

COL7160 : Quantum Computing
Lecture 4: Unitary Operations and Quantum Gates

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1 Fundamental Laws of Quantum Mechanics

- **Linearity of Operations:**

- Every valid quantum operation U must be linear.
- Linearity allows operations to be represented as matrix multiplication.
- For an n -qubit state, U is represented by a $2^n \times 2^n$ complex matrix.
- Quantum Operation $U : |\psi_{in}\rangle \rightarrow |\psi_{out}\rangle$

- **Preservation of Normalization:**

- A quantum operation must take a valid quantum (normalized) state and produce another valid quantum (normalized) state.
- This implies $\langle \psi_{in} | \psi_{in} \rangle = \langle \psi_{out} | \psi_{out} \rangle = \langle \psi_{in} | U^\dagger U | \psi_{in} \rangle$.
- For this to hold for every $|\psi_{in}\rangle$, the condition $U^\dagger U = I$ must be satisfied.
- Such matrices U are called **unitary** matrices.

2 Measurement vs. Quantum Operations

- **Quantum Operations:**

- These are reversible and deterministic.
- Determinism means that given a fixed $|\psi_{in}\rangle$ and U , you always get a fixed $|\psi_{out}\rangle$.

- **Measurement:**

- Unlike unitaries, measurement is probabilistic and irreversible.
- The inclusion of measurement makes quantum algorithms inherently probabilistic.

3 Structure of Quantum Algorithms

- **Basic Workflow:**

- Algorithms typically start with all qubits in the $|0\rangle$ state.
- They apply a sequence of Unitary operations and Measurements.

- **Operational Rules:**

- Multiple consecutive unitaries can be combined into a single unitary matrix.
- The input to the algorithm determines which unitaries are applied.

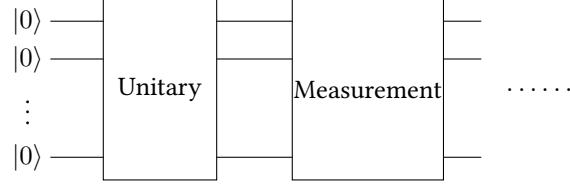


Figure 1: General structure of a quantum algorithm.

Example 1: Hadamard Transform

- **Matrix:** $H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$
- **Action on Computational Basis:**
 - $H|0\rangle = |+\rangle$
 - $H|1\rangle = |-\rangle$
- **Action on Hadamard Basis:**
 - $H|+\rangle = |0\rangle$
 - $H|-\rangle = |1\rangle$
- **Property:** $H^\dagger = H$ (Self-adjoint).

Usage: Sampling a random bit

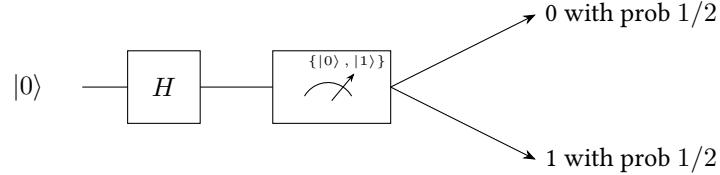


Figure 2: Quantum circuit for sampling a random bit.

Example 2: Rotation Matrix $R(\theta)$

- The rotation matrix $R(\theta)$ rotates a state by an angle of $\theta/2$ on a single application:

$$R(\theta) = \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2) \\ \sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

- Let's focus on the case where $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, where $\alpha, \beta \in \mathbf{R}$ and $\alpha^2 + \beta^2 = 1$.

