PRACTICAL QUANTUM C FOR SCIENTISTS

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Topics

We will learn

- Quantum Computing and IBM Qiskit

- Quantum Mechanisms for Computing

- Quantum Algorithms and Applications

- Hands-on Exercise on IBM Q.

Quantum Computing

A host of new computer technologies has emerged within the last few years, and quantum computing is arguably the technology requiring the greatest paradigm shift on the part of developers.

Quantum computers were proposed in the 1980s by Richard Feynman and Yuri Manin.

Quantum computers are here, the next big challenge: A quantum skills shortage. The quantum computing industry will be a $65 billion market by 2030; others anticipate that up to 20% of organizations could be budgeting for quantum computing in 2023, up from 1% in 2018 Gartner

Source: Microsoft Azure Quantum

Quantum Computing

- The intuition behind quantum computing stemmed from what was often seen as one of the greatest embarrassments of physics: remarkable scientific progress faced with an inability to model even simple systems.

- Quantum mechanics was developed between 1900 and 1925 and it remains the cornerstone on which chemistry, condensed matter physics, and technologies ranging from computer chips to LED lighting ultimately rests.

- Yet despite these successes, even some of the simplest systems seemed to be beyond the human ability to model with quantum mechanics. This is because simulating systems of even a few dozen interacting particles requires more computing power than any conventional computer can provide over thousands of years!

Source: Microsoft Azure Quantum

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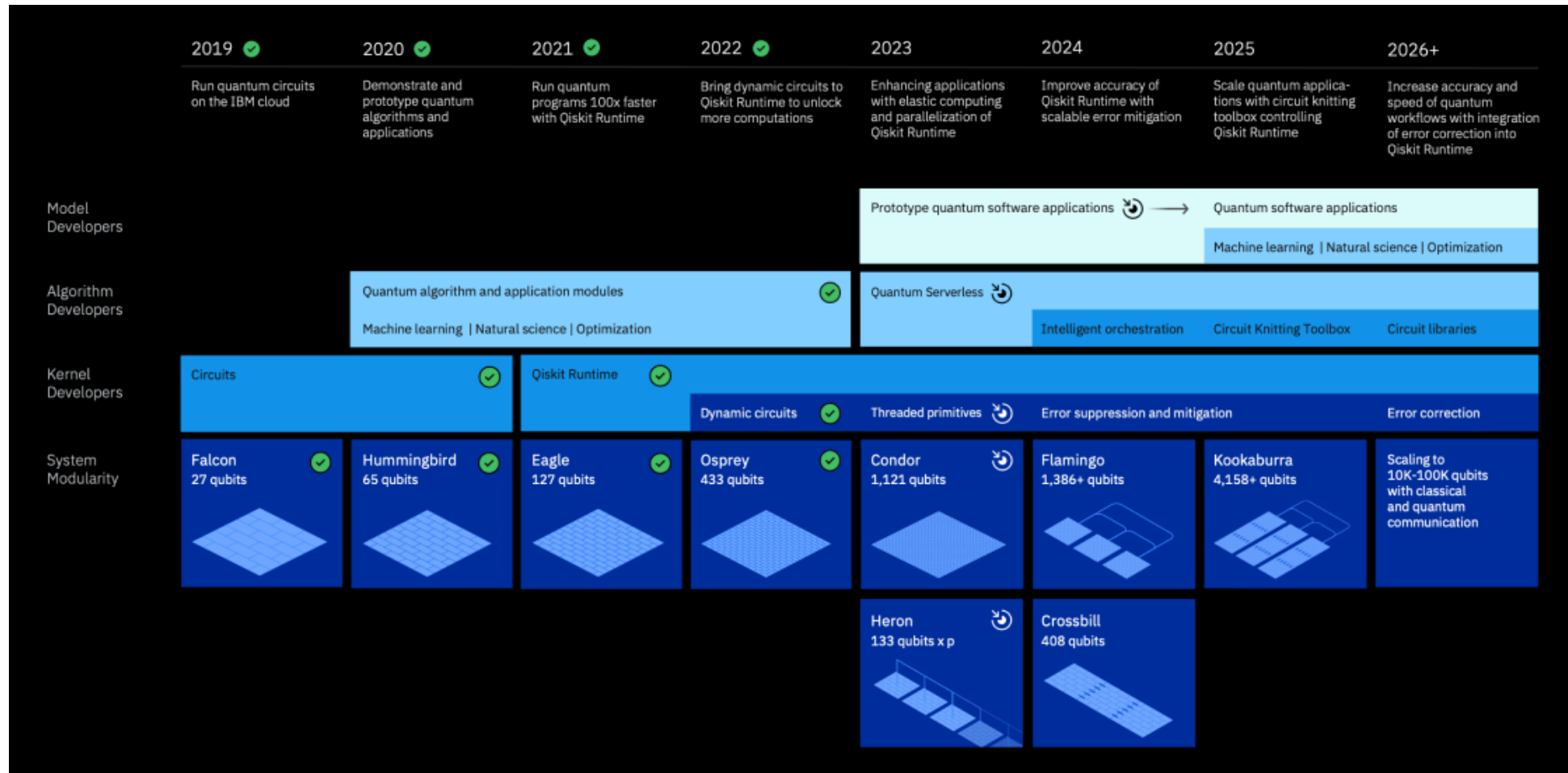
Quantum Computing

