Introduction to Quantum Computing

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Quantum chemistry and quantum dynamics simulations

During my PhD work: computationally expensive simulations of molecular interactions.

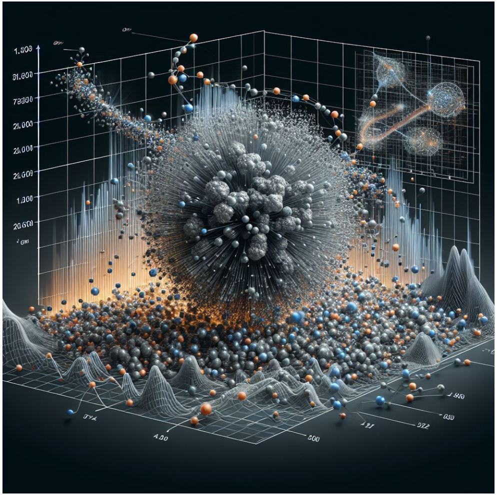


Image credit: Taha Selim, AI-generated image.

How does a quantum computer look like?

How does a quantum computer look like?

Quantum System One, a quantum computer by IBM from 2019 with 20 superconducting qubits

Photo credit: IBM Research

Quantum mechanics and quantum computing

Quantum Computing leverages the principles of quantum mechanics to perform computations:

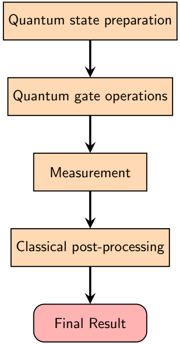
- **Superposition**: a quantum system can exist in multiple states at the same time.
- **Entanglement**: two or more quantum systems can be connected in such a way that the state of one system is dependent on the state of the other system.
- **Quantum interference**: quantum systems can interfere with each other, leading to constructive or destructive interference.
- **Quantum parallelism**: quantum systems can perform multiple computations simultaneously.

Let's learn how to perform computations using quantum computing.

Quantum mechanics and quantum computing

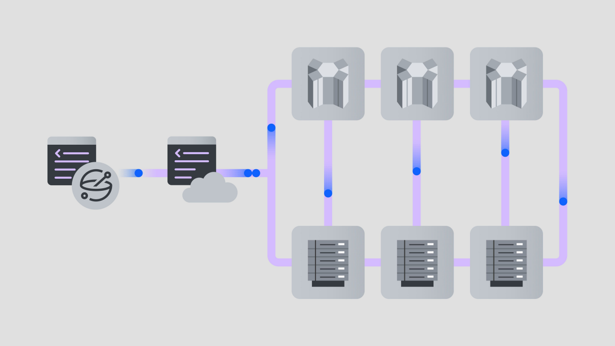
Typically, quantum computers are systems composed, in a nutshell, of:

- A quantum system, register of qubits, that exist in a ground state or specific initial state.
- Operators, quantum gates, that act on the quantum system to perform computations by altering the state of the qubits.
- Measurements, that are performed on the quantum system to obtain the outcome of the computation.
- Post-processing, that is performed on the measurement outcomes to obtain the final result.



Quantum Software Progress: Qiskit Functions

Qiskit Serverless sets the stage for Qiskit Functions in the cloud.



With Qiskit Serverless, users can build, deploy, and run workloads remotely using the compute resources of IBM Quantum™ platform.

Source: IBM Quantum

Demand for Fast Computing

Financial Sector:

- Real-time fraud detection
- High-frequency trading
- Risk assessment and management

Transportation Sector:

- Real-time traffic management
- Autonomous vehicle navigation
- Supply chain optimization

Healthcare Sector:

- Genomic data analysis
- Medical imaging processing
- Drug discovery simulations

Entertainment Sector:

- Real-time rendering and graphics
- Personalized content recommendations
- Virtual and augmented reality applications

Quantum computing vs. classical computing

Let's learn about the action of classical gates on data bits. Data in classical digital computers are in a form of bits, each bit can be in a state of 0 or 1. Basically anything that can be represented as a sequence of bits.

