



# IITSEC 2024



## Introduction to Quantum Computing (It'll be "Fine Man")



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# Learning Objectives

- ***Identify*** the three aspects of quantum information science
- ***Describe*** the difference between a quantum bit (qubit) and a classical (0/1) bit
- ***Explain*** how superposition facilitates quantum cryptography and makes quantum computing relevant today
- ***Explain*** how entanglement facilitates quantum teleportation and makes quantum computing relevant today
- ***Tell*** the truths about quantum computing myths
- ***Identify*** different computational models for quantum optimization and their applications
- ***Describe*** the four families of quantum machine learning and variations of quantum neural networks

# Outline

- **Introduction**
  - Why should I care, quantum info science, physical implementations and challenges, software interfaces, concepts from quantum mechanics and important properties, various computational models, and myths
- **Single Qubits and Cryptography**
  - The qubit and the Bloch sphere, the property of superposition, operators for gate-based QC, cryptography application
- **Multiple Qubits and Teleportation**
  - Multiple qubits, the property of entanglement, more operators for gate-based QC, teleportation application
- **Quantum Optimization**
  - Quantum Unconstrained Binary Optimization (QUBO) and the Ising model, adiabatic QC and gate-based quantum annealing, Quantum Approximate Optimization Algorithm (QAOA), Variational Quantum Eigensolver (VQE), and Grover's adaptive search
- **Quantum Machine Learning**
  - Quantum Neural Networks (QNN)
- **Closing**
  - More Information and references

# Introduction



Introduction

Single Qubit

Multiple Qubits

Quantum Optimization

Quantum Machine Learning

Closing

**Concepts from Quantum Mechanics**  
**Quantum Computing: Who Cares?**  
**Quantum Information Science**  
**Physical Implementations/Challenges**  
**Software Interfaces**  
**Computational Models**  
**Myths**





1927 Solvay Conference on Quantum Mechanics

# Concepts from Quantum Mechanics

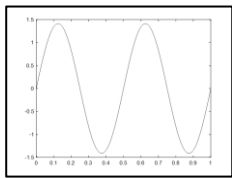
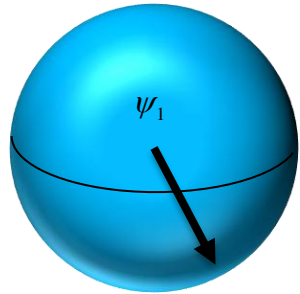
- **Quantization of Matter – Max Planck (photon), Albert Einstein (photoelectric effect)**
  - Quantum bits (qubits) operate using the properties of subatomic particles
- **Wave Function Collapse – The Copenhagen Interpretation of Neils Bohr and Max Born**
  - A qubit may be in a superposed state, but when a qubit is measured, the result is always either 0 or 1
- **Eigenstates and Eigenvalues – Linear Algebra**
  - Used to determine if an operator is Unitary (reversible gate) and/or Hermitian (irreversible measurement)
- **Exclusion Principle – Wolfgang Pauli**
  - The Pauli Exclusion Principle defines the conduct of qubits; X, Y, and Z operators (gates) are the Pauli matrices
- **Quantum Superposition and Entanglement - Spooky action at a distance (Einstein)**
  - Superposition: qubits exist in multiple states simultaneously, offering an exponential increase in computational power
  - Entanglement: qubits linked in such a way that the state of one (no matter the distance) instantly influences its partner, enabling unparalleled data synchronization
  - Interference uses the probability nature of quantum mechanics to reinforce or cancel out pathways, guiding algorithms towards the correct solution

**“If you think you understand quantum mechanics, you don’t understand quantum mechanics.” – Feynman**



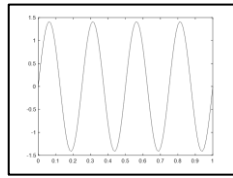
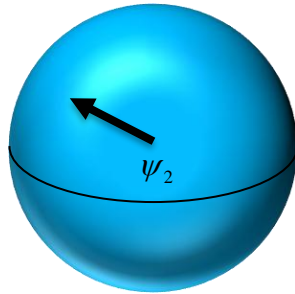
# Quantum Properties

$P(0)=15\%$   
 $P(1)=85\%$



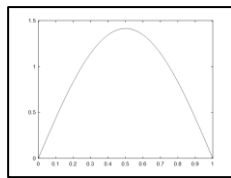
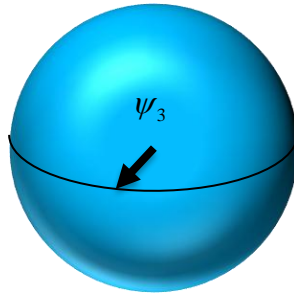
$\psi_1$

$P(0)=70\%$   
 $P(1)=30\%$



$\psi_2$

$P(0)=50\%$   
 $P(1)=50\%$

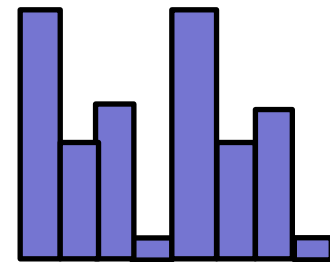
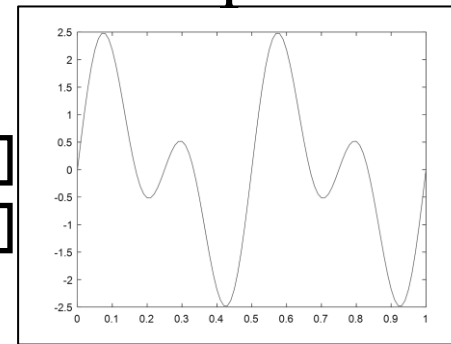


$\psi_3$

← Superposition without entanglement

=

$\Psi$

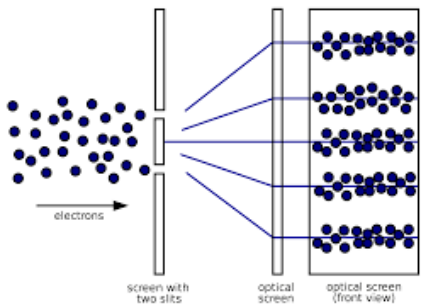


000  
001  
010  
011  
100  
101  
110  
111

Classical computers can be in any state, but they can only be in one state at a given time

Quantum computers are in a superposition of all states at a given time

Individual wavefunctions constructively/destructively interfere



- Quantum Algorithm**
1. Create superposition
  2. Entangle qubits
  3. Apply interference
  4. Measure result

Entangled probabilities - If you change the state of one qubit, the probability of all other states changes

# Quantum Computing: Who Cares?

- **Recent quantum technological breakthroughs not achievable by classical (digital) computing**
  - Quantum cryptography (implemented/fielded)
  - Quantum teleportation
- **Department of Energy (DOE) exploring applications of quantum simulation (energetics)**
- **Modeling, Simulation, and Training**
  - Optimization applications to MS&T (e.g., training and human performance optimization)
  - I/ITSEC Knowledge Repository returned 1618 papers with keyword “machine learning”
  - Quantum optimization leads to quantum machine learning

**“For the intelligence community, some areas “where you might be able to take advantage of quantum computing” include operations research, decision-making and optimization, ...”  
- Algorithmic Warfare by Josh Luckenbaugh, National Defense Magazine 2024**



# Quantum Information Science

- “Military confrontation capabilities have been upgraded to basic research related to synthetic biology, quantum information science, cognitive neuroscience, human behavior modeling, and new engineering materials.” – Integrated Human-Machine Intelligence: Beyond Artificial Intelligence, Wei Liu 2023

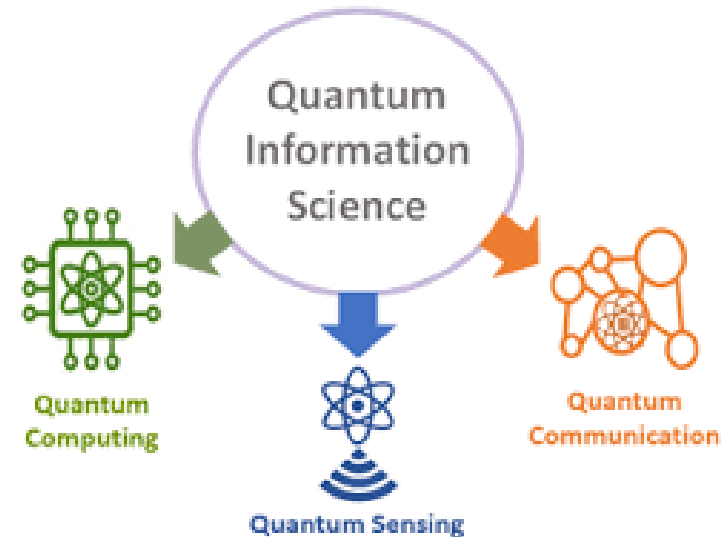
- **Quantum Sensing**

- Quantum devices for PNT
- For use in GPS-denied environments
- Also, electromagnetic and gravitational field sensing

- **Quantum Communication (Networking)**

- Cryptography
- Teleportation

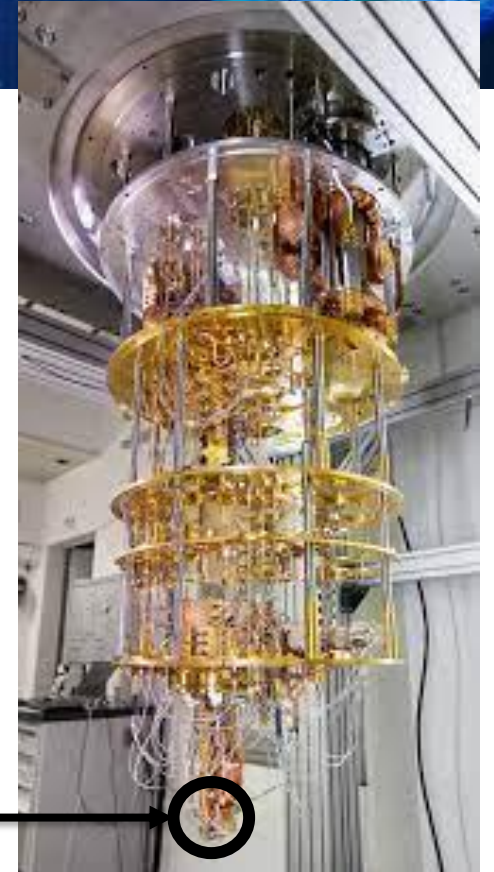
- **Quantum Computation**



The focus of this presentation will be quantum computing, with networking examples of quantum cryptography and quantum teleportation

# Physical Implementations

Company	Technology	Encoding	State
Xanadu PsiQuantum	Nanophotonics	Polarization	Polarization filters
Honeywell IonQ	Trapped Ions	Energy Levels	Spin (up/down)
IBM Intel Google D-Wave	Superconducting Josephson Junction	Charge Current	Charged/uncharged Current (CW/CCW) Ground state/first excited state
Microsoft	Hypothetical	quasi-particle (anyon)	No hardware at this time



Xanadu's nanophotonic chip powered by laser pulses



# Quantum Computers - Challenges

- Noise – In the sense of error (not audio or signal-to-noise ratio)
- Noise and Decoherence
  - At the subatomic level, electromagnetic field fluctuations and radiation result in environmental changes
  - Most of today's quantum computers are Noisy Intermediate-Scale Quantum (NISQ) computers
  - Quantum cryptography can be performed with single qubits, which is why there are commercial applications

## ➤ Quantum Error Correction

- Because of the fragility (incoherence) of qubits, ~100 physical qubits make up one logical qubit
- Physical qubits are necessary for error checking and error correction (checksum)
- IBM announced Condor, with 1121 physical qubits, the world's largest quantum chip (Jan 2024)
- Compare with the bits in an average laptop (8 core) numbering about 24,576
- We're sort of at the equivalent of the Babbage stage when it comes to quantum computers

**Notional Example**  
3 physical qubits for  
1 logical qubit

PQ	LQ
000	→ 0
001	→ 0
010	→ 0
011	→ 1
100	→ 0
101	→ 1
110	→ 1
111	→ 1

# Software Interfaces

## ➤ Software

- QDK/Q# (Microsoft)
- Cirq/Python (Google)
- Qiskit/Python (IBM)
- PennyLane/Python (Xanadu)
- Ocean/Python (D-Wave)

## ➤ Personal Experience

- Qiskit for Quantum Optimization
- PennyLane for Quantum ML
- Python can be problematic: deprecations because the technology is moving so fast!