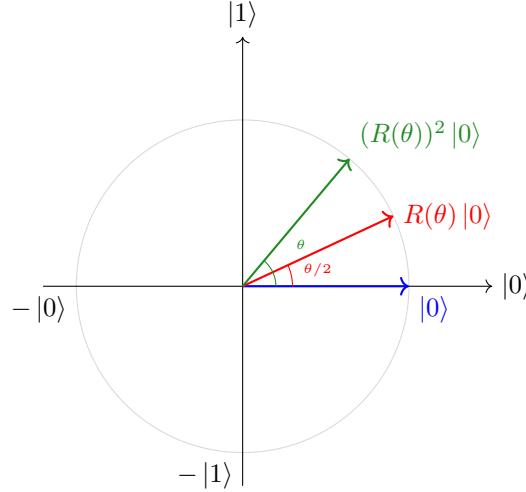


Figure 3: Rotation of a quantum state on the real unit circle.

Observation: $(R(\pi/2))^2 |0\rangle = |1\rangle$. This follows because applying $R(\pi/2)$ twice results in a total rotation of $\pi/2$ (or 90°).

4 Elitzur-Vaidman Bomb Testing

- **Setup:**

- There is a bomb that is either functional (working) or non-functional (not working).
- We can send a single qubit state $|\psi\rangle$ to the bomb to test its status without exploding it.
- **Functional Bomb:** Measures the qubit in the computational basis.
 - * If the measurement result is 1, the bomb explodes.
 - * If the result is 0, it returns the state $|0\rangle$.
- **Non-functional Bomb:** Acts as an identity operation; it takes input $|\psi\rangle$ and outputs the same state $|\psi\rangle$ without any interaction.

Protocol and Feedback Circuit

The protocol involves a sequence of rotations and interactions with the bomb. If the bomb does not explode, the output is fed back as the input for the next iteration.

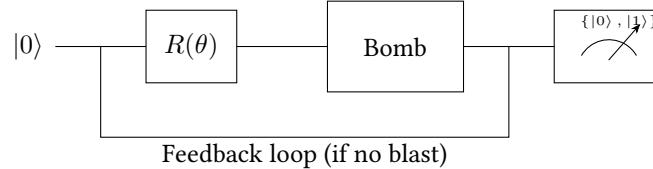


Figure 4: Feedback circuit for Elitzur-Vaidman bomb testing.

Detailed Analysis

One Iteration (Functional Bomb)

- Starting with $|0\rangle$, we apply $R(\theta)$ to get: $R(\theta)|0\rangle = \cos(\theta/2)|0\rangle + \sin(\theta/2)|1\rangle$.

- The functional bomb measures this state.
- **Probability of Blast:** $P(\text{blast}) = |\sin(\theta/2)|^2 = \sin^2(\theta/2)$.
- **Probability of No Blast:** $P(\text{no blast}) = |\cos(\theta/2)|^2 = \cos^2(\theta/2)$.
- If there is no blast, the bomb returns state $|0\rangle$, which is fed back into the next iteration.

Multi-Iteration Analysis (n iterations)

- **Case 1: Bomb is Functional**
 - The probability that the bomb does not explode after n iterations is $(\cos^2(\theta/2))^n = \cos^{2n}(\theta/2)$.
 - **Total Blast Probability:** $P(\text{at least 1 blast}) = 1 - (\cos^2(\theta/2))^n$.
 - Using $\cos^2(\theta/2) = 1 - \sin^2(\theta/2)$, we get:
$$P(\text{blast}) = 1 - (1 - \sin^2(\theta/2))^n \approx 1 - (1 - n \sin^2(\theta/2)) = n \sin^2(\theta/2)$$
 - If the bomb does not explode, the final measurement in the standard basis will yield 0 with probability 1.
- **Case 2: Bomb is Non-functional**
 - The state simply rotates n times: $(R(\theta))^n |0\rangle = R(n\theta) |0\rangle$.
 - We choose $n = \pi/\theta$ so that the total rotation is $\pi/2$.
 - The final state is $R(\pi) |0\rangle = |1\rangle$.
 - The final measurement in the standard basis will yield 1 with probability 1.

Efficiency and Success

- For $n = \pi/\theta$, we can distinguish a functional bomb from a non-functional one if the bomb did not explode.
- The blast probability is $P(\text{blast}) \approx \frac{\pi}{\theta} \cdot \sin^2(\theta/2) \leq \frac{\pi}{\theta} \cdot \frac{\theta^2}{4} = \frac{\pi\theta}{4}$.
- By decreasing θ (and increasing n), the probability of exploding the bomb during testing can be made arbitrarily small.