0	1	1	0	1	0	1	0	1	0	1	0	1

Example: ascii text to binary converter (to be checked)

Word	Binary
Hello	01001000 01100101 01101100 01101100 01101111
World	01010111 01101111 01110010 01101100 01100100

Classical gates operate on those bits.

What is a qubit?

A qubit is the basic unit of quantum information.

Qubit is a quantum system that can exist in a superposition of states. Number of states that a qubit can exist in is infinite:

$$|\psi\rangle = \alpha |0\rangle + \beta |1\rangle \,, \text{ where } \alpha, \beta \text{ are complex numbers.}$$

A quantum system of n qubits can exist in a superposition of 2^n states.
Hence, more data can be stored in a quantum system compared to a classical system.

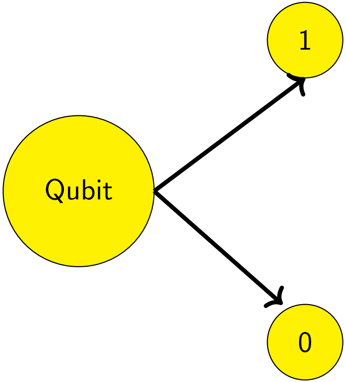
Differences between classical bits and quantum bits:

- **Classical bits**: can be in a state of 0 or 1.
- **Quantum bits**: can be in a superposition of states.
- **Classical gates**: operate on classical bits.
- **Quantum gates**: operate on quantum bits.

- **Classical computers**: use classical bits.
- **Quantum computers**: use quantum bits.
- **Classical algorithms**: operate on classical bits.
- **Quantum algorithms**: operate on quantum bits.

Qubit vs. classical bit

Qubit is a quantum bit.
Classical bit: can be in one of two states: 0 or 1.
Qubit: can be in a superposition of 0 and 1.



Quantum states and their representation

A given state of a quantum system is represented using a function called a wavefunction or a state vector that contains all the information about the quantum system.

- In case of analytical representation, we call it Ψ,
- In case of numerical or vector representation, we call it $|\Psi\rangle$.

Examples,

Analytical representation: $\Psi(x) = A\sin(kx) + B\cos(kx)$, where A and B are constants.

The vector representation: $|\Psi\rangle = \begin{bmatrix} A \\ B \end{bmatrix}$. In this case, $\sin(kx)$ and $\cos(kx)$ are the basis states.

We can write the vector representation as $|\Psi\rangle = A\,|\sin(kx)\rangle + B\,|\cos(kx)\rangle$. This is called the **bra-ket** notation, we will review it in the next slide.

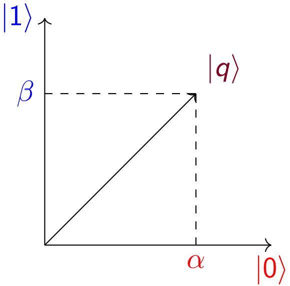
Useful information can be obtained from the wavefunction, such as the probability of finding the quantum system in a specific state.

Representing a qubit state

A qubit is a quantum bit. It is similar to a classical bit, but it can be in a superposition of states.

In analogy to vectors, we can write the wavefunction as a ket $|q\rangle$:

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



In a vector notation:

$|q\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$, where α and β are complex coefficients,

and

$\alpha|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\alpha|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, normalization: $|\alpha|^2 + |\beta|^2 = 1$.

Probability of finding an outcome during measurements

Amplitudes give the probability of finding the system in a given state when performing a measurement.

The probability of finding the system in state $|0\rangle$ is $|\alpha|^2$, and the probability of finding the system in state $|1\rangle$ is $|\beta|^2$.

The sum of the probabilities of finding the system in the two states must be equal to 1.

Hence,

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

Examples:

Question: Find the probability of finding the system in state $|0\rangle$ if the state of the system is given by $|q\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle$.

Solution:
The probability of finding the system in state $|0\rangle$ is $|\frac{1}{\sqrt{2}}|^2 = \frac{1}{2}$.