The image shows two screenshots. The top screenshot is the IBM Quantum Platform dashboard. It features a navigation bar with 'Dashboard', 'Compute resources', and 'Jobs'. The main content area has a large 'IBM Quantum' logo, a sign-in section with 'Continue with IBMid' and social media icons, and a 'Platform' section with a 'Copy your API token' button. A small inset window shows a 'Recent jobs' table with columns for Job ID, Status, Created, Completed, and Compute resources. The bottom screenshot is the PennyLane website. It has a navigation bar with 'Learn', 'Documentation', 'Get involved', 'Datasets', 'Blog', and 'Support'. The main heading is 'Discover new ideas faster.' with three sub-sections: 'Program quantum computers', 'Integrate with machine learning', and 'Master quantum chemistry'. There are 'Install PennyLane' and 'Learn more' buttons at the bottom.

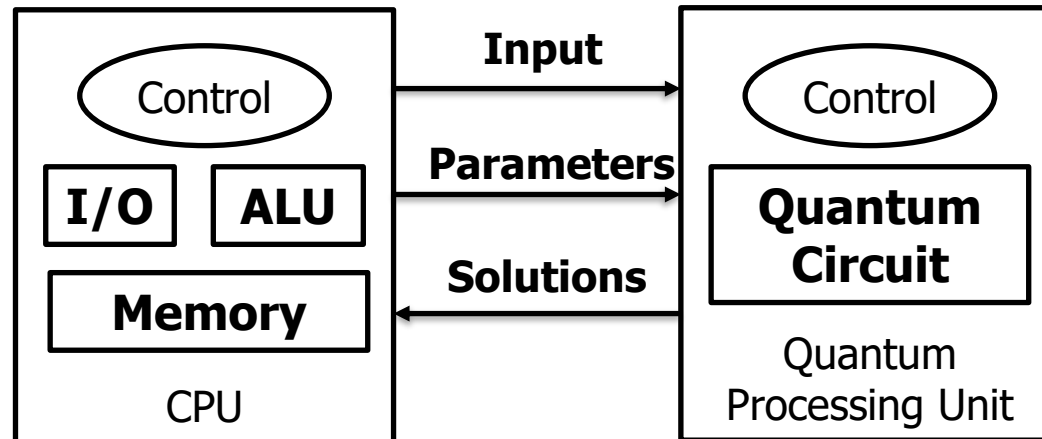


# Computational Models

- **Quantum Circuit Model (Quantum Cryptography & Quantum Teleportation)**
  - Application of quantum gates (universal quantum computing)
- **Adiabatic Quantum Computing (Quantum Optimization and Quantum Machine Learning)**
  - Adiabatic evolution: begin in ground state, not enough energy added to jump to excited state
  - Implemented as quantum annealing, it's restricted, therefore not universal quantum computing
- **Other**
  - Quantum Turing Machines
  - Measurement-Based Quantum Computing (One-Way Quantum Computing)
  - MBQC has given way to Fusion-Based QC, as pursued by PsiQuantum

# Debunking Myths

- **Myth: Quantum computers will render classical computers obsolete**
  - **Truth: For most tasks running on your personal computer, a quantum computer performs no better**
  - **Only very specific classes of algorithms are currently known to benefit from quantum computing**
- **From a programmer's perspective, a quantum computer is but a co-processor**
  - **Classical computers handle input and output and call the "QPU" for specific tasks**



- **Quantum computers excel at optimization problems and since AI/ML is nothing more than fancy curve-fitting (Judea Pearl), quantum computing may play a significant role in AI/ML**

**Today, all quantum computing (hardware) is hybrid, i.e., quantum computers receive input from classical computers and provide output to classical computers; plus, some software applications are hybrid too (classical/quantum algorithms)**

# Debunking Myths

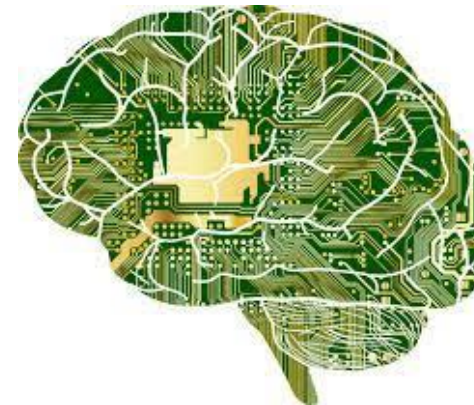
➤ **Myth: There is no practical use for quantum computers**

- Truth: Even with NISQ QCs, there are already applications (as will be shown)
- Think of Radio Shack's TRS-80 (Z-80, 2 MHz processor with 4K RAM), we did a lot with it!
- However, practical advantages? Not really.

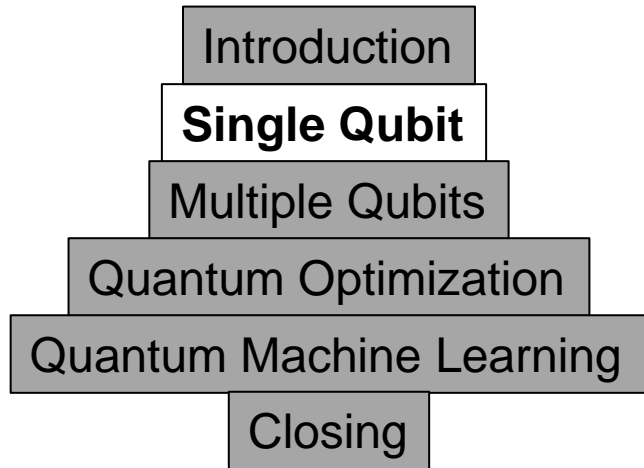


➤ **Myth: Quantum computers will develop their own minds**

- Truth: We've heard this (for a while now) about AI/ML
- For quantum computing (and AI/ML for that matter), how can this be if humans do not fully understand how consciousness works?
- For that matter, can AI reflect on a decision it has made?



# Single Qubits



**Qubits**

**Superposition**

**Bloch Sphere**

**Operators/Gates**

**Application: Cryptography**



# Single Qubits

## ➤ Classical Bit

- Either 0 or 1

## ➤ Quantum Bit (Qubit)

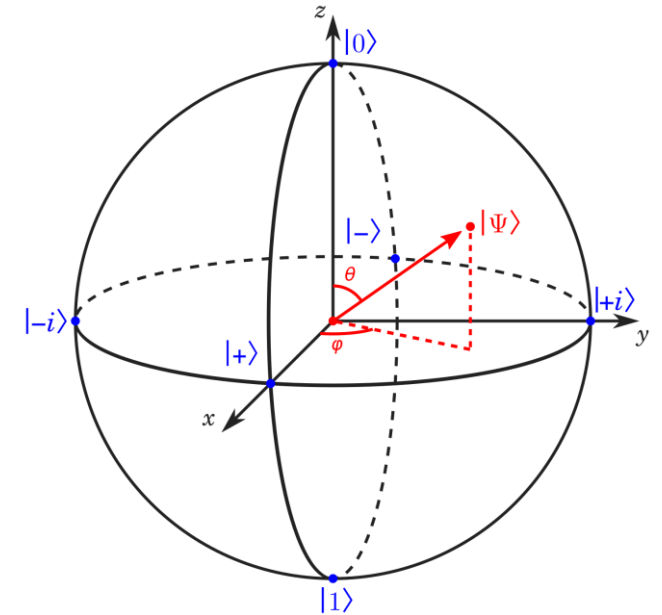
- Superposition of pure states 0 and 1
- Dirac's  $\langle bra | ket \rangle$  notation

$$|0\rangle \equiv \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad |1\rangle \equiv \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \leftarrow \text{Standard (Computational) Basis}$$

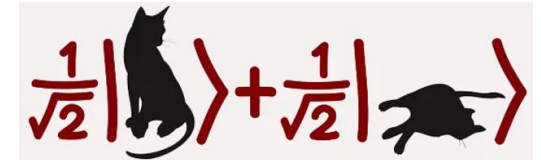
- Some qubits could be an equal superposition of 0 and 1
- These states are on the “equator” of the Bloch sphere
- While the superpositions are equal in magnitude, in some cases, their phase differs

$$|+\rangle \equiv \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) \quad |-\rangle \equiv \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$$

$$|+i\rangle \equiv \frac{1}{\sqrt{2}} (|0\rangle + i|1\rangle) \quad |-i\rangle \equiv \frac{1}{\sqrt{2}} (|0\rangle - i|1\rangle)$$