The foundational core of quantum computing is to store information in quantum states of matter and to use quantum gate operations to compute on that information, by harnessing and learning to "program" quantum interference.
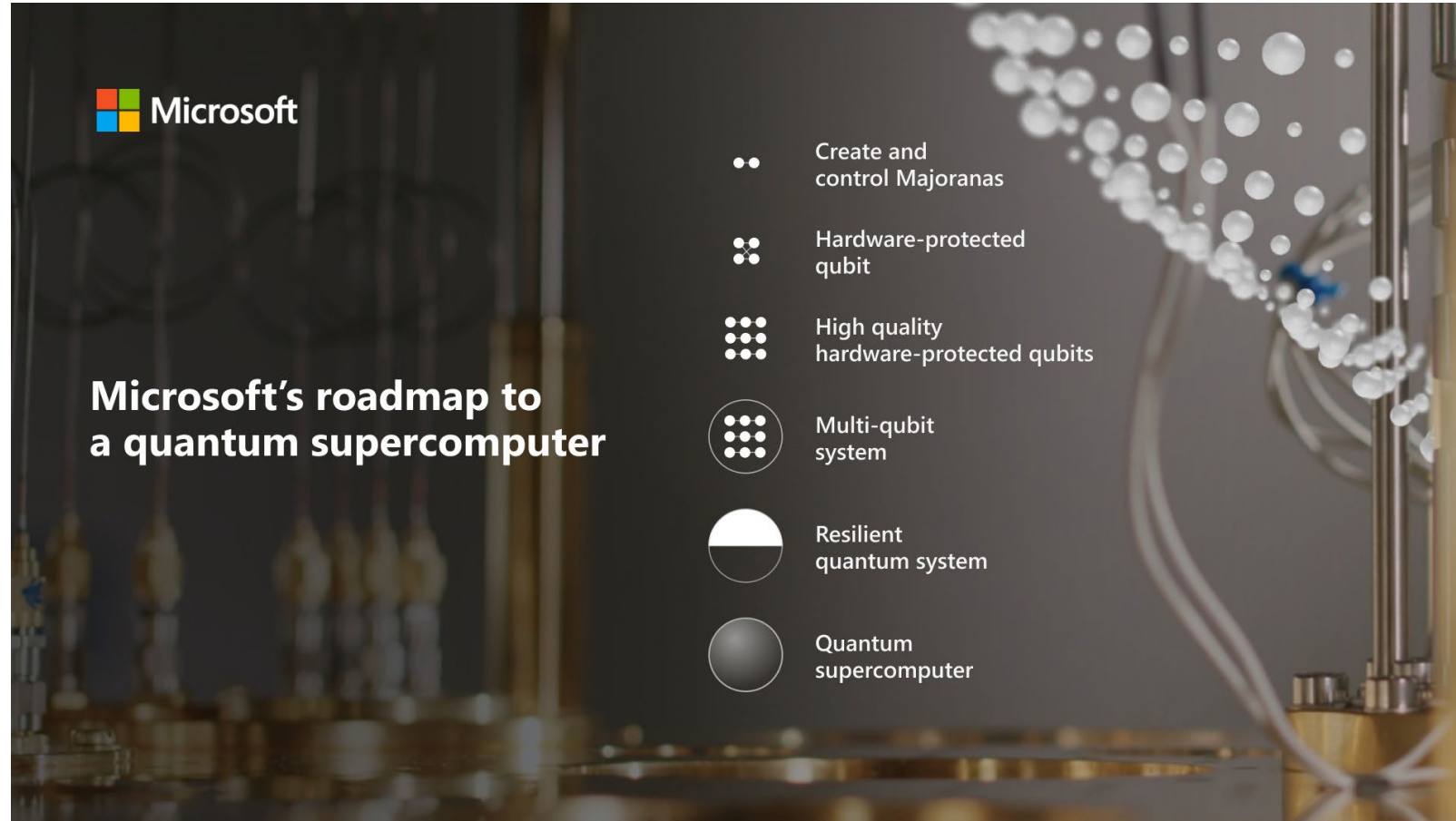
Quantum Computing

Quantum Computing harnesses the laws of quantum mechanics to solve problems to complex for classical computers

- Model the behavior of individual atoms in a molecule

- Identify subtle patterns of fraud in financial transactions

- Combinatorial problems (Travelling Salesman, Maximum Independent Vertex Set)

- Process large data sets for AI and Data Science

IBM Quantum Computing Roadmap

Microsoft Quantum Computing Roadmap

Quantum Computing Challenges

Many Challenges

- **Hardware Development**

  - Developing high-quality quantum hardware, such as qubits and control electronics, is a major challenge.

  - Qubits are highly susceptible to noise and interference- decoherence

- **Error Correction**

  - Most experts would consider this the biggest challenge. Quantum computers are extremely sensitive to noise and errors caused by interactions with their environment. This can cause errors to accumulate and degrade the quality of computation.

- **Quantum Software Development**

  - Quantum algorithms and software development tools are still in their infancy, and there is a need for new programming languages, compilers, and optimization tools that can effectively utilize the power of quantum computers.

- **Scalability**

  - Scaling up quantum computers to hundreds or thousands of qubits while maintaining high levels of coherence and low error rates remains a major challenge.

Others:
- Classical computer interface
- Standards and protocols
- Trained Talent and workforce
- Overall expense

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Quantum Computing Modality

Quantum Computing harnesses the laws of quantum mechanics to solve problems to complex for classical computers

- Superconducting qubits
  - IBM, Google, Rigetti, Oxford Quantum Circuits
- Trapped-ion
  - IONQ, Quantinuum, Oxford Ionics (electronic control)
- Neutral Atoms
  - QuEra, Pasqal, Infleqtion, Atom Computing,
- Photonic
  - PsiQuantum, Quandela, Xanadu,QuiX, ORCA
- Silicon Spin/Quantum Dots
  - Intel, diraq, Silicon Quantum Computing, Quantum Motion
- Dimond NV (Nitrogen-vacancy) Center
  - Quantum Brilliance, Quantum Dimond Tech,Diatope

Quantum Computing Platforms

Most Quantum Computing through Cloud

- IBM Quantum (IBM Q system)
- Microsoft Azure Quantum (Quantinum, IONQ, TOSHIBA, PASQAL, QCI, Rigetti)
- Amazon Braket (IonQ, Rigetti, Xanadu, QuEra, Oxford Quantum Circuits, D-WAVE)
- qBraid
- Quandela Cloud
- Qmware cloud
- Oxford Quantum Circuits Private Cloud

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Quantum Software SDK and IBM Qiskit

A tool for developing quantum algorithms for quantum computers or simulators and emulators

- IBM Qiskit (Quantum Gate Model)
- Google Cirq (Quantum Gate Model)
- Microsoft Q## and QDK
- Xanadu PennyLane
- QuEra Bloqade (Neutral atoms)
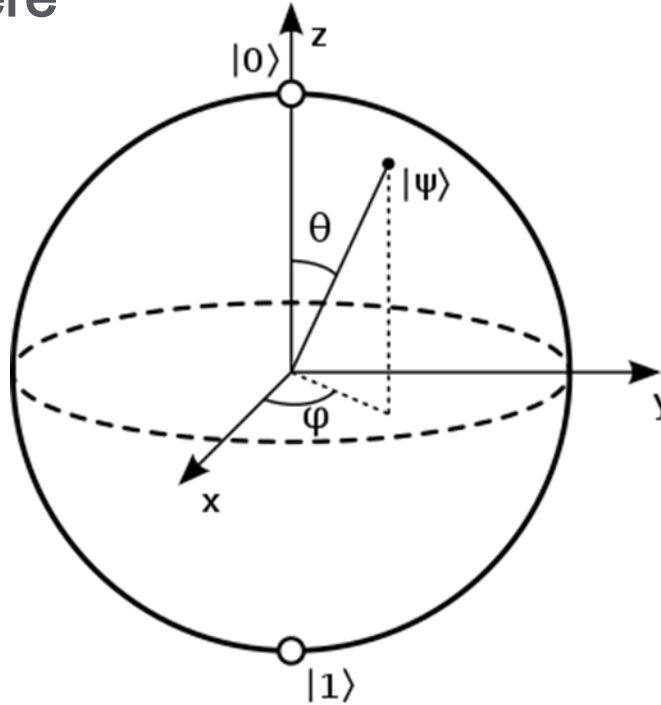- Qmware basiq SDK
- D-WAVE Ocean (Quantum Annealer)