5 Properties of Unitary Maps

In this section, we explore the fundamental relationship between unitary matrices and orthonormal bases.

Lemma 1. *Let U be a linear map on \mathbf{C}^d . Then U is unitary ($U^\dagger U = I$) iff the columns of U form an orthonormal basis.*

Proof. Let the columns of U be denoted by $|v_1\rangle, |v_2\rangle, \dots, |v_d\rangle$. The entry at row i and column j of the product $U^\dagger U$ is given by the inner product of the i -th row of U^\dagger (which is the conjugate transpose of the i -th column of U) and the j -th column of U . Thus, $(U^\dagger U)_{ij} = \langle v_i | v_j \rangle$.

- **Lemma 1.1 (\implies):** If U is unitary, then $U^\dagger U = I$. This implies $(U^\dagger U)_{ij} = \delta_{ij}$, where δ_{ij} is the Kronecker delta. Therefore, $\langle v_i | v_j \rangle = 1$ if $i = j$ and 0 if $i \neq j$, meaning the columns are orthonormal. Since there are d such vectors in \mathbf{C}^d , they form an orthonormal basis.
- **Lemma 1.2 (\impliedby):** If the columns form an orthonormal basis, then $\langle v_i | v_j \rangle = \delta_{ij}$. It follows that $(U^\dagger U)_{ij} = \delta_{ij}$, so $U^\dagger U = I$, making U unitary.

□

Lemma 2. *U is unitary iff it transforms any orthonormal basis of \mathbf{C}^d into an orthonormal basis.*

Proof. Let $\{|e_1\rangle, \dots, |e_d\rangle\}$ be an arbitrary orthonormal basis. The transformed basis is $\{|f_i\rangle\}$ where $|f_i\rangle = U|e_i\rangle$.

- **Lemma 2.1 (\implies):** Suppose U is unitary. The inner product of the transformed vectors is:

$$\langle f_i | f_j \rangle = (U | e_i \rangle)^\dagger (U | e_j \rangle) = \langle e_i | U^\dagger U | e_j \rangle$$

Since $U^\dagger U = I$, this simplifies to $\langle e_i | e_j \rangle = \delta_{ij}$. Thus, the transformed vectors remain orthonormal and form a basis.

- **Lemma 2.2 (\iff):** If U transforms any orthonormal basis into an orthonormal basis, let it act on the standard basis $\{|0\rangle, |1\rangle, \dots, |d-1\rangle\}$. The columns of U are exactly the images of the standard basis vectors. Since these images must be orthonormal by assumption, the columns of U are orthonormal. By Lemma 1.2, U is unitary.

□

Lemma 3. *If U transforms a specific orthonormal basis of \mathbf{C}^d into another orthonormal basis, then U transforms each orthonormal basis of \mathbf{C}^d into some orthonormal basis.*

Proof. Let $B_1 = \{|v_1\rangle, |v_2\rangle, \dots, |v_d\rangle\}$ be a specific orthonormal basis that U transforms into another orthonormal basis $B_2 = \{|w_1\rangle, |w_2\rangle, \dots, |w_d\rangle\}$. By definition, $U |v_i\rangle = |w_i\rangle$ for all i .

1. **Preservation of Inner Product for Basis Vectors:** Since B_2 is an orthonormal basis, the inner product of the transformed vectors satisfies:

$$\langle Uv_i | Uv_j \rangle = \langle w_i | w_j \rangle = \delta_{ij}$$

Since B_1 is also orthonormal, we have $\langle v_i | v_j \rangle = \delta_{ij}$. Thus, $\langle Uv_i | Uv_j \rangle = \langle v_i | v_j \rangle$ for all i, j .

