Quantum computing fundamentals: Composition, Dynamics

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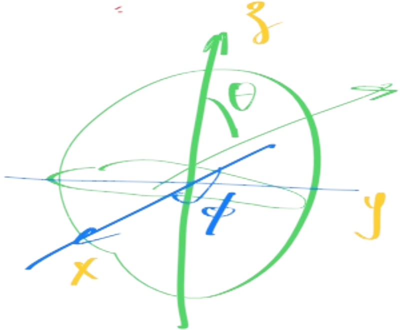
$$|\psi\rangle = e^{i\gamma}\left(\cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle\right)$$

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

$$|e^{i\gamma}| = 1$$



Postulates of quantum mechanics

closed
$|\psi\rangle$

environment
bath

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 2: Composite systems

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

Multiple qubits: the tensor product

$$|+\rangle \otimes |1\rangle = \left(\frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|1\rangle\right) \otimes |1\rangle = \frac{1}{\sqrt{2}}|01\rangle + \frac{1}{\sqrt{2}}|11\rangle$$

Tensor product of unitary matrices

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

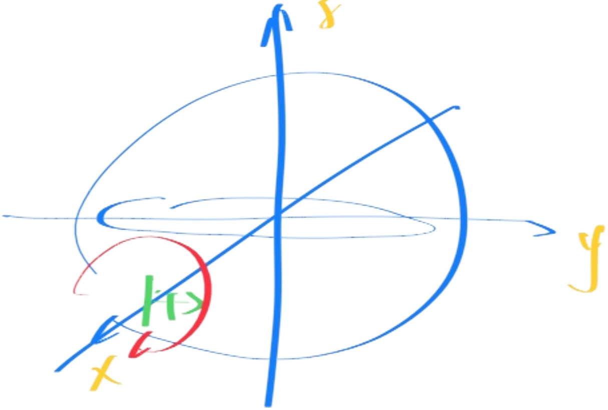
$$\begin{bmatrix} 0\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & 1\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \\ 1\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} & 0\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \end{bmatrix}\begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{\sqrt{2}}|01\rangle + \frac{1}{\sqrt{2}}|11\rangle$$

Circuit diagram representation:

$$X|+\rangle = |+\rangle$$

$$X|+\rangle$$

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



$$X = R_x(\pi)$$

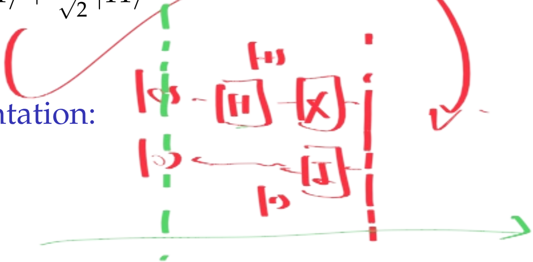
Multiple qubits: the tensor product

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:



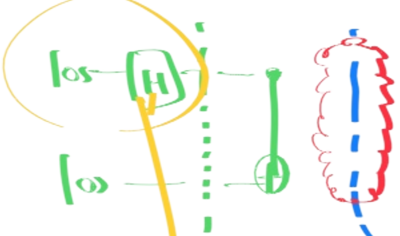
The CNOT gate

Matrix representation of CNOT operator: $\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

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

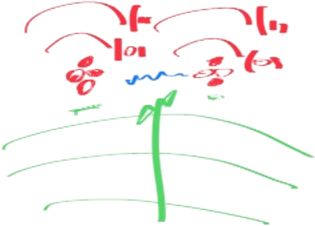
$|00\rangle \to |00\rangle$
$|01\rangle \to |01\rangle$
$|10\rangle \to |11\rangle$
$|11\rangle \to |10\rangle$

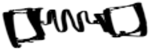
Circuit diagram representation:



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

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





state

dynamics

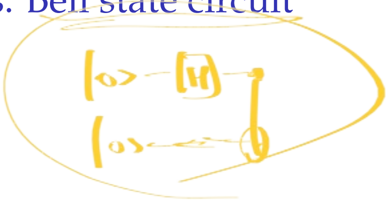
composition

$$\frac{1}{\sqrt{2}}|00\rangle + \frac{1}{\sqrt{2}}|11\rangle = |a\rangle \otimes |b\rangle$$

$$= (\alpha|0\rangle + \beta|1\rangle) \otimes (\gamma|0\rangle + \delta|1\rangle)$$

$$= \alpha\gamma|00\rangle + \alpha\delta|01\rangle + \beta\gamma|10\rangle + \beta\delta|1$$

Entangled states: Bell state circuit



Bell state circuit

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

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

no

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

Bell state circuit

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

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

No.

Bell states form an orthogonal basis set

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

$|\Phi^+\rangle \cdot |\Psi^+\rangle$

$= \underbrace{\langle\Psi^+|\Phi^+\rangle}_{\text{bra ket}}$

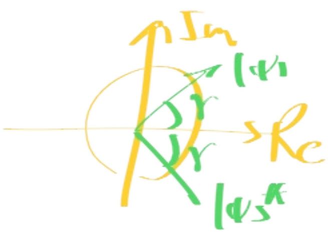
$\langle\Psi^+| = |\Psi^+\rangle^\dagger$

$|\Psi^+\rangle = \begin{bmatrix} 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix}$, $|\Psi^+\rangle^\dagger = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{bmatrix}$

$\langle\Psi^+|\Phi^+\rangle = |\Psi^+\rangle^\dagger|\Phi^+\rangle = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ 0 \\ 0 \\ \frac{1}{\sqrt{2}} \end{bmatrix}$

$= 0$

$$(e^{i\gamma})^* = e^{-i\gamma}$$



$$|\psi\rangle = \begin{bmatrix} i \\ 0 \end{bmatrix}$$

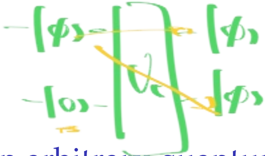
$$|\psi\rangle \cdot |\psi\rangle = 1$$

$$|\psi\rangle^\dagger |\psi\rangle = \begin{bmatrix} -i & 0 \end{bmatrix} \begin{bmatrix} i \\ 0 \end{bmatrix} = +1$$

Bell states form an orthogonal basis set

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

No-cloning theorem



$$\langle \omega | \omega \rangle = |\omega\rangle^{\dagger} |\omega\rangle$$

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:

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

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 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.

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

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

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: $H^\dagger = H$

Universal classical computation

Toffoli (CCNOT) gate can represent all classical computation

(How?)

Functional completeness

All computation on binary variables can be represented as

$$f(x) = y$$

$$x \in \{0,1\}^n; y \in \{0,1\}^m$$

All Boolean expressions can be phrased as either CNF (and of ors) or DNF (or of ands).

Various sets of logic gates are functionally complete

- {NOT,AND,OR}
- {NAND}
- {NOR}

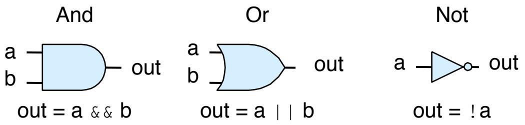

Figure: Source: CS:APP

Reversible operations

Toffoli (CCNOT) gate can represent all classical computation

CCNOT implements NAND

- Write down truth table for NAND.
- Write down truth table for CCNOT.
- Feed $|1\rangle$ into target qubit.

Creating classical computers out of purely reversible logic is a way to push the extremes of computing energy efficiency.