Module 2 : Mathematical Foundations of Quantum Mechanics

(Lecture Notes for Engineering Physics : BAPHY105)

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Disclaimer

These lecture notes do not claim originality. They are an assimilation of existing materials from various standard textbooks and lecture notes, compiled and reorganized to suit the structure and requirements of the course syllabus.

Note

These lecture notes are continuously updated based on classroom discussions and questions asked by students. There may still be mistakes, and if you find any, please feel free to write to me at vishnudath.kn@vit.ac.in.

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Module 2

Mathematical Foundations of Quantum Mechanics

Why study this module?

Quantum mechanics is based on a mathematical language that's quite different from what we use in classical physics. Instead of working with positions, velocities and forces, quantum mechanics uses states, operators and probabilities.

To actually do quantum mechanics (not just talk about it), we need to learn that language. That's what this module is about. It gives you the essential mathematical tools of quantum theory. We start with linear algebra and build up to something called Hilbert space.

You already know what a vector is, like in 3D space. In this module, we generalize that idea to:

- Vectors with complex components (because quantum amplitudes are complex)
- Vector spaces that can have infinite dimensions (like spaces of functions)
- Operations like inner products, orthogonality and projections, which are key to understanding how quantum systems evolve and how we measure them

If classical mechanics is geometry with vectors and forces, then quantum mechanics is geometry in an abstract space of possibilities.

This module helps you get comfortable with that new space. It's not just math in the background, it's the actual framework that quantum mechanics lives in.

2.1 Linear Vector Spaces and Basis

- A **vector space** is a collection of vectors (like $|\alpha\rangle, |\beta\rangle, |\gamma\rangle$, etc.) along with a set of scalars (like $a, b, c, \ldots$).
- The space is **closed** under two operations:
  - **Vector addition:** Adding two vectors gives another vector in the same space:

$$|\alpha\rangle + |\beta\rangle = |\gamma\rangle \tag{2.1}$$

  - **Scalar multiplication:** Multiplying a vector by a scalar gives another vector in the space:

$$a\,|\alpha\rangle = |\gamma\rangle \tag{2.2}$$

- **Vector addition** satisfies the following rules:
  - **Commutative:**

$$|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle \tag{2.3}$$

  - **Associative:**

$$|\alpha\rangle + (|\beta\rangle + |\gamma\rangle) = (|\alpha\rangle + |\beta\rangle) + |\gamma\rangle \tag{2.4}$$

  - There exists a **zero vector** $|0\rangle$ such that:

$$|\alpha\rangle + |0\rangle = |\alpha\rangle \tag{2.5}$$

  - Every vector has an **additive inverse** (or negative) such that:

$$|\alpha\rangle + (-\,|\alpha\rangle) = |0\rangle \tag{2.6}$$

- **Scalar multiplication** satisfies:
  - **Distributivity over vector addition:**

$$a(|\alpha\rangle + |\beta\rangle) = a\,|\alpha\rangle + a\,|\beta\rangle \tag{2.7}$$

  - **Distributivity over scalar addition:**

$$(a+b)\,|\alpha\rangle = a\,|\alpha\rangle + b\,|\alpha\rangle \tag{2.8}$$

  - **Associativity of scalar multiplication:**

$$a(b\,|\alpha\rangle) = (ab)\,|\alpha\rangle \tag{2.9}$$

  - Multiplying by 1 and 0 gives:

$$1\,|\alpha\rangle = |\alpha\rangle\,, \quad 0\,|\alpha\rangle = |0\rangle \tag{2.10}$$

- A **linear combination** means multiplying vectors by scalars and adding them:

$$a\,|\alpha\rangle + b\,|\beta\rangle + c\,|\gamma\rangle + \cdots \tag{2.11}$$

- A vector is **linearly independent** if it cannot be written as a linear combination of other vectors.
- A set of vectors is **linearly independent** if no vector in the set can be expressed as a combination of the others.
- A set of vectors **spans** the space if every vector in the space can be written as a linear combination of them.
- A **basis** is a set of vectors that are:

  - Linearly independent, and
  - Span the entire space.

- The **dimension** of a vector space is the number of vectors in any basis of that space.

- Any vector $|v\rangle$ can be written uniquely as a linear combination of basis vectors:

$$|v\rangle = \sum_i c_i |e_i\rangle \tag{2.12}$$

  where $|e_i\rangle$ are the basis vectors and c_i are the components of the vector in that basis.

- This means a vector is represented by a list (or tuple) of its components:

$$|\alpha\rangle \leftrightarrow (a_1, a_2, \ldots, a_n) \tag{2.13}$$

- Operations on vectors translate to operations on their components:

$$|\alpha\rangle + |\beta\rangle \leftrightarrow (a_1 + b_1, a_2 + b_2, \ldots) \tag{2.14}$$

$$c|\alpha\rangle \leftrightarrow (ca_1, ca_2, \ldots) \tag{2.15}$$

- The **zero vector** has all components equal to zero:

$$|0\rangle \leftrightarrow (0, 0, \ldots, 0) \tag{2.16}$$

- The **negative of a vector** has all components with the opposite sign:

$$-|\alpha\rangle \leftrightarrow (-a_1, -a_2, \ldots, -a_n) \tag{2.17}$$

- Working with components is often easier, but it depends on your **choice of basis**. The same vector will have different components in different bases.

2.2 Inner Products in Vector Space

- The dot product in three-dimensional cartesian space generalizes to the **inner product**, which works in any dimension and allows complex vectors.

- The inner product between two vectors $|\alpha\rangle$ and $|\beta\rangle$ is a complex number $\langle\alpha|\beta\rangle$ satisfying:

  1. $\langle\beta|\alpha\rangle = \langle\alpha|\beta\rangle^*$
  2. $\langle\alpha|\alpha\rangle \geq 0$, and $\langle\alpha|\alpha\rangle = 0 \iff |\alpha\rangle = |0\rangle$
  3. $\langle\alpha|b\beta + c\gamma\rangle = b\langle\alpha|\beta\rangle + c\langle\alpha|\gamma\rangle$

- A vector space with an inner product is called an **inner product space**.

Vector Space Concept	**3D Cartesian Vectors**	**Polynomials of Degree ≤ 5 with real coefficients**	**Complex 2×2 Matrices**
Vectors	$\vec{v} = (x, y, z)$	$p(x) = a_0 + a_1 x + \cdots + a_5 x^5$	$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad a, b, c, d \in \mathbb{C}$
Scalars	$\mathbb{R}$	$\mathbb{R}$	$\mathbb{C}$
Addition	$(x_1, y_1, z_1) + (x_2, y_2, z_2) = (x_1 + x_2,\ y_1 + y_2,\ z_1 + z_2)$	$p(x) + q(x)$	$\begin{pmatrix} a_1 & a_2 \\ a_3 & a_4 \end{pmatrix} + \begin{pmatrix} b_1 & b_2 \\ b_3 & b_4 \end{pmatrix} = \begin{pmatrix} a_1 + b_1 & a_2 + b_2 \\ a_3 + b_3 & a_4 + b_4 \end{pmatrix}$
Scalar Multiplication	$a(x, y, z) = (ax, ay, az)$	$a \cdot p(x)$	$\lambda A = \begin{pmatrix} \lambda a & \lambda b \\ \lambda c & \lambda d \end{pmatrix}, \quad \lambda \in \mathbb{C}$
Zero Vector	$(0, 0, 0)$	$0 + 0x + \cdots + 0x^5$	$\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$
Basis	$\hat{i}, \hat{j}, \hat{k}$	$\{1, x, x^2, \ldots, x^5\}$	Standard matrices: $\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$
Dimension	3	6	4 (over $\mathbb{C}$)
Linear Independence	Vectors not in same plane	Monomials $\{1, x, x^2, \ldots\}$	Basis matrices above are linearly independent

Table 2.1: Examples of vector spaces across different contexts

- The **norm** (or length) of a vector is defined as:

$$\|\alpha\| \equiv \sqrt{\langle \alpha | \alpha \rangle} \tag{2.18}$$

- A vector with norm 1 is called **normalized** or a **unit vector**.
- Two vectors are **orthogonal** if $\langle \alpha | \beta \rangle = 0$.
- A set of vectors $\{|\alpha_i\rangle\}$ is **orthonormal** if[1]:

$$\langle \alpha_i | \alpha_j \rangle = \delta_{ij} \tag{2.19}$$

[1] δ_{ij}, known as Kronecker delta, is defined as $\delta_{ij} = 1$ if $i = j$, and 0 otherwise.

