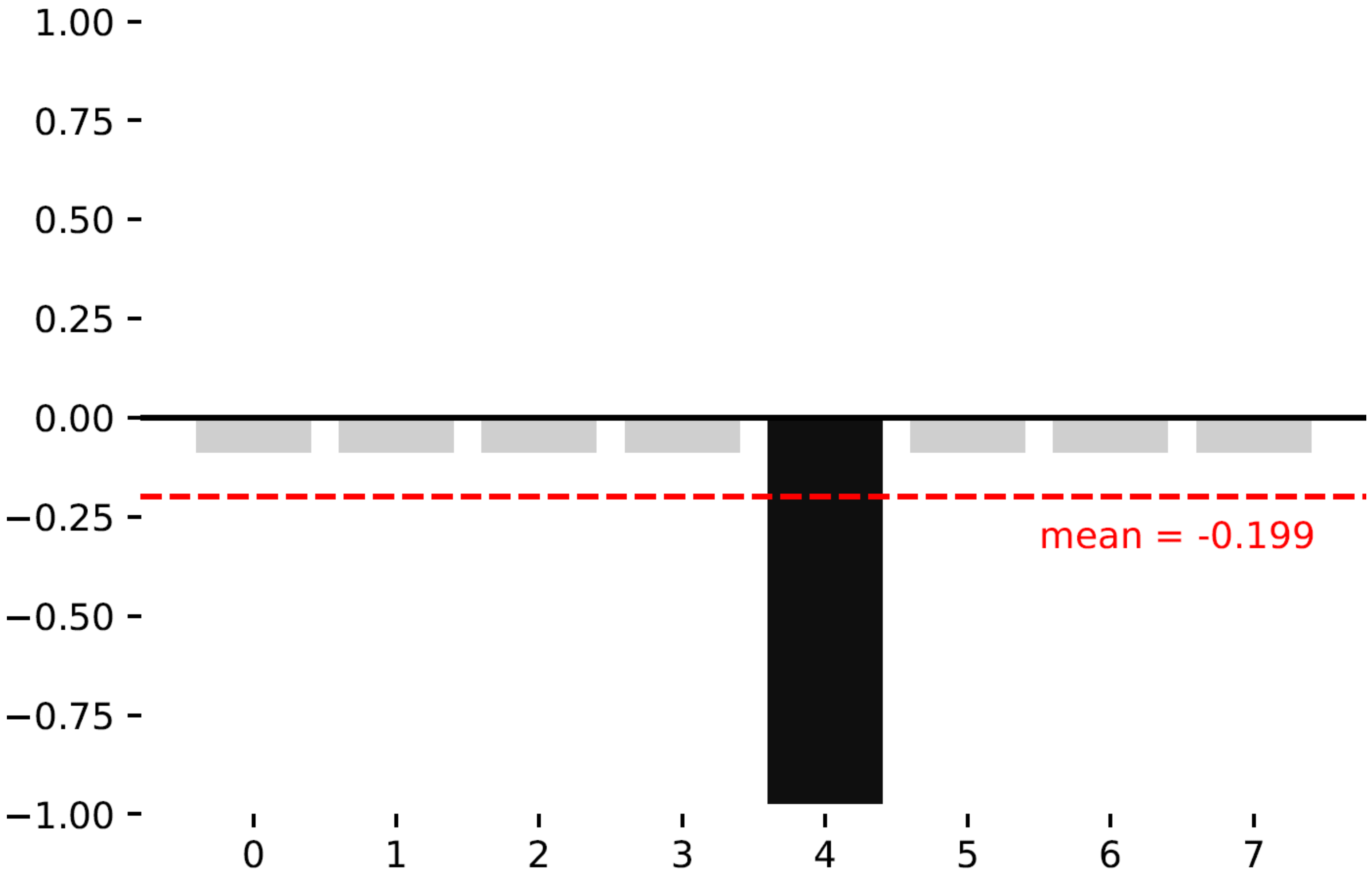
Flip again



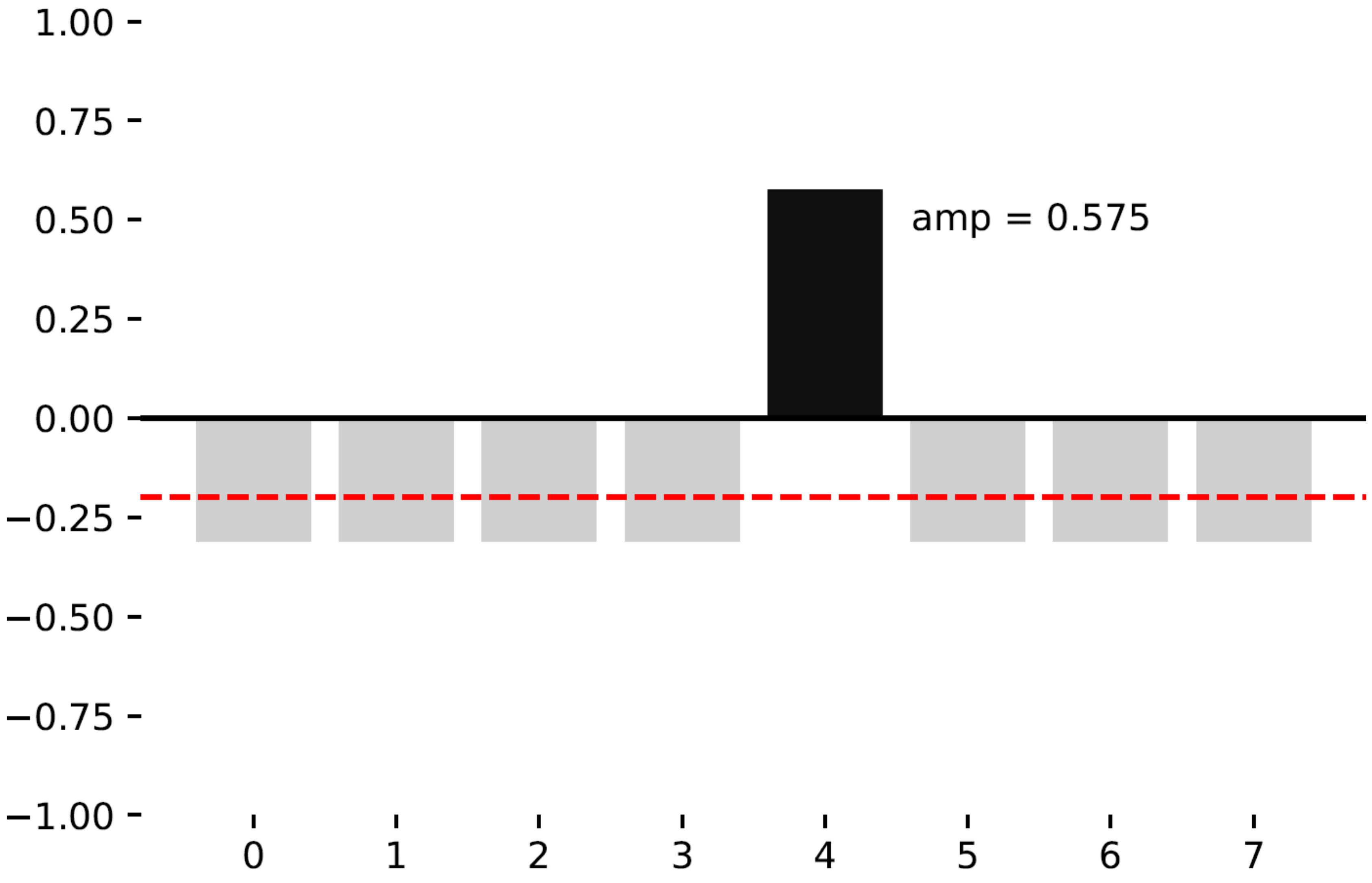
Mirror



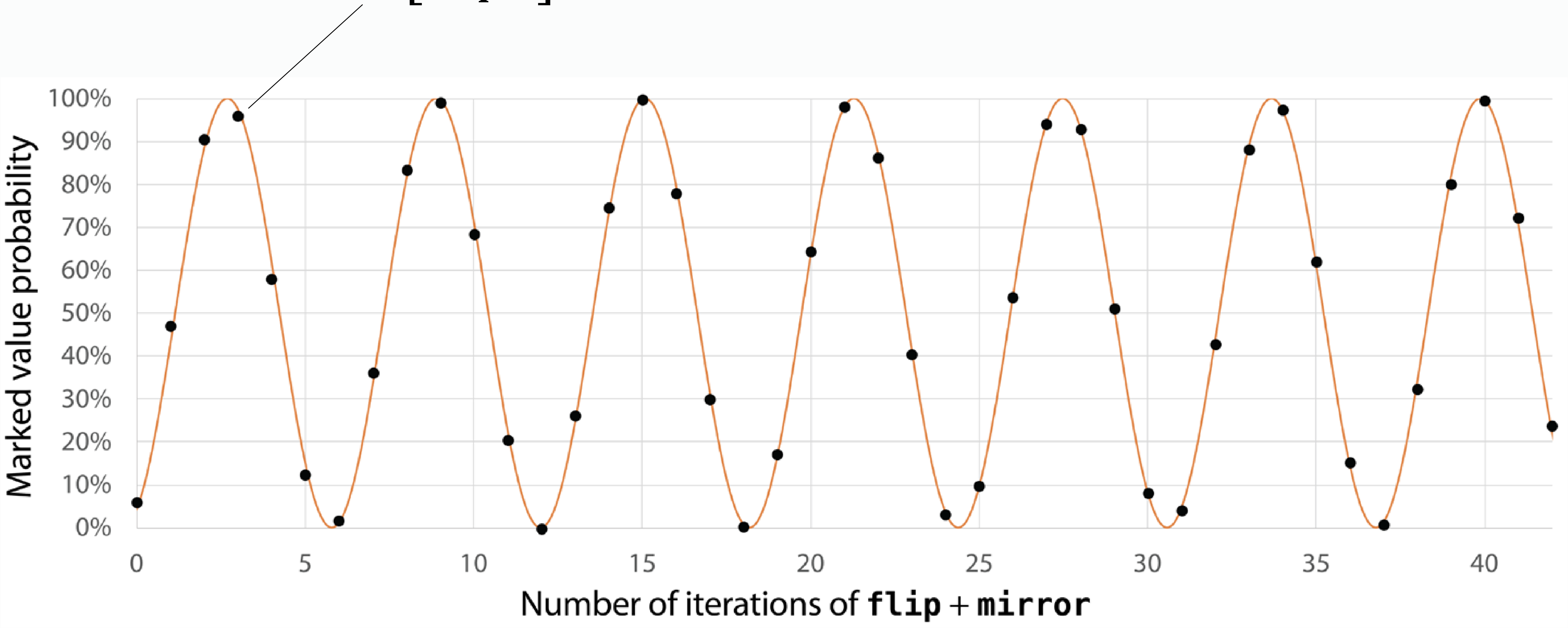
Flip



Mirror



$$N_{AA} = \left\lfloor \frac{\pi\sqrt{2^n}}{4} \right\rfloor$$



Johnston, et al. Programming Quantum Computers, 2019.

Some Quantum Algorithms

Algorithm	Description	Quantum	Classical
Quantum Fourier Transform	Frequency analysis	$O(\log^2 N)$	$O(N \log N)$
