An Introduction to Quantum Mechanics 2

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Inner Products: Definition

- An **inner product** takes two vectors $|v\rangle, |w\rangle$ and produces a complex number:

$$(|v\rangle, |w\rangle) \in \mathbb{C}$$

- Quantum mechanics uses **Dirac notation**:

$$\langle v|w\rangle$$

- $\langle v|$ is the **dual vector** (row vector form of $|v\rangle$).

$$\langle v|(|w\rangle) = \langle v|w\rangle$$

Properties of Inner Products

A function $(\cdot,\cdot) : V \times V \to \mathbb{C}$ is an inner product if:

1. **Linearity in 2nd argument:**

$$(|v\rangle, \sum_i \lambda_i |w_i\rangle) = \sum_i \lambda_i (|v\rangle, |w_i\rangle)$$

$$\langle v| \left(\sum_i \lambda_i |w_i\rangle \right) = \sum_i \lambda_i \langle v|w_i\rangle$$

2. **Conjugate symmetry:**

$$(|v\rangle, |w\rangle) = (|w\rangle, |v\rangle)^*$$

$$\langle v|w\rangle = \langle w|v\rangle^*$$

3. **Positive definiteness:**

$$(|v\rangle, |v\rangle) \geq 0, \quad = 0 \iff |v\rangle = 0$$

$$\langle v|v\rangle \geq 0, \quad = 0 \iff |v\rangle = 0$$

Inner Product Notation: Linear Algebra vs Dirac

Linear Algebra Notation	**Dirac (Quantum) Notation**
Vector v	Ket $\lvert v \rangle$
Dual vector $v^\dagger$	Bra $\langle v \rvert$
Inner product (v, w)	$\langle v \vert w \rangle$
Norm $\sqrt{(v, v)}$	$\sqrt{\langle v \vert v \rangle}$
Outer product $vw^\dagger$	$\lvert v \rangle \langle w \rvert$
Identity operator I	$\sum_i \lvert i \rangle \langle i \rvert$

Example: Inner Product in $\mathbb{C}^n$

- Vectors: $y = (y_1, \ldots, y_n)$, $z = (z_1, \ldots, z_n)$
- Inner product:

$$(y, z) = \sum_{i=1}^{n} y_i^* z_i$$

- In matrix form:

$$(y, z) = \begin{bmatrix} y_1^* & \cdots & y_n^* \end{bmatrix} \begin{bmatrix} z_1 \\ \vdots \\ z_n \end{bmatrix}$$

- Example in $\mathbb{C}^2$:

$$\langle y|z\rangle = (1+i,\ 2)^* \cdot (3,\ i) = (1-i)(3) + (2)(i) = 3 - 3i + 2i = 3 - i$$

Physical Meaning of Inner Products

- $\langle v|w\rangle$ measures the **overlap** between two states.
- If $\langle v|w\rangle = 0$: states are **orthogonal** (completely distinguishable).
- $|\langle v|w\rangle|^2$: probability of finding state $|v\rangle$ when measuring $|w\rangle$.
- In quantum mechanics, this is the core of the **Born rule**.

$$\text{Probability} = |\langle\psi|\phi\rangle|^2$$

Orthogonality

- Two vectors are **orthogonal** if their inner product is zero:

$$\langle v|w\rangle = 0$$

- Example in $\mathbb{C}^2$:

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

$$\langle v|w\rangle = (1, 0) \begin{bmatrix} 0 \\ 1 \end{bmatrix} = 0$$

Norm and Normalization

- The **norm** of a vector $|v\rangle$ is:

$$\|v\| = \sqrt{\langle v|v\rangle}$$

- A **unit vector** has $\|v\| = 1$.
- To normalize any non-zero vector:

$$|v\rangle \;\to\; \frac{|v\rangle}{\|v\|}$$

- Example: $|v\rangle = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$, $\|v\| = \sqrt{3^2 + 4^2} = 5$, normalized: $\frac{1}{5}\begin{bmatrix} 3 \\ 4 \end{bmatrix}$.

Orthonormality

- A set $\{|i\rangle\}$ is **orthonormal** if:

$$\langle i|j\rangle = \delta_{ij}$$

- Meaning:
    - $\langle i|i\rangle = 1$ (each vector has unit norm).
    - $\langle i|j\rangle = 0$ for $i \neq j$ (vectors are orthogonal).
- Example: The standard basis of $\mathbb{C}^2$:

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

Motivation: Orthonormal Bases

- We often start with an arbitrary basis $\{|w_1\rangle, \ldots, |w_d\rangle\}$.
- But in quantum mechanics, we prefer an **orthonormal basis**:

$$\langle v_i | v_j \rangle = \delta_{ij}$$

- Question: How can we systematically turn any basis into an orthonormal one?
- Answer: The **Gram–Schmidt procedure**.