- In an orthonormal basis, inner products and norms simplify (Explained later in section 2.4):

$$\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + \cdots + a_n^* b_n \tag{2.20}$$

$$\langle\alpha|\alpha\rangle = |a_1|^2 + |a_2|^2 + \cdots + |a_n|^2 \tag{2.21}$$

$$a_i = \langle e_i|\alpha\rangle\,, b_i = \langle e_i|\beta\rangle \tag{2.22}$$

- These generalize the familiar 3D formulas:

$$\vec{a}\cdot\vec{b} = a_x b_x + a_y b_y + a_z b_z, \quad |\vec{a}|^2 = a_x^2 + a_y^2 + a_z^2 \tag{2.23}$$

- The **Schwarz inequality** (also called the Cauchy–Schwarz inequality):

$$|\langle\alpha|\beta\rangle|^2 \le \langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \tag{2.24}$$

2.3 Hilbert Space

We have now understood what it means to have a complex vector space, how to define an inner product on it, and how this leads to notions of length, angles, orthogonality, and projection, even when the vectors are functions.

Let us now see how this framework becomes the natural setting for quantum mechanics.

What Is a Hilbert Space?

A **Hilbert space** is a complex vector space equipped with an inner product that satisfies an important additional condition: it is *complete* with respect to the norm defined by the inner product.

More precisely, it has the following properties:

- It is a complex vector space → we can add functions and multiply them by complex numbers.
- It has an inner product $\langle\phi|\psi\rangle$, which allows us to define notions like length, angle, and orthogonality.
- It is **complete**, meaning that certain sequences of vectors (called Cauchy sequences) always converge to a well-defined vector within the space.

Why Hilbert Space?

In quantum mechanics, the state of a particle is represented by a wavefunction $\psi(x)$, which is a complex-valued function of position. We want to treat these functions as vectors in a space where we can do linear algebra, take inner products, expand in bases, and define observables as operators (as we will see later).

However, not all functions are suitable. To interpret $|\psi(x)|^2$ as a probability density, we require[2]:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx < \infty \tag{2.25}$$

[2]This is just the condition of Normalizability that we have seen in Module 1.

Such functions are called **square-integrable**, and they form a space denoted $L^2(\mathbb{R})$. This space, together with the inner product

$$\langle\phi|\psi\rangle = \int_{-\infty}^{\infty} \phi^*(x)\psi(x)dx \tag{2.26}$$

is an example of a Hilbert space.

Summary

A Hilbert space is:

- A complex vector space
- Equipped with an inner product
- Complete with respect to the norm defined by that inner product

It provides the correct mathematical setting to describe quantum states as vectors (or more precisely, functions) with well-defined lengths, angles, and limits. From now on, when we refer to "the space of quantum states," we will mean a Hilbert space.

2.4 Geometric Meaning of the Inner Product

In quantum mechanics, the inner product $\langle\phi|\psi\rangle$ measures the "overlap" between the states $|\phi\rangle$ and $|\psi\rangle$. To build some intuition, consider an analogy with 3D vectors.

Suppose $|\psi\rangle$ is a 3-dimensional vector:

$$|\psi\rangle = a\,|i\rangle + b\,|j\rangle + c\,|k\rangle \tag{2.27}$$

where $|i\rangle, |j\rangle, |k\rangle$ are orthonormal basis vectors in Euclidean space. The coefficients are obtained using inner products:

$$\langle i|\psi\rangle = a, \quad \langle j|\psi\rangle = b, \quad \langle k|\psi\rangle = c \tag{2.28}$$

Each inner product tells us how much of $|\psi\rangle$ lies in the direction of a given basis vector, i.e., it is the projection (or shadow) of $|\psi\rangle$ along that axis.

In this sense, the inner product is a measure of directional alignment between two vectors. The full vector can be reconstructed from its projections:

$$|\psi\rangle = \langle i|\psi\rangle\,|i\rangle + \langle j|\psi\rangle\,|j\rangle + \langle k|\psi\rangle\,|k\rangle \tag{2.29}$$

We can generalize this to any discrete vector space. Suppose $\{|e_i\rangle\}$ denotes an *orthonormal basis* for any vector space. Then any vector in that space, $|\psi\rangle$, can be represented as a linear combination of the basis vectors:

$$|\psi\rangle = \sum_i c_i\,|e_i\rangle = \sum_i \langle e_i|\psi\rangle\,|e_i\rangle \tag{2.30}$$

This can be seen easily by taking

$$\langle e_j|\psi\rangle = \langle e_j|\sum_i c_i\,|e_i\rangle\rangle = \sum_i c_i\,\langle e_j|e_i\rangle = \sum_i c_i\delta_{ij} = c_j \tag{2.31}$$

where, in the last step, we have used the orthonormality property $\langle e_j|e_i\rangle = \delta_{ij}$.

2.4.1 Vectors as Column Vectors

Since any vector can be represented as $|\psi\rangle = \sum_i c_i |e_i\rangle$, we can also write $|\psi\rangle$ simply in terms of its projections along the basis vectors:

$$|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix} \tag{2.32}$$

2.5 Dirac Notation: Bras and Kets

Paul Dirac introduced a compact and powerful notation for quantum mechanics based on abstract vector spaces. He split the inner product $\langle\phi|\psi\rangle$ into two halves: a ket $|\psi\rangle$ and a bra $\langle\phi|$. In this formalism:

- A **ket** $|\psi\rangle$ represents a vector (state) in a Hilbert space.
- A **bra** $\langle\phi|$ is the Hermitian adjoint (or dual) of a ket. Thus, $\langle\phi| = (|\phi\rangle)^\dagger$. The adjoint operation is defined as

  $$(|\phi\rangle)^\dagger = (|\phi\rangle^*)^T \tag{2.33}$$

  that is, the transpose of the complex conjugate. For every vector in the ket space, there exists a corresponding bra vector (or dual vector) in the dual space. Thus, for the ket vector in Eq. 2.32,

  $$\langle\psi| = (|\psi\rangle)^\dagger = \begin{pmatrix} c_1^* & c_2^* & \cdots \end{pmatrix} \tag{2.34}$$

- The quantity $\langle\phi|\psi\rangle$ denotes the overlap between the two vectors $|\phi\rangle$ and $|\psi\rangle$. Thus in general, if $|\psi\rangle = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$ and $|\phi\rangle = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$, then,

  $$\langle\phi|\psi\rangle = (|\phi\rangle)^\dagger |\psi\rangle = b_1^* c_1 + b_2^* c_2 + b_3^* c_3. \tag{2.35}$$

Kets as Vectors, Bras as Linear Functionals

Kets live in a complex vector space, while bras live in the dual space. The bra $\langle\phi|$ acts on a ket $|\psi\rangle$ to produce a complex number:

$$\langle\phi|\psi\rangle \in \mathbb{C} \tag{2.36}$$

In infinite-dimensional spaces (such as the space of square-integrable functions), we interpret:

$$\langle\phi|\psi\rangle = \int_{-\infty}^{\infty} \phi^*(x)\psi(x)\, dx \tag{2.37}$$

This generalizes the notion of the dot product and expresses the overlap (or interference) between two states.

