

An Introduction to Quantum Mechanics 1

Dr. Hugo García Tecocoatzi

Instituto Tecnológico y de Estudios Superiores de Monterrey

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Quantum Mechanics?

- Quantum mechanics is the most accurate description of nature known.
- It forms the foundation of **quantum computation** and **quantum information**.
- Our goal: understand just enough quantum mechanics to work with quantum algorithms and information.
- No prior physics knowledge is required only **elementary linear algebra**.

Quantum Mechanics: Easier Than You Think

- Reputation: “Quantum mechanics is mysterious and difficult.”
- Reality:
 - The hard part is applying it to **complex molecules** or advanced physics.
 - The **foundations** are straightforward, once you know linear algebra.
- We focus only on concepts essential for quantum computing.

How to Learn This Chapter

- Readers with prior QM knowledge: skim for notational conventions.
- Beginners: work carefully through the material and exercises.
- Tip: If an exercise feels difficult, move on—return later.
- Key prerequisite: **linear algebra** (vectors, matrices, inner products).

Quantum Mechanics for Computing

- ➊ Review of linear algebra (vectors, inner products, operators).
- ➋ Physicists' notation (Dirac's bra-ket notation).
- ➌ Postulates of quantum mechanics.
- ➍ Simple systems: qubits and quantum states.

Linear Algebra for Quantum Mechanics

- Quantum mechanics is expressed using the language of **linear algebra**.
- Core objects:
 - **Vector spaces** (e.g. \mathbb{C}^n).
 - **Linear operations** on these spaces.
- **Dirac notation**, which looks unfamiliar at first.
- Main challenge for beginners: not the postulates of QM, but the **linear algebraic formalism**.

Vector Spaces

- The vector space of primary interest: \mathbb{C}^n .
- Elements (vectors) are n -tuples of complex numbers:

$$(z_1, z_2, \dots, z_n) \in \mathbb{C}^n$$

- Often written in column form:

$$\begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix}$$

- Vectors are the building blocks of quantum states.

Vector Addition

- In \mathbb{C}^n , vectors can be added component-wise:

$$\begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix} + \begin{bmatrix} z'_1 \\ \vdots \\ z'_n \end{bmatrix} = \begin{bmatrix} z_1 + z'_1 \\ \vdots \\ z_n + z'_n \end{bmatrix}$$

- This is the familiar vector addition you already know, extended to complex entries.

Scalar Multiplication

- A scalar (complex number z) can multiply a vector:

$$z \cdot \begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix} = \begin{bmatrix} zz_1 \\ \vdots \\ zz_n \end{bmatrix}$$

- Scalars “scale” every component of the vector.
- Together, vector addition and scalar multiplication define the structure of a vector space.

Dirac Notation: Vectors as Kets

- In quantum mechanics, vectors are written using **Dirac notation**.
- A vector is denoted as:

$$|\psi\rangle$$

- ψ is just a label (any symbol can be used).
- The vertical bar “|” and angle “)” indicate that this object is a vector.
- $|\psi\rangle$ is called a **ket**.

The Zero Vector

- Every vector space has a special element: the **zero vector**.
- Denoted simply by:

$$0$$

- Property:

$$|v\rangle + 0 = |v\rangle \quad \text{for any vector } |v\rangle$$

- Exception: we do not write $|0\rangle$ for the zero vector.
- In quantum mechanics, $|0\rangle$ means something else (a specific quantum state).

Scalar Multiplication in Dirac Notation

- For a scalar $z \in \mathbb{C}$ and vector $|\psi\rangle$:

$$z|\psi\rangle$$

is also a vector in the same space.

- For the zero vector:

$$z \cdot 0 = 0 \quad \text{for any scalar } z$$

- Example in \mathbb{C}^n :

$$z \cdot (z_1, \dots, z_n) = (zz_1, \dots, zz_n)$$

$$2 \cdot (3, 4, i) = (6, 8, 2i)$$

Dirac Notation: Vectors and Inner Products

- z^* : complex conjugate of z .
Example: $(1 + i)^* = 1 - i$.
- $|\psi\rangle$: vector (ket).
- $\langle\psi|$: dual vector (bra).
- $\langle\phi|\psi\rangle$: inner product between $|\phi\rangle$ and $|\psi\rangle$.