**Bloch Sphere**



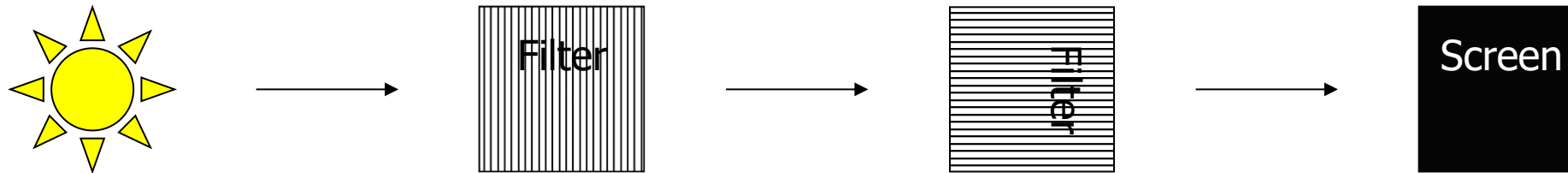
# Single Qubits

## ➤ Light polarization

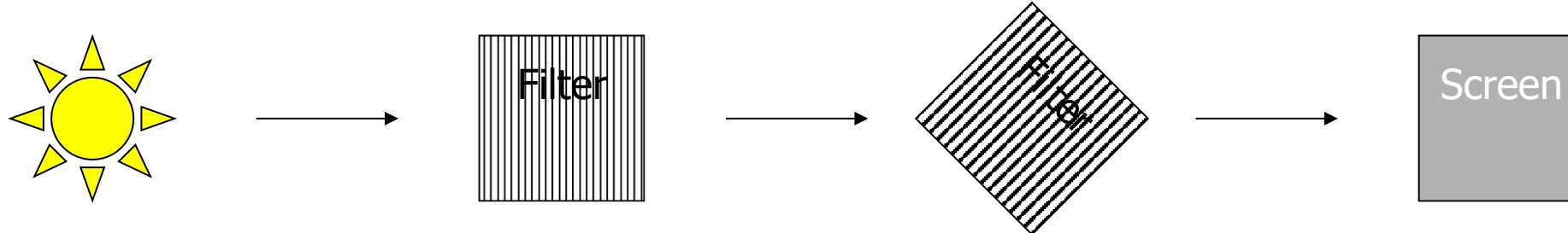
- Sunlight has no preferred polarization, however a filter can set the preferred polarization
- Let vertical polarization be represented by  $|1\rangle$  and horizontal polarization be represented by  $|0\rangle$
- Then the state of sunlight may be represented by  $|\psi\rangle = \alpha|1\rangle + \beta|0\rangle$

## ➤ Vertical polarization $|1\rangle$

- If sunlight is vertically polarized, what happens if we introduce a second perpendicular (horizontal) filter?



- If sunlight is vertically polarized, what happens if we introduce a second filter at 45 degrees?



- Vertical polarization is a superposition of  $+45^\circ$  diagonal and  $-45^\circ$  diagonal filtering  $|1\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle$
- Since the  $|+\rangle$  state is only one term in the superposition, half of the light gets through to the screen

# Single Qubits

➤ **Myth: A qubit is both 0 and 1 at the same time**

- **Truth: A qubit is a superposition of both states**

➤ **Quantum Bit (qubit)**

- In general, a qubit may lie *anywhere* on the surface of the (Bloch) sphere

$$|\Psi\rangle = \cos\left(\frac{\theta}{2}\right) |0\rangle + e^{i\varphi} \sin\left(\frac{\theta}{2}\right) |1\rangle \quad 0 \leq \theta \leq \pi \quad 0 \leq \varphi < 2\pi$$

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

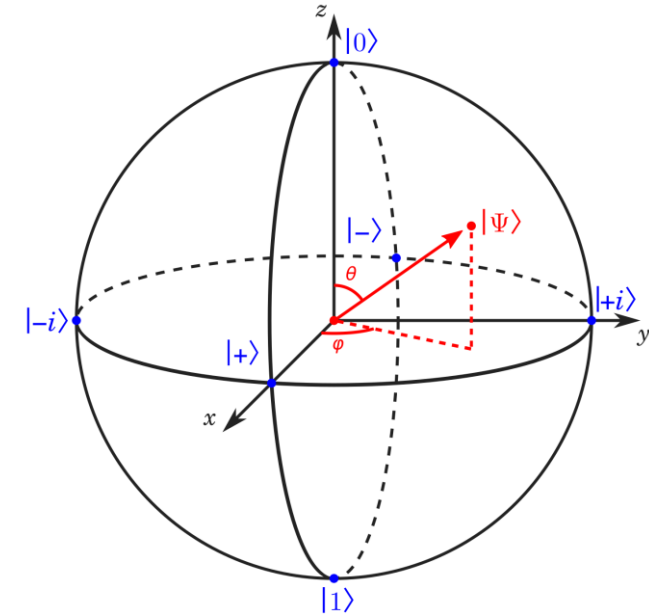
- **Note:** The coefficients ( $\alpha$  and  $\beta$ ) are amplitudes, and their squares (complex norm or modulus) are the probabilities associated with each state
- $|\alpha|^2$  is the probability of  $|\Psi\rangle$  being in the  $|0\rangle$  state
- $|\beta|^2$  is the probability of  $|\Psi\rangle$  being in the  $|1\rangle$  state
- $|\alpha|^2 + |\beta|^2 = 1$
- If  $\alpha > \beta$ ,  $P(|0\rangle) > P(|1\rangle)$
- **Note:** In general, the coefficients are complex numbers. As such they have phase. Relative phase between the complex coefficients plays a role in quantum computing.

$$\alpha = a_1 + ia_2$$

$$\beta = b_1 + ib_2$$

$$\phi_\alpha = \tan^{-1} \frac{a_2}{a_1}$$

$$\phi_\beta = \tan^{-1} \frac{b_2}{b_1}$$



**Bloch Sphere**

# Quantum Gates

- Digital computers have finite logic gates (AND, OR, etc.)
- The situation is similar with quantum computing
- There are different operations applied to qubits
  - When initializing a qubit, the process is irreversible (Hermitian)
  - When performing quantum computations, the process is reversible (Unitary)
  - When measuring qubits, the process is irreversible (Hermitian)
- Because the systems are linear, the operators are matrix multiplications



# Quantum Gates

## ➤ Hadamard Gate (Unitary)

- Used to create a superposed state
- When applied to  $|0\rangle$ , the result is  $|+\rangle$
- When applied to  $|1\rangle$ , the result is  $|-\rangle$
- $|+\rangle$  and  $|-\rangle$  comprise the **Hadamard Basis**

$$|0\rangle = \frac{1}{\sqrt{2}}|+\rangle + \frac{1}{\sqrt{2}}|-\rangle \quad |1\rangle = \frac{1}{\sqrt{2}}|+\rangle - \frac{1}{\sqrt{2}}|-\rangle$$

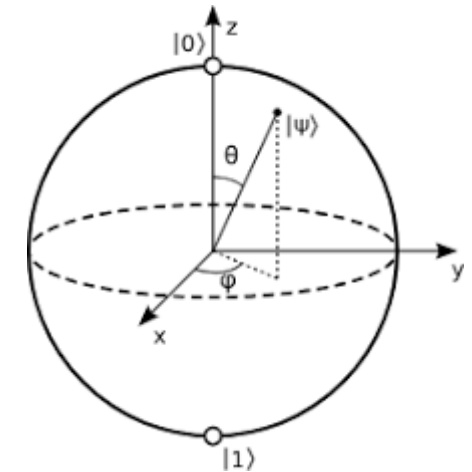
## ➤ X, Y, and Z (Pauli) Gates (Unitary)

- X is referred to as the “not” gate  
 $X|0\rangle = |1\rangle \quad X|1\rangle = |0\rangle$
- Z is referred to as the **phase shift** gate  
 It's a rotation about Z of the Bloch sphere, i.e.,  $\varphi$
- Y completes the trio  
 $iY|+\rangle = |-\rangle \quad iY|-\rangle = -|+\rangle$

$$\left\{ \begin{array}{l} X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \\ Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \\ Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \end{array} \right.$$

$$\left\{ \begin{array}{l} H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \\ H|0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) = |+\rangle \\ H|1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) = |-\rangle \end{array} \right.$$

$\begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ 1 \end{bmatrix}$   
 $\downarrow$



# Quantum Gates

- **X, Y, and Z (Pauli) Gates (Unitary)**
  - X, Y, and Z are all rotations of  $\pi$  radians (180 deg)

- **Generalized Rotations**

$$R_X(\theta) = \begin{bmatrix} \cos \frac{\theta}{2} & -i \sin \frac{\theta}{2} \\ -i \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{bmatrix}$$

$$R_Y(\theta) = \begin{bmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{bmatrix}$$

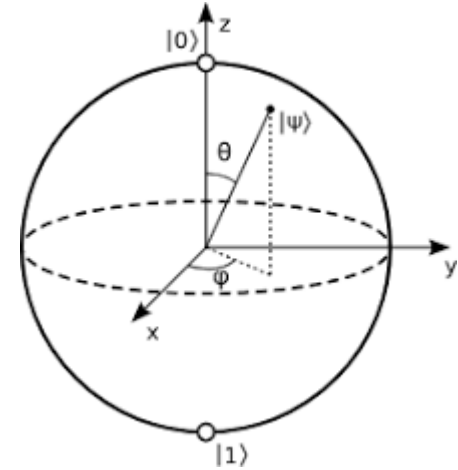
$$R_Z(\theta) = \begin{bmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{bmatrix}$$

$$R_X(\pi) = -iX \equiv X$$

$$R_Y(\pi) = iY \equiv Y$$

$$R_Z(\pi) = Z$$

$\equiv$  denotes equivalent action up to a global phase



# True Random Number Generator



➤ **Random Byte (no need for *pseudo-random* number generators)**

- $H|0\rangle$  produces a superposition, with a 50/50 chance of resulting in a 0 or a 1
- $1*Meas0 + 2*Meas1 + 4*Meas2 + 8*Meas3 + 16*Meas4 + 32*Meas5 + 64*Meas6 + 128*Meas7$

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$$

```
from qiskit import QuantumCircuit, QuantumRegister, ClassicalRegister, Aer
from qiskit.tools.visualization import circuit_drawer
from qiskit.visualization import plot_histogram
```