Summary

- $|\psi\rangle$ (ket vector): abstract state vector
- $\langle\phi|$ (bra vector): Hermitian adjoint of a ket
- $\langle\phi|\psi\rangle$: complex number (measure of overlap)

2.5.1 From Geometry to Quantum Mechanics

In mathematics, the inner product between two vectors measures their "directional overlap" in an abstract vector space. In quantum mechanics, the inner product $\langle e_i|\psi\rangle$ between a basis vector $|e_i\rangle$ and a state vector $|\psi\rangle$ has a more specific interpretation: it is the **probability amplitude** for obtaining the outcome corresponding to $|e_i\rangle$ when the system is measured in that basis. The modulus squared $|\langle e_i|\psi\rangle|^2$ gives the probability of finding the system in the state $|e_i\rangle$ upon measurement.

Suppose we have a quantum state $|\psi\rangle$ in a space spanned by some orthonormal basis $\{|e_i\rangle\}$. Then we can express the state as:

$$|\psi\rangle = \sum_i \langle e_i|\psi\rangle\, |e_i\rangle \tag{2.38}$$

Thus, just as in geometry the inner product measures "directional overlap," in quantum mechanics it simultaneously encodes projection and the probability of obtaining a particular measurement outcome.

Example: Spin-$\frac{1}{2}$ System in the $\{|e_1\rangle, |e_2\rangle\}$ Basis

Consider a spin-$\frac{1}{2}$ particle (such as an electron). In the standard basis, we can take

$$|e_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |e_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

These could represent, for example, *spin-up* and *spin-down* along the z-axis.

A general state $|\psi\rangle$ in this basis can be written as:

$$|\psi\rangle = c_1 |e_1\rangle + c_2 |e_2\rangle = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix},$$

where c_1 and c_2 are complex numbers called **probability amplitudes**.

Probability Amplitudes and Probabilities

The inner products with the basis vectors give:

$$\langle e_1|\psi\rangle = c_1, \quad \langle e_2|\psi\rangle = c_2.$$

- c_1 is the probability amplitude for finding the particle in the state $|e_1\rangle$ when measured in this basis.
- c_2 is the probability amplitude for $|e_2\rangle$.

The **probabilities** are:

$$P(e_1) = |c_1|^2, \quad P(e_2) = |c_2|^2.$$

Normalization Condition

Since the system must be found in one of these two basis states upon measurement, the probabilities must sum to 1:

$$|c_1|^2 + |c_2|^2 = 1.$$

This condition is equivalent to:

$$\langle\psi|\psi\rangle = 1.$$

From the column-vector form:

$$\langle\psi|\psi\rangle = \begin{pmatrix} c_1^* & c_2^* \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = |c_1|^2 + |c_2|^2.$$

What If the State is Not Normalized?

Suppose we have

$$\langle\psi|\psi\rangle = N = |c_1|^2 + |c_2|^2,$$

where $N > 1$ but finite. To **normalize** the state, we define:

$$|\psi'\rangle = \frac{|\psi\rangle}{\sqrt{N}} = \frac{c_1}{\sqrt{N}} |e_1\rangle + \frac{c_2}{\sqrt{N}} |e_2\rangle .$$

Now:

$$\langle\psi'|\psi'\rangle = \frac{|c_1|^2 + |c_2|^2}{N} = 1,$$

and the probabilities become:

$$P(e_1) = \frac{|c_1|^2}{N}, \quad P(e_2) = \frac{|c_2|^2}{N}.$$

Worked Example

Let

$$|\psi\rangle = \begin{pmatrix} 2+i \\ 1 \end{pmatrix}.$$

First compute:

$$|c_1|^2 = |2+i|^2 = (2)^2 + (1)^2 = 5, \quad |c_2|^2 = |1|^2 = 1.$$

Thus:

$$N = |c_1|^2 + |c_2|^2 = 5 + 1 = 6.$$

The normalized state is:

$$|\psi'\rangle = \frac{1}{\sqrt{6}} \begin{pmatrix} 2+i \\ 1 \end{pmatrix}.$$

Probabilities are:

$$P(e_1) = \frac{5}{6}, \quad P(e_2) = \frac{1}{6}.$$

These now sum to 1, as required.

Practice Problems

1. **Linear Combination and Basis**

   Let $|e_1\rangle = (1,0)$ and $|e_2\rangle = (0,1)$ be an orthonormal basis for a 2D complex vector space. Let

$$|\psi\rangle = 3\,|e_1\rangle + (1+i)\,|e_2\rangle$$

   (a) Write $|\psi\rangle$ as a column vector.

   (b) Is this a linear combination of $\{|e_1\rangle, |e_2\rangle\}$?

   (c) What are the components $c_1 = \langle e_1|\psi\rangle$ and $c_2 = \langle e_2|\psi\rangle$?

2. **Linear Independence in a 2D Vector Space**

   Check if the following vectors are linearly independent :

$$|v_1\rangle = \begin{bmatrix} 2 \\ 3 \end{bmatrix}, \qquad |v_2\rangle = \begin{bmatrix} 4 \\ 6 \end{bmatrix}.$$

   Hint.

   - Two vectors in $\mathbb{R}^2$ (or $\mathbb{C}^2$) are linearly dependent iff one is a scalar multiple of the other.
   - To test this, try to find a scalar c such that $|v_2\rangle = c\,|v_1\rangle$. Equate components and check consistency:

$$c = \frac{(v_2)_1}{(v_1)_1}, \qquad c = \frac{(v_2)_2}{(v_1)_2},$$

     provided the denominators are nonzero. If both equal the same c, the vectors are dependent. If the components give a contradiction, they are independent.
   - Handle zero components carefully: if a component of $|v_1\rangle$ is zero, use the other component to determine c, and then check the zero-component equation for consistency.

   Solution.

$$\frac{(v_2)_1}{(v_1)_1} = \frac{4}{2} = 2, \qquad \frac{(v_2)_2}{(v_1)_2} = \frac{6}{3} = 2.$$

   Both components give the same scalar $c = 2$. Hence $|v_2\rangle = 2\,|v_1\rangle$, so $\{|v_1\rangle, |v_2\rangle\}$ is *linearly dependent.*

3. **Linear Independence in 3D**

   Check if the following vectors are linearly independent :

$$|v_1\rangle = \begin{bmatrix} 1 \\ 0 \\ 2 \end{bmatrix}, \qquad |v_2\rangle = \begin{bmatrix} 0 \\ 1 \\ 3 \end{bmatrix}, \qquad |v_3\rangle = \begin{bmatrix} 2 \\ 1 \\ 7 \end{bmatrix}.$$

Hint.

Direct-combination approach: try to express one column as a linear combination of the others. For example attempt

$$|v_3\rangle = a\ |v_1\rangle + b\ |v_2\rangle .$$

This gives a small linear system for a, b obtained by equating components:

$$\begin{cases} a \cdot 1 + b \cdot 0 = 2, \\ a \cdot 0 + b \cdot 1 = 1, \\ a \cdot 2 + b \cdot 3 = 7. \end{cases}$$

Solve the first two equations for a, b and then check the third for consistency. If consistent, the columns are dependent and you have an explicit relation.[3]

Solution From the first two component equations:

$$a = 2, \qquad b = 1.$$

Check the third component:

$$2 \cdot a + 3 \cdot b = 2 \cdot 2 + 3 \cdot 1 = 4 + 3 = 7,$$

which matches the third component of $|v_3\rangle$. Therefore

$$|v_3\rangle = 2\ |v_1\rangle + 1\ |v_2\rangle ,$$

so the three kets are *linearly dependent.* [4]

4. **Norm and Normalization**

   Given a vector $|\alpha\rangle = (2, i)$ in a 2D complex vector space with inner product

   $$\langle\alpha|\beta\rangle = \alpha_1^*\beta_1 + \alpha_2^*\beta_2$$

   (a) Compute $\langle\alpha|\alpha\rangle$ and hence find $\|\alpha\|$.

