

QUANTUM COMPUTING

MCS 2025 - Sheffield

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LECTURE 2: • Some Complex Linear Algebra

- Unitary Matrices - Quantum Operators
- Hermitian Matrices - Observables

A quantum state is represented as a complex linear combination of $|0\rangle$ and $|1\rangle$

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

The field of complex numbers is obtained by adding a square root of -1 to the real numbers: $i = \sqrt{-1}$

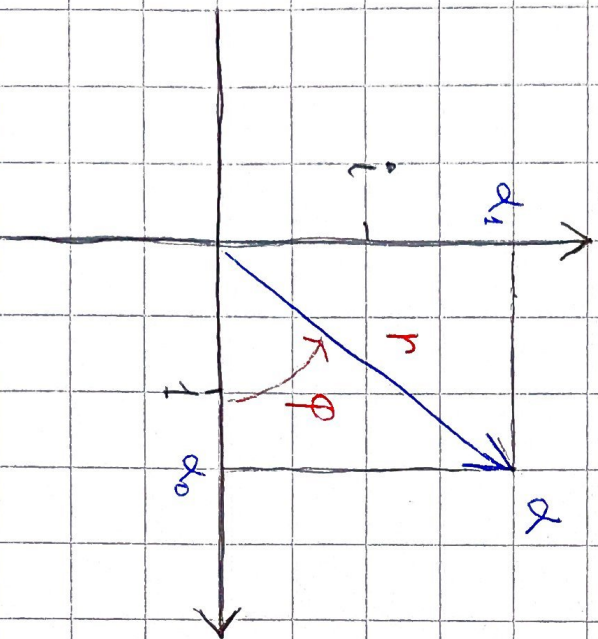
$$\alpha = \alpha_0 + \alpha_1 i$$

$$\beta = \beta_0 + \beta_1 i$$

with $\alpha_0, \alpha_1, \beta_0, \beta_1$ real

Cartesian Coordinates:

$$\alpha = \alpha_0 + \alpha_1 i$$



Polar Coordinates:

$$\alpha = r \cdot e^{i\phi}$$

So a quantum one-bit state has the form: $|\psi\rangle = r_1 \cdot e^{i\phi_1} |0\rangle + r_2 \cdot e^{i\phi_2} |1\rangle$

States that differ by a complex unit factor (global phase) are indistinguishable, so we identify them.

Therefore the quantum state can be written with a purely real coefficient for $|0\rangle$:

$$|\psi\rangle = r_1 e^{i\phi_1} |0\rangle + r_2 e^{i\phi_2} |1\rangle \equiv r_1 |0\rangle + r_2 e^{i(\phi_2 - \phi_1)} |1\rangle$$

There are two degrees of freedom:

- r_1 (r_2 is determined by $r_1^2 + r_2^2 = 1$)
- $\phi = \phi_2 - \phi_1$ (relative phase)

We can express r_1 and r_2 as: $r_1 = \cos(\theta/2)$, $r_2 = \sin(\theta/2)$, $0 \leq \theta \leq \pi$

Standard form of a quantum state:

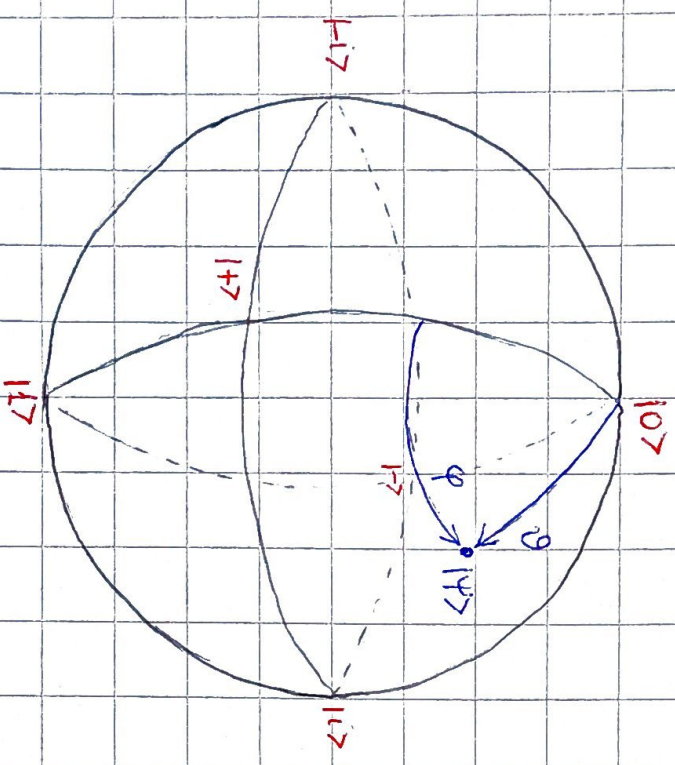
$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right) |0\rangle + \sin\left(\frac{\theta}{2}\right) e^{i\phi} |1\rangle$$

