### where $p_i$ are probabilities.

### The State of a Quantum System

- In quantum mechanics, the state of a system represents all possible information about the system.
- Unlike classical systems (where a particle has a definite position and velocity), in quantum systems the state is probabilistic and described using state vectors or wave functions.

## 2. Mathematical Representation

- The state is represented as a **vector in Hilbert space**.
- For a single qubit (two-level system), the general state is:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$$

where:

- $\circ$   $\alpha$  and  $\beta$  are complex numbers.
- O Normalization condition:  $|\alpha|^2 + |\beta|^2 = 1$ .
- For multi-qubit systems, states are described using tensor products. Example:

$$|\psi\rangle = |0\rangle \otimes |1\rangle = |01\rangle$$

# 3. Superposition Principle

- A quantum state can exist in a linear combination of basis states.
- Example:

$$|\psi\rangle = (1/\sqrt{2})(|0\rangle + |1\rangle)$$

 $\rightarrow$  the system is in superposition of both  $|0\rangle$  and  $|1\rangle$ .

#### 4. Measurement and Probabilities

- Measurement collapses the state into one of the basis states
- The probability of observing a particular outcome is given by the square of the amplitude:
  - o Probability of measuring  $|0\rangle = |\alpha|^2$
  - Probability of measuring  $|1\rangle = |\beta|^2$
- Example: For  $|\psi\rangle = (1/\sqrt{2})(|0\rangle + |1\rangle)$ ,
  - $\circ$  Probability( $|0\rangle$ ) = 1/2
  - $\circ$  Probability( $|1\rangle$ ) = 1/2

#### 5. Types of Quantum States

- Pure State:
  - o Described by a single state vector  $|\psi\rangle$ .
  - $\circ \quad \text{Example: } |0\rangle, (1/\sqrt{2})(|0\rangle + |1\rangle).$
- Mixed State:
  - Represents statistical uncertainty over pure states.
  - o Described by a **density matrix**:

$$\rho = \sum p_i |\psi_i\rangle\langle\psi_i|$$

#### 8. Example of a Quantum State

- Consider an electron spin (spin-1/2 particle):
  - State can be  $|\uparrow\rangle$  (spin-up) or  $|\downarrow\rangle$  (spin-down).
  - General state:

$$|\psi\rangle = \alpha |\!\uparrow\rangle + \beta |\!\downarrow\rangle$$

• Measurement along z-axis gives outcomes with probabilities  $|\alpha|^2$  and  $|\beta|^2$ .

## Time-Evolution of a Closed Quantum System

- A **closed quantum system** is one that does not interact with the environment.
- Its time evolution is governed entirely by its **Hamiltonian** (energy operator).
- The evolution is **deterministic** and **reversible**.

### 2. Schrödinger Equation

 The dynamics of a closed quantum system are described by the time-dependent Schrödinger equation:

$$i\hbar (d/dt)|\psi(t)\rangle = H |\psi(t)\rangle$$

where:

- $|\psi(t)\rangle$  = state of the system at time t
- H = Hamiltonian operator (represents energy of system)
- ħ = reduced Planck's constant
- $\circ$  I = imaginary unit.

#### 3. Solution of Schrödinger Equation

• The general solution is:

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle$$

where U(t) is the **time-evolution operator**:

$$U(t) = \exp(-iHt / \hbar)$$

• U(t) is a **unitary operator** (U†U = I), which ensures probability conservation.

### 4. Key Properties of Time Evolution

- 1. **Unitary**: Evolution preserves total probability (norm of state vector remains 1).
- 2. **Reversible**: Given  $|\psi(t)\rangle$ , one can always recover  $|\psi(0)\rangle$
- 3. **Deterministic**: Unlike measurement, time evolution does not involve randomness.
- 4. **Depends on Hamiltonian**: The Hamiltonian fully determines how the system evolves.

#### 6. Importance

- Time evolution explains how isolated quantum systems behave over time.
- Foundation for quantum simulation, quantum gates, and quantum algorithms.
- Ensures **unitary evolution** before measurement collapses the state.

### Composite Quantum Systems

- A **composite system** is a quantum system made up of two or more subsystems.
- The total state is described in a **larger Hilbert space**, which is the **tensor product** of the individual subsystem spaces.
- Composite systems allow the study of **entanglement**, one of the most important features of quantum mechanics.