   (b) Normalize $|\alpha\rangle$ to get a unit vector $|\tilde{\alpha}\rangle$.

5. **Inner Product and Orthogonality**

   Let $|\phi\rangle = (1, -1)$, $|\chi\rangle = (1, 1)$. Consider the standard complex inner product.

   (a) Compute $\langle\phi|\chi\rangle$.

   (b) Are $|\phi\rangle$ and $|\chi\rangle$ orthogonal?

[3] An equivalent shortcut in $\mathbb{R}^3$ is to form the matrix $M = [|v_1\rangle\ \ |v_2\rangle\ \ |v_3\rangle]$ and compute $\det M$: if $\det M = 0$, the vectors are dependent; if $\det M \neq 0$, they are independent.

[4] Equivalently, $\det M = 0$.

6. **Orthonormal Basis Expansion**

   Let $\{|e_1\rangle, |e_2\rangle\}$ be an orthonormal basis and a state is given by

   $$|\psi\rangle = \frac{1}{\sqrt{2}}|e_1\rangle + \frac{i}{\sqrt{2}}|e_2\rangle$$

   (a) Find the norm of $|\psi\rangle$.

   (b) What is the probability of measuring the state $|e_2\rangle$?

7. **Hilbert Space and Square-Integrability**

   Which of the following functions $\psi(x)$ are square-integrable on $\mathbb{R}$? (meaning $\int_{-\infty}^{\infty} |\psi(x)|^2 dx < \infty$?)

   (a) $\psi(x) = \frac{1}{1+x^2}$

   (b) $\psi(x) = \sin(x)$

   (c) $\psi(x) = e^{-x^2}$

   Justify your answers qualitatively.

2.6 Matrix Representations and Operators

Once we fix a basis, we can represent all the objects in Dirac notation concretely using matrices and vectors.

We have already seen that in a finite-dimensional Hilbert space, we can write a ket $|\psi\rangle$ as a column vector:

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_n \end{pmatrix} \tag{2.39}$$

and the corresponding bra $\langle\psi|$ is the Hermitian adjoint (conjugate transpose):

$$\langle\psi| = \begin{pmatrix} \psi_1^* & \psi_2^* & \cdots & \psi_n^* \end{pmatrix} \tag{2.40}$$

Thus the inner product becomes a matrix multiplication:

$$\langle\phi|\psi\rangle = \begin{pmatrix} \phi_1^* & \cdots & \phi_n^* \end{pmatrix} \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_n \end{pmatrix} = \sum_{i=1}^{n} \phi_i^* \psi_i \tag{2.41}$$

2.6.1 Operators as Matrices

Linear operators as matrices

A linear operator $\hat{A}$ is just a mathematical rule that takes one vector and gives you another vector in the same vector space. If our space has dimension n, we can write both the input and output vectors as columns with n numbers. In that case, $\hat{A}$ can be represented by an $n \times n$ square matrix.

In symbols:

$$\hat{A}\,|\psi\rangle = \begin{pmatrix} A_{11} & \cdots & A_{1n} \\ \vdots & \ddots & \vdots \\ A_{n1} & \cdots & A_{nn} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \vdots \\ \psi_n \end{pmatrix} = |\phi\rangle \tag{2.42}$$

This means: apply the matrix to the column representing $|\psi\rangle$ to get a new column representing $|\phi\rangle$.

Example: 2D case

Think of a 2D vector $|\psi\rangle$ like

$$|\psi\rangle = \begin{pmatrix} 2 \\ 3 \end{pmatrix}$$

This might represent a point in the x-y plane.

Now let the operator $\hat{A}$ be represented by the matrix

$$\hat{A} = \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}$$

When $\hat{A}$ acts on $|\psi\rangle$:

$$\hat{A}\,|\psi\rangle = \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 2 \\ 3 \end{pmatrix} = \begin{pmatrix} 1 \times 2 + 2 \times 3 \\ 0 \times 2 + 1 \times 3 \end{pmatrix} = \begin{pmatrix} 8 \\ 3 \end{pmatrix} = |\phi\rangle$$

Here, $\hat{A}$ has transformed the vector $|\psi\rangle$ into a new vector $|\phi\rangle$ in the same space.

In short:

- The vector is the “input”
- The matrix is the “machine” (operator)
- The output is another vector in the same space

2.6.2 Matrix operations:

- **Transpose:** Denoted T^{T}, obtained by swapping rows and columns.
- **Symmetric matrix:** $T^{\mathrm{T}} = T$.
- **Antisymmetric matrix:** $T^{\mathrm{T}} = -T$.
- **Complex conjugate:** Denoted T^*, obtained by taking the complex conjugate of each entry.
- **Real matrix:** $T^* = T$, **Purely imaginary matrix:** $T^* = -T$.
- **Hermitian conjugate (adjoint):** Denoted $T^\dagger$, defined as $T^\dagger = (T^*)^{\mathrm{T}}$.
- **Hermitian matrix:** $T^\dagger = T$.
- **Skew-Hermitian matrix:** $T^\dagger = -T$.

- **Inverse:** Denoted T^{-1}, defined by $TT^{-1} = T^{-1}T = I$, where I is the identity matrix. A matrix has an inverse only if it is square and its determinant is nonzero.
- The **commutator** of two matrices A and B is denoted by $[A, B]$ and is defined as $[A, B] = AB - BA$.

Useful properties:

- $(A^{\mathrm{T}})^{\mathrm{T}} = A$
- $(A^*)^* = A$
- $(A^\dagger)^\dagger = A$
- $(AB)^{\mathrm{T}} = B^{\mathrm{T}}A^{\mathrm{T}}$
- $(AB)^* = A^*B^*$
- $(AB)^\dagger = B^\dagger A^\dagger$
- $(A^{-1})^{\mathrm{T}} = (A^{\mathrm{T}})^{-1}$ (if A^{-1} exists)
- $(A^{-1})^* = (A^*)^{-1}$ (if A^{-1} exists)
- $(A^{-1})^\dagger = (A^\dagger)^{-1}$ (if A^{-1} exists)
- $(AB)^{-1} = B^{-1}A^{-1}$ (if A^{-1} and B^{-1} exist)

Practice Problems — Full Solutions

1. **Linear Combination and Basis**

   Let $|e_1\rangle = (1, 0)$ and $|e_2\rangle = (0, 1)$ be an orthonormal basis for a 2D complex vector space. Let
   $$|\psi\rangle = 3\,|e_1\rangle + (1+i)\,|e_2\rangle\,.$$

   Solution.

   (a) Writing explicitly:
   $$|\psi\rangle = 3\begin{bmatrix}1\\0\end{bmatrix} + (1+i)\begin{bmatrix}0\\1\end{bmatrix} = \begin{bmatrix}3\\0\end{bmatrix} + \begin{bmatrix}0\\1+i\end{bmatrix} = \begin{bmatrix}3\\1+i\end{bmatrix}.$$

   (b) Yes. A vector is a linear combination of a set of vectors if it can be written as
   $$|\psi\rangle = c_1\,|e_1\rangle + c_2\,|e_2\rangle$$
   for some scalars c_1, c_2. Here $c_1 = 3$ and $c_2 = 1 + i$, so by construction $|\psi\rangle$ is a linear combination of the basis vectors.

   (c) Since $\{|e_1\rangle, |e_2\rangle\}$ is orthonormal:
   $$c_1 = \langle e_1|\psi\rangle = 3, \quad c_2 = \langle e_2|\psi\rangle = 1 + i.$$
   These are the components of $|\psi\rangle$ in this basis.

2. **Linear Independence in a 2D Vector Space**
   We check whether
   $$|v_1\rangle = \begin{bmatrix}2\\3\end{bmatrix}, \qquad |v_2\rangle = \begin{bmatrix}4\\6\end{bmatrix}$$
   are linearly independent.