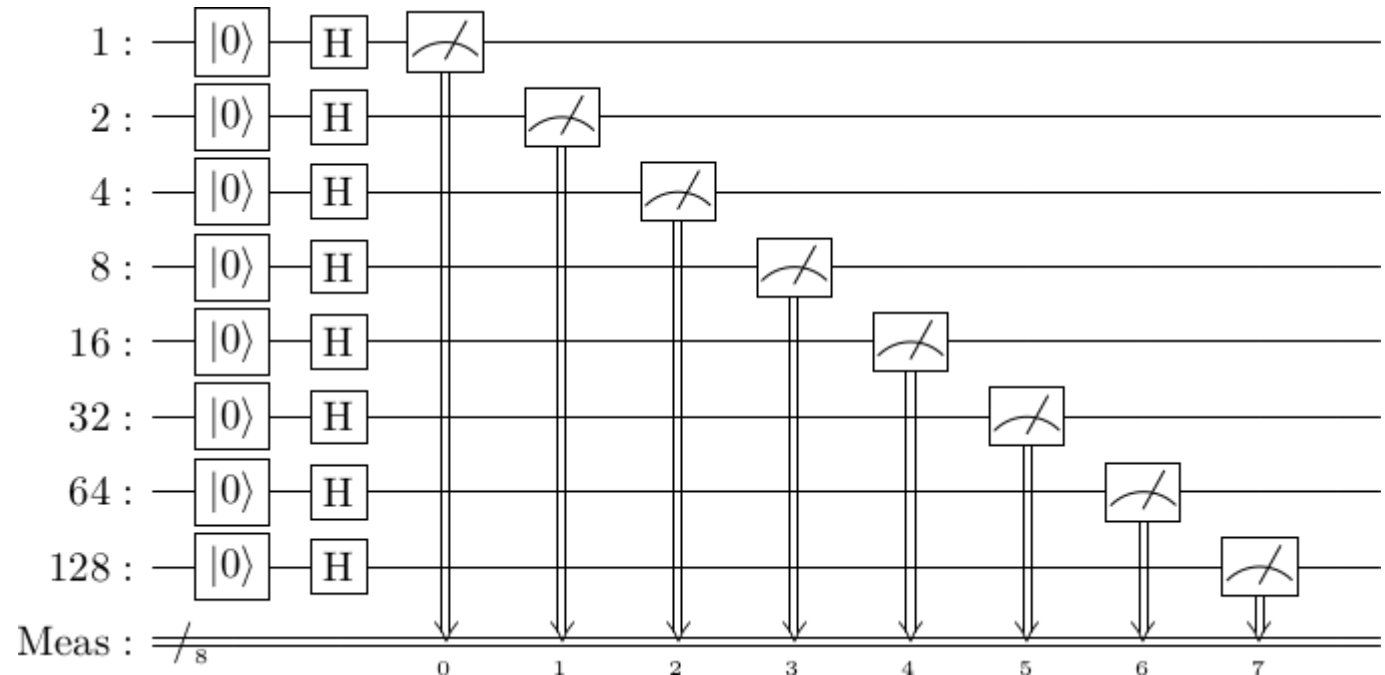
```
qr1 = QuantumRegister(1, 'qr1'), qr2 = QuantumRegister(1, 'qr2')
qr3 = QuantumRegister(1, 'qr3'), qr4 = QuantumRegister(1, 'qr4')
qr5 = QuantumRegister(1, 'qr5'), qr6 = QuantumRegister(1, 'qr6')
qr7 = QuantumRegister(1, 'qr7'), qr8 = QuantumRegister(1, 'qr8')
cr = ClassicalRegister(8, 'cr')
qc = QuantumCircuit(qr1,qr2,qr3,qr4,qr5,qr6,qr7,qr8,cr)
```

```
qc.reset(0),qc.reset(1),qc.reset(2),qc.reset(3)
qc.reset(4),qc.reset(5),qc.reset(6),qc.reset(7)
```

```
qc.h(0),qc.h(1),qc.h(2),qc.h(3)
qc.h(4),qc.h(5),qc.h(6),qc.h(7)
```

```
qc.measure(0, 0),qc.measure(1, 1),qc.measure(2, 2),qc.measure(3, 3)
qc.measure(4, 4),qc.measure(5, 5),qc.measure(6, 6),qc.measure(7, 7)
```

```
circuit_drawer(qc, output='latex', style={'backgroundcolor': '#EEEEEE'})
```



**NIST's New Quantum Method Generates Really Random Numbers - 2018**

# Qubit Summary

- Qubits are a superposition of both states simultaneously
- Because of superposition, there is a relative phase (quantum interference) between  $\alpha$  and  $\beta$ 
  - This has implications for Deutch's algorithm and Grover's algorithm
- Entanglement (to be discussed) is a property of multiple qubits
- Because of these properties, qubits are more powerful than classical bits
- <https://javafxpert.github.io/grok-bloch/>
- One drawback is the “No Cloning Theorem” which states that a qubit cannot be copied
  - This has implications for cryptography which we will explore next...

# Application: Quantum Cryptography

- A quantum computer with several thousand qubits can solve a strategic problem (encryption and decryption) that classical computers have no hope of solving
  - This is one of those “special applications” where quantum computing outperforms classical computers
  - Peter Shor’s algorithm cracks the widely used RSA encryption scheme
  - But quantum computing also has some clever ways to solve this problem with single qubits...
- Cryptography aims to hide the meaning of a message through encryption
  - BB84 was developed by Charles Bennett and Gilles Brassard in 1984
  - Goal: to share symmetric keys, securely
  - The qubits themselves are not used to send messages

# Application: Quantum Cryptography

- **Alice and Bob want to share a secret**
  - Alice generates 20 qubits and sends them to Bob
  - Eavesdropper (Eve) listens-in, makes note of the qubits, and forwards them to Bob
  - The secret has been compromised, hmmm...
  
- **But Alice and Bob know about quantum computing**
  - Alice applies the Hadamard gate before sending her qubits
  - Since the Hadamard gate is its own inverse, Bob can recover each qubit
  
- **Unfortunately, Eve knows about quantum computing too**
  - Eve applies the Hadamard gate twice, once to recover the qubits and again before forwarding them to Bob
  - Alas, Hadamard gates alone don't help, hmmm...
  
- **Unfortunately, just as Eve can't figure out what Alice meant to send, neither can Bob**
  - If Alice tells Bob which qubits had been Hadamarded, Eve could intercept that message, hmmm...



# Application: Quantum Cryptography



## ➤ BB84

- **Both Alice and Bob decide to randomly apply the Hadamard gate with two possible outcomes:**
  - They both applied the Hadamard gate, or neither applied the Hadamard gate
  - One applied the Hadamard gate, and the other didn't
- **Bob publicly announces which qubits he applied the Hadamard gate to**
  - If Eve is listening-in, the information Bob provides is or no use to her
- **Alice publicly announces which of her choices agrees with Bob**
  - If Eve is listening-in, the information Alice provides is or no use to her
- **Bob publicly announces the results of the first-half of their agreement as “test qubits”**
  - If Eve is listening-in, there is little chance that all “test qubits” match
- **The second-half of the results form the “shared secret”**

Qubit #	Alice		
1	1		
2	0	H	$\frac{1}{\sqrt{2}}( 0\rangle +  1\rangle)$
3	1	H	$\frac{1}{\sqrt{2}}( 0\rangle -  1\rangle)$
4	0	H	$\frac{1}{\sqrt{2}}( 0\rangle +  1\rangle)$
5	0		
6	1		
7	0	H	$\frac{1}{\sqrt{2}}( 0\rangle +  1\rangle)$
8	0		
9	1		
10	1	H	$\frac{1}{\sqrt{2}}( 0\rangle -  1\rangle)$
11	1	H	$\frac{1}{\sqrt{2}}( 0\rangle -  1\rangle)$
12	1		
13	0	H	$\frac{1}{\sqrt{2}}( 0\rangle +  1\rangle)$
14	1	H	$\frac{1}{\sqrt{2}}( 0\rangle -  1\rangle)$
15	1	H	$\frac{1}{\sqrt{2}}( 0\rangle -  1\rangle)$
16	1		
17	0	H	$\frac{1}{\sqrt{2}}( 0\rangle +  1\rangle)$
18	1		
19	0	H	$\frac{1}{\sqrt{2}}( 0\rangle +  1\rangle)$
20	0		

Qubit #	Bob	
1	H	?
2		?
3		?
4	H	0
5		0
6		1
7	H	0
8	H	?
9		1
10		?
11		?
12		1
13	H	0
14	H	1
15		?
16	H	?
17		?
18	H	?
19	H	0
20		0

Bob publishes all 20 of his decisions

Alice publishes when she agrees, namely qubits 4, 5, 6, 7, 9, 12, 13, 14, 19, 20

Bob publishes results of the first-half, namely [0, 0, 1, 0, 1] as "test qubits"

The second-half, namely [1, 0, 1, 0, 0] form the "shared secret"



# Application: Quantum Cryptography

- Suppose we want to encrypt the message, "LSA"
  - In ASCII L=1001100, S=1010011, A=1000001
  - The bit stream is 1001100 1010011 1000001
  - Alice repeatedly applies the XOR "shared secret" 10100 (key)
  - Then she sends the encrypted message to Bob

Message	1 0 0 1 1 0 0	1 0 1 0 0 1 1	1 0 0 0 0 0 1
Key	1 0 1 0 0 1 0	1 0 0 1 0 1 0	0 1 0 1 0 0 1
Encrypted	0 0 1 1 1 1 0	0 0 1 1 0 0 1	1 1 0 1 0 0 0

- Upon receipt, Bob repeatedly applies the XOR "shared secret" and recovers the message

Encrypted	0 0 1 1 1 1 0	0 0 1 1 0 0 1	1 1 0 1 0 0 0
Key	1 0 1 0 0 1 0	1 0 0 1 0 1 0	0 1 0 1 0 0 1
Message	1 0 0 1 1 0 0	1 0 1 0 0 1 1	1 0 0 0 0 0 1

"L"                      "S"                      "A"

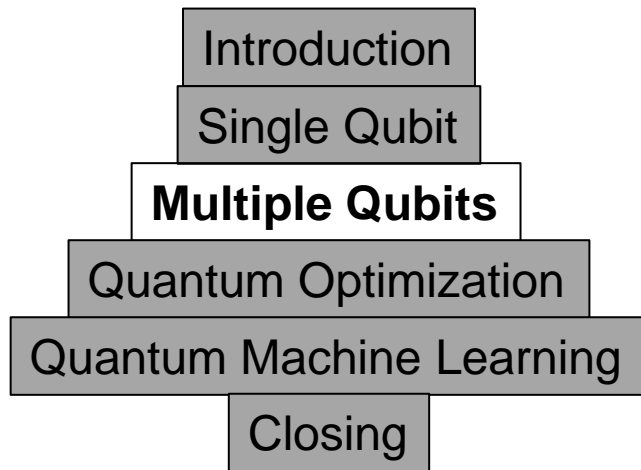
# Application: Quantum Cryptography

- **Myth: Quantum computers will put cybersecurity at risk**
  - **Truth: While the power and speed of quantum computers could crack RSA public key encryption (Shor's algorithm), there are already quantum-resistant cryptography algorithms**
- **We just showed a simple (BB84) example using only single qubits and the Hadamard gate for superposition to establish a post-quantum encryption algorithm**
  - Perhaps this could be extended for secure distributed simulation
- **What is Post-Quantum Cryptography (PQC)?**
  - The development of novel classical cryptographic schemes, believed to be resistant to future quantum computers employing Shor's algorithm
  - The NSA is taking this seriously to safeguard data against future hackers
  - Efforts are already underway to incorporate these new schemes (some of which have already been hacked)
  - **Note: Encrypted data is being collected now for future decryption (What is the “shelf-life” of your data?)**

NIST SP 1800-38B, Migration to Post-Quantum Cryptography Quantum Readiness: **Cryptographic Discovery**

NIST SP 1800-38C, Migration to Post-Quantum Cryptography Quantum Readiness: **Testing Draft Standards for Interoperability and Performance**