Gram–Schmidt Procedure

- Start with a basis $\{|w_1\rangle, \ldots, |w_d\rangle\}$.
- Step 1: Normalize the first vector:

$$|v_1\rangle = \frac{|w_1\rangle}{\| w_1 \|}$$

- Step 2: Inductive step (remove projections, then normalize):

$$|v_{k+1}\rangle = \frac{|w_{k+1}\rangle - \sum_{i=1}^{k} \langle v_i | w_{k+1}\rangle |v_i\rangle}{\| \, |w_{k+1}\rangle - \sum_{i=1}^{k} \langle v_i | w_{k+1}\rangle |v_i\rangle \|}$$

- Result: $\{|v_1\rangle, \ldots, |v_d\rangle\}$ is an orthonormal basis for V.

Gram–Schmidt Example in $\mathbb{R}^2$

- Given basis:

$$|w_1\rangle = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad |w_2\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

- Step 1: Normalize $|w_1\rangle$:

$$|v_1\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

- Step 2: Subtract projection of $|w_2\rangle$ on $|v_1\rangle$:

$$|u_2\rangle = |w_2\rangle - \langle v_1|w_2\rangle |v_1\rangle$$

$$\langle v_1|w_2\rangle = \frac{1}{\sqrt{2}} \quad \Rightarrow \quad |u_2\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} - \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

- Normalize:

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

Result of Gram–Schmidt

- The original basis:

$$|w_1\rangle = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad |w_2\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

- Produced the orthonormal basis:

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

- These vectors satisfy:

$$\langle v_i | v_j \rangle = \delta_{ij}$$

Exercise: Gram–Schmidt in $\mathbb{R}^3$

Task: Apply the Gram–Schmidt procedure to construct an orthonormal basis.

Given basis vectors

$$|w_1\rangle = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \quad |w_2\rangle = \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}, \quad |w_3\rangle = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}$$

1. Normalize $|w_1\rangle$ to obtain $|v_1\rangle$.
2. Subtract projection of $|w_2\rangle$ onto $|v_1\rangle$, then normalize to get $|v_2\rangle$.
3. Subtract projections of $|w_3\rangle$ onto $|v_1\rangle$ and $|v_2\rangle$, then normalize to get $|v_3\rangle$.

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Reminder:

$$|u_k\rangle = |w_k\rangle - \sum_{i=1}^{k-1} \langle v_i|w_k\rangle |v_i\rangle, \quad |v_k\rangle = \frac{|u_k\rangle}{\||u_k\|}$$

Inner Product in Matrix Form

Let

$$|w\rangle = \sum_i w_i |i\rangle, \quad |v\rangle = \sum_j v_j |j\rangle$$

with respect to an orthonormal basis $\{|i\rangle\}$.

$$\langle v|w\rangle = \sum_i v_i^* w_i$$

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$$\langle v|w\rangle = \begin{bmatrix} v_1^* & v_2^* & \cdots & v_n^* \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}$$

Key Point

The bra $\langle v|$ is the conjugate-transpose (row vector) of the ket $|v\rangle$.

Outer Product as Operator

Given vectors $|v\rangle \in V$ and $|w\rangle \in W$, define the operator:

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$$(|w\rangle\langle v|)\,|v'\rangle = |w\rangle\langle v|v'\rangle$$

Interpretation

- Produces scalar $\langle v|v'\rangle$ (a complex number). - Multiplies that scalar by $|w\rangle$. - Hence, $|w\rangle\langle v|$ is a matrix of rank 1.

Completeness Relation

Let $\{|i\rangle\}$ be an orthonormal basis. Any vector can be written as:

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Check:

$$\left(\sum_i |i\rangle\langle i|\right)|v\rangle = \sum_i |i\rangle\langle i|v\rangle = \sum_i v_i|i\rangle = |v\rangle$$

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Check:

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$$\boxed{\sum_i |i\rangle\langle i| = I}$$

Meaning

The identity operator can be expressed in terms of projectors onto basis states.

Operators in Outer Product Notation

Given $A : V \to W$, insert completeness twice:

$$A = I_W A I_V = \left(\sum_j |w_j\rangle\langle w_j| \right) A \left(\sum_i |v_i\rangle\langle v_i| \right)$$

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$$A = I_W A I_V = \left(\sum_j |w_j\rangle\langle w_j| \right) A \left(\sum_i |v_i\rangle\langle v_i| \right)$$

$$A = \sum_{i,j} |w_j\rangle\langle w_j|A|v_i\rangle\langle v_i|$$

Key Takeaway

- Any operator can be expressed in terms of its **matrix elements** $\langle w_j|A|v_i\rangle$.
- This is the link between matrix representation and operator formalism.