### 2. Mathematical Representation

 If system A has state space H<sub>a</sub> and system B has state space H<sub>β</sub>, then the combined system lives in:

$$H = H_a \bigotimes H_{\beta}$$

• If  $|\psi_a\rangle$  is a state of A and  $|\psi_\beta\rangle$  is a state of B, then the joint state is:

$$|\psi\rangle = |\psi_a\rangle \bigotimes |\psi_\beta\rangle$$

• Example:

If  $A = |0\rangle$  and  $B = |1\rangle$ , then:

$$|\psi\rangle = |0\rangle \otimes |1\rangle = |01\rangle$$

### 3. Superposition in Composite Systems

- Just like single systems, composite systems can exist in **superpositions** of product states.
- Example (two qubits):

$$|\psi\rangle = (1/\sqrt{2})(|00\rangle + |11\rangle)$$

# 4. Entanglement

- Some composite states cannot be written as a simple product of subsystem states. These are entangled states.
- Example (Bell state):

$$|\Phi^+\rangle = (1/\sqrt{2})(|00\rangle + |11\rangle)$$

 Entanglement shows strong correlations between subsystems, even when separated by large distances.

### 6. Examples of Composite Systems

1. **Two Qubits**: States like  $|00\rangle$ ,  $|01\rangle$ ,  $|10\rangle$ ,  $|11\rangle$ .

2. **Atom** + **Photon**: Combined system of matter and light.

#### 1. Mixed States

#### (a) Pure vs Mixed States

- **Pure state**: A quantum system described by a single state vector  $|\psi\rangle$  in Hilbert space. Example:  $|\psi\rangle = (1/\sqrt{2})(|0\rangle + |1\rangle)$ .
- **Mixed state**: Describes a system when there is **classical uncertainty** about which pure state it is in. Example: A qubit is in |0⟩ with probability 0.6 and in |1⟩ with probability 0.4.

#### (b) Density Operator Formalism

A mixed state is represented using a density matrix
 (ρ):

$$\rho = \Sigma \; p_i \; |\psi_i\rangle \langle \psi_i|$$
 where  $p_i \geq 0$  and  $\Sigma \; p_i = 1$  .

• Example: If a qubit has 50% chance of being |0\) and 50% chance of being |1\):

$$\rho = 0.5 |0\rangle\langle 0| + 0.5 |1\rangle\langle 1| = [[0.5, 0], [0, 0.5]]$$

## (c) Properties of Density Matrix

- 1. The **eigenvalues of a density matrix** lie between 0 and 1, and their sum is 1.
- 2. A density matrix is always **Hermitian**.
- 3. The **trace of a density matrix is 1**, ensuring total probability is normalized.

## (d) Importance of Mixed States

- Describes systems interacting with an **environment** (open quantum systems).
- Models **imperfect knowledge** of a system.

## 2. General Quantum Operations

A quantum operation describes how a quantum state (density matrix) evolves, not only under unitary gates, but also when noise, measurements, or open-system effects are present.

### (a) Time Evolution vs General Evolution

- In a closed system: evolution is **unitary** (UρU†).
- In an open system: need more general description because of noise, measurements, and environment effects.

### (b) Completely Positive Trace-Preserving (CPTP) Maps

A **CPTP map** is the most general mathematical description of how a quantum state evolves.

It extends beyond unitary evolution to include **noise**, **measurement**, and interactions with the environment.

$$\rho' = \sum E_i \rho E_i \dagger$$

where  $\{E_i\}$  are **Kraus operators**, satisfying:  $\Sigma E_i \dagger E_i = I$ 

### (c) Examples of Quantum Operations

1. Unitary Evolution:  $\rho' = U\rho U^{\dagger}$  (special case of CPTP).

#### 2. Measurement:

If measurement operators are  $\{M_m\}$ , then after outcome m:  $\rho'=(M_m\ \rho\ M_m\dagger)$  / P(m), where  $P(m)=Tr(M_m\ \rho\ M_m\dagger)$ .