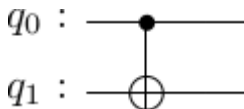
# Multiple Qubits



**Multi-Qubit Operators/Gates**  
**Entanglement**  
**Application: Teleportation**

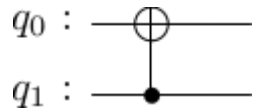
# Multiple Qubits

- The Hadamard and Pauli gates operate on a single qubit
- Some gates operate on multiple qubits in parallel
- Qubits are combined according to the tensor product  $|q_0q_1\rangle$
- **Caution!** Some literature uses different ordering
- **Controlled NOT (CNOT)**
  - If the control qubit is 0, do nothing
  - If the control qubit is 1, flip the other (target) qubit
  - Assume: left qubit  $|x\rangle$  is Control, right qubit  $|y\rangle$  is Target

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


q<sub>0</sub> : —●—  
q<sub>1</sub> : —⊕—

- **Caution!** Sometimes the control/target qubits are opposite



q<sub>0</sub> : —⊕—  
q<sub>1</sub> : —●—

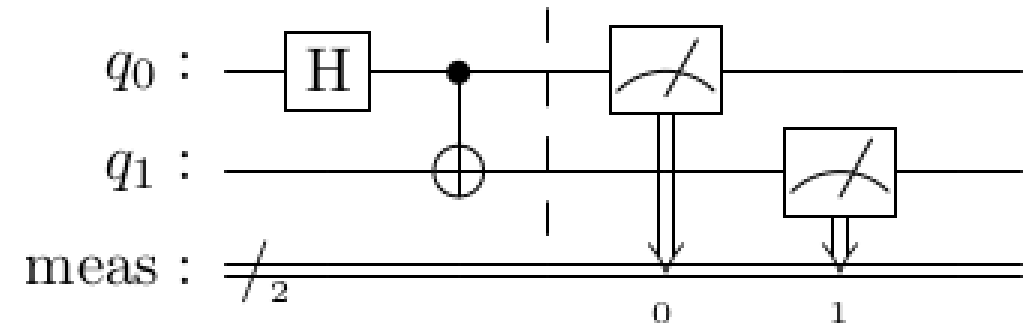
$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} |00\rangle \\ |01\rangle \\ |10\rangle \\ |11\rangle \end{bmatrix} = \begin{bmatrix} |00\rangle \\ |11\rangle \\ |10\rangle \\ |01\rangle \end{bmatrix}$$

Label		Math
↓		↓
	$ q_1q_0\rangle =  q_1\rangle \otimes  q_0\rangle$	
$ 00\rangle$	$=  0\rangle \otimes  0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} =$	$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$
$ 01\rangle$	$=  0\rangle \otimes  1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 0 \\ 1 \end{bmatrix} =$	$\begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$
$ 10\rangle$	$=  1\rangle \otimes  0\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} =$	$\begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$
$ 11\rangle$	$=  1\rangle \otimes  1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} 0 \\ 1 \end{bmatrix} =$	$\begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$



# Gate-Based/Universal Quantum Computing

- Create wires and associate qubits with them
- Gates interact with the qubits to perform calculations
  - The Hadamard gate interact with a single qubit
  - The CNOT gate interacts with multiple qubits
- In the end, measurements are made
  - **Remember:** The result is either a 0 or a 1



## ➤ Example in Qiskit

```
from qiskit import QuantumCircuit
```

```
circuit = QuantumCircuit(2)
```

```
circuit.h(0)
```

```
circuit.cnot(0,1)
```

```
circuit.measure_all()
```

```
display(circuit.draw('latex'))
```

*Import the library*

*Create a quantum circuit with two qubits,  $q_0$  and  $q_1$*

*Apply the Hadamard operator to qubit 0*

*Apply the CNOT operator  $q_0(C)$ ,  $q_1(T)$*

*Measure both qubits*

*Draw the circuit*

# Circuitry and Mathematics

- What is the result of the previous example?
- Let's "do the math..."

- Assume each qubit is in the initial pure state  $|0\rangle$

$$|q_1\rangle \otimes |q_0\rangle = |0\rangle \otimes |0\rangle = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = |00\rangle$$

← Math  
← Label

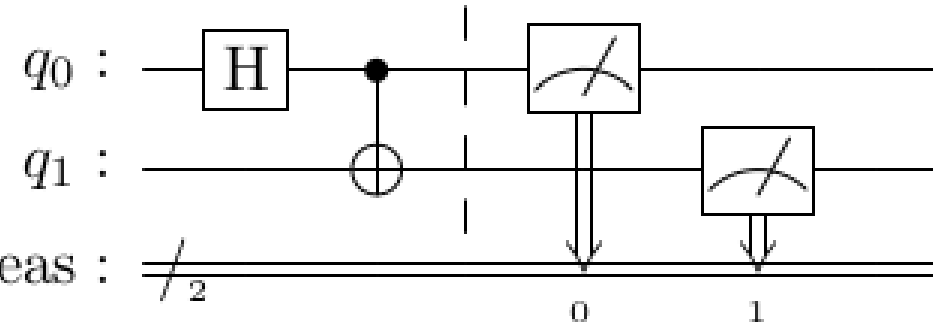
- We want to apply to Hadamard operator to  $q_0$  while maintaining  $q_1$  in parallel

$$(I \otimes H) \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \left( \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \otimes \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \right) \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}$$

- Next, we apply the CNOT operator

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$$

← Math  
← Label

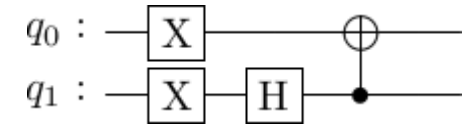
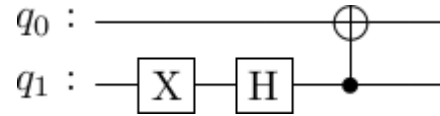
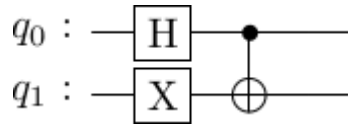
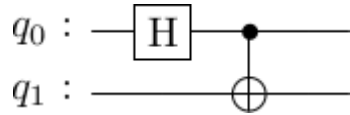
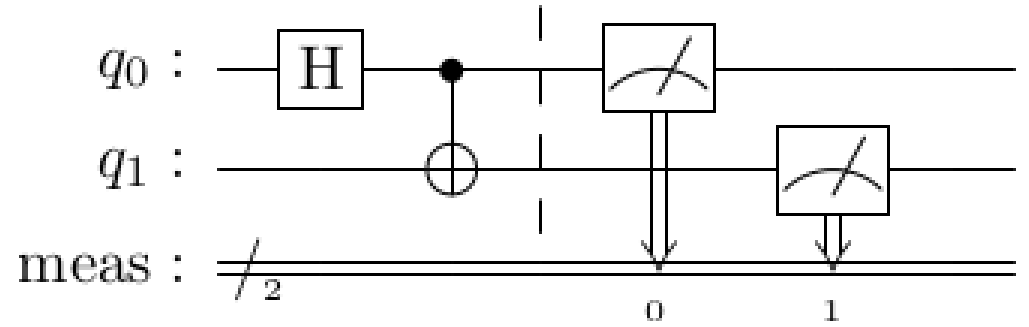


**Note: You could begin by applying the Hadamard operator to  $q_0$ , perform the tensor multiplication, then apply the CNOT operator**

# Circuitry and Mathematics

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle)$$

- At this point, the qubits are equally likely (50/50) to be in either the  $|00\rangle$  or the  $|11\rangle$  state
- If  $q_0$  is measured to be 0, then  $q_1$  must be 0; likewise, if  $q_0$  is measured to be 1,  $q_1$  must be 1
- The qubits are known to be *entangled*
- Similarly...



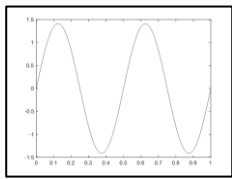
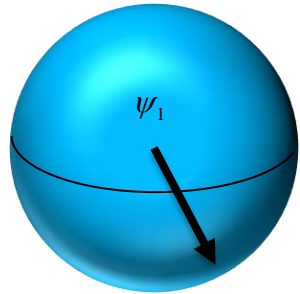
$$|\Phi^+\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle) \quad |\Psi^+\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) \quad |\Phi^-\rangle = \frac{1}{\sqrt{2}} (|00\rangle - |11\rangle) \quad |\Psi^-\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle)$$

- ...these are known as EPR\* pairs or Bell states (after John Bell who proved the EPR paradox)

\*EPR refers to a paper written by Einstein, Podolsky, and Rosen challenging the concept of entanglement (hidden variables)

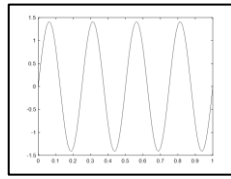
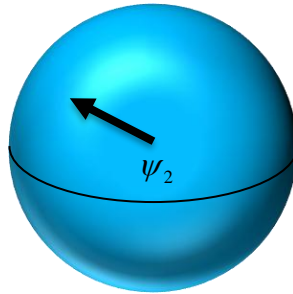
# Quantum Properties

$P(0)=15\%$   
 $P(1)=85\%$



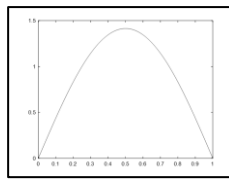
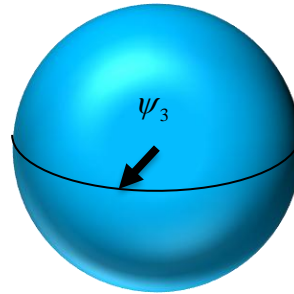
$\psi_1$

$P(0)=70\%$   
 $P(1)=30\%$



$\psi_2$

$P(0)=50\%$   
 $P(1)=50\%$

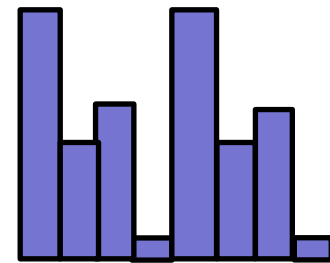
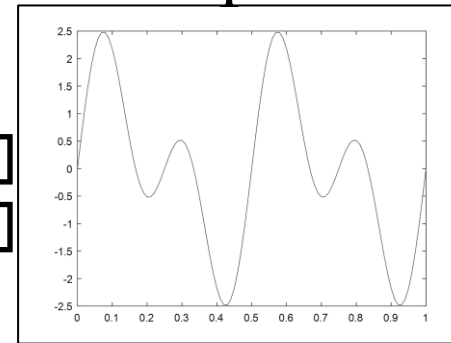


$\psi_3$

← Superposition without entanglement

=

$\Psi$

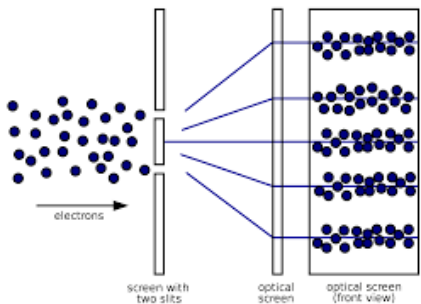


000  
001  
010  
011  
100  
101  
110  
111

Classical computers can be in any state, but they can only be in one state at a given time

