Ch3: Quantum Instruction Sets & Quantum Circuits

Quantum bit

A qubit state is a unit vector in a two-dimensional complex vector space – Hilbert space:

- Superposition: $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$
- Probability amplitudes: $\alpha, \beta \in \mathbb{C}$
- Normalization: $|\alpha|^2 + |\beta|^2 = 1$

Computational basis

The special states $|0\rangle$ and $|1\rangle$ are called computational basis states:

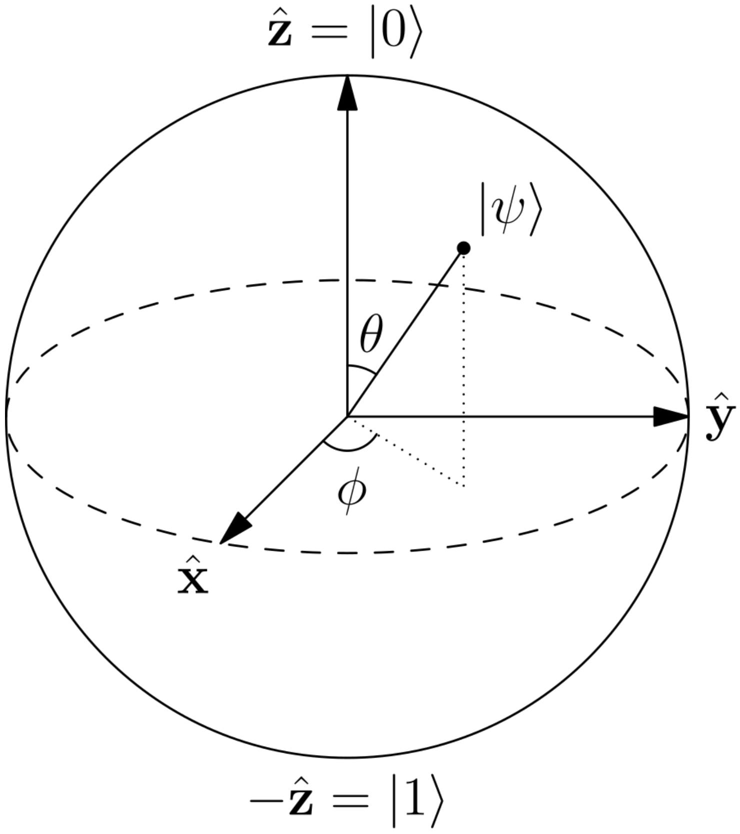
- Classical bit 0: $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$
- Classical bit 1: $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

Bloch sphere representation

A qubit state can be seen as a vector pointing at a sphere surface ($\mathbb{C}^2 \longmapsto \mathbb{R}^3$):

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

- Amplitude parameter: $0 \leq \theta \leq \pi$
- Phase parameter: $0 \leq \phi \leq 2\pi$
- Bloch vector coordinates: $\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}$



Unitary evolution

A general unitary transformation must be able to take the computational basis state $|0\rangle$ to any desired state $|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle$. That is:

$$U = \begin{pmatrix} \cos(\theta / 2) & a \\ e^{i\phi}\sin(\theta / 2) & b \end{pmatrix}$$

where a and b are complex numbers constrained such that $UU^\dagger = I$. This gives:

$$U = \begin{pmatrix} \cos(\theta / 2) & -e^{i\lambda}\sin(\theta / 2) \\ e^{i\phi}\sin(\theta / 2) & e^{i\lambda + i\phi}\cos(\theta / 2) \end{pmatrix}.$$

where $0 \leq \lambda < 2\pi$. This is the most general form of a single qubit unitary.

Physical gates

All single-qubit operations are compiled down to gates known as u1 , u2 and u3 before running on real quantum hardware. For that reason they are sometimes called the physical gates:

- u3-gate: $$u3(\theta, \phi, \lambda) = \begin{pmatrix} \cos\frac{\theta}{2} & -e^{i\lambda}\sin\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} & e^{i(\lambda+\phi)}\cos\frac{\theta}{2} \end{pmatrix}$$
- u2-gate: $$u2(\phi, \lambda) = u3(\tfrac{\pi}{2}, \phi, \lambda) = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -e^{i\lambda} \\ e^{i\phi} & e^{i(\lambda+\phi)} \end{pmatrix}$$
- u1-gate: $$u1(\lambda) = u3(0, 0, \lambda) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\lambda} \end{pmatrix}$$

Pauli operators

The simplest quantum gates are the Pauli operators: X, Y and Z. Their action is to perform a half rotation of the Bloch sphere around the x, y and z axes.