Eigenvectors and Eigenvalues

An eigenvector of a linear operator A is a non-zero vector $|v\rangle$ such that

$$A|v\rangle = \lambda|v\rangle$$

where $\lambda \in \mathbb{C}$ is called the **eigenvalue**.

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Meaning

- $|v\rangle$: direction unchanged by A. - λ: stretching (or shrinking / phase rotation) factor.

Finding Eigenvalues

To find eigenvalues of a matrix A:

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

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To find eigenvalues of a matrix A:

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- Solve this polynomial for λ. - Each solution λ is an eigenvalue. - Then solve $(A - \lambda I)|v\rangle = 0$ for the eigenvector(s).

Worked Example

Let

$$A = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}$$

Step 1: Characteristic equation

$$\det(A - \lambda I) = \det \begin{bmatrix} 2 - \lambda & 1 \\ 1 & 2 - \lambda \end{bmatrix} = (2 - \lambda)^2 - 1$$

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$$\det(A - \lambda I) = \det \begin{bmatrix} 2-\lambda & 1 \\ 1 & 2-\lambda \end{bmatrix} = (2-\lambda)^2 - 1$$

$$c(\lambda) = \lambda^2 - 4\lambda + 3 = 0 \quad \Rightarrow \quad \lambda_1 = 3,\ \lambda_2 = 1$$

Eigenvectors of A

For $\lambda_1 = 3$:

$$(A - 3I)|v\rangle = 0 \quad \Rightarrow \quad \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = 0$$

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Solution: $|v_1\rangle = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

For $\lambda_2 = 1$:

$$(A - I)|v\rangle = 0 \quad \Rightarrow \quad \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = 0$$

Eigenvectors of A

For $\lambda_1 = 3$:

$$(A - 3I)|v\rangle = 0 \quad \Rightarrow \quad \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = 0$$

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Eigenvalues in Quantum Mechanics

- In quantum mechanics, **observables** (like position, momentum, spin) are represented by operators.
- The possible outcomes of a measurement are the **eigenvalues** of the operator.
- The system collapses into the corresponding **eigenvector state**.

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Example

Measuring spin along z: Operator $\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ - Eigenvalues: ± 1 (measurement outcomes). - Eigenvectors: $|0\rangle, |1\rangle$ (spin-up, spin-down states).

Diagonal Representation

Definition

A **diagonal representation** for an operator A on a vector space V is a representation:

$$A = \sum_i \lambda_i |i\rangle \langle i|$$

where the vectors $\{|i\rangle\}$ form an **orthonormal set** of eigenvectors for A, with corresponding eigenvalues λ_i.

Diagonalizable Operators

Definition

An operator is said to be **diagonalizable** if it has a diagonal representation.

In the next section we will find a simple set of necessary and sufficient conditions for an operator on a Hilbert space to be diagonalizable.

Example: Pauli Z Matrix

Example

The Pauli Z matrix has the diagonal representation:

$$\sigma_Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = |0\rangle\langle 0| - |1\rangle\langle 1|$$

where the matrix representation is with respect to orthonormal vectors $|0\rangle$ and $|1\rangle$.

Diagonal representations are sometimes also known as **orthonormal decompositions**.

Degenerate Eigenspaces

Definition

When an eigenspace is more than one dimensional, we say that it is **degenerate**.

example

The matrix A defined by:

$$A \equiv \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

has a two-dimensional eigenspace corresponding to the eigenvalue 2.

Degenerate Eigenvectors

example

[Continued] The eigenvectors $(1, 0, 0)$ and $(0, 1, 0)$ are said to be **degenerate** because they are:

- Linearly independent eigenvectors of A
- Have the same eigenvalue (2)

Note

Degenerate eigenvectors span the eigenspace corresponding to their shared eigenvalue.

Exercise: Eigenvalues and Eigenvectors

Compute the eigenvalues and eigenvectors of

$$B = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

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1. Find the characteristic equation: $\det(B - \lambda I) = 0$.
2. Solve for the eigenvalues λ.
3. For each eigenvalue, solve $(B - \lambda I)|v\rangle = 0$ to find the eigenvector(s).
4. Normalize the eigenvectors.

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Question

B is the Pauli-X operator (quantum NOT gate). What does it do to $|0\rangle$ and $|1\rangle$?

Python + Linear Algebra in the Cloud

- We will use **Python** to explore linear algebra concepts (vectors, matrices, eigenvalues, operators, quantum gates).
- Environment: **Anaconda Cloud** at `https://anaconda.com/app`
  1. Create a free Anaconda account.
  2. Launch a **Jupyter Notebook** session in the cloud.
  3. Create a new project.
  4. From the course **Canvas Files section**, download the provided Jupyter notebook.
  5. Upload it into your Anaconda project.
- Benefits:
  - No installation required – everything runs in the cloud.
  - Interactive coding with `numpy` and `matplotlib`.
  - Directly connects theory $\leftrightarrow$ computation.