   Solution. Two vectors in $\mathbb{R}^2$ (or $\mathbb{C}^2$) are linearly dependent if one is a scalar multiple of the other. We test for a scalar c such that:
   $$|v_2\rangle = c\,|v_1\rangle\,.$$
   From the first component:
   $$4 = c \cdot 2 \quad \Rightarrow \quad c = 2.$$
   From the second component:
   $$6 = c \cdot 3 \quad \Rightarrow \quad c = 2.$$
   Both give the same scalar $c = 2$, hence:
   $$|v_2\rangle = 2\,|v_1\rangle\,.$$
   Therefore, $\{|v_1\rangle\,, |v_2\rangle\}$ is *linearly dependent*.

3. **Linear Independence in 3D**
   We check whether
   $$|v_1\rangle = \begin{bmatrix}1\\0\\2\end{bmatrix}, \qquad |v_2\rangle = \begin{bmatrix}0\\1\\3\end{bmatrix}, \qquad |v_3\rangle = \begin{bmatrix}2\\1\\7\end{bmatrix}$$
   are linearly independent.

   Solution. Assume:
   $$|v_3\rangle = a\,|v_1\rangle + b\,|v_2\rangle\,.$$
   Comparing each component:
   $$\text{(1st)}: \quad 2 = a(1) + b(0) \quad \Rightarrow \quad a = 2,$$
   $$\text{(2nd)}: \quad 1 = a(0) + b(1) \quad \Rightarrow \quad b = 1,$$
   $$\text{(3rd)}: \quad 7 = a(2) + b(3) = 2(2) + 1(3) = 4 + 3 = 7,$$
   which is consistent. Therefore:
   $$|v_3\rangle = 2\,|v_1\rangle + 1\,|v_2\rangle\,.$$
   Since one vector is a linear combination of the others, the set is *linearly dependent*. (Equivalently, $\det[|v_1\rangle \ \ |v_2\rangle \ \ |v_3\rangle] = 0$.)

4. **Norm and Normalization**

Given the vector (ket)

$$|\alpha\rangle = \begin{bmatrix} 2 \\ i \end{bmatrix}$$

in a 2D complex vector space with the standard inner product.

Solution.

(a) *Ket, bra, and inner product.* The bra associated with $|\alpha\rangle$ is the Hermitian conjugate:

$$\langle\alpha| = |\alpha\rangle^\dagger = \begin{bmatrix} 2 & -i \end{bmatrix}.$$

Compute the inner product as a bra–ket (row–column) multiplication:

$$\langle\alpha|\alpha\rangle = \begin{bmatrix} 2 & -i \end{bmatrix} \begin{bmatrix} 2 \\ i \end{bmatrix} = 2 \cdot 2 + (-i) \cdot i = 4 + 1 = 5.$$

Hence

$$\|\alpha\| = \sqrt{\langle\alpha|\alpha\rangle} = \sqrt{5}.$$

(b) *Normalization.* The normalized ket is

$$|\tilde{\alpha}\rangle = \frac{1}{\|\alpha\|} |\alpha\rangle = \frac{1}{\sqrt{5}} \begin{bmatrix} 2 \\ i \end{bmatrix} = \begin{bmatrix} \frac{2}{\sqrt{5}} \\ \frac{i}{\sqrt{5}} \end{bmatrix}.$$

Its bra is

$$\langle\tilde{\alpha}| = |\tilde{\alpha}\rangle^\dagger = \begin{bmatrix} \frac{2}{\sqrt{5}} & -\frac{i}{\sqrt{5}} \end{bmatrix},$$

and indeed

$$\langle\tilde{\alpha}|\tilde{\alpha}\rangle = \begin{bmatrix} \frac{2}{\sqrt{5}} & -\frac{i}{\sqrt{5}} \end{bmatrix} \begin{bmatrix} \frac{2}{\sqrt{5}} \\ \frac{i}{\sqrt{5}} \end{bmatrix} = \frac{4}{5} + \frac{1}{5} = 1.$$

5. **Inner Product and Orthogonality**

Let the kets be

$$|\phi\rangle = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \qquad |\chi\rangle = \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

Solution.

(a) *Bras and the inner product.* The corresponding bras are the Hermitian conjugates:

$$\langle\phi| = |\phi\rangle^\dagger = \begin{bmatrix} 1 & -1 \end{bmatrix}, \qquad \langle\chi| = |\chi\rangle^\dagger = \begin{bmatrix} 1 & 1 \end{bmatrix}.$$

Compute the inner product by multiplying the bra $\langle\phi|$ from the left with the ket $|\chi\rangle$:

$$\langle\phi|\chi\rangle = \begin{bmatrix} 1 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = 1 \cdot 1 + (-1) \cdot 1 = 1 - 1 = 0.$$

(b) Since $\langle\phi|\chi\rangle = 0$, the vectors $|\phi\rangle$ and $|\chi\rangle$ are *orthogonal.*

6. **Orthonormal Basis Expansion**

Let $\{|e_1\rangle, |e_2\rangle\}$ be an orthonormal basis and:

$$|\psi\rangle = \frac{1}{\sqrt{2}}|e_1\rangle + \frac{i}{\sqrt{2}}|e_2\rangle.$$

Solution.

(a) Norm:

$$\|\psi\|^2 = \left|\frac{1}{\sqrt{2}}\right|^2 + \left|\frac{i}{\sqrt{2}}\right|^2 = \frac{1}{2} + \frac{1}{2} = 1.$$

Hence $\|\psi\| = 1$, so the state is already normalized.

(b) The probability of measuring $|e_2\rangle$ is:

$$P(e_2) = |\langle e_2|\psi\rangle|^2 = \left|\frac{i}{\sqrt{2}}\right|^2 = \frac{1}{2}.$$

7. **Hilbert Space and Square-Integrability**

Check whether each $\psi(x)$ is square integrable, i.e. whether:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx < \infty.$$

Solution.

(a) $\psi(x) = \dfrac{1}{1+x^2}$ Then:

$$|\psi(x)|^2 = \frac{1}{(1+x^2)^2}.$$

As $|x| \to \infty$, this behaves like $1/x^4$, whose integral converges. Near $x = 0$, the function is finite. Hence it is square integrable.

(b) $\psi(x) = \sin x$ Then:

$$|\psi(x)|^2 = \sin^2 x,$$

which oscillates between 0 and 1 and does not decay as $|x| \to \infty$. The integral over $\mathbb{R}$ diverges, so it is *not* square integrable.

(c) $\psi(x) = e^{-x^2}$ Then:

$$|\psi(x)|^2 = e^{-2x^2}.$$

This is a Gaussian, which decays rapidly at infinity. The Gaussian integral:

$$\int_{-\infty}^{\infty} e^{-2x^2} dx = \sqrt{\frac{\pi}{2}}$$

is finite. Hence it is square integrable.

2.7 Eigenvectors and Eigenvalues

Geometric Intuition

An eigenvector is a vector whose *direction* does not change when a transformation is applied to it. Only its *length* may change (it may also be reversed if multiplied by a negative number).

For example, consider a rotation in 3D space about a fixed axis by an angle θ. Most vectors move in a complicated way, tracing out a cone. However, any vector lying *along* the rotation axis is unchanged by the rotation:

$$\hat{T}|\alpha\rangle = |\alpha\rangle \tag{2.43}$$

Here the vector $|\alpha\rangle$ is unchanged in direction, and the scaling factor is 1.

More generally, a linear transformation $\hat{T}$ on a vector space has special nonzero vectors that satisfy:

$$\hat{T}|\alpha\rangle = \lambda|\alpha\rangle \tag{2.44}$$

Here λ is the **eigenvalue** (possibly complex), and $|\alpha\rangle \neq 0$ is the **eigenvector**.

Note: Any scalar multiple of an eigenvector is also an eigenvector with the same eigenvalue.