Quantum computers are in a superposition of all states at a given time

Individual wavefunctions constructively/destructively interfere



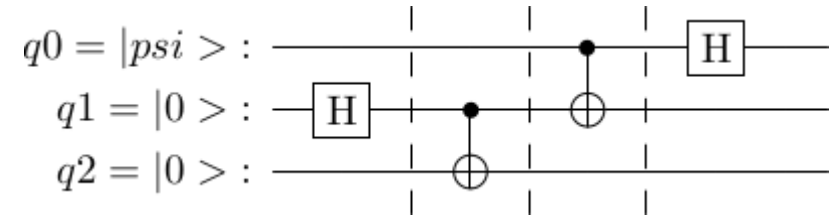
**Quantum Algorithm**  
 1. Create superposition  
 2. Entangle qubits  
 3. Apply interference  
 4. Measure result

Entangled probabilities - If you change the state of one qubit, the probability of all other states changes

# Application: Quantum Teleportation

## ➤ Practical Application: Quantum Networking

- Goal: Alice wants to send the state of her qubit  $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$  to Bob
- Problem: If Bob tries measuring Alice's qubit, he'll get either  $|0\rangle$  or  $|1\rangle$
- Problem: Because of the No Cloning Theorem, it cannot be copied
- Solution: Quantum Teleportation through an entangled EPR pair (Bell state)



## ➤ From the circuit, before applying the first CNOT operator, we need the tensor product

$$|q_2\rangle \otimes |q_1\rangle \otimes |q_0\rangle = |0\rangle \otimes H|0\rangle \otimes |\psi\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \otimes \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \frac{1}{\sqrt{2}} [\alpha \ \beta \ \alpha \ \beta \ 0 \ 0 \ 0 \ 0]$$

## ➤ $CNOT \otimes I$ with q1(C) and q2(T)

$$\frac{1}{\sqrt{2}} [\alpha \ \beta \ 0 \ 0 \ 0 \ 0 \ \alpha \ \beta]$$

## ➤ $I \otimes CNOT$ with q0(C) and q1(T)

$$\frac{1}{\sqrt{2}} [\alpha \ 0 \ 0 \ \beta \ 0 \ \beta \ \alpha \ 0]$$

## ➤ $I \otimes I \otimes H$

$$\frac{1}{\sqrt{2}} [\alpha \ \alpha \ \beta \ -\beta \ \beta \ -\beta \ \alpha \ \alpha]$$



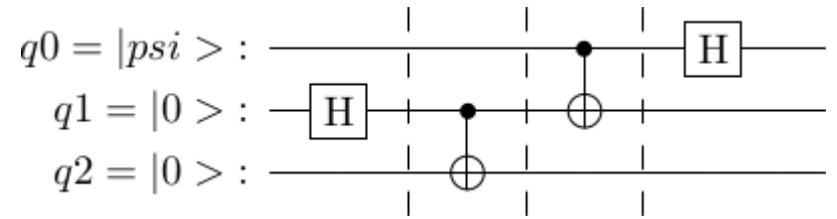
**While the term "teleportation" is used, matter is not being displaced. There's no need to call Scotty.**

# Application: Quantum Teleportation

- Recall the qubit order is  $|q_2q_1q_0\rangle$
- If Alice measures  $|q_200\rangle$ , the state is  $\alpha|0\rangle + \beta|1\rangle = |\psi\rangle$

$\alpha$	$ 000\rangle$
$\alpha$	$ 001\rangle$
$\beta$	$ 010\rangle$
$-\beta$	$ 011\rangle$
$\beta$	$ 100\rangle$
$-\beta$	$ 101\rangle$
$\alpha$	$ 110\rangle$
$\alpha$	$ 111\rangle$

$|\psi\rangle$  is the original state Alice wanted to send to Bob!  
It has been quantum teleported through entanglement.



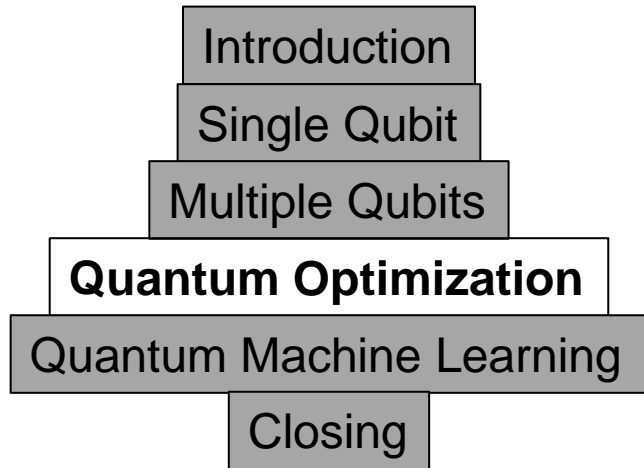
- If Alice measures  $|q_201\rangle$ , the state is  $\alpha|0\rangle - \beta|1\rangle$ , Bob just needs to apply the Z gate
- If Alice measures  $|q_210\rangle$ , the state is  $\beta|0\rangle + \alpha|1\rangle$ , Bob needs to apply the X gate
- If Alice measures  $|q_211\rangle$ , the state is  $-\beta|0\rangle + \alpha|1\rangle$ , Bob needs to apply the X gate, then the Z gate

Alice	Bob
$ 00\rangle$	$ \psi\rangle = I q_2\rangle$
$ 01\rangle$	$ \psi\rangle = Z q_2\rangle$
$ 10\rangle$	$ \psi\rangle = X q_2\rangle$
$ 11\rangle$	$ \psi\rangle = ZX q_2\rangle$

**Re: Spooky Action at a Distance, an entangled system may be separated by great distance e.g., part of the system may be in orbit and the other part may be ground-based. Since there is no communication network, there is nothing to be hacked. This is certainly an advantage over classical computing!**



# Quantum Optimization



**Quantum Unconstrained Binary Optimization**  
**Adiabatic Quantum Computing/Quantum Annealing**  
**Quantum Approximate Optimization Algorithm**  
**Variational Quantum Eigensolver**  
**Grover Adaptive Search**

# Quantum Unconstrained Binary Optimization

## ➤ Quadratic Objective Function with Linear Equality/Inequality Constraints

- Begin with Quantum Unconstrained Binary Optimization (QUBO)  $x_j \in \{0,1\}$
- Convert any Inequality Constraints to Equality Constraints via Slack Variables
- Append Equality Constraints to the Objective Function (typical Lagrangian approach)
- Change variables  $x_j = (1 - z_j) / 2$ ,  $z_j \in \{1, -1\}$  to produce the Ising model
- Objective function  $\rightarrow$  Hamiltonian (energy) and minimization determines the ground state energy
- Evaluation of the Objective Function (Hamiltonian) is the Expectation Value  $\langle \psi | H | \psi \rangle \dots$
- ...where  $|\psi\rangle$  is the state of the Ising model

Note: when applying constraints via slack variables, a suboptimal solution may give "impossible" results that don't satisfy the constraints

$$H = -\sum_{j,k} J_{jk} Z_j Z_k - \sum_j h_j Z_j$$

Hamiltonians are sums of tensor products of Z matrices

**This is mostly just recasting an optimization problem into something that resonates with physicists**

# QUBO Application

➤ **Example...**

- $\min 2 - 4x_0 - 2x_1 - 2x_2 + 4x_0x_1 + 4x_0x_2$
- **subject to**  $x_j \in \{0, 1\}$
- **Substitute**  $x_j = (1 - z_j) / 2$

- $\min z_0(z_1 + z_2)$
- **subject to**  $z_j \in \{1, -1\}$

- **Ising Hamiltonian**  $H = Z^{z_0} \otimes Z^{z_1} \otimes I + Z^{z_0} \otimes I \otimes Z^{z_2}$
- **There are three variables, therefore three qubits are needed**
- **Expectation Values based on**  $\langle \psi | H | \psi \rangle$

Diagonal tensor product of Z gates

$z_0 \quad z_1 \quad z_2 \quad z_0 \quad z_1 \quad z_2$

Orthogonality note:

$\langle x | Z_j | x \rangle = 1$  if the  $j^{\text{th}}$  bit of  $x$  is 0 and that  $\langle x | Z_j | x \rangle = -1$  otherwise

$\langle x | Z_j Z_k | x \rangle = 1$  if the  $j^{\text{th}}$  and  $k^{\text{th}}$  bits of  $x$  are equal and  $\langle x | Z_j Z_k | x \rangle = -1$  otherwise

$$\langle 011 | H | 011 \rangle = \langle 011 | Z_0 Z_1 + Z_0 Z_2 | 011 \rangle = \langle 011 | Z_0 Z_1 | 011 \rangle + \langle 011 | Z_0 Z_2 | 011 \rangle = -1 - 1 = -2$$

$$\langle 000 | H | 000 \rangle = 2$$

$$\langle 001 | H | 001 \rangle = 0$$

$$\langle 010 | H | 010 \rangle = 0$$

$$\langle 011 | H | 011 \rangle = -2$$

$$\langle 100 | H | 100 \rangle = -2$$

$$\langle 101 | H | 101 \rangle = 0$$

$$\langle 110 | H | 110 \rangle = 0$$

$$\langle 111 | H | 111 \rangle = 2$$

$$|011\rangle \rightarrow z_0 = 1, z_1 = -1, z_2 = -1$$

$$|100\rangle \rightarrow z_0 = -1, z_1 = 1, z_2 = 1$$

# Adiabatic QC and Quantum Annealing

- **Adiabatic quantum computing uses a quantum device called a quantum annealer**
  - Think of simulated annealing, where the temperature is varied
  - A simple Hamiltonian adiabatically evolves to the desired complicated Hamiltonian
  - But don't add more energy than  $\Delta E$
- **Quantum Annealing**
  - Adiabatic evolution can take too long for the process to lead to a feasible/optimal solution
  - System evolves from its initial state to the Ising model's ground state
  - Physical quantum devices based on quantum annealing are simpler to construct
  - It's possible to scale the size of these quantum annealers up to hundreds or even thousands of qubits

**There is no known computational advantage to quantum annealing  
Also, scaling will be limited by the connectivity between qubits**

# Quantum Approximate Optimization Algorithm

➤ **Quantum Approximate Optimization Algorithm (QAOA)**

- For use with gate-based quantum circuit computers, as an alternative to quantum annealers

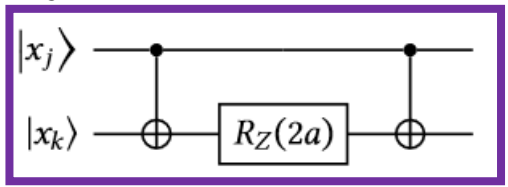
$$H_0 = \bigotimes_{i=0}^{n-1} |+\rangle = -\sum_{j=0}^{n-1} X_j \quad H_1 = -\sum_{j,k} J_{jk} Z_j Z_k - \sum_j h_j Z_j$$