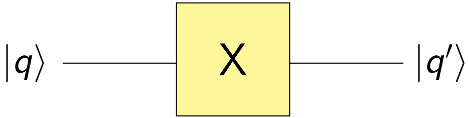
Question: Check whether the state $|q\rangle = \frac{1}{\sqrt{3}}|0\rangle + \frac{2}{\sqrt{3}}|1\rangle$ is normalized.

Solution:
Applying the normalization condition, we have $|\frac{1}{\sqrt{3}}|^2 + |\frac{2}{\sqrt{3}}|^2 = 1$.
Hence, the state is normalized.

Operations on qubits with quantum gates

We can also represent the action of a quantum gate on a qubit graphically.

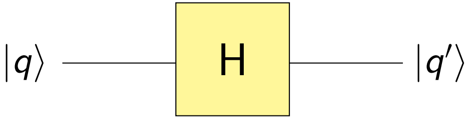
The action of the X-gate on the qubit $|0\rangle$ is represented as:



From the action of the gate, the truth table for the X-gate is:

Input	**Output**
$\vert 0\rangle$	$\vert 1\rangle$
$\vert 1\rangle$	$\vert 0\rangle$

Similarly, the action of the H-gate on the qubit $|0\rangle$ is represented as:



From the action of the gate, the truth table for the H-gate is:

Input	**Output**
$\vert 0\rangle$	$\frac{1}{\sqrt{2}}(\vert 0\rangle + \vert 1\rangle)$
$\vert 1\rangle$	$\frac{1}{\sqrt{2}}(\vert 0\rangle - \vert 1\rangle)$

Quantum circuits

A quantum circuit is typically composed of:

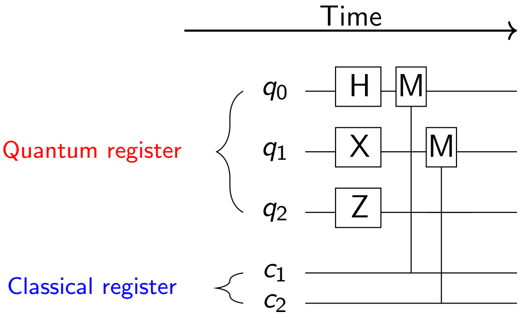
1. quantum register: ollection/stack of qubits.
2. Classical register: collection of classical bits,
3. Quantum gates: operations that act on qubits.
4. Quantum gates are arranged in a particular order/sequence to perform a specific task, a certain computation.

Quantum register: $q_0, q_1, q_2, \cdots$

Classical register: $c_0, c_1, c_2, \cdots$

Quantum gates: $H, X, Z, \cdots$

Measurement gates: M

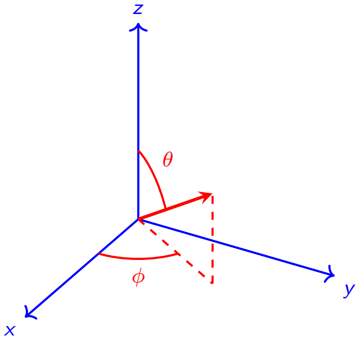


Qubit state representation on a Bloch sphere

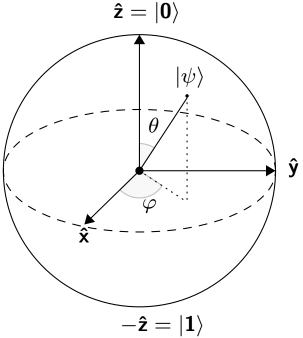
Block sphere is a geometrical representation of the state of a qubit with the aid of the Bloch vector and spherical coordinates.

The Bloch sphere is a unit sphere with radius 1, where the north pole represents the state $|0\rangle$ and the south pole represents the state $|1\rangle$.

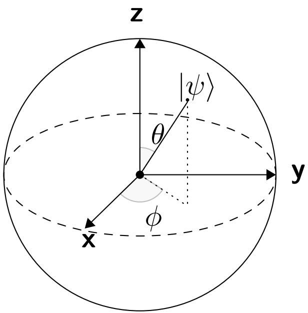
Spherical coordinates are given by $x = \sin(\theta)\cos(\phi)$, $y = \sin(\theta)\sin(\phi)$, and $z = \cos(\theta)$.