The Bloch Sphere

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

$$0 \leq \theta \leq \pi, \quad 0 \leq \varphi < 2\pi$$

θ and φ determine a point on a sphere:



$| 0 \rangle$ and $| 1 \rangle$ are the poles of the sphere:

$$| 0 \rangle : \theta = 0, \varphi = 0$$

$$| 1 \rangle : \theta = \pi, \varphi = 0$$

this is called the computational basis

Other antipodal points on the sphere correspond to alternative bases

Hadamard Basis:

$$| + \rangle = \frac{1}{\sqrt{2}} (| 0 \rangle + | 1 \rangle) : \theta = \pi/2, \varphi = 0$$

$$| - \rangle = \frac{1}{\sqrt{2}} (| 0 \rangle - | 1 \rangle) : \theta = \pi/2, \varphi = \pi$$

Circular Basis:

$$| i \rangle = | \psi \rangle = \frac{1}{\sqrt{2}} (| 0 \rangle + i | 1 \rangle) : \theta = \pi/2, \varphi = \pi/2$$

$$| -i \rangle = | \psi \rangle = \frac{1}{\sqrt{2}} (| 0 \rangle - i | 1 \rangle) : \theta = \pi/2, \varphi = 3\pi/2$$

Quantum Operations are represented by unitary matrices

- The complex conjugate of a complex number $a+bi$ is $\overline{a+bi} = a-bi$

- The conjugate transpose of a matrix $U =$

$$U = \begin{bmatrix} a_{00} & & a_{0m} \\ & \ddots & \\ a_{n0} & & a_{nm} \end{bmatrix}$$

is

$$U^* = \begin{bmatrix} \overline{a_{00}} & \dots & \overline{a_{n0}} \\ \overline{a_{01}} & \dots & \overline{a_{nm}} \end{bmatrix}$$

- A matrix is unitary if its conjugate transpose is its inverse.

square

$$U^* \cdot U = U \cdot U^* = \mathbb{I} \leftarrow \text{identity matrix}$$

It follows that the columns (and rows) of U are orthonormal:

So: U is a change of basis (rotation in the Bloch sphere) orthogonal to each other and of unit length

THE PAULI GATES

- X gate (NOT) $\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

is a rotation around the X-axis:

$$\begin{aligned} \sigma_x |0\rangle &= |1\rangle, & \sigma_x |1\rangle &= |0\rangle \\ \sigma_x |+\rangle &= |+\rangle, & \sigma_x |-\rangle &= |-\rangle \\ \sigma_x |i\rangle &= |-i\rangle, & \sigma_x |-i\rangle &= |i\rangle \end{aligned}$$

- Y gate $\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$

is a rotation around the Y-axis:

$$\begin{aligned} \sigma_y |0\rangle &= |1\rangle, & \sigma_y |1\rangle &= |0\rangle \\ \sigma_y |+\rangle &= |-\rangle, & \sigma_y |-\rangle &= |+\rangle \\ \sigma_y |i\rangle &= |i\rangle, & \sigma_y |-i\rangle &= |-i\rangle \end{aligned}$$

- Z gate
 phase flip $\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

is a rotation around the Z-axis:

$$\begin{aligned} \sigma_z |0\rangle &= |0\rangle, & \sigma_z |1\rangle &= |1\rangle \\ \sigma_z |+\rangle &= |-\rangle, & \sigma_z |-\rangle &= |+\rangle \\ \sigma_z |i\rangle &= |-i\rangle, & \sigma_z |-i\rangle &= |i\rangle \end{aligned}$$

HADAMARD GATE

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

is a change of basis between the computational and Hadamard basis

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

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

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

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

The Hadamard gate is often applied at the beginning of an algorithm to prepare the qubits into a superposition.

