

Quantum computing fundamentals: State, Composition, Dynamics

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The opportunities in quantum computing

Killer apps

- ▶ Factoring
- ▶ Search
- ▶ Optimization
- ▶ Chemistry

Chemistry

- ▶ A molecule: has n electrons that represent n electrons
- ▶ Classical computer: $O(k^n)$ bits to represent n electrons
- ▶ Quantum computer: $O(n^p)$ qubits to represent n electrons

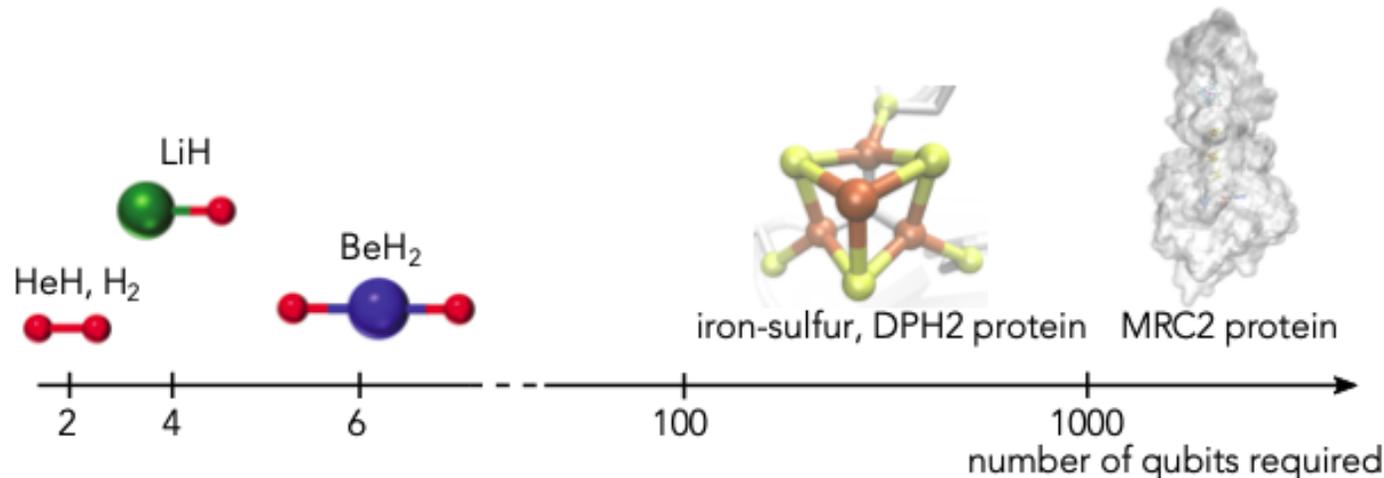


Figure: Credit: Moll et al. Quantum optimization using variational algorithms on near-term quantum devices

A simple physics experiment that classical computing cannot replicate

Algorithm

David Deutsch and Richard Jozsa. Rapid solution of problems by quantum computation. 1992.

Implementation

- ▶ Mach-Zehnder interferometer implementation.

`https://www.st-andrews.ac.uk/physics/quvis/simulations_html5/sims/SinglePhotonLab/SinglePhotonLab.html`

Mathematical description of the algorithm

$$|0\rangle \xrightarrow{H} |+\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \left\{ \begin{array}{ll} I \rightarrow |+\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} & \xrightarrow{H} |0\rangle \\ Z \rightarrow |-\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{bmatrix} & \xrightarrow{H} |1\rangle \\ -Z \rightarrow -|-\rangle = \begin{bmatrix} \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} & \xrightarrow{H} -|1\rangle \\ -ZZ=-I \rightarrow -|+\rangle = \begin{bmatrix} \frac{-1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{bmatrix} & \xrightarrow{H} -|0\rangle \end{array} \right.$$

QC current status: Verge of quantum advantage & quantum utility?