The Bloch sphere representation of a qubit state $|q\rangle$ is given by the Bloch vector $\vec{r} = (x, y, z)$.
where θ is the polar angle and ϕ is the azimuthal angle.



Qubit state representation on a Bloch sphere



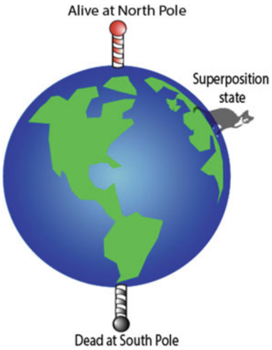
- The spherical coordinates are (r, θ, ϕ).
- The unit sphere is defined by the equation $x^2 + y^2 + z^2 = 1$.
- Spherical coordinates are related to the Cartesian coordinates by the following equations:

$$x = r\sin(\theta)\cos(\phi)$$
$$y = r\sin(\theta)\sin(\phi)$$
$$z = r\cos(\theta)$$

Schrödinger's cat on a Blochsphere

Schrödinger's cat is determined to be alive.What location on the Earth in the figure could the cat have been before the quantum measurement?

1. Russia.
2. North Pole.
3. Australia.
4. All the above.



Question source: Hughes et al. (2021), Springer. Quantum Computing for the Quantum Curious.

Blochsphere

The state of a qubit can be represented by a point on the Blochsphere.
This point is defined by the spherical coordinates (θ, ϕ).
It also gives us an idea about the superposition of the qubit.

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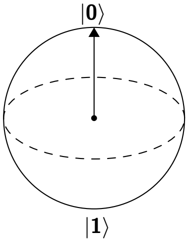

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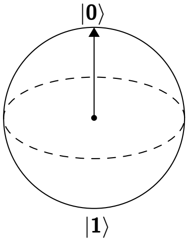

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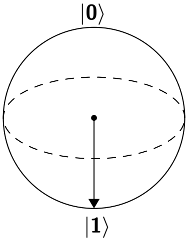

$|\psi\rangle = |1\rangle$

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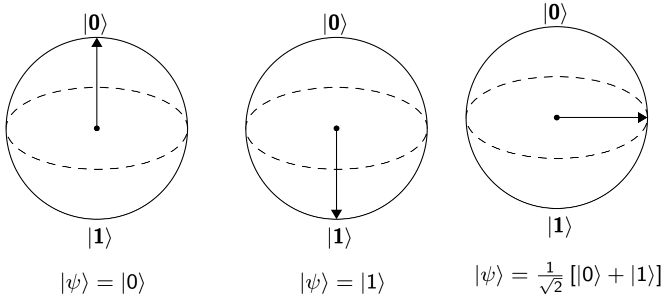

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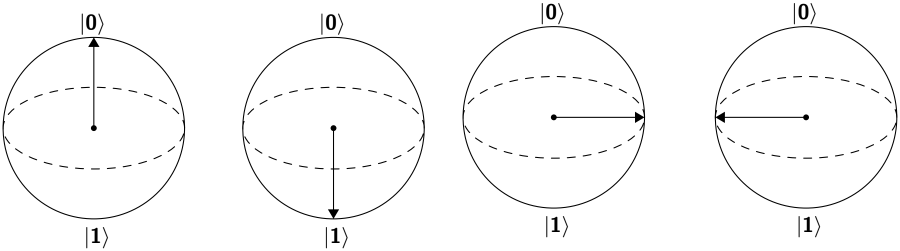

$|\psi\rangle = |0\rangle$ $\quad$ $|\psi\rangle = |1\rangle$ $\quad$ $|\psi\rangle = \frac{1}{\sqrt{2}}\left[|0\rangle + |1\rangle\right]$ $\quad$ $|\psi\rangle = \frac{1}{\sqrt{2}}\left[|0\rangle - |1\rangle\right]$

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Applications

Let's have a look on IBM quantum composer platform:

`https://quantum.cloud.ibm.com/composer`

Programming a quantum computer

Let's do some quantum coding!