Grover's Search	Satisfiability (etc.)	$O(\sqrt{N})$	$O(N)$
HHL	Linear Systems	$O(\log(N) s^2 \kappa^2 / \varepsilon)$	$O(N s \kappa \log(1/\varepsilon))$
Shor's	Factoring	$O(n^2 \log n)$	$O(\exp n^{1/3})$

$N = 2^n$ = problem size, n = # qubits/bits

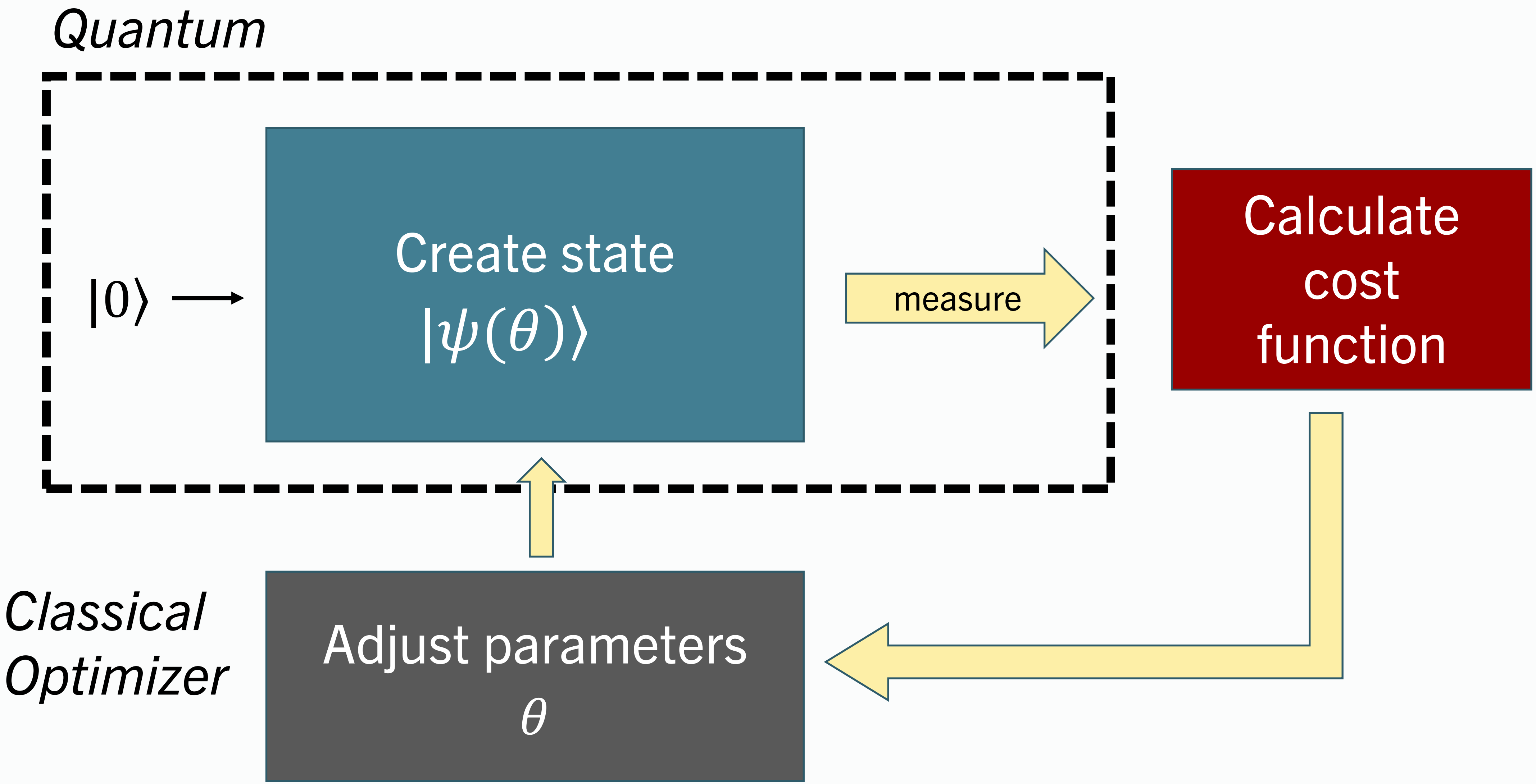
Quantum Algorithm Challenges

1. **Large number of qubits**
   - Binary representation of data
2. **Deep circuits**
   - Lots of gates
   - Decoherence (and other noise) becomes a problem