Example

For $|\psi\rangle = \begin{bmatrix} 1 \\ i \end{bmatrix}$, $\langle\psi| = [1 \quad -i]$.

Tensor Products

- $|\phi\rangle \otimes |\psi\rangle$: tensor product of two vectors.
- Often abbreviated as $|\phi\rangle|\psi\rangle$.
- Forms a larger vector space: $\mathbb{C}^m \otimes \mathbb{C}^n$.

Example

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

Spanning Sets

- A set of vectors $\{|v_1\rangle, |v_2\rangle, \dots, |v_n\rangle\}$ is a **spanning set** if any vector $|v\rangle$ can be written as:

$$|v\rangle = \sum_i a_i |v_i\rangle$$

- Example: In \mathbb{C}^2 , the standard spanning set is:

$$|v_1\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |v_2\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- Any vector

$$|v\rangle = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$$

can be written as:

$$|v\rangle = a_1 |v_1\rangle + a_2 |v_2\rangle$$

Alternative Spanning Sets

- A vector space may have many different spanning sets.
- Example: Another spanning set for \mathbb{C}^2 is

$$|v_1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad |v_2\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

- Any vector $|v\rangle = (a_1, a_2)$ can be written as:

$$|v\rangle = \frac{a_1 + a_2}{\sqrt{2}} |v_1\rangle + \frac{a_1 - a_2}{\sqrt{2}} |v_2\rangle$$

Linear Dependence and Independence

- A set of nonzero vectors $\{|v_1\rangle, \dots, |v_n\rangle\}$ is **linearly dependent** if there exist complex numbers a_1, \dots, a_n , not all zero, such that:

$$a_1|v_1\rangle + a_2|v_2\rangle + \dots + a_n|v_n\rangle = 0$$

- Otherwise, the vectors are **linearly independent**.
- Independence \Rightarrow no vector in the set can be written as a linear combination of the others.

Basis and Dimension

- A **basis** is a spanning set of linearly independent vectors.
- Any two bases of the same vector space contain the same number of elements.
- This number is the **dimension** of the vector space.
- Example: \mathbb{C}^2 has dimension 2.
- Standard basis:

$$\{|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}\}$$

- Alternative basis:

$$\{|+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, |-\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}\}$$

Basis and Qubits

- A **basis** is a spanning set of linearly independent vectors.
- Any vector in the space can be written uniquely as a linear combination of basis vectors.
- For a single qubit, the vector space is \mathbb{C}^2 .

Computational Basis

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

- Any qubit state can be written as:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad \alpha, \beta \in \mathbb{C}, \quad |\alpha|^2 + |\beta|^2 = 1$$

- Other useful bases exist, e.g. the **Hadamard basis**:

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \quad |-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$$

What is an Operator?

- Mathematically: A linear operator A maps vectors to vectors

$$A : |v\rangle \mapsto A|v\rangle = |w\rangle$$

- Physically: An operator represents an **action** or a **transformation**.
 - Example: Translation, rotation, reflection
 - In quantum mechanics: **observables** (measurable quantities) are represented by operators
- Operators encode how a system evolves or how measurements are made.

Operators as Physical Actions

- Think of a vector $|v\rangle$ as a **state of a system**.
- An operator A acts like a machine: it takes one state and produces another.

$$|v'\rangle = A|v\rangle$$

- Examples:
 - **Translation Operator**: shifts a particle in space.
 - **Rotation Operator**: rotates spin or spatial orientation.
 - **Hamiltonian Operator**: generates time evolution.

Operators and Observables

- In quantum mechanics, every measurable property (**observable**) corresponds to an operator.

Observable \longleftrightarrow Hermitian operator

- Examples:
 - Position \hat{x} operator
 - Momentum \hat{p} operator
 - Energy (Hamiltonian) \hat{H}
- Measurement: applying the operator corresponds to asking "what value does this physical property have?"