- X-gate: $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = u3(\pi, 0, \pi)$
- Y-gate: $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = u3(\pi, \frac{\pi}{2}, \frac{\pi}{2})$
- Z-gate: $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = u1(\pi)$

$$[X, Y] = XY - YX = 2iZ$$
$$[Y, Z] = 2iX$$
$$[Z, X] = 2iY$$

$$\{X, Y\} = XY + YX = 0$$
$$\{Y, Z\} = 0$$
$$\{Z, X\} = 0$$

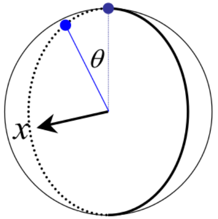
$$X^2 = Y^2 = Z^2 = I$$

Rotation operators

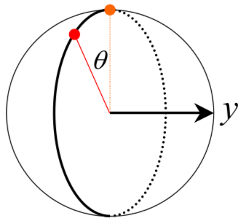
The Pauli operators give rise to three useful classes of unitary operators when they are exponentiated, the rotations operators about the x, y and z axes of the Bloch sphere:

$$R_P(\theta) = e^{-i\theta P} = \cos\tfrac{\theta}{2} I - i\sin\tfrac{\theta}{2} P$$

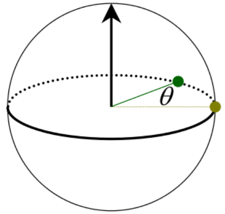
- $\mathrm{R_x}$-gate: $$R_X(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} = u3(\theta, -\tfrac{\pi}{2}, \tfrac{\pi}{2})$$



- $\mathrm{R_Y}$-gate: $$R_Y(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} = u3(\theta, 0, 0)$$



- $\mathrm{R_z}$-gate: $$R_Z(\theta) = \begin{pmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{pmatrix} = u1(\theta)$$



Clifford gates

The Clifford gates are the elements of the Clifford group, a set of mathematical transformations which effect permutations of the Pauli operators:

- H-gate: $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = u2(0, \frac{\pi}{2})$
- S-gate: $S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix} = u1(\frac{\pi}{2})$
- T-gate: $T = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\frac{\pi}{4}} \end{pmatrix} = u1(\frac{\pi}{4})$

$$HXH = Z$$
$$HYH = -Y$$
$$HZH = X$$

$$SXS^\dagger = iY$$
$$SYS^\dagger = iX$$
$$SZS^\dagger = Z$$

Computational basis

To describe the state of a two-qubit system, by convention, we use the computational basis states $\{00, 10, 01, 11\}$:

$$|00\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}1\begin{pmatrix}1\\0\end{pmatrix}\\0\begin{pmatrix}1\\0\end{pmatrix}\end{pmatrix} = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}$$

$$|01\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}1\begin{pmatrix}0\\1\end{pmatrix}\\0\begin{pmatrix}0\\1\end{pmatrix}\end{pmatrix} = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}$$

$$|10\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix}0\begin{pmatrix}1\\0\end{pmatrix}\\1\begin{pmatrix}1\\0\end{pmatrix}\end{pmatrix} = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}$$

$$|11\rangle = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}0\begin{pmatrix}0\\1\end{pmatrix}\\1\begin{pmatrix}0\\1\end{pmatrix}\end{pmatrix} = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

Product states

Consider two non-interacting systems A and B, with respective Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. The Hilbert space of the composite system is the tensor product: $\mathcal{H}_A \otimes \mathcal{H}_B$.

If the first system is in state $|\psi\rangle_A$ and the second in state $|\phi\rangle_B$, the state of the composite system is: $|\psi\rangle_A \otimes |\phi\rangle_B$.

States of the composite system that can be represented in this form are called separable states, or product states. An example of separable states is given by:

$$\frac{|00\rangle + |10\rangle + |01\rangle + |11\rangle}{2}$$

where $|\psi\rangle_A = \dfrac{|0\rangle + |1\rangle}{\sqrt{2}}$ and $|\phi\rangle_B = \dfrac{|0\rangle + |1\rangle}{\sqrt{2}}$.

Entangled states

Not all states are separable states (and thus product states). If a state is inseparable, it is called an entangled state. See for instance the so-called Bell states:

$$\begin{cases} |\phi\pm\rangle_{AB} = \dfrac{|00\rangle \pm |11\rangle}{\sqrt{2}} \\ |\psi\pm\rangle_{AB} = \dfrac{|10\rangle \pm |01\rangle}{\sqrt{2}} \end{cases}$$

Such states are examples of maximally entangled states.

In a quantum computer, entanglement leads to correlations between the qubit systems, even though they are spatially separated.

Controlled operations

Most of the two-qubit gates are of the controlled type (the SWAP gate being the exception). In general, a controlled two-qubit gate C_U acts to apply the single-qubit unitary U to the second qubit when the state of the first qubit is in $|1\rangle$. Suppose U has a matrix representation:

$$U = \begin{pmatrix} u_{00} & u_{01} \\ u_{10} & u_{11} \end{pmatrix}$$

Then the action of C_U is in matrix form:

$$C_U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & u_{00} & u_{01} \\ 0 & 0 & u_{10} & u_{11} \end{pmatrix}$$

Controlled-NOT gate

A critical operator for quantum computing is the controlled NOT gate. We use it to entangle two qubits.