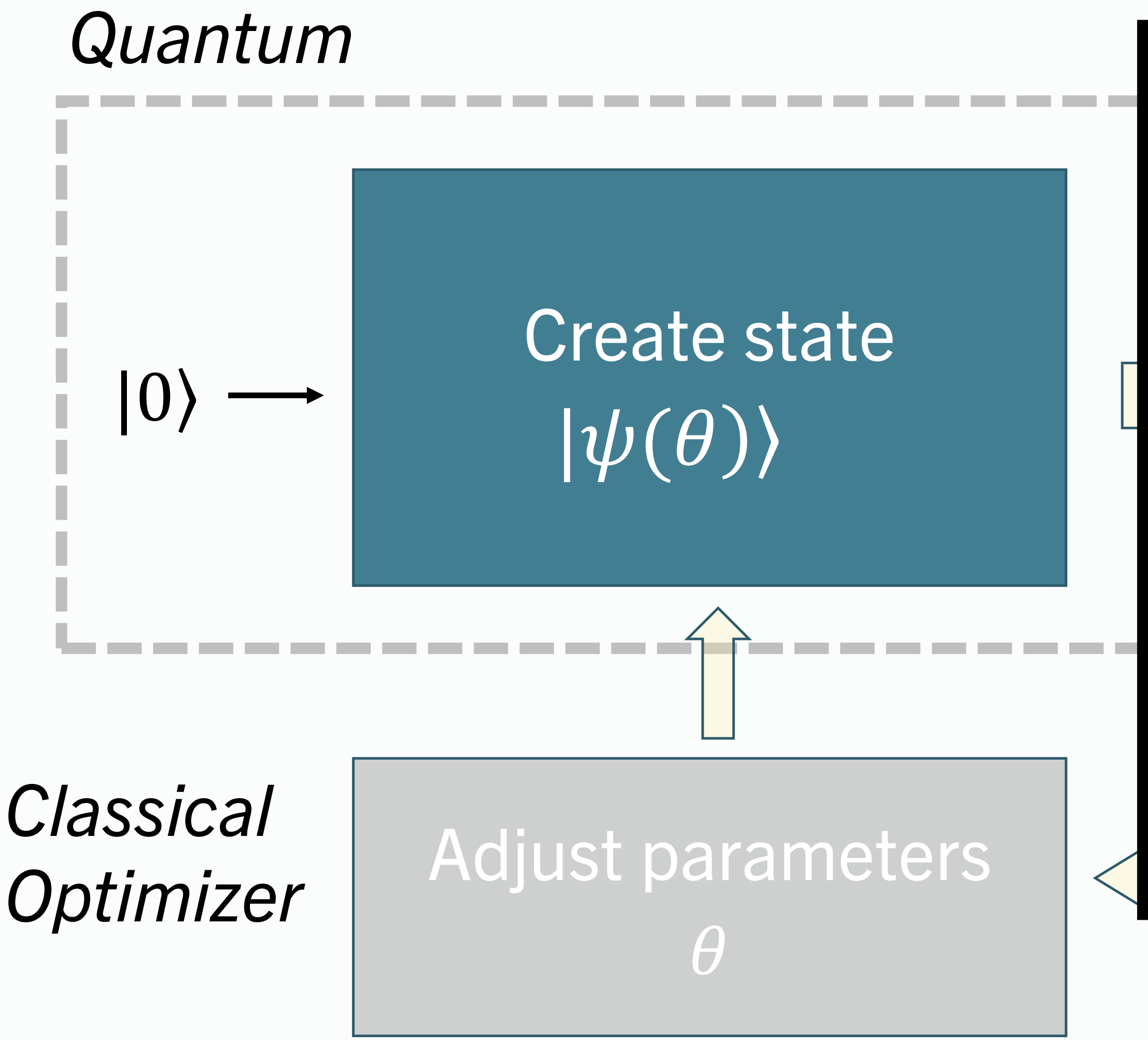
Variational Quantum Algorithms

Photo by Conny Schneider on Unsplash

Variational Algorithm



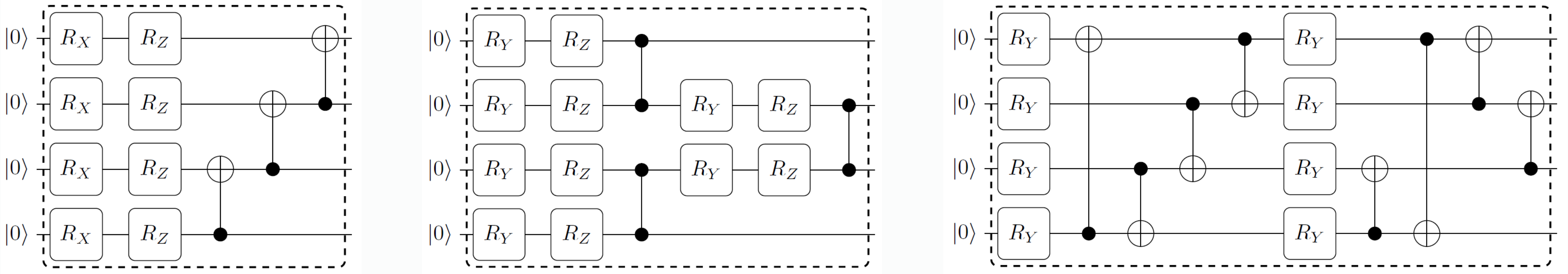
Variational Algorithm

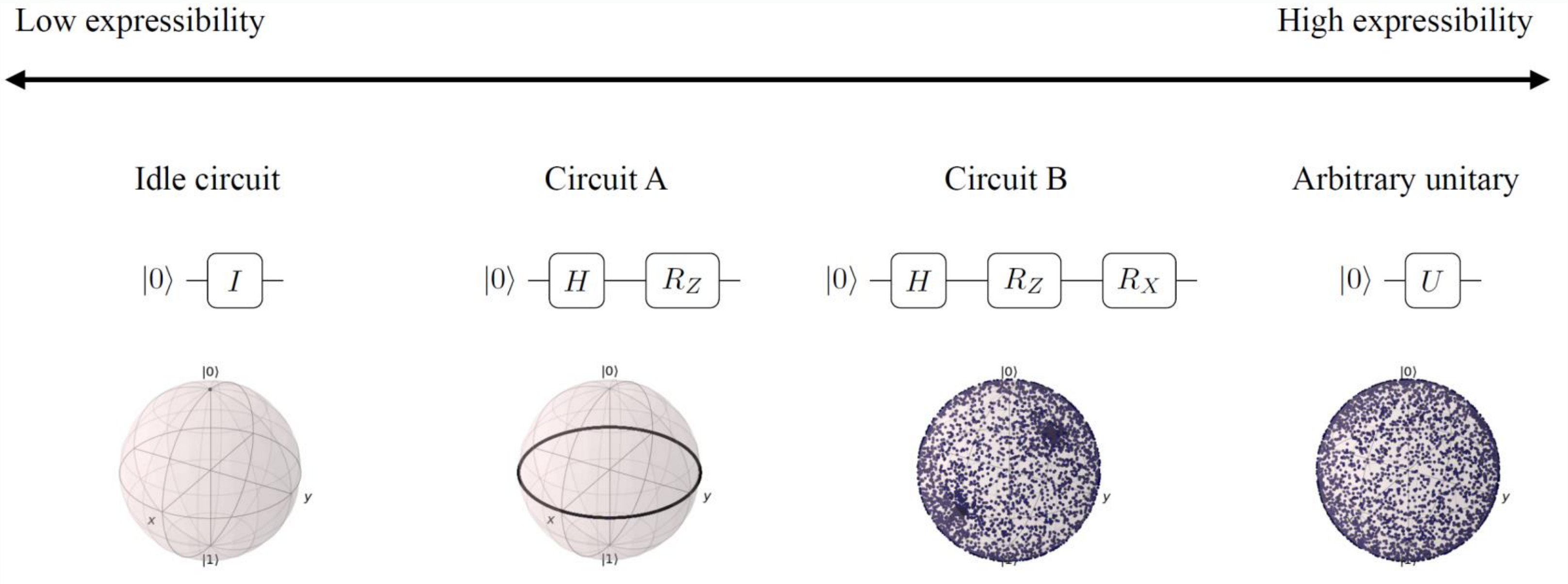


Parameterized Quantum Circuit

- Rx/Ry/Rz gate with angle of rotation specified as a parameter
- Entangling gates: CNOT, CZ
- Vector of parameters (θ) for different gates
- Allows controlled exploration of state space
- Also known as an "ansatz"