Qubits

Basic Information Unit

- A qubit (quantum bit) is the basic unit of information in quantum computing.
- A qubit (or quantum bit) is the quantum mechanical analogue of a classical bit.
- A general -pure- qubit state is expressed as: $\psi = \alpha|0\rangle + \beta|1\rangle$
- $|0\rangle$ and $|1\rangle$ basis
- α and β are the complex probability amplitudes
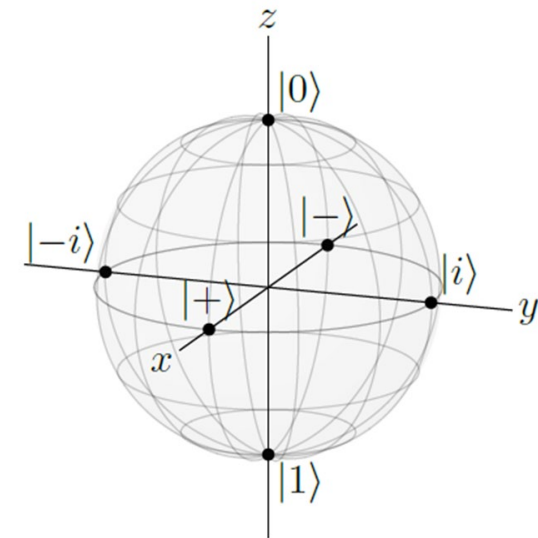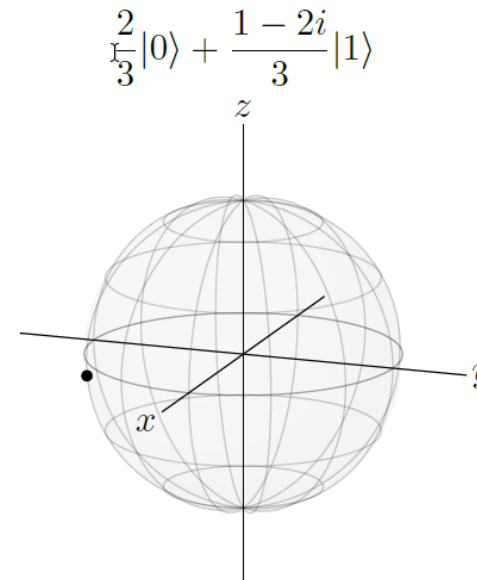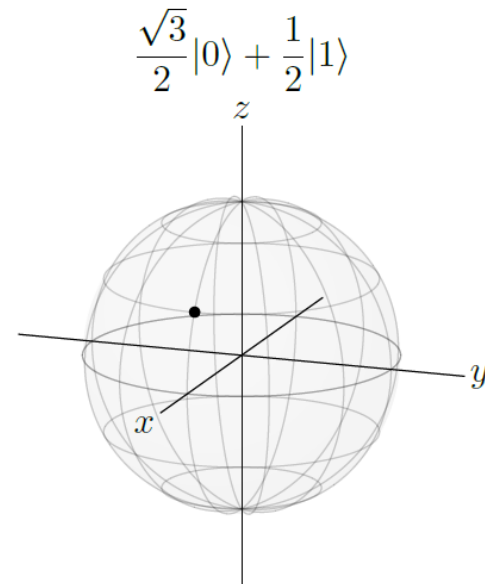
A single qubit by Bloch Sphere

$$|\psi\rangle = \cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle = \cos(\theta/2)|0\rangle + (\cos\phi + i\sin\phi)\sin(\theta/2)|1\rangle, \text{ where } 0 \le \theta \le \pi \text{ and } 0 \le \phi < 2\pi.$$

Measure Qubits

At end of a computation, we read (measure) the qubit

- The qubit "collapse" to either |0> or |1> with some probability
- Probability is the norm-square of each amplitude.

$$\frac{\sqrt{3}}{2}|0\rangle + \frac{1}{2}|1\rangle$$

$$\frac{2}{3}|0\rangle + \frac{1-2i}{3}|1\rangle$$

One-Qubit Quantum Gates

At end of a computation, we read (measure) the qubit

Identity Gate I

Pauli X gate

$$X|0\rangle = |1\rangle,$$
$$X|1\rangle = |0\rangle.$$

Pauli Y gate

$$Y|0\rangle = i|1\rangle,$$
$$Y|1\rangle = -i|0\rangle.$$

Pauli Z gate

$$Z|0\rangle = |0\rangle,$$
$$Z|1\rangle = -|1\rangle.$$

- Phase Gate S

$$S|0\rangle = |0\rangle,$$
$$S|1\rangle = i|1\rangle.$$

- Hadamard gate turns $|0\rangle$ into $|+\rangle$, and $|1\rangle$ into $|-\rangle$:

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

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

- Column Vectors

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

- Row Vectors

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}^{\mathsf{T}} = (\alpha \ \beta). \qquad\qquad \begin{pmatrix} \alpha \\ \beta \end{pmatrix}^{\dagger} = (\alpha^* \ \beta^*).$$

- Bra $\langle\psi| = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}^{\dagger} = (\alpha^* \ \beta^*).$

- Ket $|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$

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- Inner Products Are Scalars

$$|\psi\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \quad \text{and} \quad |\phi\rangle = \begin{pmatrix} \gamma \\ \delta \end{pmatrix}.$$

$$\langle\psi||\phi\rangle = \begin{pmatrix} \alpha^* & \beta^* \end{pmatrix} \begin{pmatrix} \gamma \\ \delta \end{pmatrix}.$$

$$\langle\psi|\phi\rangle = \alpha^*\gamma + \beta^*\delta.$$

Gates as Matrices

Gate	Action on Computational Basis	Matrix Representation
Identity	$I\lvert 0\rangle = \lvert 0\rangle$ $I\lvert 1\rangle = \lvert 1\rangle$	$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$
Pauli X	$X\lvert 0\rangle = \lvert 1\rangle$ $X\lvert 1\rangle = \lvert 0\rangle$	$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$
Pauli Y	$Y\lvert 0\rangle = i\lvert 1\rangle$ $Y\lvert 1\rangle = -i\lvert 0\rangle$	$Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
Pauli Z	$Z\lvert 0\rangle = \lvert 0\rangle$ $Z\lvert 1\rangle = -\lvert 1\rangle$	$Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$
Phase S	$S\lvert 0\rangle = \lvert 0\rangle$ $S\lvert 1\rangle = i\lvert 1\rangle$	$S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}$
T	$T\lvert 0\rangle = \lvert 0\rangle$ $T\lvert 1\rangle = e^{i\pi/4}\lvert 1\rangle$	$T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}$
Hadamard H	$H\lvert 0\rangle = \frac{1}{\sqrt{2}}(\lvert 0\rangle + \lvert 1\rangle)$ $H\lvert 1\rangle = \frac{1}{\sqrt{2}}(\lvert 0\rangle - \lvert 1\rangle)$	$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

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$$HSTH|0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}\begin{pmatrix} 1 \\ e^{i\pi/4} \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 1 \\ e^{i3\pi/4} \end{pmatrix}$$

$$= \frac{1}{2}\begin{pmatrix} 1 + e^{i3\pi/4} \\ 1 - e^{i3\pi/4} \end{pmatrix}.$$

All Quantum Operations must be reversible

A matrix that satisfies this property $U^{\dagger}U = I$ (and $UU^{\dagger} = I$) is called *unitary*.