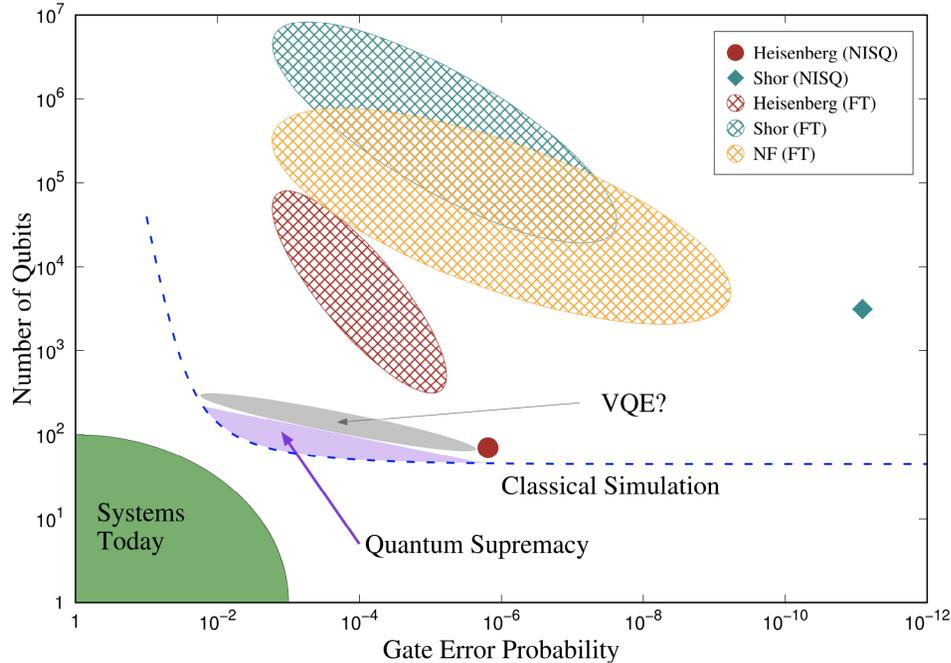


Figure: Credit: Maslov, Nam, and Kim. An Outlook for Quantum Computing. Proceedings of the IEEE. 2019.

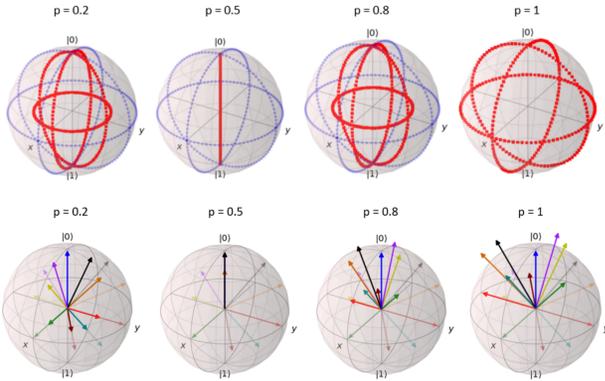
Fig. 2. Performance space of quantum computers, measured by the error probability of each entangling gate in the horizontal axis (roughly inversely proportional to the total number of gates that can be executed on a NISQ machine), and the number of qubits in the system in the vertical axis. Blue dotted line approximately demarcates quantum systems that can be simulated using best classical computers, while the green colored region shows where the existing quantum computing systems with verified performance numbers lie (as of September 2018). Purple shaded region indicates computational tasks that accomplish the so-called “quantum supremacy,” where the computation carried out by the quantum computer defies classical simulation regardless of its usefulness. The different shapes illustrate resource counts for solving various problems, with solid symbols corresponding to the exact entangling gate counts and number of qubits in NISQ machines, and shaded regions showing approximate gate error requirements and number of qubits for an FT implementation (not pictured are the regions where the error gets too close to the known fault-tolerance thresholds): cyan diamond and shaded region correspond to factoring a 1024-bit number using Shor’s algorithm [14], magenta circle and shaded region represent simulation of a 72-spin Heisenberg model [20], and orange shaded region illustrates NF simulation [21].

Quantum computer building blocks are unreliable

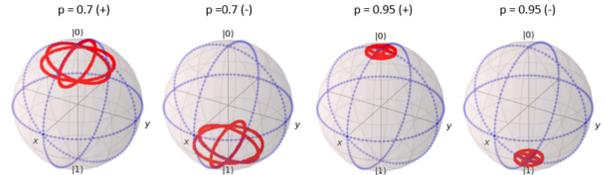
Quantum circuits are an ideal abstraction with simple rules, except:

- ▶ Depolarizing noise (not ideal, but fortunately uniform).
- ▶ Bit flip and phase flip noise (not uniform, but fortunately balanced).
- ▶ Amplitude and phase damping noise (not balanced, but fortunately contained).
- ▶ Leakage noise (not contained, but fortunately independent).
- ▶ Correlated noise (not independent?!).