Parameterized Quantum Circuit





Expressibility
Entanglement
Trainability
H/W Compatibility
Layers

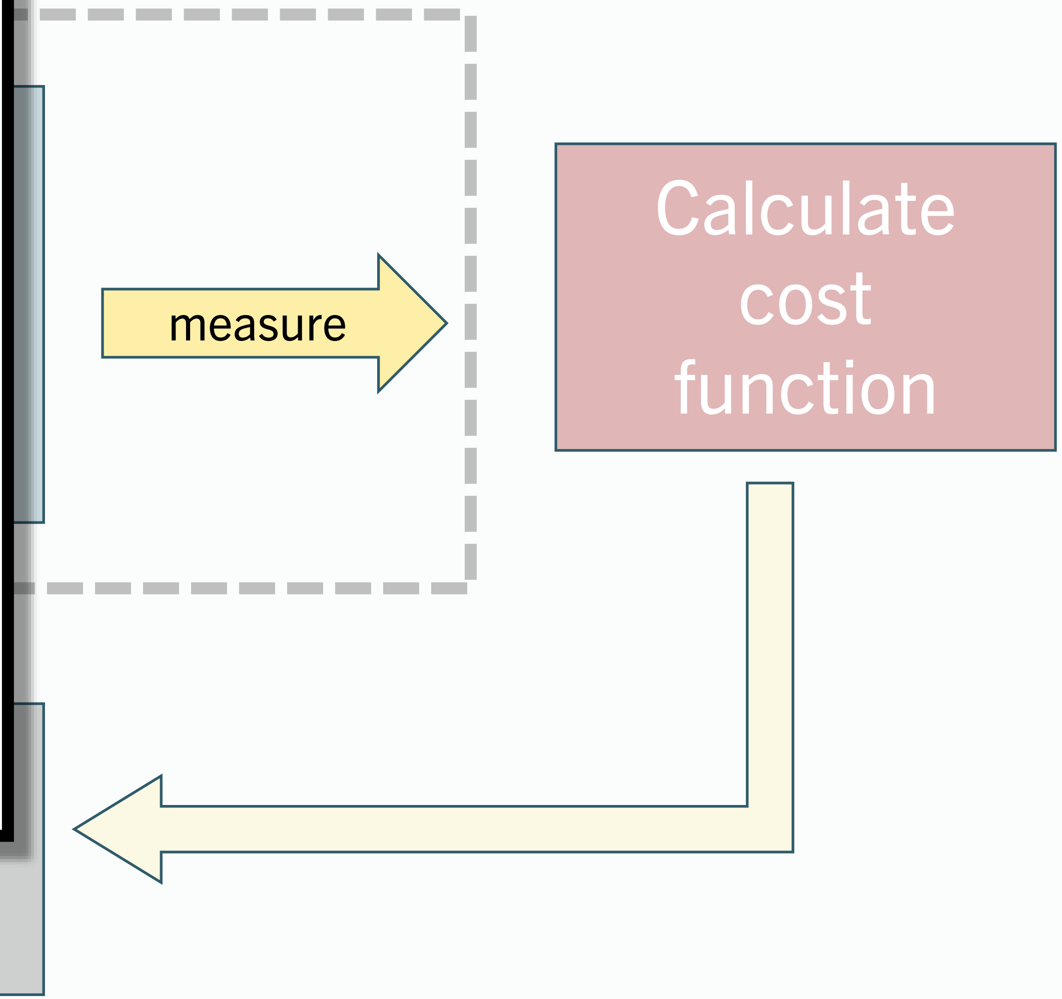
afternoon tutorial

S. Sim, et al. https://doi.org/10.1002/qute.201900070

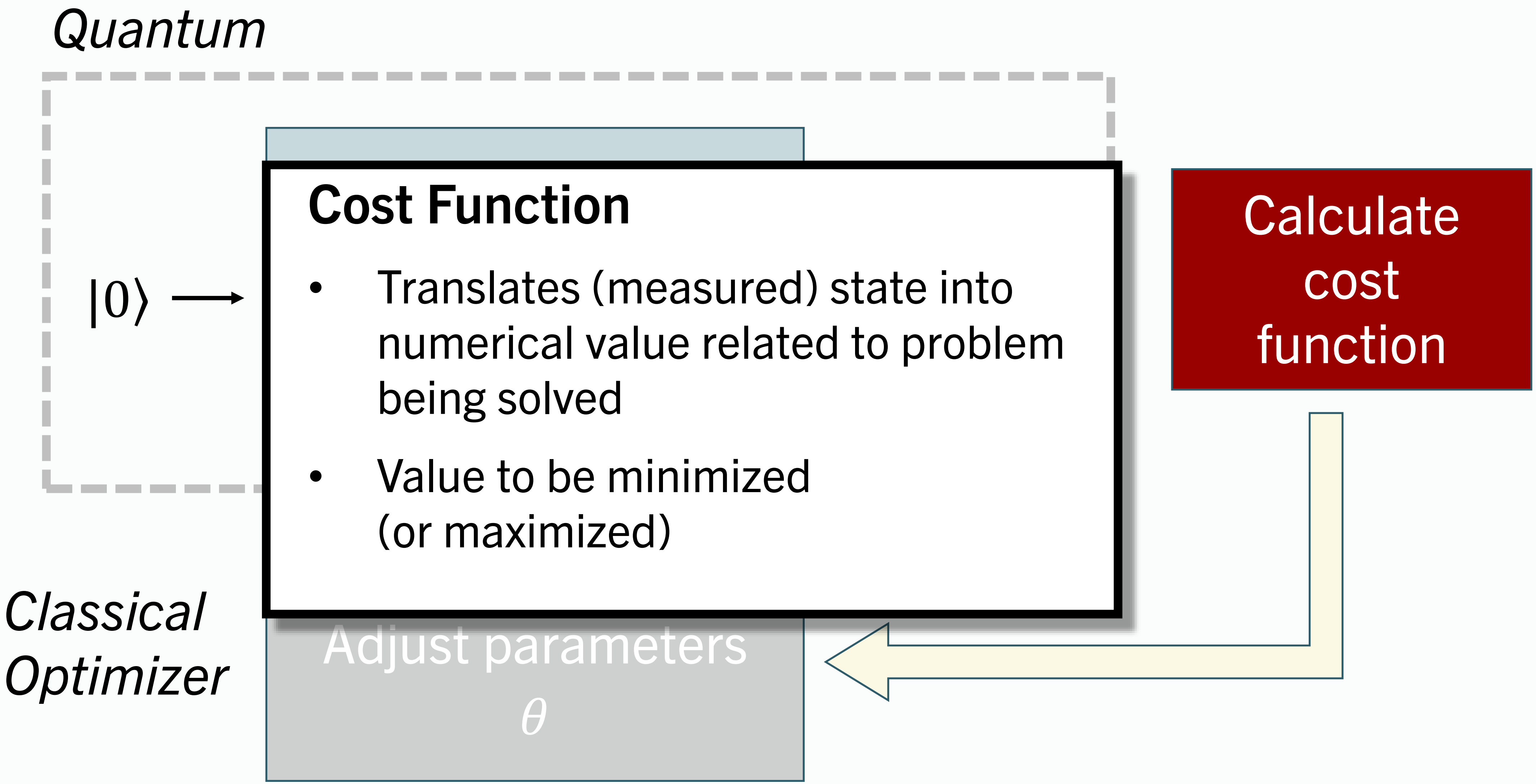
Variational Algorithm

Measurements

- Lots of measurements to extract / estimate statistics of quantum state