Quantum gates are unitary matrices, and unitary matrices are quantum gates.

Quantum Mechanism

Quantum Computing Depends on Quantum Mechanism

- Quantum Superposition
- Quantum Entanglement
- Quantum Interference

Quantum Superposition

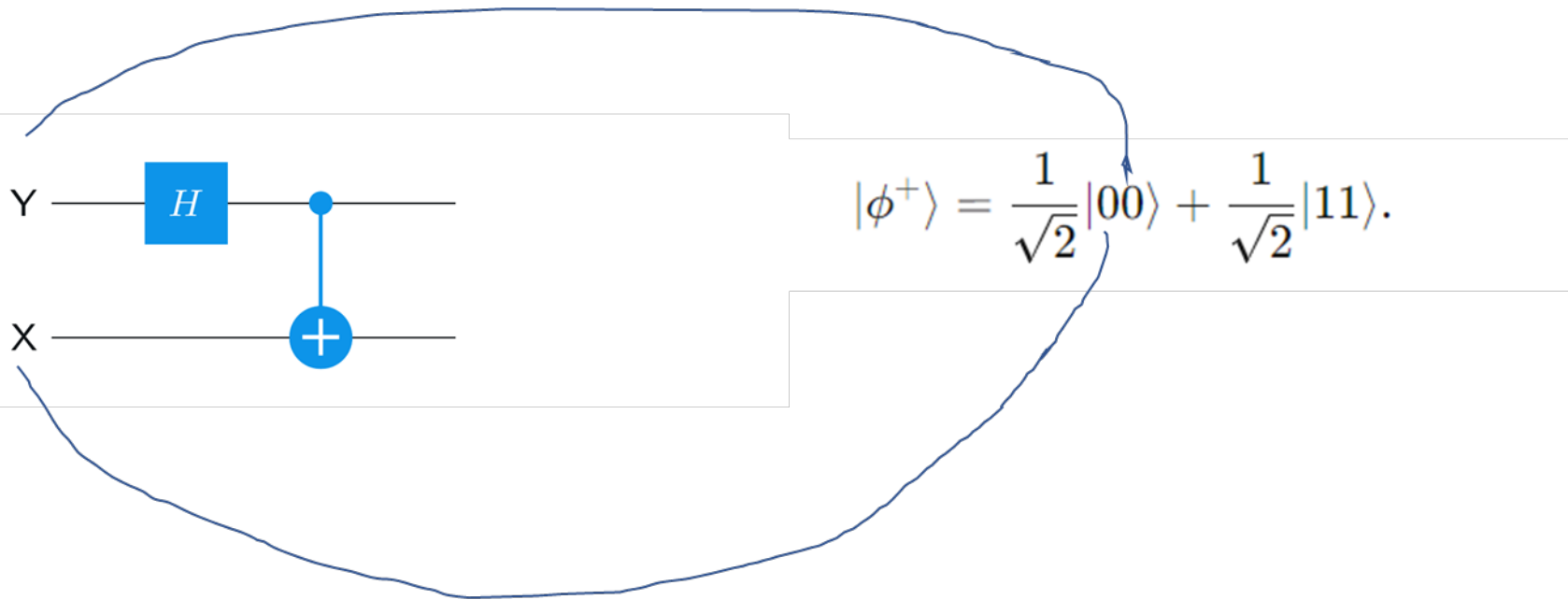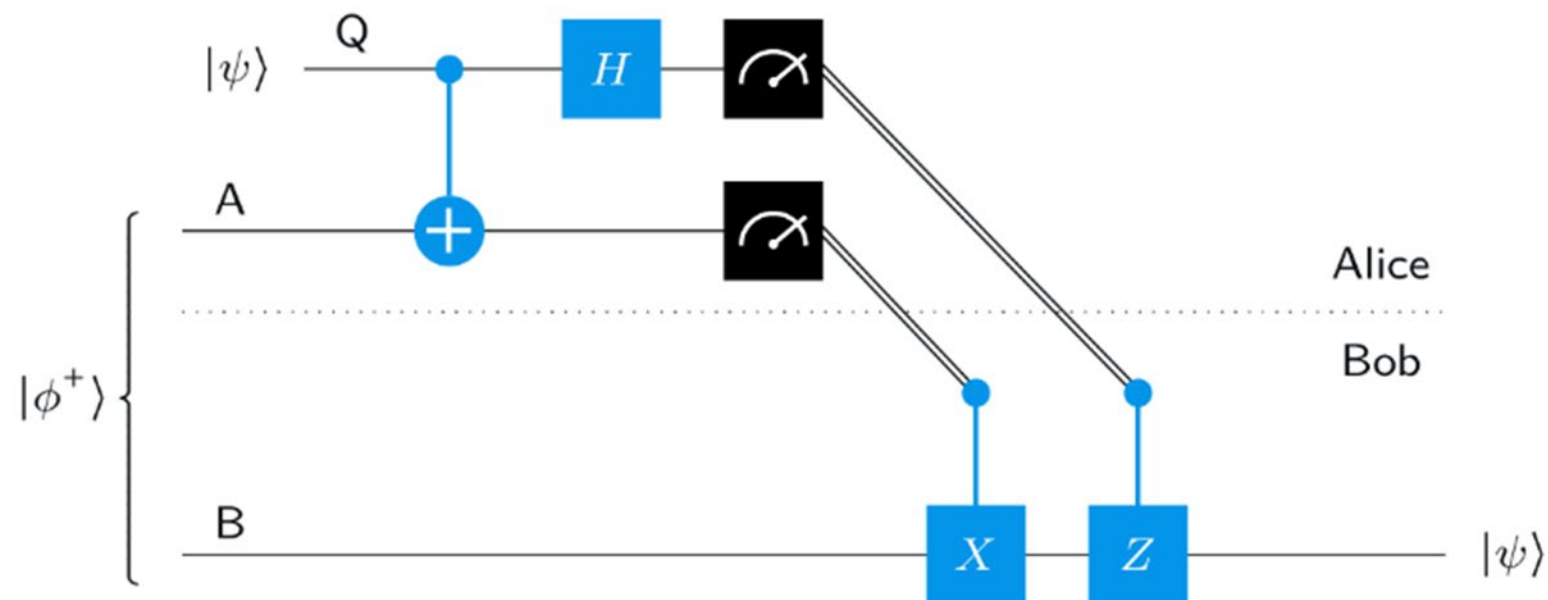Superposition is the ability of a quantum system to be in multiple states at the same time until it is measured.
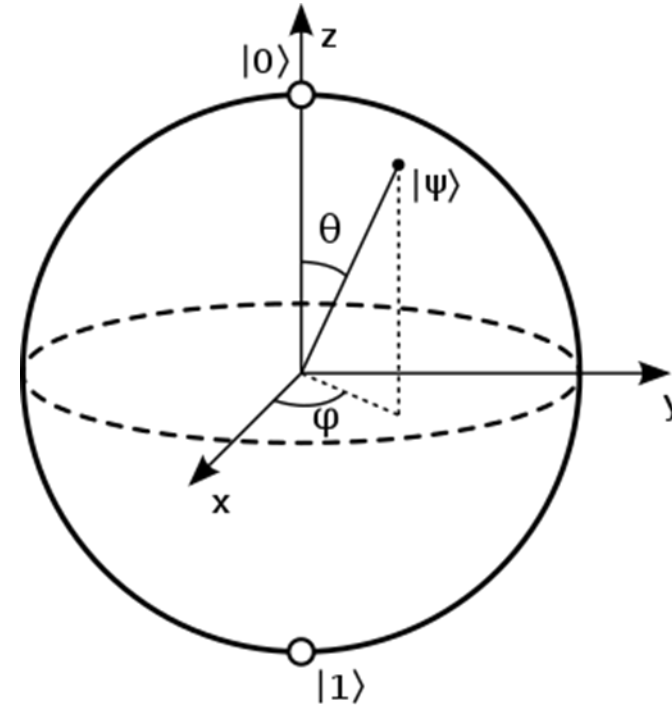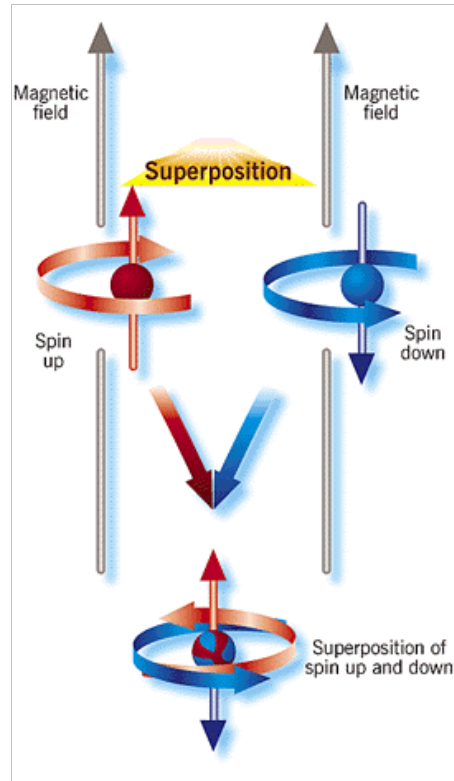