4. Phase Damping Channel



5. Amplitude Damping Channel



Need many building blocks to create error correction codes

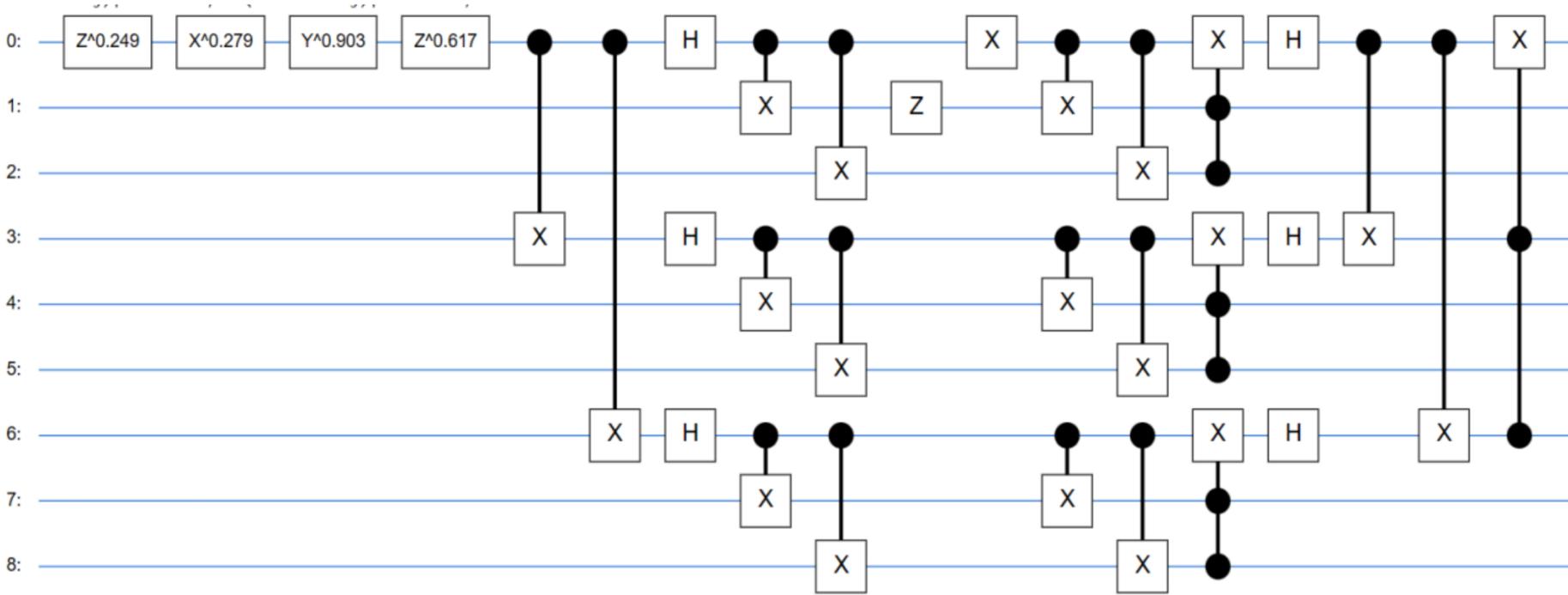


Figure 3.1: Example circuit from our implementation

Quantum computer state quickly exceeds classical simulation

Why is simulating quantum computing hard?

$d \backslash n$	2	4	8	16
2	128 B	2 kB	512 kB	32 GB
3	648 B	51.26 kB	328.42 MB	13.17 PB
5	4.88 kB	2.98 MB	1.11 TB	157.77 ZB
7	51.26 kB	328.42 MB	241.8 TB	7.14 RB

Figure 1: RAM for single precision $d^n \times d^n$ matrix ($2 \cdot 4d^{2n}$ bytes)