- Could be different kinds of measurements
- Related to the cost function, based on the problem to be solved



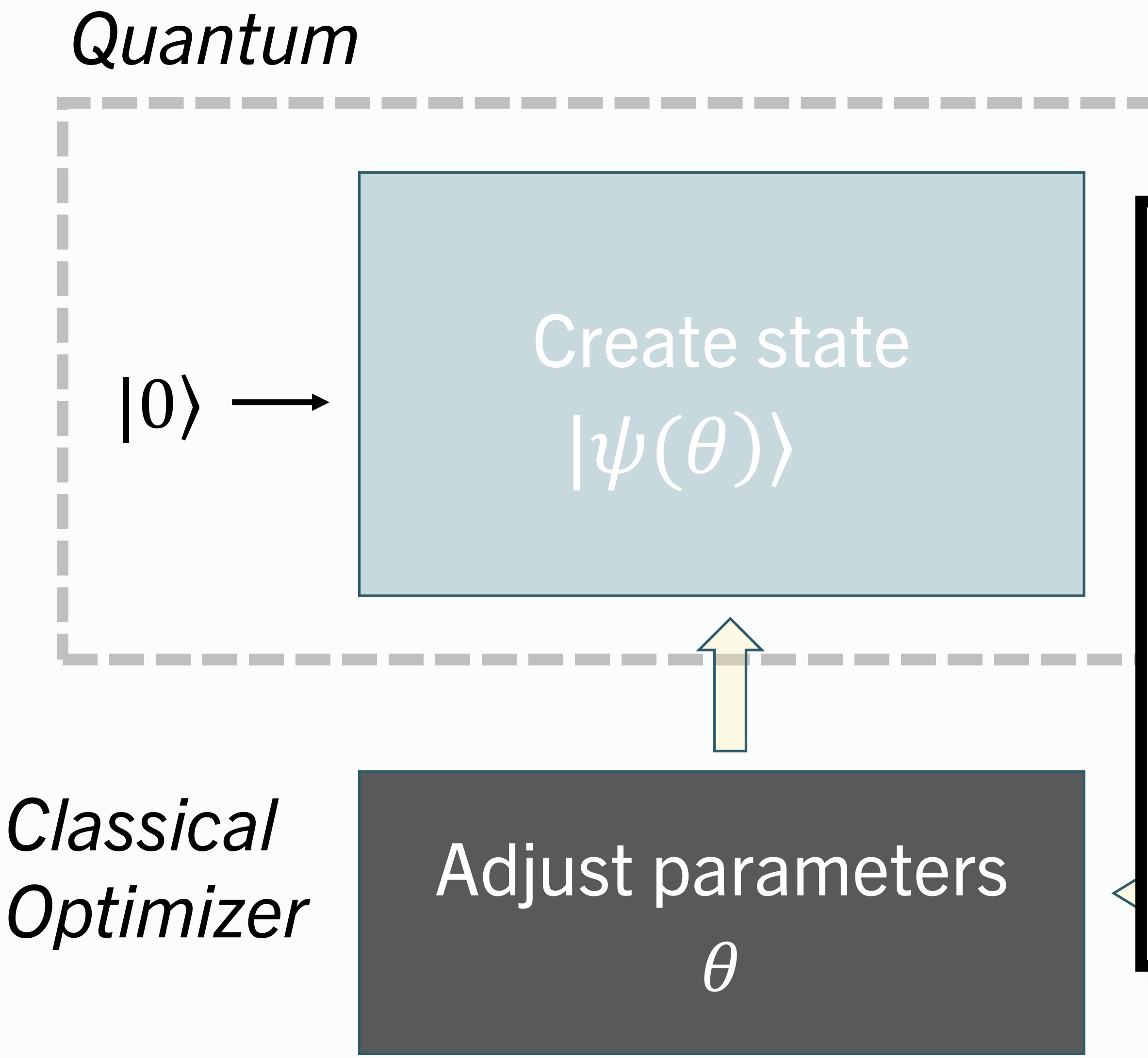
Variational Algorithm



Cost Function

- Translates (measured) state into numerical value related to problem being solved
- Value to be minimized (or maximized)