#### 3. Noise Channels:

- o Bit-flip channel
- o Phase-damping channel
- Depolarizing channel

### (d) Importance of Quantum Operations

- Needed to describe **realistic systems** (not perfectly isolated).
- Provide the mathematical framework for **quantum algorithms under noise**.
- Essential for quantum error correction and faulttolerant quantum computing.

#### Universal Sets of Quantum Gates

- In classical computing, any computation can be built from a small set of logic gates (e.g., AND, OR, NOT).
- Similarly, in **quantum computing**, there exists a small set of **quantum gates** from which any unitary operation can be constructed.
- Such a collection is called a Universal Set of Quantum Gates.

#### 2. Quantum Gates Basics

- A quantum gate is a unitary operator acting on one or more qubits.
- They transform quantum states while preserving normalization.
- Examples:
  - Single-qubit gates: Pauli-X, Y, Z; Hadamard (H).
  - Multi-qubit gates: CNOT, Toffoli, Controlledphase.

### 3. Definition of Universality

- A set of quantum gates is universal if it can approximate any arbitrary unitary operation U on n qubits to any desired accuracy.
- Universal gates allow construction of all quantum algorithms.

#### 4. Common Universal Gate Sets

#### (a) {H, T, CNOT}

- Hadamard (H): Creates superposition.
- T-gate ( $\pi$ /8 gate): Adds a specific quantum phase.
- **CNOT** (**Controlled-NOT**): Introduces entanglement.
- This set is **universal** because:
  - o H + T generate arbitrary single-qubit rotations.
  - o CNOT adds entanglement between qubits.

### (b) {Clifford + T}

The **Clifford group** is a special set of gates that map **Pauli operators** (**X**, **Y**, **Z**) to other Pauli operators under conjugation.

When you combine **Clifford gates** with the **T gate**, you get a **universal gate set**.

This means **any unitary transformation** on qubits can be approximated to arbitrary precision using just H, S, CNOT, and T.

#### (c) Toffoli + Hadamard

• Toffoli gate (controlled-controlled-NOT) + H can also form a universal set.

| ☐ Toffoli gate alone is <b>classically universal</b> , but not |
|--|
| quantum universal (no superpositions).                         |
|  |

☐ Hadamard introduces **superposition and interference**, enabling access to the full power of quantum mechanics.

☐ Together, **Toffoli** + **H** form a universal gate set:

- Toffoli provides nonlinear classical control.
- Hadamard provides quantum parallelism.

# 6. Importance of Universal Gate Sets

- 1. Provide the **building blocks** for quantum algorithms (Shor's, Grover's, QFT, etc.).
- 2. Allow implementation of **arbitrary unitary operations** on qubits.
- 3. Simplify hardware design: only need to implement a small set of gates in physical quantum computers.
- 4. Essential for **fault-tolerant quantum computing** (error correction works best with certain universal sets).

### 1. Quantum Measurement

- Measurement in quantum mechanics is the process of extracting classical information from a quantum system.
- Unlike classical measurement, quantum measurement **disturbs** the state being measured.
- Quantum measurement is fundamentally **probabilistic**, unlike classical measurement.
- It is described by a set of **measurement operators** {Mm}, where each operator corresponds to a possible outcome.

#### Postulates of Measurement

#### 1. **Probabilities**:

If state is  $|\psi\rangle$ , the probability of measuring outcome m is:

$$P(m) = \langle \psi | P_m | \psi \rangle$$

where P<sub>m</sub> is the projector onto the eigenstate.

# 2. State Collapse:

After measurement, the system collapses to the eigenstate corresponding to the observed outcome.

### (c) Types of Measurements

- $\begin{array}{lll} \hbox{1.} & \textbf{Projective} & \textbf{(von Neumann)} & \textbf{Measurement:} \\ & \text{Standard measurement with projection operators } P_m. \end{array}$
- 2. **POVM** (**Positive Operator-Valued Measure**): Generalized measurement, useful in noisy or practical systems.

### (d) Example

- Measuring a qubit  $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$  in the computational basis:
  - o Probability(0) =  $|\alpha|^2$ , collapses to  $|0\rangle$ .
  - o Probability(1) =  $|\beta|^2$ , collapses to  $|1\rangle$ .

### (e) Importance

- Connects the quantum world to classical information.
- Essential for running quantum algorithms (final output must be measured).
- Provides randomness in quantum systems.