Figure: Memory footprint

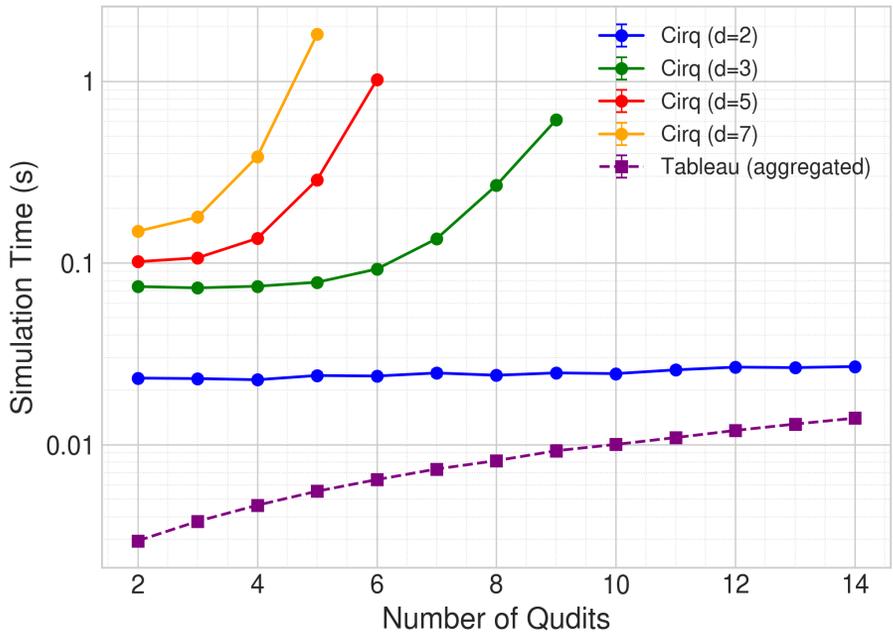


Figure: Compute time

QC current status: Verge of quantum advantage & quantum utility?

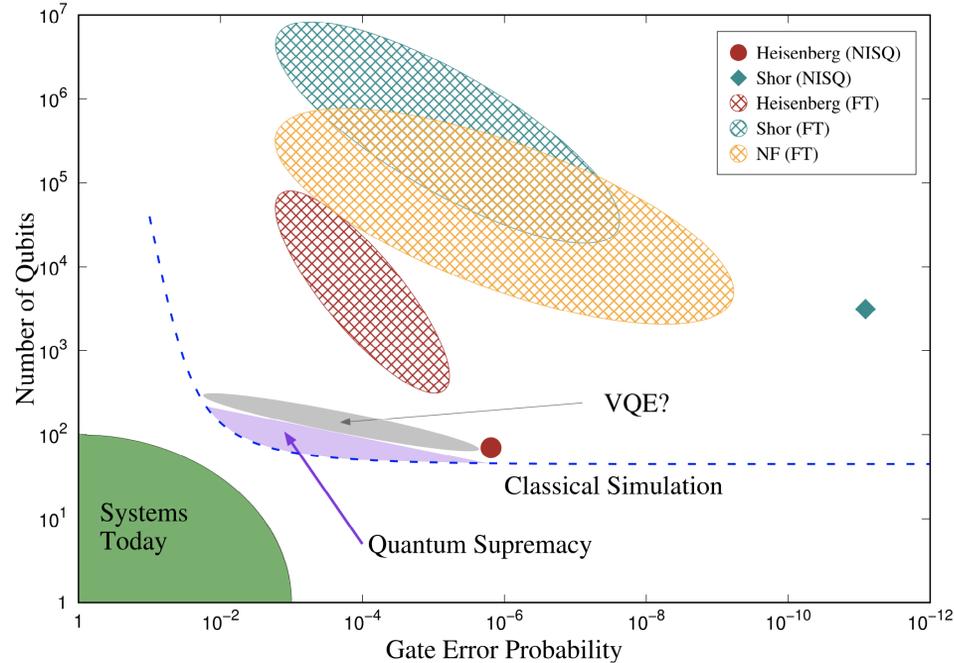


Figure: Credit: Maslov, Nam, and Kim. An Outlook for Quantum Computing. Proceedings of the IEEE. 2019.

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The state of a single qubit

Superposition

Bloch sphere

The state of multiple qubits

Tensor product

Entanglement

No-cloning theorem

The evolution of qubit states

Postulates of quantum mechanics

1. State space
2. Composite systems
3. Evolution
4. Quantum measurement

1, 2, and 3 are linear and describe closed quantum systems. 4 is nonlinear and describes open quantum systems.