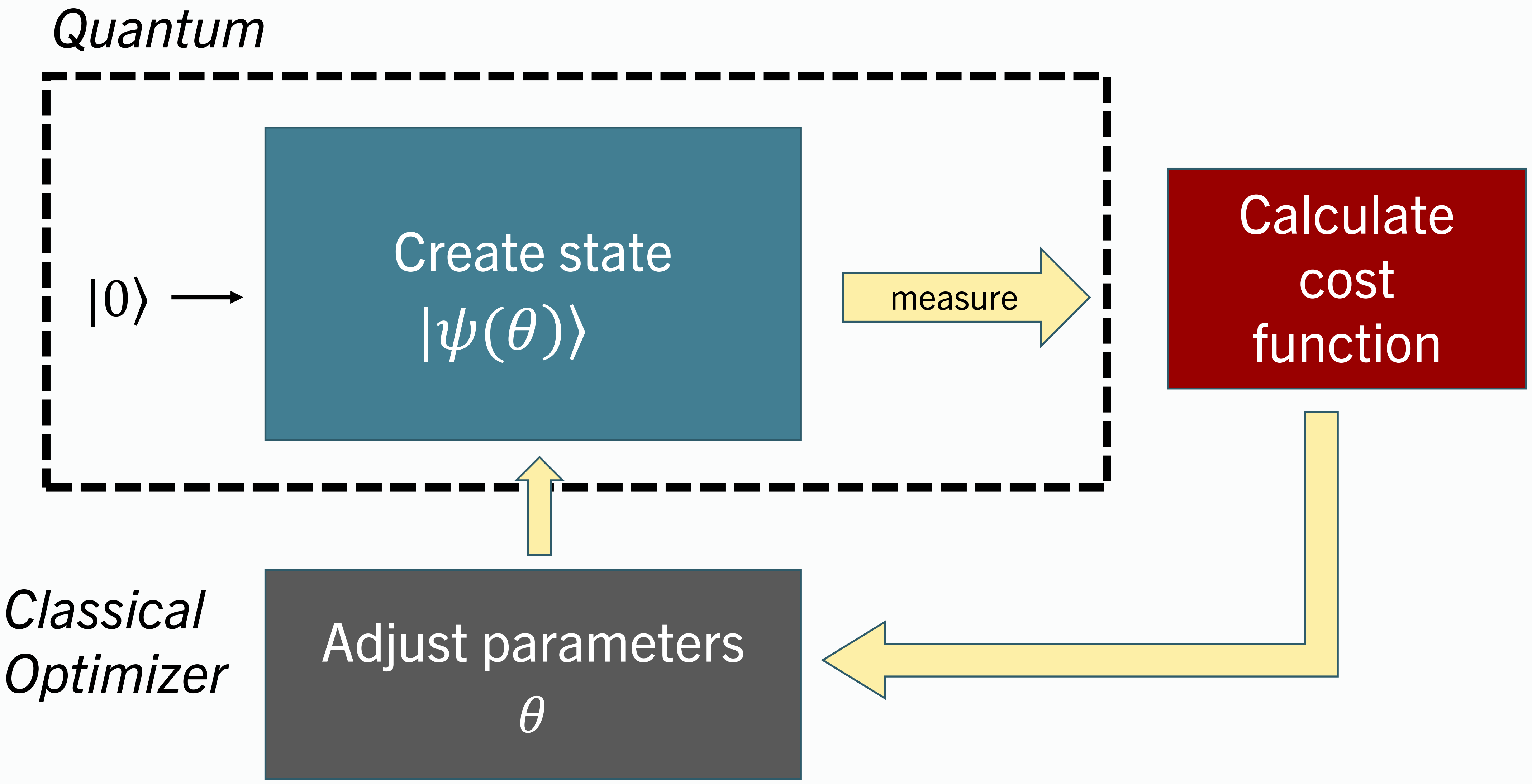
Variational Algorithm



Optimizer

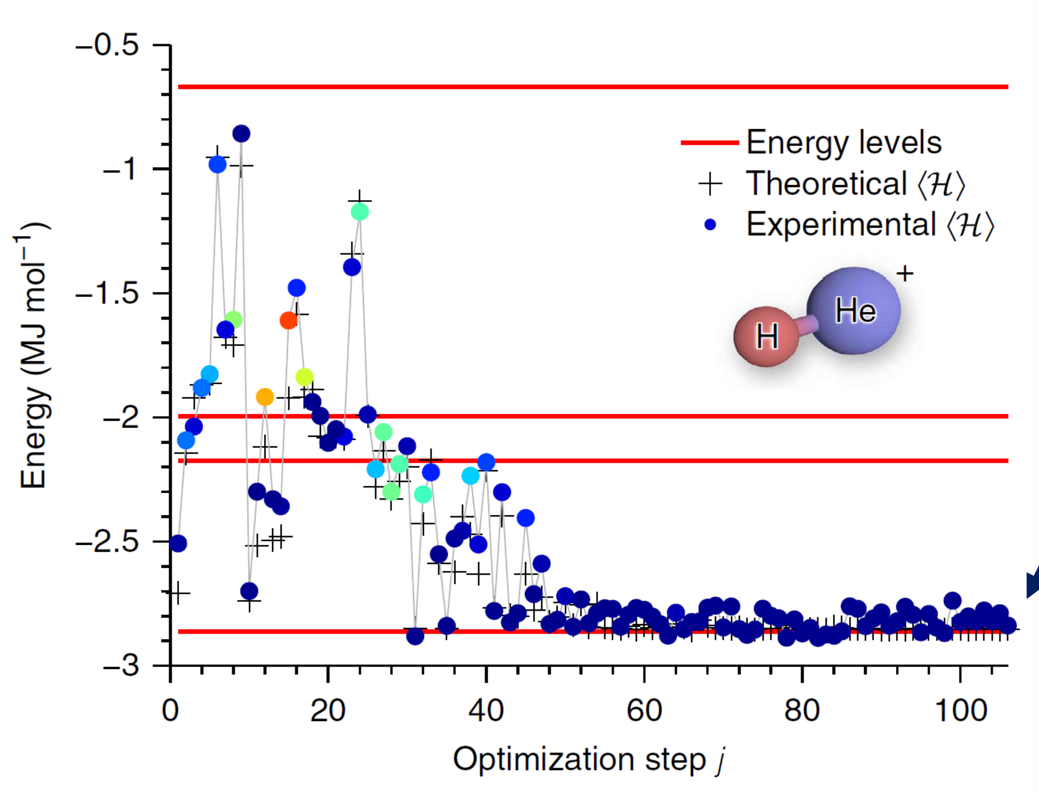
- Adjust parameters to minimize cost function
- Lots of options:
  Gradient descent, COBYLA, SQSLP, SPSA, CMA-ES, hyperparameters, ...
- Influenced by our understanding of cost function properties

Variational Algorithm



VQE: Variational Quantum Eigensolver

2014



Goal: Find ground state (lowest) energy level of a particular molecule.

Energy described by Hamiltonian $\mathcal{H}$.

Ground state is eigenstate of $\mathcal{H}$ with the lowest eigenvalue.

Use PQC to create state that minimizes expectation $\langle \mathcal{H} \rangle$.

A. Peruzzo, et al. Nature Comm, 2014

Eigenstates, Eigenvalues

For matrix A, state $|\psi\rangle$ is an **eigenstate** if:

$$A|\psi\rangle = \lambda|\psi\rangle$$

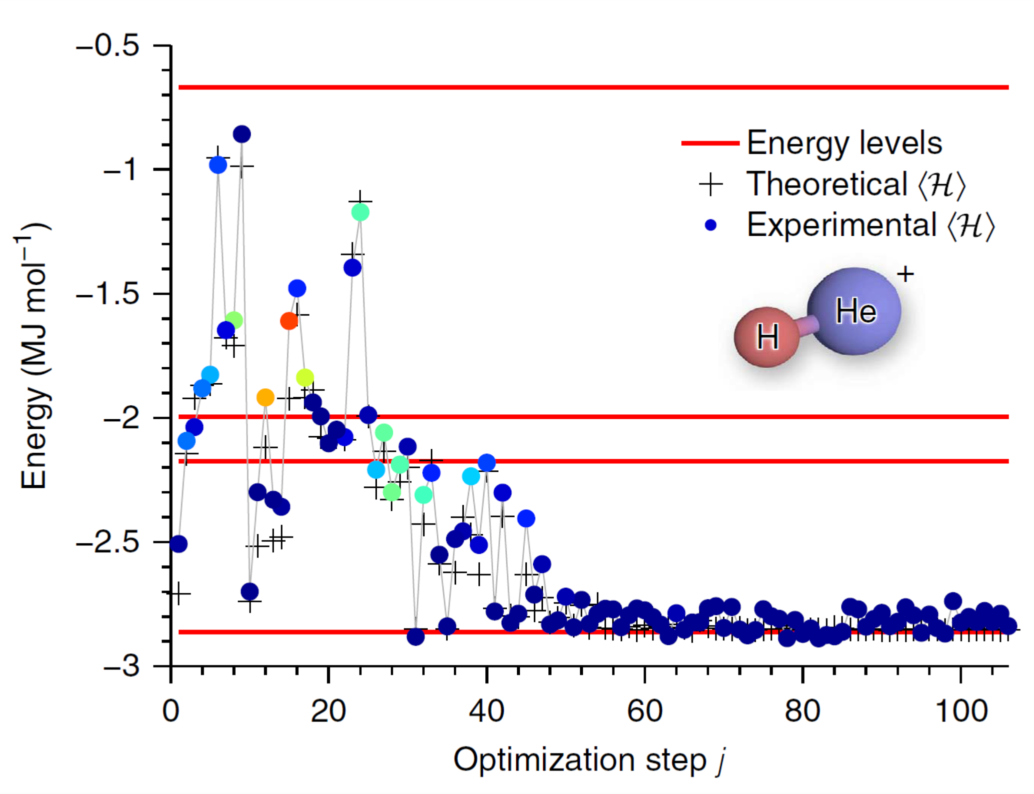
*scalar, known as the **eigenvalue** of $|\psi\rangle$*

Energy level is a (real) eigenvalue of Hamiltonian $\mathcal{H}$, and the ground state has the lowest energy level.

$$\mathcal{H}|e_0\rangle = E_0|e_0\rangle$$

Measurement and Eigenvalues

For any observable (measurable) quantity,
there is an associated Hermitian matrix,
and the result of any measurement is an eigenvalue of that matrix.