- CNOT-gate: $$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

SWAP gate

The SWAP gate exchanges the states of the two qubits.

- SWAP-gate: $$SWAP = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Universal get set

Any unitary can be decomposed using:

- Arbitrary single qubit gates
- The 2-qubit CNOT gate

Problem: it is not realistic to be able to perform arbitrary single-qubit gates with infinite precision. We would like a finite gate set.

3.5 Universality of simple gate sets

Kitaev-Solovay theorem

The following sets allow to approximate any unitary arbitrary well:

- CNOT, Hadamard, T-gate
- Hadamard and Toffoli (3-qubit CCNOT gate) if the unitary have only real entries

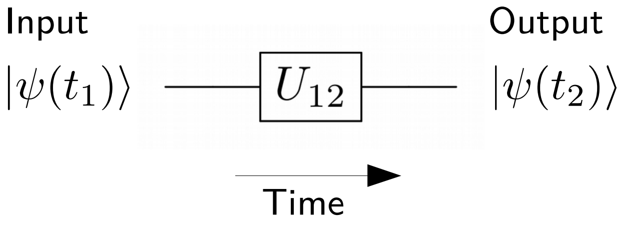
Kitaev-Solovay: any 1 or 2-qubit unitary can be approximated up to an error using polylog(1/) gates from the set.

3.6 Quantum circuit diagrams

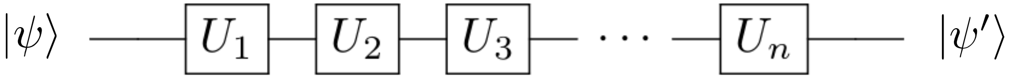
Quantum registers

Circuit diagrams are to be read from left to right. Each qubit is represented by a single horizontal wire and most gates are represented by boxes:

- A quantum register of one qubit with a single single qubit operation:



- Successive implementation:

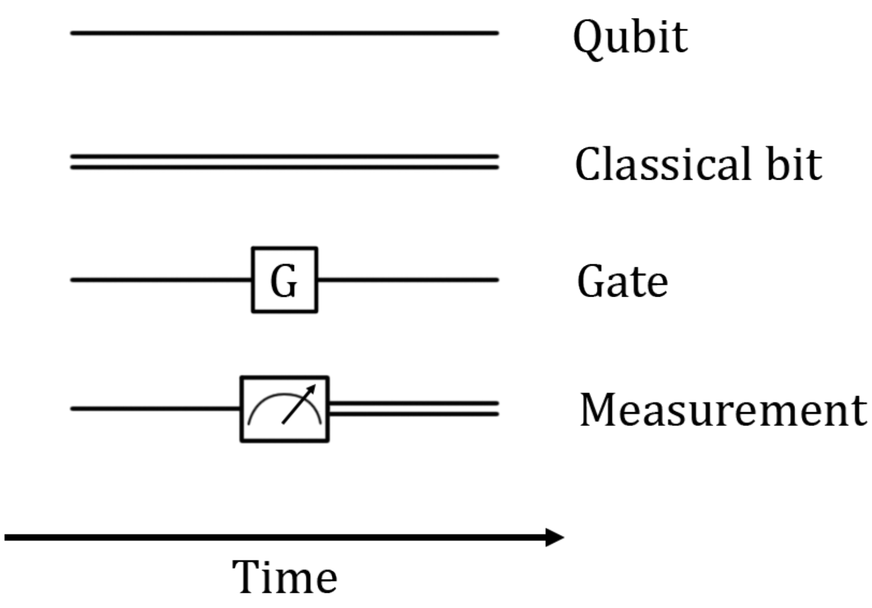


$$|\psi'\rangle = U_n \cdots U_3 U_2 U_1 |\psi\rangle$$

Time

Classical registers

We also need classical registers, represented by doubled horizontal wires, to get the measurement result after completion of a computation.



Building blocks

Operator	Gate(s)		Matrix
Pauli-X (X)	X	$\oplus$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H		$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	S		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	T		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
Controlled Z (CZ)	Z		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$
SWAP			$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$
Toffoli (CCNOT, CCX, TOFF)			$\begin{bmatrix} 1&0&0&0&0&0&0&0 \\ 0&1&0&0&0&0&0&0 \\ 0&0&1&0&0&0&0&0 \\ 0&0&0&1&0&0&0&0 \\ 0&0&0&0&1&0&0&0 \\ 0&0&0&0&0&1&0&0 \\ 0&0&0&0&0&0&0&1 \\ 0&0&0&0&0&0&1&0 \end{bmatrix}$