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Quantum postulate 1: State space

The position or momentum of a physical system is described as a wavefunction

- ▶ Assuming continuous state space:

$$|\psi\rangle = \int_{-\infty}^{\infty} \psi(x) |x\rangle dx$$
$$|x\rangle$$

are orthonormal

$$\psi(x) \in \mathbb{C}$$

- ▶ Assuming discrete state space:

$$|\psi\rangle = \sum_{i=0}^{\infty} \psi(x_i) |x_i\rangle$$

$$\psi(x) \in \mathbb{C}$$

Quantum postulate 1: State space

The position or momentum of a physical system is described as a wavefunction

- ▶ Assuming discrete state space:

$$|\psi\rangle = \sum_{i=0}^{\infty} \psi(x_i) |x_i\rangle$$

$$\psi(x) \in \mathbb{C}$$

- ▶ Assuming discrete binarized state space:

$$|\psi\rangle = \sum_{i=0}^1 \psi(x_i) |x_i\rangle$$

$$\psi(x) \in \mathbb{C}$$

The binary abstraction

High, low voltage

Adds resilience against noise.

Representation as a state vector

- ▶ $\begin{bmatrix} 1 \\ 0 \end{bmatrix} = |0\rangle$ We pronounce this "ket" 0
- ▶ $\begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle$ We pronounce this "ket" 1

The NOT gate

Matrix representation of NOT operator: $X = \sigma_X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

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

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

Circuit diagram representation:

The Hadamard gate

Matrix representation of Hadamard operator: $H = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}$

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

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

Circuit diagram representation:

Interference

Amplitudes can positively and negatively interfere

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

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

Circuit diagram representation:

Superposition

Single qubit state

- ▶ $\alpha |0\rangle + \beta |1\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$
- ▶ Amplitudes $\alpha, \beta \in \mathbb{C}$
- ▶ $|\alpha|^2 + |\beta|^2 = 1$
- ▶ The above constraints require that qubit operators are unitary matrices.

Many physical phenomena can be in superposition and encode qubits

- ▶ Polarization of light in different directions
- ▶ Electron spins (Intel solid state qubits)
- ▶ Atom energy states (UMD, IonQ ion trap qubits)
- ▶ Quantized voltage and current (IBM, Google superconducting qubits)

If multiple discrete values are possible (e.g., atom energy states, voltage and current), we pick (bottom) two for the binary abstraction.