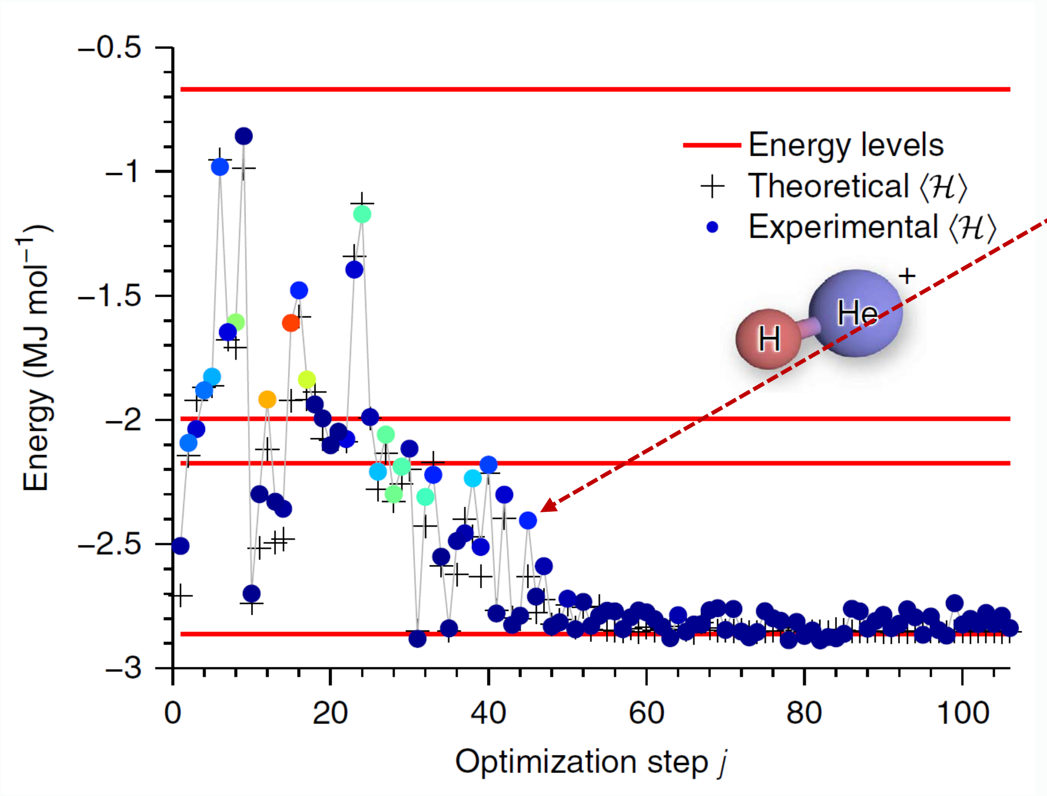


$$\mathcal{H} = \sum E_i \, |e_i\rangle\langle e_i|$$

Expectation of Measurement

Expectation is average of all possible measurements, weighted by their likelihood.

$$\langle \mathcal{H} \rangle_\psi = \langle \psi | \mathcal{H} | \psi \rangle$$



Since we don't know $|\psi\rangle$, make lots of measurements to estimate probability of each result.

$$E_{\exp} = \sum p(E_i) \cdot E_i$$

How do we measure $\mathcal{H}$?

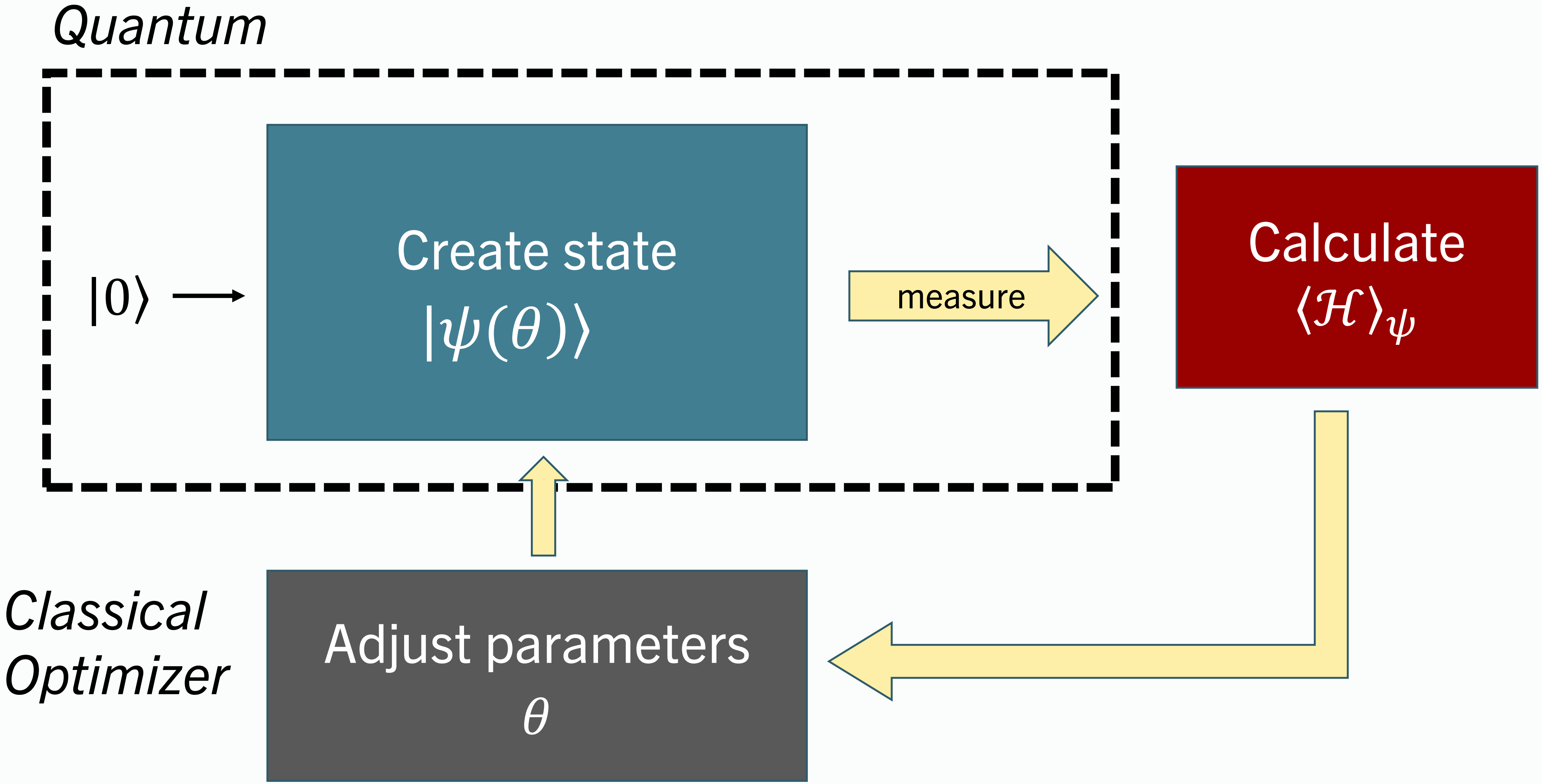
In a quantum computer, we can generally only measure Z.
Any Hamiltonian $\mathcal{H}$ can be written as a sum of X, Y, Z components.