## 2. Quantum Entanglement

- **Entanglement** is a uniquely quantum phenomenon where the state of one particle is **inseparably linked** to the state of another, even when separated by large distances.
- An entangled state cannot be written as a product of single-qubit states.

### (b) Example: Bell States (Maximally Entangled States)

Four common entangled two-qubit states:

$$|\Phi^{+}\rangle = (1/\sqrt{2})(|00\rangle + |11\rangle)$$

$$|\Phi^{-}\rangle = (1/\sqrt{2})(|00\rangle - |11\rangle)$$

$$|\Psi^{+}\rangle = (1/\sqrt{2})(|01\rangle + |10\rangle)$$

$$|\Psi^{-}\rangle = (1/\sqrt{2})(|01\rangle - |10\rangle)$$

### (c) Properties of Entanglement

- Non-local correlations: Measurement outcomes are correlated, even across distance.
- 2. **No classical counterpart**: Cannot be explained by classical probability.
- 3. **Non-separability**: Entangled states cannot be factored into independent subsystems.

## (d) Applications of Entanglement

- 1. **Quantum teleportation** (transfer of quantum state using entanglement + classical communication).
- 2. **Superdense coding** (sending 2 classical bits with 1 qubit).
- 3. **Quantum cryptography** (security from entanglement correlations).
- 4. Quantum algorithms and quantum error correction.

### The Quantum Fourier Transform (QFT)

- The Quantum Fourier Transform (QFT) is the quantum analogue of the Discrete Fourier Transform (DFT).
- It transforms quantum states from the **computational basis** to the **frequency basis**.
- QFT is a central tool in many quantum algorithms such as **Shor's Algorithm** and **Phase Estimation**.

#### 2. Mathematical Definition

For an **n-qubit system**, let

- The number of possible states be  $N = 2^n$
- A computational basis state be  $|x\rangle$ , where  $x \in \{0,1,...,N-1\}$

Then the Quantum Fourier Transform is defined as:

QFT(
$$|\mathbf{x}\rangle$$
) = (1 /  $\sqrt{N}$ )  $\Sigma$  (from y = 0 to N-1) [  $e^{(2\pi \mathbf{i} \cdot \mathbf{x} \cdot \mathbf{y} / \mathbf{N})}$  |y $\rangle$ ]

#### 3. Matrix Form of QFT

The QFT is represented by an  $N \times N$  unitary matrix:

QFT = 
$$(1 / \sqrt{N})$$
  $\begin{bmatrix} 1, 1, 1, ..., 1 \\ 1, \omega, \omega^2, ..., \omega^{\wedge}(N-1) \\ 1, \omega^2, \omega^4, ..., \omega^{\wedge}(2(N-1)) \\ ... \\ 1, \omega^{\wedge}(N-1), \omega^{\wedge}(2(N-1)), ..., \omega^{\wedge}((N-1)(N-1)) \end{bmatrix}$ 

where

 $\omega = e^{(2\pi i / N)}$  (the primitive N-th root of unity).

### 4. Properties of QFT

- 1. **Unitary**  $\rightarrow$  QFT  $\cdot$  QFT $\dagger$  = I
- Efficient → Implemented with O(n²) quantum gates vs. O(N²) in classical DFT.
- 3. **Reversible**  $\rightarrow$  Inverse QFT exists, given by:

QFT<sup>-1</sup>(|x)) =  $(1 / \sqrt{N}) \Sigma$  (from y=0 to N-1) [ e^(-2 $\pi$ i·x·y/N) |y) ]

### 5. Circuit Implementation

For an **n-qubit register**  $|x_1x_2...x_n\rangle$ :

- Apply a **Hadamard** (**H**) on the first qubit.
- Apply controlled **phase shift gates (Rk)**:

 $R_k = |0\rangle\langle 0| + e^{(2\pi i/2^k)} |1\rangle\langle 1|$ 

- Repeat for all qubits.
- Apply **SWAP gates** at the end to reverse qubit order.

### 6. Example (QFT on 2 qubits, N=4)

Let input =  $|x\rangle = |1\rangle$  (binary 01, decimal 1).