Example in 2D

Let

$$T = \begin{pmatrix} 2 & 0 \\ 0 & 3 \end{pmatrix}$$

and consider the vector

$$\mathbf{a} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

We find

$$T\mathbf{a} = \begin{pmatrix} 2 \\ 0 \end{pmatrix} = 2\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

So $\mathbf{a}$ is an eigenvector with eigenvalue $\lambda = 2$.

Similarly, $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ is an eigenvector with eigenvalue $\lambda = 3$.

2.7.1 Matrix Representation and Characteristic Equation

In matrix form, the eigenvalue equation can be written as:

$$T\mathbf{a} = \lambda\mathbf{a}, \quad \mathbf{a} \neq 0 \tag{2.45}$$

Rearranging:

$$(T - \lambda I)\mathbf{a} = 0 \tag{2.46}$$

This is a homogeneous system of linear equations. A nonzero solution for $\mathbf{a}$ exists only if the determinant of $(T - \lambda I)$ is zero:

$$\det(T - \lambda I) = 0 \tag{2.47}$$

This determinant equation is called the **characteristic equation**. Expanding it gives:

$$C_n\lambda^n + C_{n-1}\lambda^{n-1} + \cdots + C_1\lambda + C_0 = 0 \tag{2.48}$$

where the coefficients C_i depend on the elements of T. By the fundamental theorem of algebra, an $n\times n$ matrix has exactly n (possibly repeated) complex eigenvalues. The set of all eigenvalues is called the **spectrum**. If more than one linearly independent eigenvector corresponds to the same eigenvalue, that eigenvalue is said to be **degenerate**.

Example: Finding Eigenvalues and Eigenvectors of a 2×2 Matrix

Let us take a simple 2×2 matrix:

$$T = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}$$

The eigenvalue equation is:

$$T\mathbf{a} = \lambda\mathbf{a}$$

Rewriting:

$$(T - \lambda I)\mathbf{a} = 0$$

For nonzero $\mathbf{a}$, we must have:

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

That is:

$$\det\begin{pmatrix} 2-\lambda & 1 \\ 1 & 3-\lambda \end{pmatrix} = 0$$

Expanding the determinant:

$$(2-\lambda)(3-\lambda) - (1)(1) = 0$$

$$\lambda^2 - 5\lambda + 5 = 0$$

Solving the quadratic equation:

$$\lambda = \frac{5 \pm \sqrt{25-20}}{2} = \frac{5 \pm \sqrt{5}}{2}$$

So the two eigenvalues are:

$$\lambda_1 = \frac{5+\sqrt{5}}{2}, \quad \lambda_2 = \frac{5-\sqrt{5}}{2}$$

Finding eigenvectors:

For $\lambda_1 = \frac{5+\sqrt{5}}{2}$, substitute into $(T - \lambda I)\mathbf{a} = 0$:

$$\begin{pmatrix} 2-\lambda_1 & 1 \\ 1 & 3-\lambda_1 \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = 0$$

This gives a relation between a_1 and a_2:

$$(2-\lambda_1)a_1 + a_2 = 0$$

We can set $a_1 = 1$ and solve for a_2:

$$a_2 = \lambda_1 - 2$$

So one eigenvector is:

$$\mathbf{a}^{(1)} = \begin{pmatrix} 1 \\ \lambda_1 - 2 \end{pmatrix}$$

Similarly, for $\lambda_2 = \frac{5-\sqrt{5}}{2}$, we find:

$$a_2 = \lambda_2 - 2$$

So the second eigenvector is:

$$\mathbf{a}^{(2)} = \begin{pmatrix} 1 \\ \lambda_2 - 2 \end{pmatrix}$$

Note that we can multiply an eigenvector by any nonzero constant and it will still be an eigenvector. In practice, we often normalise eigenvectors to have unit length.

2.8 Hermitian Transformations

A linear transformation $\hat{T}$ is **Hermitian** if

$$\langle\alpha|\hat{T}|\beta\rangle = \langle\beta|\hat{T}^\dagger|\alpha\rangle^* \tag{2.49}$$

for all $|\alpha\rangle, |\beta\rangle$. In matrix representation, this corresponds to:

$$T^\dagger = T \tag{2.50}$$

where $T^\dagger$ is the Hermitian conjugate (complex conjugate, then transpose).

Hermitian matrices are important in quantum mechanics because they represent physical observables. Their eigenvalues and eigenvectors have the following important properties.

1. Eigenvalues of Hermitian Operators are Real

Let $\hat{T}|\alpha\rangle = \lambda|\alpha\rangle$ with $|\alpha\rangle \neq 0$. Then:

$$\langle\alpha|\hat{T}|\alpha\rangle = \langle\alpha|\lambda|\alpha\rangle = \lambda\langle\alpha|\alpha\rangle \tag{2.51}$$

Since $\hat{T}$ is Hermitian, $\hat{T}^\dagger = \hat{T}$, we also have:

$$\langle\alpha|\hat{T}|\alpha\rangle = \langle\alpha|\hat{T}^\dagger|\alpha\rangle = \langle\alpha|\hat{T}|\alpha\rangle^* = \lambda^*\langle\alpha|\alpha\rangle \tag{2.52}$$

Because $\langle\alpha|\alpha\rangle \neq 0$, we conclude:

$$\lambda = \lambda^* \quad \Rightarrow \quad \lambda \in \mathbb{R} \tag{2.53}$$

QED: Eigenvalues of Hermitian operators are real.

2. Eigenvectors with Distinct Eigenvalues are Orthogonal

Suppose $\hat{T}|\alpha\rangle = \lambda|\alpha\rangle$ and $\hat{T}|\beta\rangle = \mu|\beta\rangle$ with $\lambda \neq \mu$. Then:

$$\langle\alpha|\hat{T}|\beta\rangle = \mu\langle\alpha|\beta\rangle \tag{2.54}$$

and

$$\langle\beta|\hat{T}|\alpha\rangle = \lambda\langle\beta|\alpha\rangle \tag{2.55}$$

Since $\hat{T}$ is Hermitian:

$$\langle\alpha|\hat{T}|\beta\rangle = \langle\beta|\hat{T}|\alpha\rangle^* \tag{2.56}$$

Therefore:

$$\mu\langle\alpha|\beta\rangle = \lambda\langle\alpha|\beta\rangle \tag{2.57}$$

which implies:

$$(\mu - \lambda)\langle\alpha|\beta\rangle = 0 \tag{2.58}$$

Since $\lambda \neq \mu$, we must have:

$$\langle\alpha|\beta\rangle = 0 \tag{2.59}$$

QED: Eigenvectors with distinct eigenvalues of a Hermitian operator are orthogonal.

3. Eigenvectors Span the Space

A Hermitian operator can always be diagonalized. This means its eigenvectors form a complete basis for the vector space. Any vector in the space can be written as a linear combination of these eigenvectors.

This fact is fundamental to quantum mechanics because it ensures that any quantum state can be expressed in terms of eigenstates of a Hermitian observable.

Note: The above results are guaranteed in finite-dimensional vector spaces. In infinite-dimensional Hilbert spaces, diagonalization and completeness require more careful treatment using the spectral theorem.

Example: Eigenvalues and Eigenvectors of a 2×2 Hermitian Matrix

Consider the Hermitian matrix:

$$A = \begin{pmatrix} 2 & 1+i \\ 1-i & 3 \end{pmatrix}$$

The characteristic equation is:

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

That is:

$$\begin{vmatrix} 2-\lambda & 1+i \\ 1-i & 3-\lambda \end{vmatrix} = (2-\lambda)(3-\lambda) - (1+i)(1-i) = (2-\lambda)(3-\lambda) - 2$$

Simplifying:

$$\lambda^2 - 5\lambda + 4 = 0$$

which gives:

$$\lambda_1 = 1, \quad \lambda_2 = 4$$

For $\lambda_1 = 1$, solve $(A - I)\vec{v} = 0$:

$$\begin{pmatrix} 1 & 1+i \\ 1-i & 2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 0$$

From the first row: $x + (1+i)y = 0 \Rightarrow x = -(1+i)y$. Choosing $y = 1$, we have $\vec{v}_1 = \begin{pmatrix} -(1+i) \\ 1 \end{pmatrix}$.