$$|\psi\rangle = \cos(\theta/2)|0\rangle + e^{i\phi}\sin(\theta/2)|1\rangle = \cos(\theta/2)|0\rangle + (\cos\phi + i\sin\phi)\sin(\theta/2)|1\rangle, \text{ where } 0 \le \theta \le \pi \text{ and } 0 \le \phi < 2\pi.$$

Quantum Entanglement

Quantum entanglement explains how two subatomic particles can be intimately linked to each other even if separated by billions of light -years of space. A change induced in one will affect the other, even if they are separated by a large distance.

$$|\phi^+\rangle = \frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle.$$

Quantum Interference

Superposition is the ability of a quantum system to be in multiple states at the same time until it is measured.

Light Source

Metal Sheet

Screen
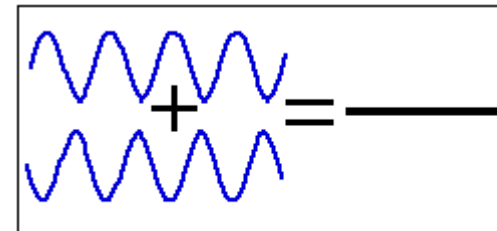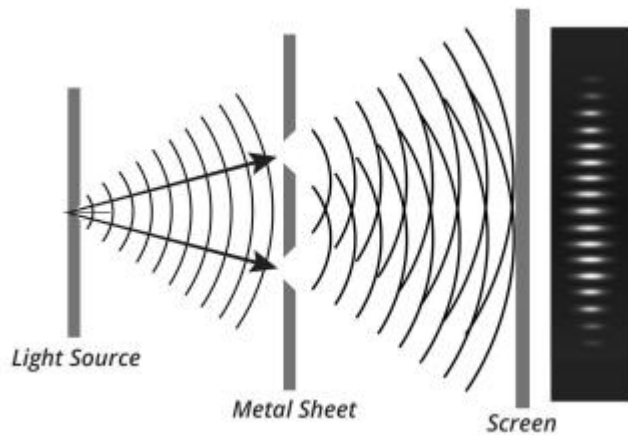
Destructive Interference

https://www.discovery.com/science/Double -Slit-Experiment

Quantum Teleportation

Quantum Superdense Coding

$$|\phi^+\rangle \mapsto |00\rangle$$
$$|\phi^-\rangle \mapsto |01\rangle$$
$$|\psi^+\rangle \mapsto |10\rangle$$
$$|\psi^-\rangle \mapsto -|11\rangle$$