Why Operators Matter

- Operators connect the abstract math (linear algebra) to the real physics.
- They tell us:
 - How states evolve (dynamics)
 - What outcomes measurements can produce (eigenvalues)
 - Probabilities of outcomes (through inner products)
- **Keep in mind:** Operators are the bridge between quantum states and physical reality.

Matrix Representation of Operators

- Let $A : V \rightarrow W$, with bases $\{|v_1\rangle, \dots, |v_m\rangle\}$ for V and $\{|w_1\rangle, \dots, |w_n\rangle\}$ for W .
- Then for each j :

$$A|v_j\rangle = \sum_i A_{ij}|w_i\rangle$$

- The matrix with entries A_{ij} is the **matrix representation** of A .
- Thus:
 - Operators \Leftrightarrow Matrices
 - Vectors \Leftrightarrow Column vectors
 - Composition \Leftrightarrow Matrix multiplication

Operators as Matrices

- Any $m \times n$ matrix A with entries A_{ij} acts as a linear operator:

$$A \left(\sum_i a_i |v_i\rangle \right) = \sum_i a_i A|v_i\rangle$$

- Action = matrix multiplication on column vectors.
- Example: $A = \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix}$, $|v\rangle = \begin{bmatrix} x \\ y \end{bmatrix}$, $A|v\rangle = \begin{bmatrix} x + 2y \\ y \end{bmatrix}$

Linear Operators

- A linear operator $A : V \rightarrow W$ is a function satisfying:

$$A \left(\sum_i a_i |v_i\rangle \right) = \sum_i a_i A|v_i\rangle$$

- Acts linearly on vectors in V .
- If $A : V \rightarrow V$, we simply say " A is defined on V ."
- Important operators:
 - Identity operator: $I|v\rangle = |v\rangle$
 - Zero operator: $0|v\rangle = 0$

Matrices and Hermitian Conjugates

- A^* : element-wise complex conjugate of matrix A .
- A^T : transpose of A .
- A^\dagger : Hermitian conjugate (adjoint): $A^\dagger = (A^T)^*$.

Example

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix}^\dagger = \begin{bmatrix} a^* & c^* \\ b^* & d^* \end{bmatrix}$$

- $\langle \phi | A | \psi \rangle$: inner product between $|\phi\rangle$ and $A|\psi\rangle$. Equivalently $\langle A^\dagger \phi | \psi \rangle$.

Composition of Operators

- If $A : V \rightarrow W$ and $B : W \rightarrow X$, then their composition is:

$$(BA)(|v\rangle) = B(A(|v\rangle))$$

- Abbreviated as: $BA|v\rangle$
- Operators can be chained just like functions.
The matrix multiplication.

Composition \Rightarrow Matrix Multiplication 1

Setup

$$A = \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad |v\rangle = \begin{bmatrix} x \\ y \end{bmatrix}$$

Step 1: Apply A

$$A|v\rangle = \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} x + 2y \\ y \end{bmatrix}$$

Step 2: Apply B to the result

$$B(A|v\rangle) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x + 2y \\ y \end{bmatrix} = \begin{bmatrix} y \\ x + 2y \end{bmatrix}$$

Composition \Rightarrow Matrix Multiplication 2

Compute the composite matrix BA

$$BA = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 \cdot 1 + 1 \cdot 0 & 0 \cdot 2 + 1 \cdot 1 \\ 1 \cdot 1 + 0 \cdot 0 & 1 \cdot 2 + 0 \cdot 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 2 \end{bmatrix}$$

Check (matrix–vector in one shot)

$$(BA)|v\rangle = \begin{bmatrix} 0 & 1 \\ 1 & 2 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} y \\ x + 2y \end{bmatrix}$$

$$\Rightarrow B(A|v\rangle) = (BA)|v\rangle$$

Exercise: Composition = Matrix Multiplication

- Show that applying two operators in sequence is the same as multiplying their matrices.
- Method:
 - 1 Apply the first matrix to the vector, then the second.
 - 2 Multiply the matrices first, then apply the result to the vector.
 - 3 Verify that both give the same answer.

Operators:

$$A = \begin{bmatrix} 1 & 2 \\ 0 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

Vector:

$$|v\rangle = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$$

Evaluate:

$$BA|v\rangle$$