Bloch sphere

Representation of pure states of a single qubit

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

- ▶ θ polar angle
- ▶ ϕ azimuthal angle

Euler's formula

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

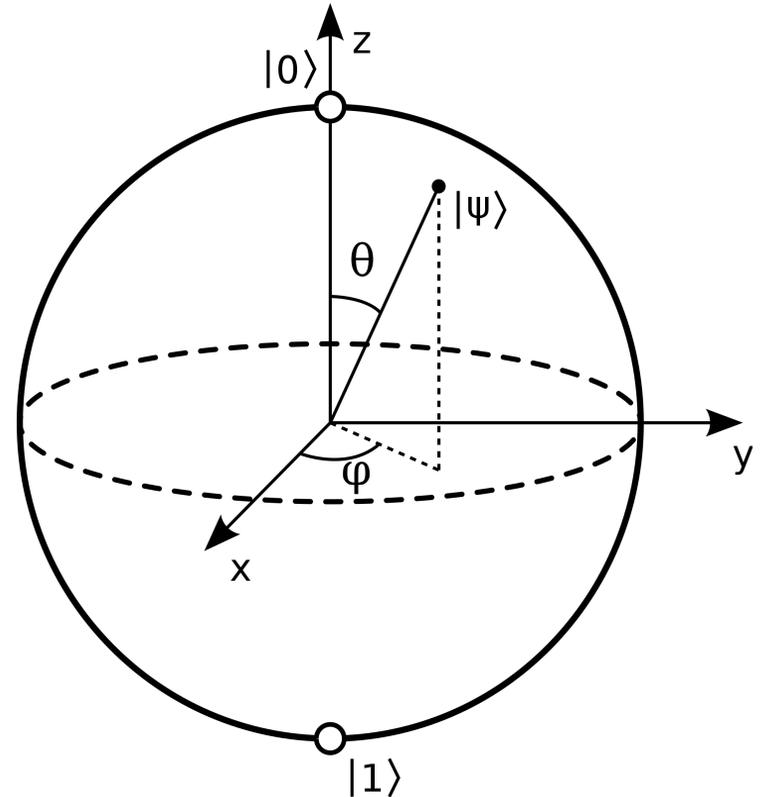


Figure: Source: Wikimedia

Bloch sphere

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

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

Important locations on the Bloch sphere

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

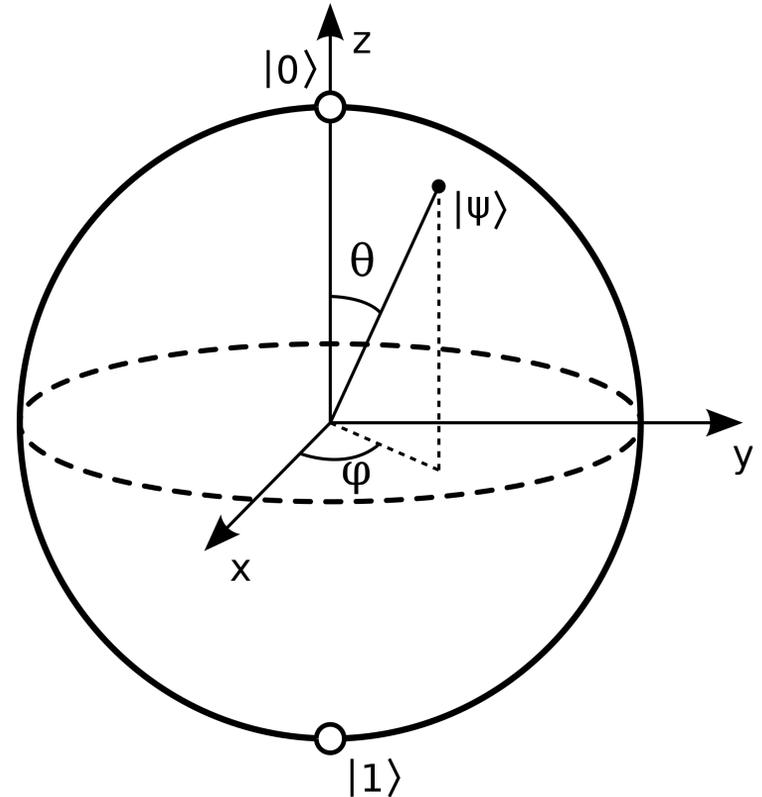


Figure: Source: Wikimedia

Bloch sphere

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

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

Rotations around the Bloch sphere



$$R_x(\theta) = \cos\frac{\theta}{2} I - i\sin\frac{\theta}{2} X$$



$$R_y(\theta) = \cos\frac{\theta}{2} I - i\sin\frac{\theta}{2} Y$$



$$R_z(\theta) = \cos\frac{\theta}{2} I - i\sin\frac{\theta}{2} Z$$

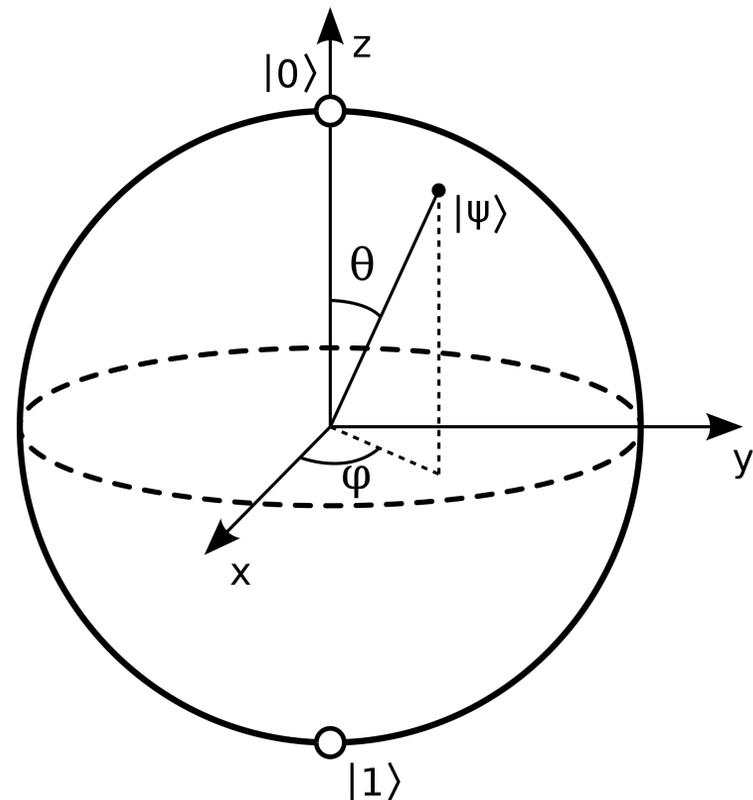


Figure: Source: Wikimedia

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Quantum postulate 2: Composite systems

The state space of composite systems is the tensor product of state space of component systems.

Multiple qubits: the tensor product

Tensor product (also known as Kronecker product) of state vectors

$$|+\rangle \otimes |-\rangle = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ 1 \\ \frac{1}{\sqrt{2}} \end{bmatrix} \otimes \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -1 \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -1 \\ \frac{1}{\sqrt{2}} \end{bmatrix} \\ \frac{1}{\sqrt{2}} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -1 \\ \frac{1}{\sqrt{2}} \end{bmatrix} \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ -\frac{1}{2} \\ \frac{1}{2} \\ -\frac{1}{2} \end{bmatrix} = \frac{1}{2} |00\rangle - \frac{1}{2} |01\rangle + \frac{1}{2} |10\rangle - \frac{1}{2} |11\rangle$$

Multiple qubits: the tensor product

Tensor product of unitary matrices

$$X \otimes I \left(\frac{1}{\sqrt{2}} |01\rangle + \frac{1}{\sqrt{2}} |11\rangle \right) = \left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \right) \begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} =$$
$$\begin{bmatrix} 0 & \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\ 1 & \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \end{bmatrix} \begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{\sqrt{2}} |01\rangle + \frac{1}{\sqrt{2}} |11\rangle$$