For $\lambda_2 = 4$, solve $(A - 4I)\vec{v} = 0$:

$$\begin{pmatrix} -2 & 1+i \\ 1-i & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 0$$

From the first row: $-2x + (1+i)y = 0 \Rightarrow x = \frac{1+i}{2}y$. Choosing $y = 1$, we have $\vec{v}_2 = \begin{pmatrix} \frac{1+i}{2} \\ 1 \end{pmatrix}$.

The eigenvectors can then be normalized, and since A is Hermitian, these eigenvectors will be orthogonal (Please verify!).

2.9 Unitary Operators

A linear operator U on a Hilbert space is called **unitary** if

$$U^\dagger U = UU^\dagger = I,$$

where $U^\dagger$ is the Hermitian adjoint of U and I is the identity operator.

Key properties:

- **Norm-preserving:** Unitary operators preserve the length of vectors:

$$\|U|\psi\rangle\| = \||\psi\rangle\|.$$

- **Inner-product preserving:** Let

$$|\phi'\rangle = U|\phi\rangle, \quad |\psi'\rangle = U|\psi\rangle.$$

  Then the inner product between vectors is preserved:

$$\langle\phi'|\psi'\rangle = \langle\phi|\psi\rangle.$$

  This shows that the "overlap" or "angle" between vectors does not change under a unitary transformation.

- Examples include rotation matrices in 2D

Unitary operators are important in quantum mechanics because they describe **evolution of isolated quantum states**, which must preserve probabilities.

2.10 Outer Product

So far, we have introduced kets $|\psi\rangle$ as vectors, bras $\langle\phi|$ as their duals (adjoint), and inner products $\langle\phi|\psi\rangle$ as complex numbers. There is another extremely useful construction that combines a ket and a bra to form a **linear operator** (which is in fact just a matrix!): the *outer product*.

Definition: Outer Product

Given two vectors $|v\rangle$ (in space V) and $|w\rangle$ (in space W), we define the *outer product* $|w\rangle\langle v|$ to be the linear operator from V to W whose action is

$$(|w\rangle\langle v|)\,|x\rangle \;=\; \langle v|x\rangle\;|w\rangle\,, \qquad \forall\,|x\rangle \in V.$$

That is, $|w\rangle\langle v|$ takes any input vector $|x\rangle$ from V, projects it onto $|v\rangle$ (via the inner product $\langle v|x\rangle$), and then outputs a multiple of $|w\rangle$.

Be careful not to confuse the outer product $|w\rangle\langle v|$ (an operator) with the inner product $\langle w|v\rangle$ (a complex number).

Example 1

If $|v\rangle$ and $|w\rangle$ are both vectors in $\mathbb{C}^2$ (2-dimensional complex space), say

$$|v\rangle = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \quad |w\rangle = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix},$$

then the operator $|w\rangle\langle v|$ is represented as a 2×2 matrix:

$$|w\rangle\langle v| = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} \begin{pmatrix} v_1^* & v_2^* \end{pmatrix} = \begin{pmatrix} w_1 v_1^* & w_1 v_2^* \\ w_2 v_1^* & w_2 v_2^* \end{pmatrix}.$$

Example 2: Outer Product Between Different Spaces

Suppose we have two vector spaces: $\mathbb{C}^2$ and $\mathbb{C}^3$ (3-dimensional complex space).

Let

$$|v\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \in \mathbb{C}^2, \quad |w\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \in \mathbb{C}^3.$$

The outer product

$$|w\rangle\langle v|$$

is a linear operator from $\mathbb{C}^2 \to \mathbb{C}^3$ and is represented as a 3×2 matrix:

$$|w\rangle\langle v| = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

Acting on an arbitrary vector $|x\rangle \in \mathbb{C}^2$, say $|x\rangle = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$, gives

$$(|w\rangle \langle v|) |x\rangle = \begin{pmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 \\ x_1 \\ 0 \end{pmatrix} \in \mathbb{C}^3.$$

Thus, the operator $|w\rangle \langle v|$ *projects* onto $|v\rangle$ in $\mathbb{C}^2$ and maps the result to the direction of $|w\rangle$ in $\mathbb{C}^3$.

If $|v\rangle \in \mathbb{C}^n$ and $|w\rangle \in \mathbb{C}^m$, then $|w\rangle \langle v|$ is an $m \times n$ matrix.

Linearity

We can take linear combinations of outer products in the obvious way. For example,

$$\sum_i a_i |w_i\rangle \langle v_i|$$

is the linear operator which, when acting on a vector $|x\rangle$, produces

$$\sum_i a_i \langle v_i|x\rangle \; |w_i\rangle .$$

2.11 Projection Operators

A special case of the outer product is when a vector is paired with itself. If $|i\rangle$ is a normalized vector (i.e. $\langle i|i\rangle = 1$), we define the **projection operator** onto the direction of $|i\rangle$ as

$$P = |i\rangle \langle i| .$$

More generally, for a non-normalized vector $|u\rangle$, the projector is

$$P = \frac{|u\rangle \langle u|}{\langle u|u\rangle},$$

which ensures the correct properties of a projection operator.

Action of a Projection Operator

For any vector $|v\rangle$, we have

$$P |v\rangle = |i\rangle \langle i|v\rangle ,$$

which means P projects $|v\rangle$ onto the direction of $|i\rangle$.

Properties of Projection Operators

- $P^2 = P$ (projecting twice is the same as projecting once)
- $P^\dagger = P$ (projection operators are Hermitian)

Example: Projection Operator in 2D

Consider the normalized vector

$$|i\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \in \mathbb{R}^2.$$

The projection operator onto the direction of $|i\rangle$ is

$$P = |i\rangle \langle i| = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

Now let an arbitrary vector in 2D be

$$|v\rangle = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}.$$

Then

$$P|v\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} v_1 \\ 0 \end{pmatrix}.$$

So P *projects any vector onto the x-axis.*

Completeness Relation

Let $\{|e_i\rangle\}$ be an orthonormal basis for a Hilbert space V. We have already seen that any vector can be expanded as (Eq. (2.30))

$$|v\rangle = \sum_i c_i |e_i\rangle, \qquad c_i = \langle e_i|v\rangle,$$

where the summations is over all the basis vectors. Now consider the operator

$$\sum_i |e_i\rangle \langle e_i|.$$

Acting this on an arbitrary vector $|v\rangle$ gives

$$\left(\sum_i |e_i\rangle \langle e_i| \right) |v\rangle = \sum_i \langle e_i|v\rangle |e_i\rangle = |v\rangle.$$

Since this holds for all $|v\rangle$, we conclude

$$\sum_i |e_i\rangle \langle e_i| = I,$$

where I is the identity operator. This is known as the **completeness relation**.

2.12 Matrix Representation from Completeness

Let $\{|e_i\rangle\}_{i=1}^n$ be an orthonormal basis of an n-dimensional Hilbert space. The completeness relation states that

$$I = \sum_{i=1}^n |e_i\rangle\langle e_i|.$$

Given a linear operator $\hat{A}$, we can insert this resolution of the identity on both sides:

$$\hat{A} = I\hat{A}I = \Big(\sum_{i=1}^{n} |e_i\rangle\langle e_i|\Big)\hat{A}\Big(\sum_{j=1}^{n} |e_j\rangle\langle e_j|\Big).$$

Expanding, we obtain

$$\hat{A} = \sum_{i,j=1}^{n} |e_i\rangle\langle e_i|\hat{A}|e_j\rangle\langle e_j|.$$

Thus, the coefficients

$$A_{ij} = \langle e_i|\hat{A}|e_j\rangle$$

are the matrix elements of $\hat{A}$ in this basis, and the operator can be written as

$$\hat{A} = \sum_{i,j=1}^{n} A_{ij}\,|e_i\rangle\langle e_j|.$$

Now, let

$$|\psi\rangle = \sum_{k=1}^{n} c_k|e_k\rangle$$

be a general state. Acting with $\hat{A}$ gives

$$\hat{A}|\psi\rangle = \sum_{i,j=1}^{n} A_{ij}\,|e_i\rangle\langle e_j|\psi\rangle = \sum_{i,j=1}^{n} A_{ij}c_j\,|e_i\rangle.$$

Therefore, the coefficients transform as

$$c_i' = \sum_{j=1}^{n} A_{ij}c_j,$$

which is exactly the standard matrix multiplication rule.