PHASE-CHANGE GATES

are a generalization of Pauli Z gate that change the relative phase of the qubit by an arbitrary angle φ :

$$R_\varphi^Z = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\varphi} \end{bmatrix} \text{ for } 0 \leq \varphi < 2\pi$$

$$R_0^Z = I_2$$

$$R_\pi^Z = Z$$

$$S = R_{\pi/2}^Z$$

$$T = R_{\pi/4}^Z$$

DENSITY MATRICES

The density matrix of a quantum state $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$ is an alternative representation of the state.

$$\rho = |\psi\rangle\langle\psi| = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}^* \begin{bmatrix} \alpha & \beta \end{bmatrix} = \begin{bmatrix} |\alpha|^2 & \alpha\bar{\beta} \\ \bar{\alpha}\beta & |\beta|^2 \end{bmatrix}$$

If we represent $|\psi\rangle$ in standard form: $|\psi\rangle = r_1|0\rangle + r_2 e^{i\varphi_i}|1\rangle$, $r_1, r_2 \in \mathbb{R}_0$, $0 \leq \varphi < 2\pi$

Then
$$\rho = \begin{bmatrix} r_1^2 & r_1 r_2 e^{-i\varphi_i} \\ r_1 r_2 e^{i\varphi_i} & r_2^2 \end{bmatrix}, \text{ so } r_1 = \sqrt{\rho_{00}}, r_2 = \sqrt{\rho_{11}}, e^{i\varphi_i} = \rho_{10}/r_1 r_2$$

ρ completely determines $|\psi\rangle$ (up to global phase)
The diagonal elements of ρ are the probabilities of observing $|0\rangle$ and $|1\rangle$

Ex. Density matrix of $|0\rangle$: $|0\rangle\langle 0| = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} =: M_0$, of $|1\rangle$: $|1\rangle\langle 1| = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} =: M_1$

For any $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$:

$$\langle\psi|M_0|\psi\rangle = |\alpha|^2$$

$$\langle\psi|M_1|\psi\rangle = |\beta|^2$$

MEASUREMENTS

We can set up a measuring device to measure a quantum state along any basis, not just $|0\rangle$ and $|1\rangle$ for example along the Hadamard basis $|+\rangle, |-\rangle$

- Choose the value that the measurement should return is a certain state is observed:
For example:
 - return 1 if we observe $|+\rangle$
 - return -1 if we observe $|-\rangle$

- The measurement can be fully characterized by a single matrix: sum of the density matrices of the observed states with the return values as coefficients.

$$M = 1 \cdot |+\rangle\langle +| - 1 \cdot |-\rangle\langle -| = \dots = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

We can recover the values and states from M :

- Observed values = eigenvalues of M
- Observed states = eigenvectors of M

This is the same as the σ_x operator, but it has a different meaning when used as a measurement

OBSERVABLES : an observable is a matrix which:

- is Hermitian : $A = A^*$
- The eigenvectors of A form a basis of the quantum state space

An eigenvector is a state that is mapped by A to a multiple of itself

$$A \cdot | \psi \rangle = \lambda \cdot | \psi \rangle$$

↑
eigenvector
↑
eigenvalue

We can compute the eigenvalues by solving the equation

$$\det(A - \lambda I) = 0$$

and then compute the eigenvectors by substituting the values for λ in.

Several unitary matrices (quantum operations) are also Hermitian (observables)

For example σ_x , σ_y , σ_z , H

Exercise 1: Determine what we are observing (eigenvalues) and what the results of the observation are (eigenvalues)

In a real quantum computer we can only observe $|0\rangle$ and $|1\rangle$

~~Show~~

Exercise 2: Show how we can measure any observable by composing with unitary matrices.