Circuit diagram representation:

Multiple qubits: the tensor product

Tensor product of state vectors

$$X\left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right) \otimes I|1\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \otimes \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \otimes \begin{bmatrix} 0 \\ 1 \end{bmatrix} =$$
$$\begin{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\ \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{\sqrt{2}}|01\rangle + \frac{1}{\sqrt{2}}|11\rangle$$

Circuit diagram representation:

Multiple qubits: the tensor product

Exercise: proof by induction about the Hadamard transform

Show that $|+\rangle^{\otimes n} = \frac{1}{2^{n/2}} \sum_{m=0}^{2^n-1} |m\rangle$

Entangled states: Bell state circuit

Bell state circuit

$$|00\rangle \xrightarrow{H \otimes I} \frac{1}{\sqrt{2}} \left(|00\rangle + |10\rangle \right) \xrightarrow{CNOT} \frac{1}{\sqrt{2}} \left(|00\rangle + |11\rangle \right) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix} = |\Phi^+\rangle$$

Can $|\Phi^+\rangle$ be treated as the tensor product (composition) of two individual qubits?

Prove that the Bell state cannot be factored into two single-qubit states

Bell state circuit

$$|00\rangle \xrightarrow{H \otimes I} \frac{1}{\sqrt{2}} \left(|00\rangle + |10\rangle \right) \xrightarrow{CNOT} \frac{1}{\sqrt{2}} \left(|00\rangle + |11\rangle \right) = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix} = |\Phi^+\rangle$$

Can $|\Phi^+\rangle$ be treated as the tensor product (composition) of two individual qubits?

No.

Bell states form an orthogonal basis set

1. $|00\rangle \xrightarrow{H \otimes I} \frac{1}{\sqrt{2}} \left(|00\rangle + |10\rangle \right) \xrightarrow{CNOT} \frac{1}{\sqrt{2}} \left(|00\rangle + |11\rangle \right) = |\Phi^+\rangle$
2. $|01\rangle \xrightarrow{H \otimes I} \frac{1}{\sqrt{2}} \left(|01\rangle + |11\rangle \right) \xrightarrow{CNOT} \frac{1}{\sqrt{2}} \left(|01\rangle + |10\rangle \right) = |\Psi^+\rangle$
3. $|10\rangle \xrightarrow{H \otimes I} \frac{1}{\sqrt{2}} \left(|00\rangle - |10\rangle \right) \xrightarrow{CNOT} \frac{1}{\sqrt{2}} \left(|00\rangle - |11\rangle \right) = |\Phi^-\rangle$
4. $|11\rangle \xrightarrow{H \otimes I} \frac{1}{\sqrt{2}} \left(|01\rangle - |11\rangle \right) \xrightarrow{CNOT} \frac{1}{\sqrt{2}} \left(|01\rangle - |10\rangle \right) = |\Psi^-\rangle$