Alice

Bob
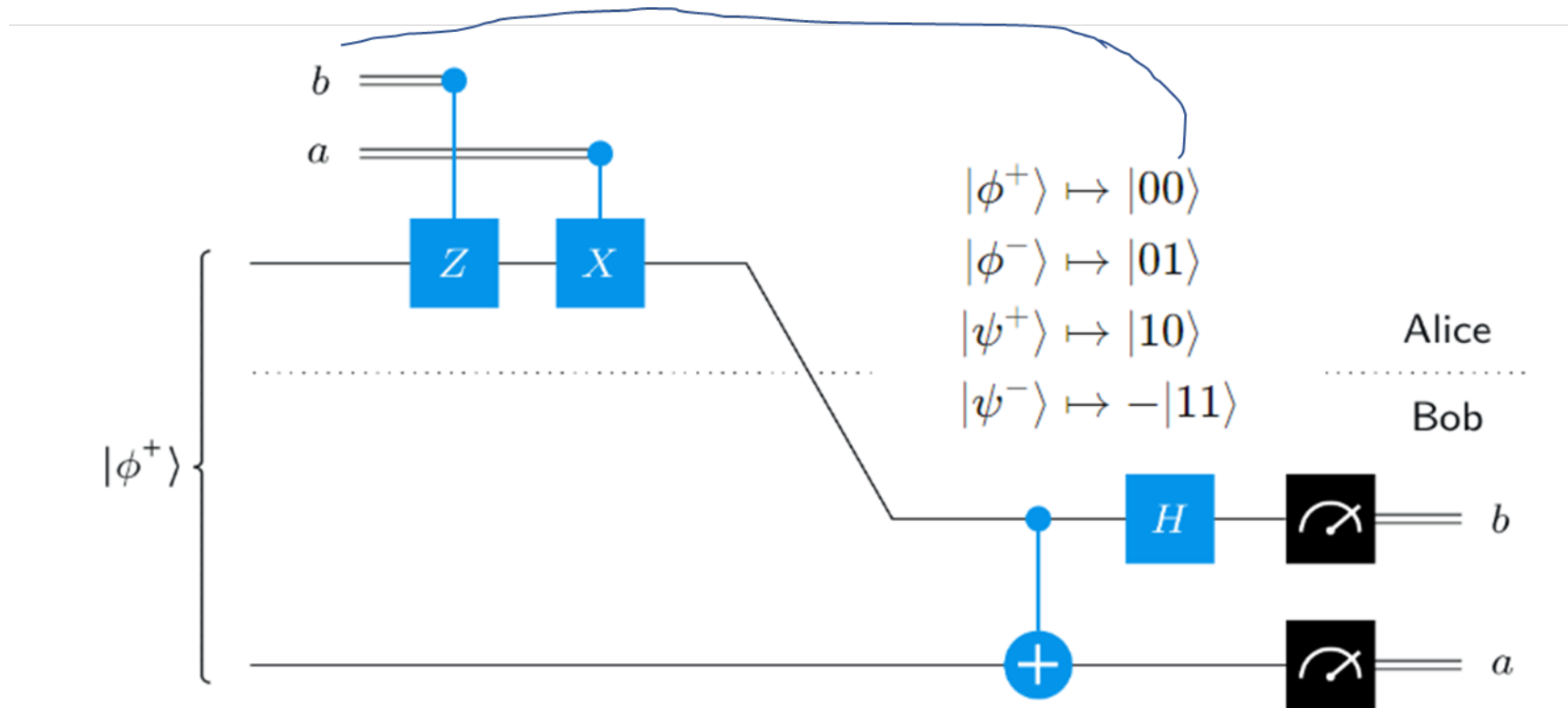
Quantum Algorithms

A tool for developing quantum algorithms for quantum computers or simulators and emulators

- Quantum Phase Kickback
- Grover's Algorithm
- Phase Estimation
- Shor's Algorithm
- Quantum Fourie Transform

Quantum Phase Kickback

Quantum phase kickback is a quantum phenomenon that uses entanglement properties to transfer phase information from a target register to a control qubit. A vital role:

- Grover's Algorithm
- The Phase Estimation
- Shor's Algorithm
- Simon's Algorithm
- Deutsch-Jozsa algorithm
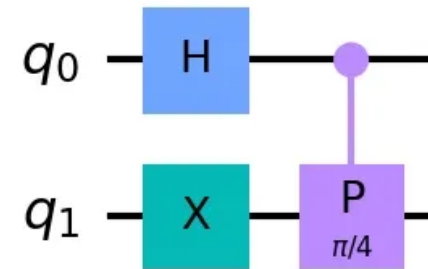
$$\frac{1}{\sqrt{2}}(|01\rangle + e^{i\frac{\pi}{4}}|11\rangle) = \frac{1}{\sqrt{2}}(|0\rangle + e^{i\frac{\pi}{4}}|1\rangle) \otimes |1\rangle$$

Grover's Algorithm

solves one of the complex scenarios in the area of computing. It's the second major algorithm proposed for quantum computing. It solves the problem of searching through unstructured data. (1996)

Quadratical Speed up over classical algorithm
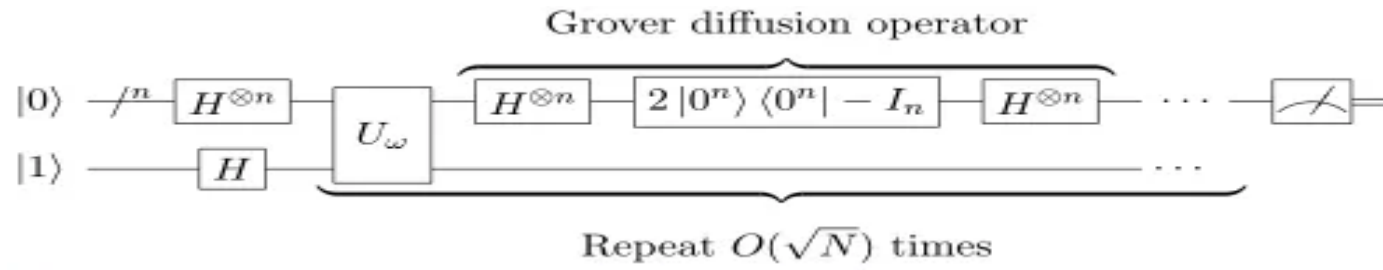
Shor's Algorithm

finding the **prime factors** of an integer (1994)

Exponential Speedup to best known classical algorithm

With sufficient qubits and high quantum coherence, this algorithm can break public-key cryptography

- RSA Scheme

- Diffe-Hellman Key Exchange

- Elliptic Curve Diffie-Hellman Key Exchange

1. turns the factoring problem into the problem of finding the period of a function, and may be implemented classically.