- ...such that

$$\exp(i\beta_k H_0) = \exp(i\beta_k \sum_{j=0}^{n-1} X_j) = \prod_{j=0}^{n-1} \exp(-i\beta_k X_j) \quad R_X(2\beta)$$

$$\exp(i\gamma_l H_1) = \exp(i\gamma_l \sum_{j,k} J_{jk} Z_j Z_k + \sum_j h_j Z_j) = \prod_{j,k} \exp(-i\gamma_l J_{jk} Z_j Z_k) \prod_j \exp(-i\gamma_l h_j Z_j) \quad R_Z(2\gamma)$$

- Let  $a = \gamma_l J_{jk}$
- If  $|x\rangle$  is a computational basis state in which j and k have the same value, then  $\exp(-iaZ_j Z_k) |x\rangle = \exp(-ia) |x\rangle$
- If j and k have different values, then  $\exp(-iaZ_j Z_k) |x\rangle = \exp(ia) |x\rangle$



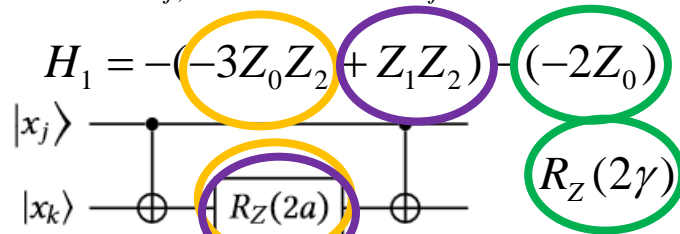
# Quantum Approximate Optimization Algorithm

➤ Quantum Approximate Optimization Algorithm (QAOA)

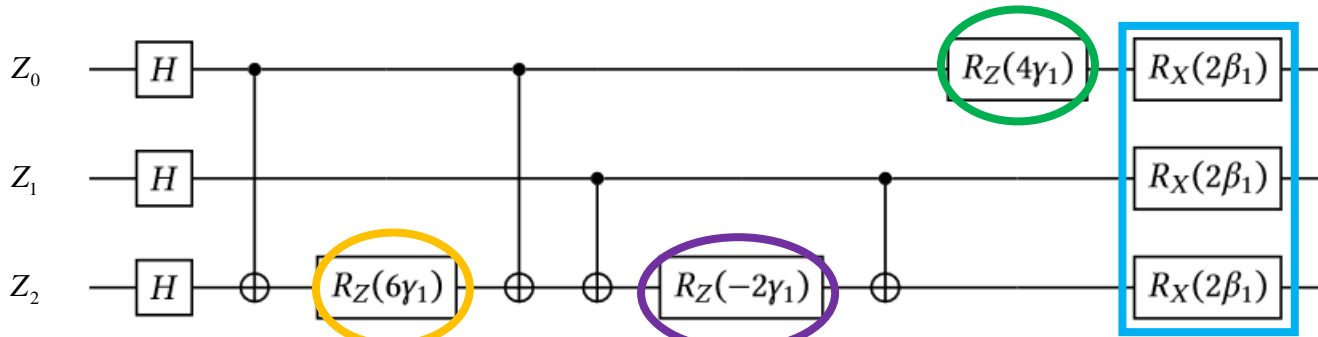
- Example: Let  $H = 3Z_0Z_2 - Z_1Z_2 + 2Z_0$   
 $H_0 = \otimes_{i=0}^{n-1} |+\rangle = -\sum_{j=0} X_j$        $H_1 = -\sum_{j,k} J_{jk} Z_j Z_k - \sum_j h_j Z_j$

$$H_0 = -X_0 - X_1 - X_2$$

$$R_X(2\beta) \ R_X(2\beta) \ R_X(2\beta)$$



- The quantum circuit implementation (for p=1) is



**There is no known computational advantage to QAOA**

- As seen with QUBO,  $\langle x|Z_j|x\rangle = 1$  if the  $j$ th bit of  $x$  is 0 and that  $\langle x|Z_j|x\rangle = -1$  otherwise
- $\langle x|Z_j Z_k|x\rangle = 1$  if the  $j$ th and  $k$ th bits of  $x$  are equal and  $\langle x|Z_j Z_k|x\rangle = -1$  otherwise

$$\langle 101 | H | 101 \rangle = \langle 101 | 3Z_0Z_2 - Z_1Z_2 + 2Z_0 | 101 \rangle = 3\langle 101 | Z_0Z_2 | 101 \rangle - \langle 101 | Z_1Z_2 | 101 \rangle + 2\langle 101 | Z_0 | 101 \rangle = 3 + 1 - 2 = 2$$



# Variational Quantum Eigensolver

➤ Measurements in quantum mechanics are represented by Hermitian operators (observables), e.g., Z matrix

➤ The expectation value of any Hermitian operator (observable) A is given by

$$\langle A \rangle_\psi = \sum_{j,k} \left| \langle \lambda_j^k | \psi \rangle \right|^2 \lambda_j = \langle \psi | A | \psi \rangle$$

➤ An observable can be expressed as a linear combination of tensor products of Pauli matrices, I, X, Y, Z

▪ **Example**  $A = \frac{1}{2}Z \otimes I \otimes X - 3I \otimes Y \otimes Y + 2Z \otimes X \otimes Z$

$$\langle \psi | A | \psi \rangle = \frac{1}{2} \langle \psi | Z \otimes I \otimes X | \psi \rangle - 3 \langle \psi | I \otimes Y \otimes Y | \psi \rangle + 2 \langle \psi | Z \otimes X \otimes Z | \psi \rangle$$

- The eigenvectors of Z are  $|0\rangle$  with eigenvalue 1 and  $|1\rangle$  with eigenvalue -1
- The eigenvectors of X are  $|+\rangle$  with eigenvalue 1 and  $|-\rangle$  with eigenvalue -1
- The eigenvectors of Y are  $|i\rangle = \frac{1}{\sqrt{2}}(|0\rangle + i|1\rangle)$  with eigenvalue 1 and  $|-i\rangle = \frac{1}{\sqrt{2}}(|0\rangle - i|1\rangle)$  with eigenvalue -1
- Any (non-null) state is an eigenvector of I with eigenvalue 1

ZIX	Eigenvalue
$ 0\rangle 0\rangle +\rangle$	1
$ 0\rangle 0\rangle -\rangle$	-1
$ 0\rangle 1\rangle +\rangle$	-1
$ 0\rangle 1\rangle -\rangle$	1
$ 1\rangle 0\rangle +\rangle$	-1
$ 1\rangle 0\rangle -\rangle$	1
$ 1\rangle 1\rangle +\rangle$	1
$ 1\rangle 1\rangle -\rangle$	-1

IYY	Eigenvalue
$ 0\rangle i\rangle i\rangle$	1
$ 0\rangle i\rangle -i\rangle$	-1
$ 0\rangle -i\rangle i\rangle$	-1
$ 0\rangle -i\rangle -i\rangle$	1
$ 1\rangle i\rangle i\rangle$	-1
$ 1\rangle i\rangle -i\rangle$	1
$ 1\rangle -i\rangle i\rangle$	1
$ 1\rangle -i\rangle -i\rangle$	-1

ZXZ	Eigenvalue
$ 0\rangle +\rangle 0\rangle$	1
$ 0\rangle +\rangle 1\rangle$	-1
$ 0\rangle -\rangle 0\rangle$	-1
$ 0\rangle -\rangle 1\rangle$	1
$ 1\rangle +\rangle 0\rangle$	-1
$ 1\rangle +\rangle 1\rangle$	1
$ 1\rangle -\rangle 0\rangle$	1
$ 1\rangle -\rangle 1\rangle$	-1

# Variational Quantum Eigensolver

- **Example (continued)**

- Recall  $H|0\rangle = |+\rangle$  and  $H|1\rangle = |-\rangle$  such that  $|0\rangle = H|+\rangle$  and  $|1\rangle = H|-\rangle$
- Also,  $SH|0\rangle = |i\rangle$  and  $SH|1\rangle = |-i\rangle$  such that  $|0\rangle = (SH)^\dagger|i\rangle$  and  $|1\rangle = (SH)^\dagger|-i\rangle$
- Therefore...
- H takes the eigenvectors of X to the standard/computational basis
- SH takes the eigenvectors of Y to the standard/computational basis
- I takes the eigenvectors of Z to the standard/computational basis

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$S \equiv \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$$

$$Z \otimes I \otimes X \rightarrow I \otimes I \otimes H \qquad I \otimes Y \otimes Y \rightarrow I \otimes (SH)^\dagger \otimes (SH)^\dagger \qquad Z \otimes X \otimes Z \rightarrow I \otimes H \otimes I$$

$$\langle \psi | A | \psi \rangle = \frac{1}{2} \langle \psi | Z \otimes I \otimes X | \psi \rangle - 3 \langle \psi | I \otimes Y \otimes Y | \psi \rangle + 2 \langle \psi | Z \otimes X \otimes Z | \psi \rangle$$

$$\langle \psi | A | \psi \rangle = \frac{1}{2} \langle \psi | I \otimes I \otimes H | \psi \rangle - 3 \langle \psi | I \otimes (SH)^\dagger \otimes (SH)^\dagger | \psi \rangle + 2 \langle \psi | I \otimes H \otimes I | \psi \rangle$$

- Bottom line: For any Hermitian operator A, there is always a unitary transformation that takes any basis of eigenvectors of A to the computational basis, and vice versa

- **Note: Everything we have done, so far, is to find the ground state (minimum) of the Hamiltonian**
- **However, the Hamiltonian may be augmented to find excited states with Physical Chemistry applications**

**There is no known computational advantage to VQE**

# Grover's Algorithm

- Grover's algorithm is  $O(\sqrt{n})$

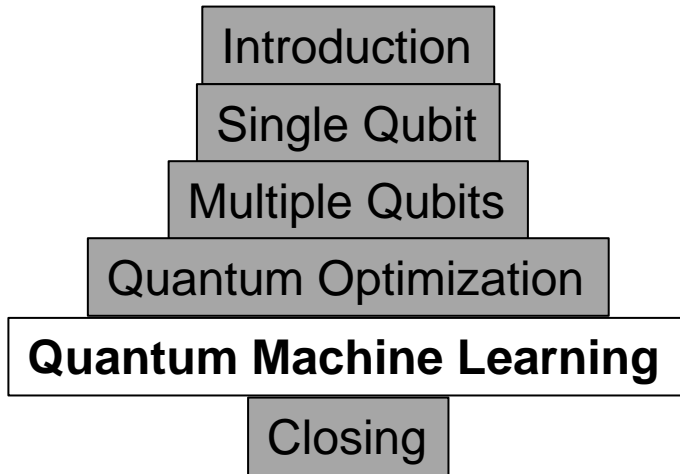
## Hacking a 13-character (alpha only) password

- $26^{13} = 2.5 \times 10^{18}$  combinations
- At one guess/nanosecond, that's  $2.5 \times 10^9$  sec (~80 years)
- Grover solves it in  $\sqrt{n} = \sqrt{2.5 \times 10^9} = 50,000$  sec
- If QC advances like today's Intel chips, i.e., at 50,000X...
- ...then the password will be hacked in 1 sec