No-cloning theorem

There is no way to duplicate an arbitrary quantum state

Suppose a cloning operation U_c exists. Then:



$$U_c(|\phi\rangle \otimes |\omega\rangle) = |\phi\rangle \otimes |\phi\rangle,$$

$$U_c(|\psi\rangle \otimes |\omega\rangle) = |\psi\rangle \otimes |\psi\rangle,$$

for arbitrary states $|\phi\rangle, |\psi\rangle$ we wish to copy.

▶ The overlap of the initial states is:

$$\langle\phi| \otimes \langle\omega| |\psi\rangle \otimes |\omega\rangle = \langle\phi| |\psi\rangle \cdot \langle\omega| |\omega\rangle = \langle\phi| |\psi\rangle$$

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for arbitrary states $|\phi\rangle, |\psi\rangle$ we wish to copy.

▶ The overlap of the final states is:

$$\langle\phi| \otimes \langle\phi| |\psi\rangle \otimes |\psi\rangle = \langle\phi| |\psi\rangle \cdot \langle\phi| |\psi\rangle = (\langle\phi| |\psi\rangle)^2$$

▶ The overlap of the final states is also:

$$\langle\phi| \otimes \langle\phi| |\psi\rangle \otimes |\psi\rangle = \langle\phi| \otimes \langle\omega| U^\dagger U |\psi\rangle \otimes |\omega\rangle = \langle\phi| \otimes \langle\omega| |\psi\rangle \otimes |\omega\rangle = \langle\phi| |\psi\rangle$$

▶ $(\langle\phi| |\psi\rangle)^2 = \langle\phi| |\psi\rangle$, so $\langle\phi| |\psi\rangle = 0$, or $\langle\phi| |\psi\rangle = 1$, $|\phi\rangle$ and $|\psi\rangle$ cannot be arbitrary states as claimed.

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Quantum postulate 3: Evolution

The time evolution of a state follows the Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle$$

- ▶ Comes from the conservation of total energy in the closed system, one of the observables from the system state.
- ▶ Itself reflects a time-invariance.

$$\frac{\partial}{\partial t} |\psi(t)\rangle = \frac{-iH}{\hbar} |\psi(t)\rangle$$

$$|\psi(t)\rangle = e^{\frac{-iH}{\hbar} t} |\psi(0)\rangle$$

Quantum postulate 3: Evolution

The evolution of a closed quantum system is a unitary transformation.

$$|\psi(t = t_1)\rangle = U |\psi(t = t_0)\rangle$$

- ▶ $|\psi_1\rangle = U |\psi_0\rangle$
- ▶ In a closed quantum system, $\langle\psi_1| |\psi_1\rangle = \langle\psi_0| U^\dagger U |\psi_0\rangle = \langle\psi_0| |\psi_0\rangle = 1$
- ▶ $U^\dagger U = I, U^\dagger = U^{-1}$; Such matrices U are unitary

Quantum postulate 3: Evolution

From unitary transformations we can show Hamiltonians in closed quantum systems must be hermitian

- ▶ $U |\psi\rangle = e^{\frac{-iH}{\hbar}} |\psi\rangle$
- ▶ $U^\dagger |\psi\rangle = e^{\frac{-(iH)^\dagger}{\hbar}} |\psi\rangle$
- ▶ $U^\dagger |\psi\rangle = U^{-1} |\psi\rangle = e^{\frac{iH}{\hbar}} |\psi\rangle$
- ▶ $(iH)^\dagger = -iH$, $A = iH$; such matrices A are called anti-Hermitian a.k.a. skew-Hermitian
- ▶ If iH is skew-Hermitian, H is Hermitian a.k.a. self-adjoint: $H^\dagger = H$