2. finds the period using the quantum Fourier transform, and is responsible for the quantum speedup.
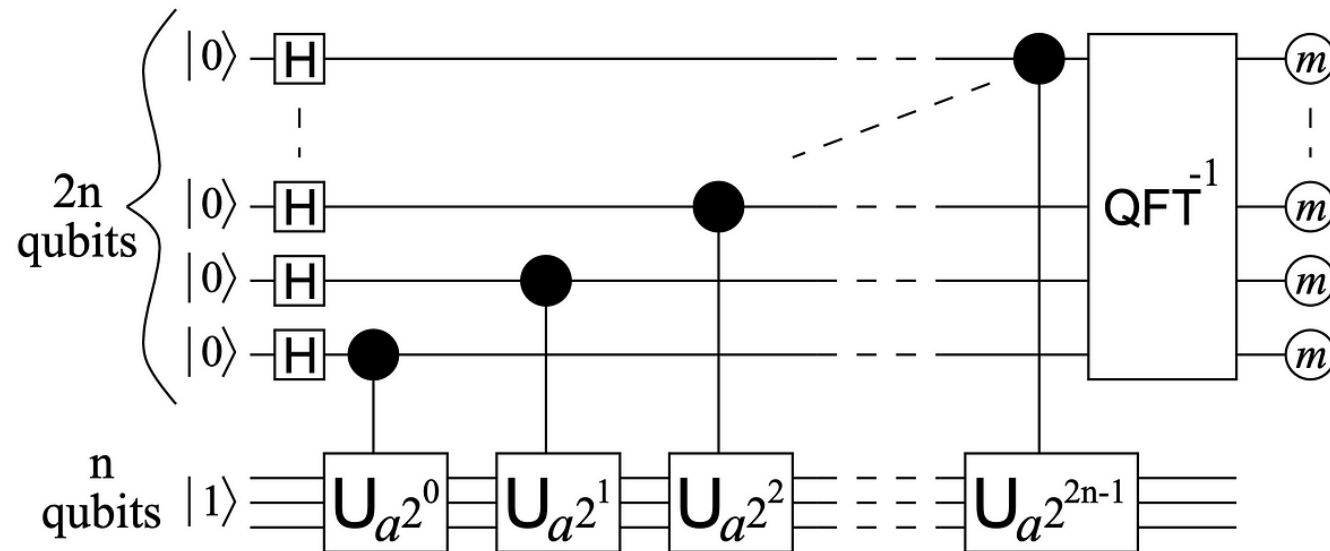
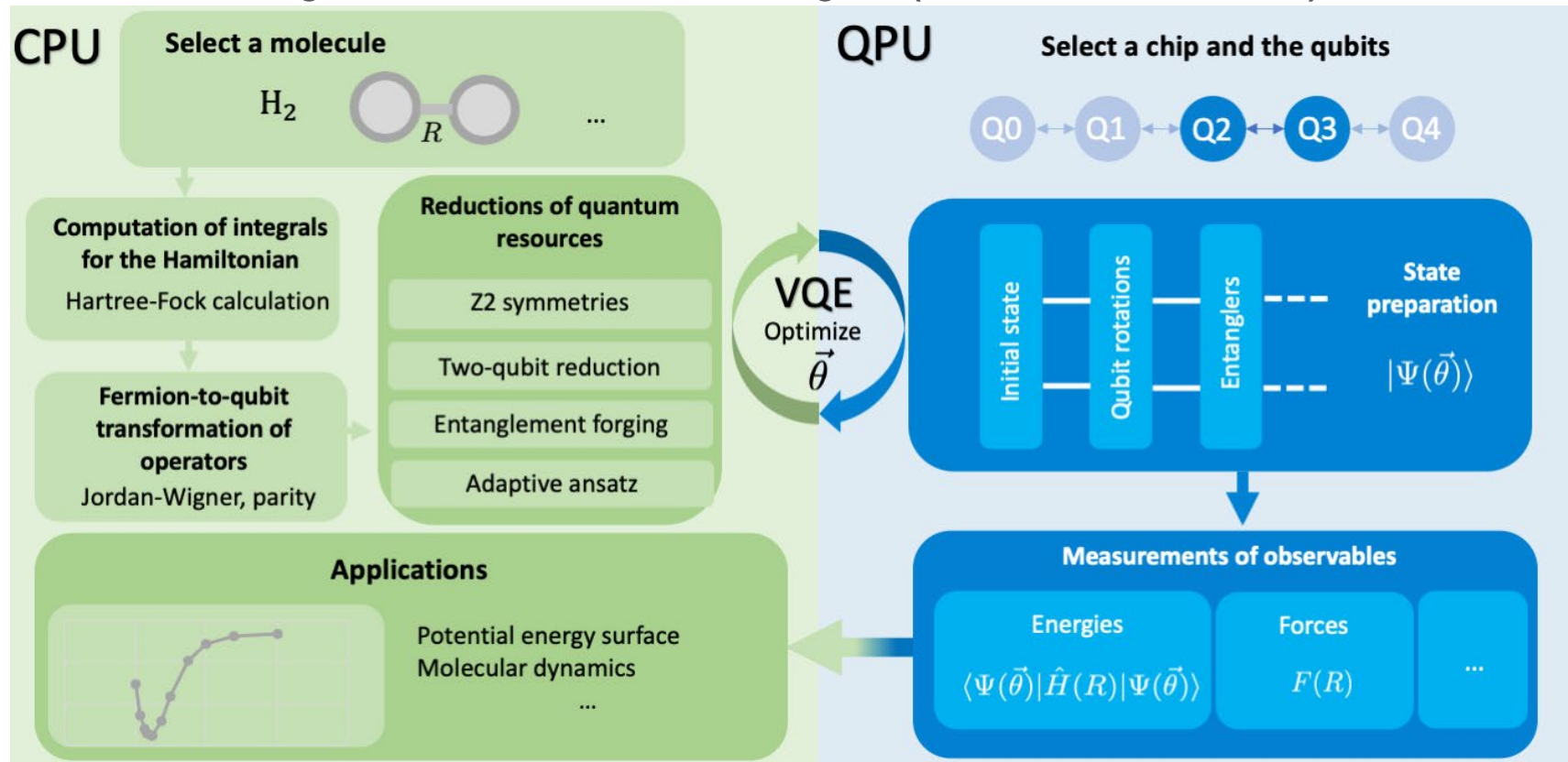# Quantum Speedups in Finance (Price Options)

Traditional Monte Carlo methods generally require extensive computational resources.

Quantum Mechanism: Amplitude Estimation, quadratic speed-up
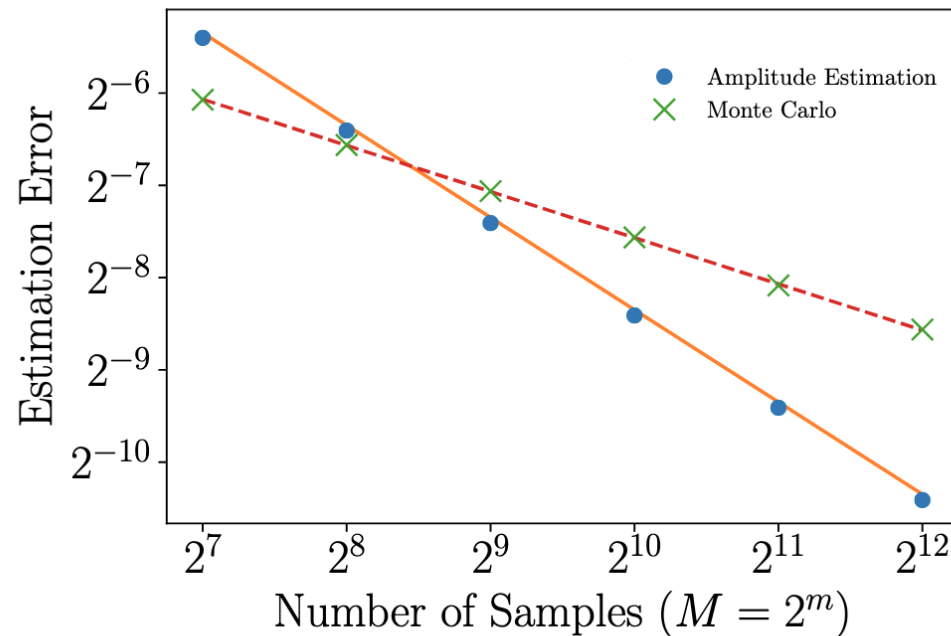
# Quantum Chemistry. Electronic Structure Calculations