- Caveats:

- It provides only a quadratic speedup
- You need to know the number of solutions (or be patient in guessing)
- It can be adapted to optimization via a binary search of cost function values
- Classical algorithms, such as Schoening's algorithm, offer a better speedup for satisfiability problems
- A quantum version may offer further enhancement

# Quantum Machine Learning



## Quantum Machine Learning Application: Quantum Neural Networks

**Many machine learning problems can be reduced to the minimization of a loss function through some optimization algorithm on a suitable model**

# Quantum Machine Learning (QML)

## ➤ Quantum Machine Learning

- Use a quantum computer in some part a model that you wish to train
- Use data generated by some quantum process
- Use a quantum computer to process quantum-generated data

## ➤ Four families of QML

- CQ – classical data training a quantum algorithm
- QQ – quantum technologies still immature

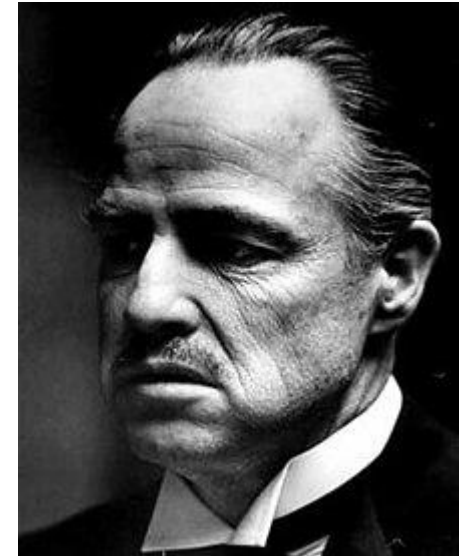
	Classical Algorithm	Quantum Algorithm
Classical Data	CC	CQ
Quantum Data	QC	QQ

## ➤ Quantum algorithms

- Quantum model and quantum optimization (hardware not currently ready)
- Quantum model and classical optimization (available on NISQ devices)

## ➤ Models

- Quantum Support Vector Machines (SVM): quantum computers mapping data to quantum states
- Quantum Neural Networks: a full quantum model running on a quantum computer

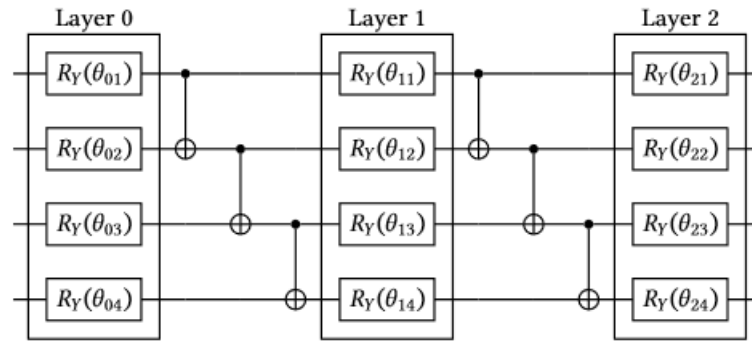


# Quantum Neural Networks

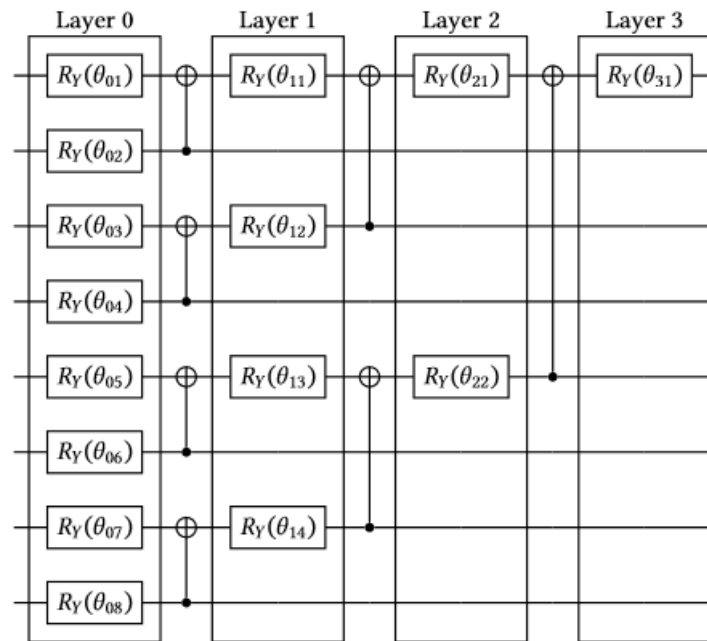
- **CQ – Classical data training a quantum algorithm**
  - Classical computing for the preparation of circuits and the statistical analysis of measurements
  - Quantum neural networks are “purely quantum” models
- **Data input: Input nodes**
  - Classical inputs mapped to quantum states through a feature map
- **Data processing: Network**
  - Architecture is a variational circuit dependent on optimizable parameters
- **Data output: Output nodes**
  - Output is the result of a measurement operation on the final state

# Quantum Neural Networks

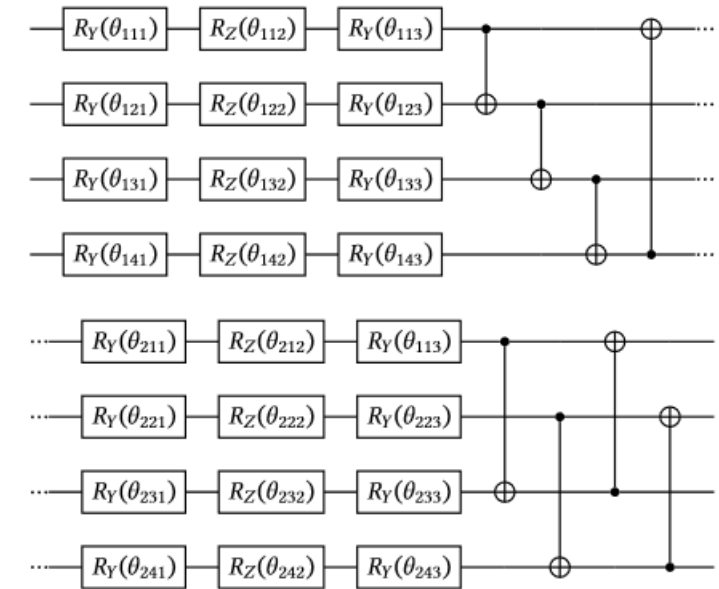
## ➤ Variational forms



Two-local Variational Form



Tree Tensor Variational Form



Strongly Entangling Layers

These variational circuits have the same “black box” explainability challenges as classical neural nets



# Quantum Neural Networks

## ➤ Measurements (classification problems)

- The M operator associates the eigenvalues 1 and 0 to the qubit's value being 0 and 1
- The Z operator associates the eigenvalues 1 and -1 to the qubit's value being 0 and 1

$$M \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad Z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

## ➤ Training/Optimization (Adam algorithm)

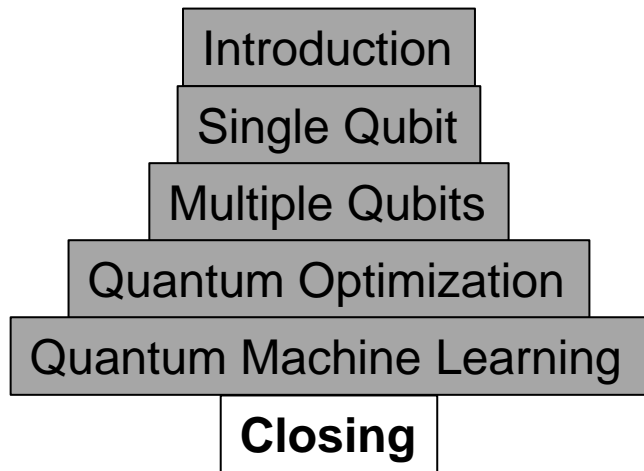
- Numerical approximation
- Automatic differentiation
- Parameter shift rule

## ➤ Tips

- Feature map → variational form → measurement operation
- Variational form: too many optimizable parameters → overfitting, too few → underfitting
- Small learning rate → accurate/slower, higher batch size → effective optimization/slower
- Normalize the data and consider dimensionality reduction techniques

**QML provides a larger state space with the potential benefit of requiring less data**

# Closing



**Recap**  
**Learning Objectives**  
**More Information**  
**References**

# Learning Objectives

- **Identify** the three aspects of quantum information science
- **Describe** the difference between a quantum bit (qubit) and a classical (0/1) bit
- **Explain** how superposition facilitates quantum cryptography and makes quantum computing relevant today
- **Explain** how entanglement facilitates quantum teleportation and makes quantum computing relevant today
- **Tell** the truths about quantum computing myths
- **Identify** different computational models for quantum optimization and their applications
- **Describe** the four families of quantum machine learning and variations of quantum neural networks

# For More Information on...

- **...the algorithms**
  - Linear algebra (almost any college text will suffice)
- **...the science underlying quantum computing**
  - Quantum mechanics (Griffiths' Intro to QM, Weinberg's Lectures on QM)
- **...the engineering challenges**
  - Noise and decoherence, error detection, and error correction (Mike & Ike)
- **...practicing quantum computing code**
  - Qiskit, Penny Lane, and D-Wave documentation pages
  - OpenQASM, Q#, Cirq, Bracket
  - Qirk (web-based simulator)
  - Virtual Quantum Optics Lab (quantum objects experiments) [vqol.org](http://vqol.org)

# Quantum Computing References

## ➤ Textbooks

- Quantum Computation and Quantum Information (Michael Nielsen & Isaac Chuang aka “Mike & Ike”)
- Quantum Computing: An Applied Approach (Hidary), complementary to Mike & Ike
- Quantum Computer Science (Mermin)
- Quantum Computing Algorithms (Burd)
- A Practical Guide to Quantum Machine Learning and Quantum Optimization (Combarro & Gonzalez-Castillo)
- Programming Quantum Computers (Johnston, Harrigan, Gimeno-Segovina)
- E-book <https://www.thomaswong.net> (Thomas Wong)

## ➤ Udemy

- Quantum Computing Made Simple
- QC101 Quantum Computing and Intro to Quantum Machine Learning
- QC201 Advanced Math for Quantum Computing

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**The University of Texas at Austin**

- **Where are the quantum computers? Can I order one from Dell or pick one up at Best Buy?**
  - Research institutions, NSA, etc.
- **What do the experts think? Progress, roadblocks, etc.**
  - 10, 20, 50 years? Nobody knows at this time. An over-night breakthrough may occur.
- **What are the implications for managers?**
  - Workforce development
  - Quantum education
  - Quantum programming jobs
- **My question to you...**
  - This material has been essentially at the “101” level
  - Would you like another tutorial at the “201” level?
  - Would you like an IITSEC Workshop with hands-on quantum computing?
- **Your questions...?**