QFT(
$$|1\rangle$$
) = (1/2) [  $|0\rangle$  +  $i|1\rangle$  -  $|2\rangle$  -  $i|3\rangle$  ]

This spreads amplitudes in the frequency basis.

#### 7. Applications of QFT

- 1. Shor's Algorithm  $\rightarrow$  integer factoring.
- 2. Quantum Phase Estimation (QPE)  $\rightarrow$  finding eigenvalues of unitary operators.
- 3. **Period Finding**  $\rightarrow$  crucial for factoring.
- 4. **Hidden Subgroup Problem** → general algorithmic framework.

#### 8. Importance

- Provides **exponential speedup** compared to classical Fourier transform.
- The backbone of many powerful quantum algorithms.
- Showcases quantum parallelism.

#### 1. Definition

Quantum Phase Estimation (QPE) is a quantum algorithm used to estimate the **phase**  $(\phi)$  in the eigenvalue equation of a unitary operator.

If  $U | u \rangle = e^{(2\pi i \cdot \phi)} | u \rangle$ , then the goal of QPE is to find the value of  $\phi$ , where  $0 \le \phi < 1$ .

#### 2. Basic Idea

- QPE uses two quantum registers:
  - First register (m qubits): stores the phase information.
  - 2. **Second register:** contains the eigenvector  $|u\rangle$ .
- The algorithm encodes  $\varphi$  into the first register using controlled operations, then applies the **Inverse Quantum Fourier Transform (QFT**<sup>-1</sup>) to extract the binary digits of  $\varphi$ .

### 3. Steps of the Algorithm

1. Initialize:

State =  $|0...0\rangle \otimes |u\rangle$ 

2. **Hadamard** Gates: Apply H to each qubit in the first register → creates superposition:

 $(1/\sqrt{(2^m)}) \Sigma$  (k=0 to 2<sup>m</sup>-1) |k $\rangle \otimes$  |u $\rangle$ 

3. Controlled-U operations: Apply controlled-U^(2^j)  $\rightarrow$  introduces phase shift:  $(1/\sqrt{(2^m)}) \Sigma$  (k=0 to 2<sup>m</sup>-1)  $e^(2\pi i \cdot \phi \cdot k)$  |k\rangle  $\otimes$  |u\rangle

Inverse QFT:
 Apply QFT<sup>-1</sup> on first register → converts phase information into binary representation.

5. Measurement:

Measure first register  $\rightarrow$  gives an **m-bit** approximation of  $\varphi$ .

# 4. Formula

- Eigenvalue relation:  $U |u\rangle = e^{(2\pi i \cdot \phi)} |u\rangle$
- Final superposition before inverse QFT:  $(1/\sqrt{(2^m)}) \Sigma$  (k=0 to 2<sup>m</sup>-1)  $e^{(2\pi i \cdot \phi \cdot k)} |k\rangle \otimes |u\rangle$
- After QFT<sup>-1</sup>:  $PT^{-1} = PT^{-1} = PT^{-1$

### 5. Example

If  $U|u\rangle = e^{(2\pi i \cdot (3/8))} |u\rangle$ , then  $\varphi = 3/8$ .

- Binary expansion:  $\varphi = 0.011_2$
- QPE with 3 qubits in the first register gives output 011.

• Hence measurement result  $\approx 3/8$ .

#### 6. Applications

- Shor's Algorithm → used for order finding and factoring.
- 2. **Quantum Simulation** → estimating energy levels of molecules.
- 3. **Quantum Chemistry** → eigenvalue computation of Hamiltonians.
- 4. **Hidden Subgroup Problems** and **Discrete Logarithms**.

#### Order-Finding and Factoring in Quantum Computing

#### 1. Introduction

- **Factoring**: The problem of finding prime factors of a large integer **N**.
- Order-finding: A related mathematical problem, used as a subroutine in Shor's algorithm for factoring.
- Classical algorithms for factoring are slow (subexponential), while quantum algorithms using order-finding are exponentially faster.

# 2. Order-Finding Problem

#### Definition

Given two integers:

- A positive integer N
- An integer  $\mathbf{a}$ , where  $gcd(\mathbf{a}, \mathbf{N}) = 1$

The **order r of a modulo N** is the smallest positive integer r such that:

$$a^r \equiv 1 \pmod{N}$$

### Example

Let N = 15, a = 2.