Quantum computing holds promise to revolutionize high -performance computing and possesses enormous potential for transforming various fields beyond the current capabilities of classical computing. Quantum Approach: Variational Quantum Eigensolver (VQE) and quantum Equation of Motion to calculate H2O ground and excited state energies (Source: IBM Quantum)
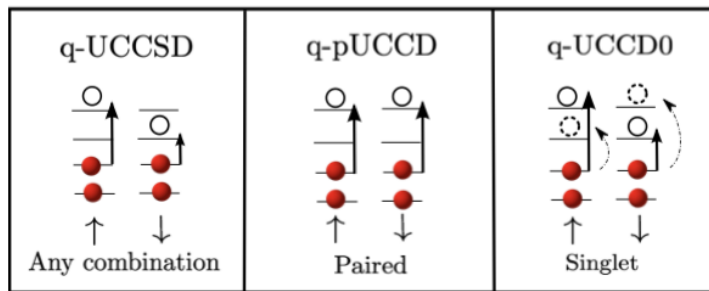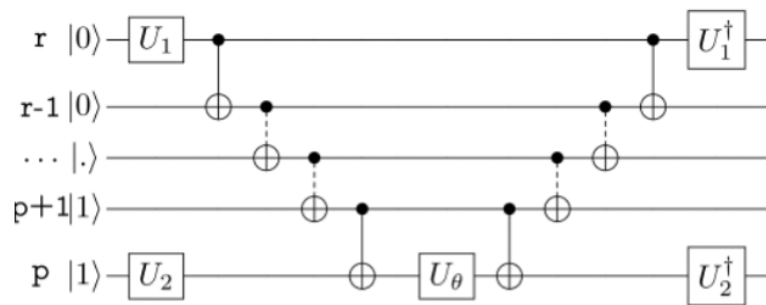
q-UCC ansatze
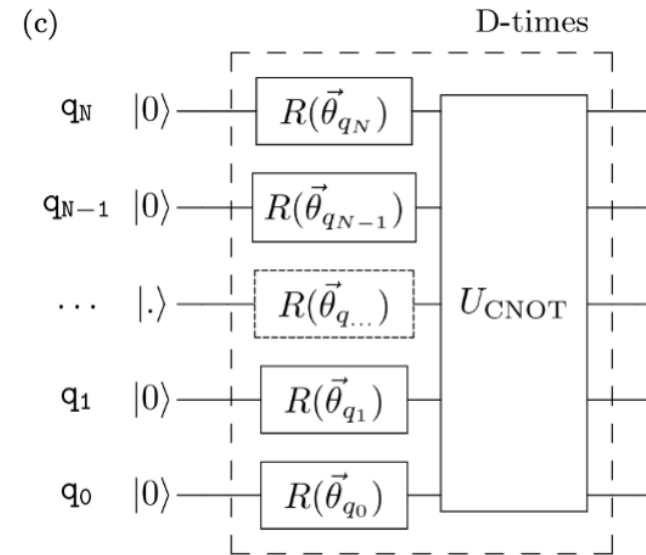
Heuristic (TwoLocal)

Hands-on Quantum Chemistry Simulation

Quantum Chemistry Simulation, adapted from IBM Quantum Challenge Fall 2022
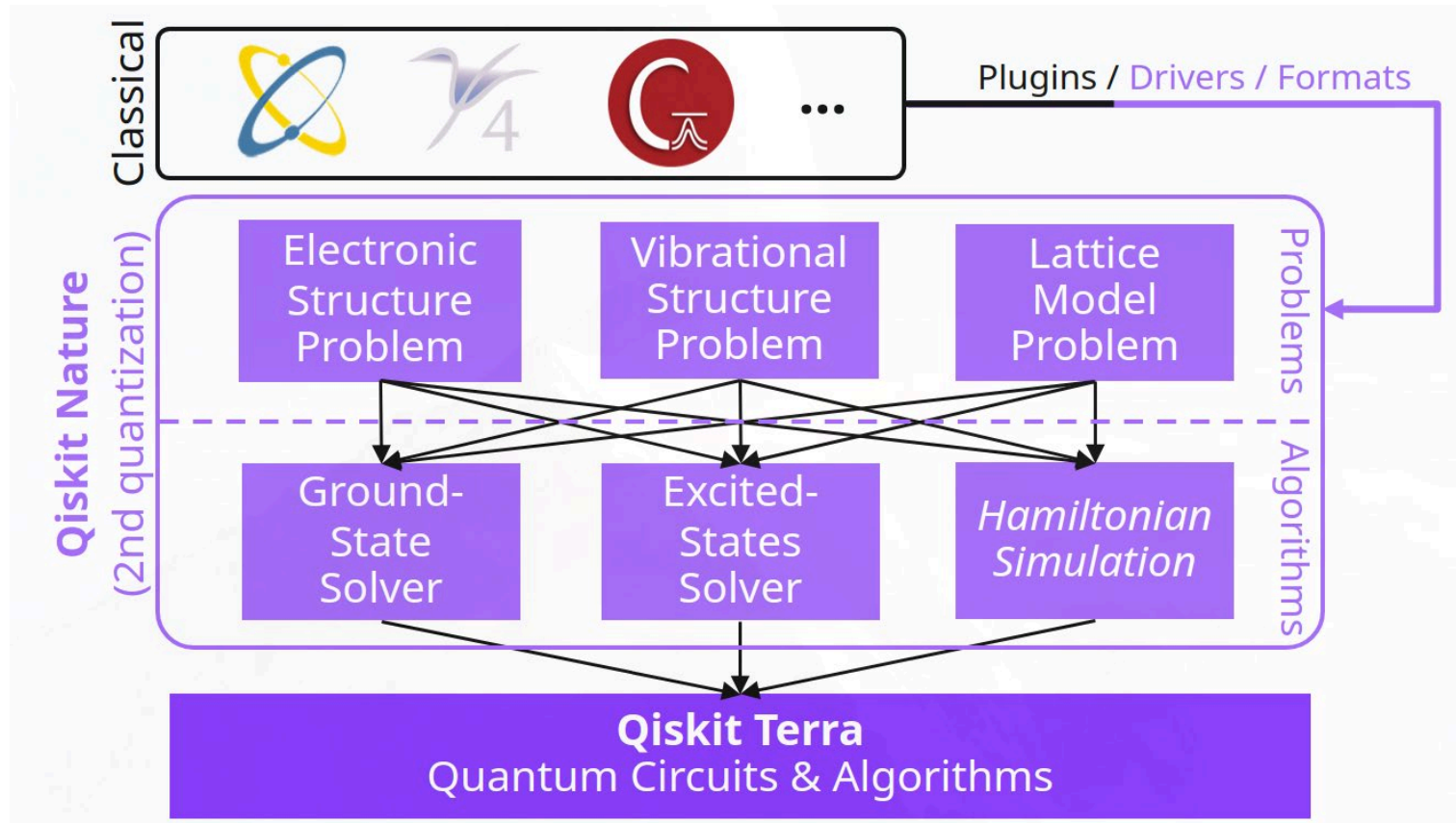
Use Quantum Computers to Explore Interstellar Space!

https://github.com/qiskit -community/ibm -quantum-challenge-fall-22

Quantum Support Vector Classification

A tool for developing quantum algorithms for quantum computers or simulators and emulators

Qiskit Nature is an open-source framework which supports solving quantum mechanical natural science problems using quantum computing algorithms.

source: https://github.com/qiskit -community/qiskit -nature

THANK YOU

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