$$\mathcal{H} = g_0 I + g_1 Z_0 + g_2 Z_1 + g_3 Z_0 Z_1 + g_4 Y_0 Y_1 + g_5 X_0 X_1$$

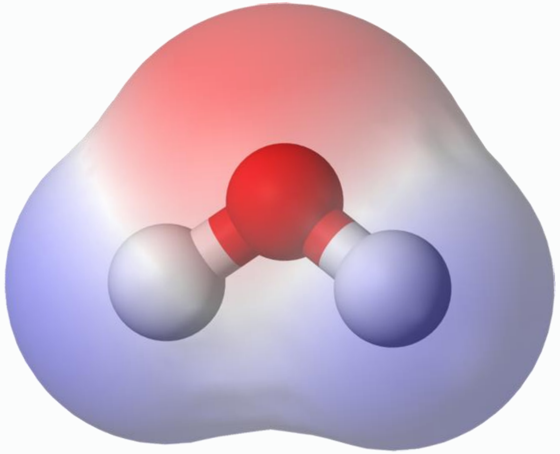
$$\langle \mathcal{H} \rangle = g_0 + \underbrace{g_1 \langle Z_0 \rangle + g_2 \langle Z_1 \rangle}_{\text{single-qubit measurements}} + g_3 \underbrace{\langle Z_0 Z_1 \rangle + g_4 \langle Y_0 Y_1 \rangle + g_5 \langle X_0 X_1 \rangle}_{\text{two-qubit measurements}}$$

Example Hamiltonian for H2 molecule
O'Malley, et al. PRX, 2016.

VQE


Quantum
$|0\rangle$
Create state
$|\psi(\theta)\rangle$
measure
Calculate
$\langle \mathcal{H} \rangle_\psi$
Classical
Optimizer
Adjust parameters
θ

Applications of VQE

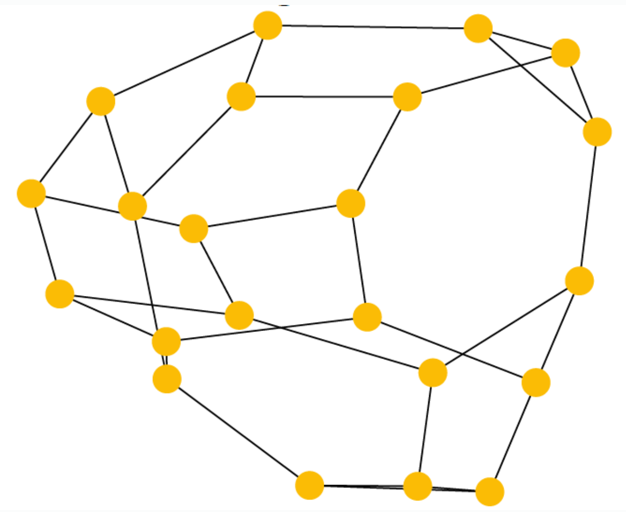


Quantum Simulation

- chemistry, physics, materials, ...

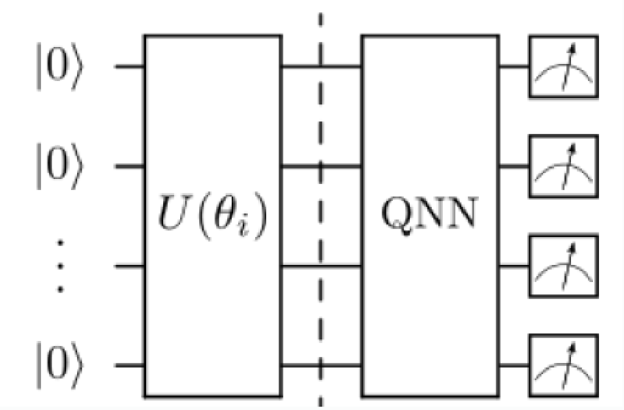
Optimization

- express problem as a Hamiltonian
- MaxCut, Traveling Salesman, Min Vertex Cover...



Quantum Machine Learning

- creating quantum datasets (M. Cerezo tutorial)



QAOA

2014

Quantum Approximate Optimization Algorithm

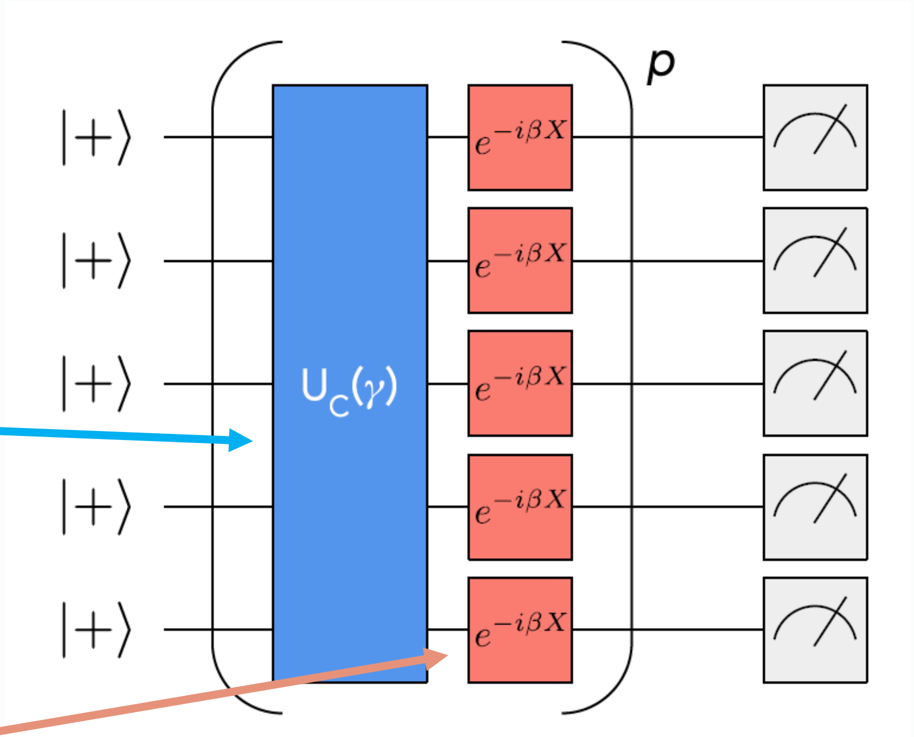
Designed to find approximate solutions to combinational optimization problems.

Ansatz is based on cost function

$$C = \sum_{j<k} w_{jk} Z_j Z_k \qquad U_C(\gamma) = e^{-i\gamma C}$$

and mixer

$$B = \sum_{j} X_j \qquad U_B(\beta) = e^{-i\beta B}$$



Farhi, Goldstone. arXiv: 1411.4028, 2014.
Google AI, et al. arXiv: 2004.04197, 2020.

VQA Examples

VQE: Variational Quantum Eigensolver

Quantum chemistry, quantum physics, optimization

QAOA: Quantum Approximate Optimization Algorithm

Combinatorial optimization

VQF: Variational Quantum Factoring

Integer factorization

Variational Algorithms

1. Reasonably shallow circuits
2. More noise-tolerant (perhaps)
3. Broad range of applications