2. **General Unitarity:** Any arbitrary vectors $|a\rangle, |b\rangle \in \mathbf{C}^d$ can be expanded in the basis B_1 as $|a\rangle = \sum_i a_i |v_i\rangle$ and $|b\rangle = \sum_j b_j |v_j\rangle$. Due to the linearity of U :

$$\langle Ua | Ub \rangle = \sum_{i,j} a_i^* b_j \langle Uv_i | Uv_j \rangle = \sum_{i,j} a_i^* b_j \delta_{ij} = \sum_i a_i^* b_i = \langle a | b \rangle$$

This identity $\langle a | U^\dagger U | b \rangle = \langle a | I | b \rangle$ for all $|a\rangle, |b\rangle$ implies $U^\dagger U = I$. Therefore, U is unitary.

3. **Transformation of Any Basis:** By Lemma 2.1, we have already established that if U is unitary, it transforms *any* orthonormal basis into another orthonormal basis. Thus, the property holds universally.

□

6 Elementary Quantum Gates

6.1 Single Qubit Gates

- **Hadamard (H):**

- **Matrix:** $H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$

- **Action on Computational Basis:**

- $H |0\rangle = |+\rangle$
- $H |1\rangle = |-\rangle$

- **Action on Hadamard Basis:**

- $H |+\rangle = |0\rangle$
- $H |-\rangle = |1\rangle$

- **Property:** $H^\dagger = H$ (Self-adjoint).

- **Pauli-X (Bit Flip):**

- **Matrix:** $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

- **Action:**

- * $X |0\rangle = |1\rangle$
 - * $X |1\rangle = |0\rangle$

- **Pauli-Z (Phase Flip):**

- **Matrix:** $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

- **Action on Computational Basis:**

- * $Z |0\rangle = |0\rangle$
 - * $Z |1\rangle = -|1\rangle$

- **Action on Hadamard Basis:** (Acts as bit flip in Hadamard basis)

- * $Z |+\rangle = |-\rangle$
 - * $Z |-\rangle = |+\rangle$

- **Pauli-Y:**

- **Matrix:** $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

- **Relation:** $Y = iXZ$

- **Action:**

- * $Y |0\rangle = i |1\rangle$
 - * $Y |1\rangle = -i |0\rangle$

- **Phase Gate (R_φ):**

- **Matrix:** $R_\varphi = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{pmatrix}$

- **Action:**

- * $R_\varphi |0\rangle = |0\rangle$
 - * $R_\varphi |1\rangle = e^{i\varphi} |1\rangle$

- **Note:** The Z gate is a special case where $Z = R_\pi$.

6.2 Multi-Qubit Gates

- **CNOT (Controlled-NOT):**

- A 2-qubit gate with a control qubit and a target qubit.

- **Matrix Representation:**

$$\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

- **Operational Mapping:**

- * $\text{CNOT} |0\rangle |b\rangle = |0\rangle |b\rangle$
 - * $\text{CNOT} |1\rangle |b\rangle = |1\rangle |1 \oplus b\rangle$

- **Qubit Roles:**

- * First qubit \rightarrow Control qubit
 - * Second qubit \rightarrow Target qubit

- **CCNOT (Toffoli Gate):**

- A 3-qubit gate where the third qubit (target) is flipped if and only if the first two qubits (controls) are both in the $|1\rangle$ state.

- **Matrix Representation:**

$$\text{CCNOT} = \left(\begin{array}{c|cc} I_{6 \times 6} & 0 \\ \hline 0 & 0 & 1 \\ 1 & 1 & 0 \end{array} \right)$$

- **Logic:**

- $|x, y, z\rangle \rightarrow |x, y, z \oplus (x \wedge y)\rangle$

7 Exercises

1. **Conditional Unitary Construction:** Construct a matrix for a $2n$ qubit state that applies unitary U to the last n qubits only when the first n qubits are all 1.
2. **Universal Logic:** Construct classical AND, OR, and NOT gates using only the Toffoli gate.