• Compute powers: 
$$2^1 = 2 \mod 15$$
  $2^2 = 4 \mod 15$   $2^3 = 8 \mod 15$   $2^4 = 16 \equiv 1 \mod 15$ 

So, order r = 4.

### 3. Factoring Using Order-Finding

#### Key Idea

Factoring a number N can be reduced to finding the order of a random number a modulo N.

- 1. Choose random  $\mathbf{a} < \mathbf{N}$  with  $gcd(\mathbf{a}, \mathbf{N}) = 1$ .
- 2. Find order **r** of **a mod N** using **Quantum Phase** Estimation + modular exponentiation.
- 3. If **r** is even, compute:

$$\begin{array}{lll} p &=& gcd(a^{\wedge}(r/2) & & - & & 1, & & N) \\ q &=& gcd(a^{\wedge}(r/2)+1, N) & & & & \end{array}$$

These give non-trivial factors of N.

## Example (Factoring N = 15)

- 1. Pick a = 2.
- 2. Order r = 4 (as shown earlier).
- 3. Compute:

$$\circ$$
  $a^{(r/2)} = 2^2 = 4$ 

$$\gcd(4-1, 15) = \gcd(3, 15) = 3$$

$$\circ$$
 gcd(4 + 1, 15) = gcd(5, 15) = 5

Thus, factors of 15 are 3 and 5.

### 4. Quantum Algorithm for Order-Finding

- Superposition: Create uniform superposition of states.
- Modular Exponentiation: Apply U: |x⟩ → |a<sup>x</sup> mod N⟩.
- 3. **Quantum Phase Estimation (QPE)**: Extract the phase related to order **r**.
- 4. Classical Post-Processing: Use continued fractions to recover r from measured phase.

### 5. Importance

- Order-finding is the core quantum subroutine of Shor's factoring algorithm.
- Factoring large integers is hard for classical computers (basis of RSA cryptography).
- Quantum order-finding allows efficient factoring, breaking RSA security.

#### Applications of the Quantum Fourier Transform (QFT)

The QFT is a key mathematical tool in quantum computing. Its main applications arise from its ability to **detect periodicity** in quantum states. Many important quantum algorithms are built upon this property.

#### 1. Period-Finding

### Concept

- Period-finding means determining the repeating pattern (period) in a function.
- If a function f(x) is periodic with period r, then f(x) = f(x + r).
- The QFT helps to extract this period efficiently from a quantum state encoding the function values.

#### Steps

- 1. Encode function f(x) into quantum states.
- 2. Apply **superposition** over inputs.
- Perform QFT to convert the state into frequency space.
- 4. Measurement gives information about the **period r**.

#### Importance

- **Shor's Algorithm** for factoring integers uses period-finding.
- Classical methods for period-finding are exponential time, but QFT makes it polynomial time.

### 2. Discrete Logarithms

### Concept

- The **discrete logarithm problem**: Given g and h =  $g^x \pmod{p}$ , find the integer x.
- This is very hard for classical computers (basis of many cryptosystems).
- QFT helps solve it by turning it into a hidden period problem.

## Steps

- 1. Encode powers of g into quantum states.
- 2. Use QFT to find the hidden periodicity between powers of g and the value h.
- 3. From the period, extract the discrete logarithm x.

#### Importance

- Breaks cryptographic systems like **Diffie–Hellman key exchange** and **ElGamal encryption**.
- Shows how quantum computing threatens classical cryptography.

## 3. Hidden Subgroup Problem (HSP)

### Concept

- A general problem in group theory: Suppose we have a function f defined on a group G.
- The function is constant on cosets of a **hidden** subgroup **H** ⊆ G, and different on different cosets.

• Goal: Find the hidden subgroup H.

#### Steps

- 1. Encode the group elements into quantum states.
- 2. Apply superposition over the group.
- 3. Use **QFT** to reveal information about the subgroup structure.
- Measurement yields generators of the hidden subgroup.

#### Importance

- Period-finding and discrete logarithms are special cases of HSP.
- Shor's algorithm and many other quantum algorithms can be understood as solving HSP.
- Generalizing HSP helps design new quantum algorithms.