In words: the bra $\langle e_j|$ extracts the j-th component of the input, the matrix element A_{ij} weights it, and the ket $|e_i\rangle$ reinserts it into the i-th output direction.

2.13 Tensor Product of Vector Spaces

The **tensor product** is a way of combining two vector spaces into a larger space. In quantum mechanics this is important for describing *composite systems* (for example, two particles or two qubits together).

Definition

Suppose V has dimension m with basis $\{|e_i\rangle\}$, and W has dimension n with basis $\{|f_j\rangle\}$. Then the tensor product space $V \otimes W$ has dimension $m \cdot n$ with basis

$$\{|e_i\rangle \otimes |f_j\rangle \;\;|\;\; i = 1, \ldots, m;\; j = 1, \ldots, n\}.$$

For short, we often write $|e_i\rangle \otimes |f_j\rangle$ as $|e_i f_j\rangle$ or just $|ij\rangle$.

Tensor Product Between Two Vectors

Suppose

$$|\psi\rangle = \begin{pmatrix} a \\ b \end{pmatrix}, \quad |\phi\rangle = \begin{pmatrix} c \\ d \end{pmatrix} \in \mathbb{C}^2.$$

Then

$$|\psi\rangle \otimes |\phi\rangle = \begin{pmatrix} ac \\ ad \\ bc \\ bd \end{pmatrix} \in \mathbb{C}^4.$$

Numeric Example

$$|\psi\rangle = \begin{pmatrix} 1 \\ 2 \end{pmatrix}, \quad |\phi\rangle = \begin{pmatrix} 3 \\ 4 \end{pmatrix}, \quad |\psi\rangle \otimes |\phi\rangle = \begin{pmatrix} 3 \\ 4 \\ 6 \\ 8 \end{pmatrix}.$$

Operators on Tensor Product Spaces

If A acts on V and B acts on W, then the combined operator $A \otimes B$ acts as

$$(A \otimes B)(|v\rangle \otimes |w\rangle) = (A\,|v\rangle) \otimes (B\,|w\rangle).$$

Example: Two Qubits

Each qubit is a vector in $\mathbb{C}^2$ with basis $\{|0\rangle, |1\rangle\}$. Two qubits together live in $\mathbb{C}^2 \otimes \mathbb{C}^2 = \mathbb{C}^4$ with basis

$$|00\rangle, \quad |01\rangle, \quad |10\rangle, \quad |11\rangle.$$

A general two-qubit state is

$$|\Psi\rangle = c_{00}\,|00\rangle + c_{01}\,|01\rangle + c_{10}\,|10\rangle + c_{11}\,|11\rangle.$$

2.14 Pauli Matrices

The **Pauli matrices** are three important 2×2 matrices:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

They act on two-dimensional vectors, such as qubit states.

Basic Properties

- $\sigma_i^2 = I$ (squaring gives the identity matrix).
- $\mathrm{Tr}(\sigma_i) = 0$ (the diagonal entries add to zero).
- Each σ_i is Hermitian: $\sigma_i^\dagger = \sigma_i$ (so they correspond to observable quantities).

Commutators and Anticommutators

For matrices A, B:

$$[A, B] = AB - BA, \quad \{A, B\} = AB + BA.$$

$[A, B]$ is called the commutator and $\{A, B\}$ the anticommtator.
The Pauli matrices satisfy:

$$[\sigma_i, \sigma_j] = 2i\,\epsilon_{ijk}\,\sigma_k, \qquad \{\sigma_i, \sigma_j\} = 2\delta_{ij} I.$$

Here: - δ_{ij} is the **Kronecker delta**, equal to 1 if $i = j$ and 0 otherwise. - ϵ_{ijk} is the **Levi-Civita symbol**, defined by

$$\epsilon_{ijk} = \begin{cases} +1 & \text{if } (i, j, k) \text{ is an even permutation of } (x, y, z), \\ -1 & \text{if } (i, j, k) \text{ is an odd permutation of } (x, y, z), \\ 0 & \text{if any indices are repeated.} \end{cases}$$

Example: Commutator Calculation

$$[\sigma_x, \sigma_y] = \sigma_x \sigma_y - \sigma_y \sigma_x = 2i\sigma_z.$$

Connection to Spin

For a spin-$\frac{1}{2}$ particle (like the electron), we use the z-basis $\{|0\rangle_z, |1\rangle_z\}$, where

$$|0\rangle_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle_z = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

These states represent "spin-up" and "spin-down" along the z-axis. The Pauli matrix σ_z acts on them as

$$\sigma_z |0\rangle_z = +|0\rangle_z, \qquad \sigma_z |1\rangle_z = -|1\rangle_z.$$

The physical spin operator is

$$S_z = \tfrac{\hbar}{2}\sigma_z,$$

so the eigenvalues of S_z are $\pm\frac{\hbar}{2}$.

This corresponds exactly to the two outcomes observed in the **Stern–Gerlach experiment**, where a beam of silver atoms split into two distinct spots: one for spin-up $(+\frac{\hbar}{2})$ and one for spin-down $(-\frac{\hbar}{2})$.

Appendix

A1. The Position Basis and the Wavefunction

The expansion

$$|\psi\rangle = \sum_i \langle e_i|\psi\rangle\ |e_i\rangle \tag{2.60}$$

is valid whenever the basis $\{|e_i\rangle\}$ is orthonormal and complete. When the basis is *continuous* rather than discrete—for example, when labeling by position $x \in \mathbb{R}$—the sum becomes an integral.

The Hilbert space is then spanned by a continuum of orthonormal basis states $\{|x\rangle\}$, satisfying:[5]

$$\langle x|x'\rangle = \delta(x - x')\,. \tag{2.61}$$

Analogous to the discrete case, we can now write:

$$|\psi\rangle = \int_{-\infty}^{\infty} \langle x|\psi\rangle \; |x\rangle \; dx \tag{2.62}$$

The quantity

$$\psi(x) := \langle x|\psi\rangle$$

is the **wavefunction** in the position representation. It plays the same role as the components $\langle e_i|\psi\rangle$ in the discrete case, and its squared modulus $|\psi(x)|^2\,dx$ gives the probability of finding the particle between x and $x + dx$.

Thus, the familiar $\psi(x)$ is not the state itself, but the *representation* of the abstract state $|\psi\rangle$ in the position basis. In Dirac notation:

$$\psi(x) = \langle x|\psi\rangle \tag{2.63}$$

This unifies the geometric and probabilistic perspectives: the wavefunction is a collection of inner products with position basis vectors, just as coordinates are projections onto axes in classical vector spaces.

[5] $\delta(x - x')$ is the *Dirac delta*, which is *not* a function in the ordinary sense but a *distribution*. It is defined by its action under integration:

$$\int_{-\infty}^{\infty} \delta(x - x')f(x')\,dx' = f(x)$$

for any smooth test function f. It is zero whenever $x \neq x'$, and is "infinite" at $x = x'$ in such a way that its total integral equals 1. In quantum mechanics, it plays the role of the Kronecker delta δ_{ij} for continuous indices.