An Introduction to Quantum Mechanics 3

Dr. Hugo García Tecocoatzi

Instituto Tecnológico y de Estudios Superiores de Monterrey

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Operators in Outer Product Notation

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

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

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

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.

Outer Product Representation

- Given vectors $|v\rangle$ and $|w\rangle$, the **outer product** is:

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

- It defines a linear operator:

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

- Example: For basis vectors in $\mathbb{C}^2$,

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

- Outer product: $|0\rangle\langle 1| = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$

Matrix Elements of $|0\rangle\langle 1|$

- Recall: matrix elements are defined as

$$A_{ij} = \langle i|A|j\rangle$$

- For the outer product $A = |0\rangle\langle 1|$:

$$A_{ij} = \langle i|(|0\rangle\langle 1|)|j\rangle$$

- Step 1: Apply $|0\rangle\langle 1|$ to $|j\rangle$:

$$(|0\rangle\langle 1|)|j\rangle = \langle 1|j\rangle\,|0\rangle$$

- Step 2: Take overlap with $\langle i|$:

$$A_{ij} = \langle i|0\rangle\,\langle 1|j\rangle$$

- Explicit calculation:

$$A = \begin{bmatrix} \langle 0|0\rangle\langle 1|0\rangle & \langle 0|0\rangle\langle 1|1\rangle \\ \langle 1|0\rangle\langle 1|0\rangle & \langle 1|0\rangle\langle 1|1\rangle \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$$

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**.

To find eigenvalues of a matrix A:

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

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

Diagonal Representation

Definition

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

Example: A Non-Diagonalizable Matrix

Consider

$$A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}.$$

Step 1: Characteristic polynomial

$$c(\lambda) = \det(A - \lambda I) = \det \begin{bmatrix} 1-\lambda & 0 \\ 1 & 1-\lambda \end{bmatrix} = (1-\lambda)^2.$$

Result: The only eigenvalue is $\lambda = 1$, with *algebraic multiplicity* 2.

Step 2: Eigenvectors for $\lambda = 1$

$$A - I = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad (A - I)\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ x \end{bmatrix} = 0.$$

Thus, $x = 0$, and y is free.

Kernel (null space): The set of all solutions to $(A - I)\vec{v} = 0$:

$$\ker(A - I) = \left\{ \begin{bmatrix} 0 \\ y \end{bmatrix} : y \in \mathbb{C} \right\}.$$

Span: This is written as

$$\ker(A - I) = \text{span}\left\{ \begin{bmatrix} 0 \\ 1 \end{bmatrix} \right\}.$$

Dimension of eigenspace: 1.

Adjoint of an Operator

- Let A be a linear operator on a Hilbert space V.
- There exists a unique operator $A^\dagger$ (the **adjoint** of A) such that:

$$(|v\rangle, A|w\rangle) = (A^\dagger|v\rangle, |w\rangle) \quad \forall |v\rangle, |w\rangle \in V$$

- $A^\dagger$ is also called the **Hermitian conjugate**.
- In matrix representation:

$$A^\dagger = (A^*)^T$$

(conjugate transpose).

Properties of the Adjoint

- $(AB)^\dagger = B^\dagger A^\dagger$
- $(A^\dagger)^\dagger = A$
- $(\alpha A + \beta B)^\dagger = \alpha^* A^\dagger + \beta^* B^\dagger$
- For vectors:

$$(A|v\rangle)^\dagger = \langle v|A^\dagger$$

Hermitian Operators

- An operator A is **Hermitian** if:

$$A^\dagger = A$$

- Properties:
  - All eigenvalues are real.
  - Eigenvectors corresponding to different eigenvalues are orthogonal.
- Physical significance:
  - Observables in quantum mechanics (e.g., position, momentum, energy) are represented by Hermitian operators.

Example

- Consider the matrix
$$A = \begin{bmatrix} 2 & i \\ -i & 3 \end{bmatrix}$$
- Compute the adjoint:
$$A^\dagger = \begin{bmatrix} 2 & i \\ -i & 3 \end{bmatrix}^\dagger = \begin{bmatrix} 2 & -i \\ i & 3 \end{bmatrix}^T = \begin{bmatrix} 2 & i \\ -i & 3 \end{bmatrix} = A$$
- Therefore, A is Hermitian.

Projectors: An Important Class of Hermitian Operators

Setting

Suppose W is a k-dimensional vector subspace of the d-dimensional vector space V.

Using the Gram-Schmidt procedure, we can construct an orthonormal basis $|1\rangle, \ldots, |d\rangle$ for V such that $|1\rangle, \ldots, |k\rangle$ is an orthonormal basis for W.

Definition of a Projector

Definition

The **projector** onto the subspace W is defined as:

$$P \equiv \sum_{i=1}^{k} |i\rangle \langle i|$$

Key Property

This definition is **independent** of the particular orthonormal basis $|1\rangle, \ldots, |k\rangle$ used for W.

Hermitian Property of Projectors

Theorem

Projectors are Hermitian operators: $P^\dagger = P$

Proof.

From the definition, we know that $|v\rangle\langle v|$ is Hermitian for any vector $|v\rangle$. Since:

$$P = \sum_{i=1}^{k} |i\rangle\langle i|$$

and each term $|i\rangle\langle i|$ is Hermitian, their sum P is also Hermitian. $\square$

Notation Convention

Vector Space Shorthand

We will often refer to the '**vector space**' P as shorthand for the vector space onto which P is a projector.

This notation is convenient when discussing properties and operations involving the subspace associated with a projector.

Orthogonal Complement Projector

Definition

The **orthogonal complement** of projector P is defined as:

$$Q \equiv I - P$$

where I is the identity operator on V.

Properties of the Orthogonal Complement

Theorem

Q is a projector onto the vector space spanned by $|k+1\rangle, \ldots, |d\rangle$

Notation

We refer to this space as the **orthogonal complement** of P, and may denote it by Q.

The basis $|k+1\rangle, \ldots, |d\rangle$ completes the orthonormal basis for the entire space V.

Key Properties Summary

- Projectors are **Hermitian operators**: $P^\dagger = P$
- Projectors are **idempotent**: $P^2 = P$
- The identity minus a projector gives the **orthogonal complement**
- P and Q project onto **orthogonal subspaces**
- $P + Q = I$ (completeness relation)
- P projects vectors onto subspace W
- Q projects onto the orthogonal complement
- Any vector can be decomposed as $|\psi\rangle = P|\psi\rangle + Q|\psi\rangle$

Normal Operators

Definition

An operator A is said to be **normal** if it commutes with its adjoint:

$$AA^{\dagger} = A^{\dagger}A$$

Immediate Observation

Any **Hermitian** operator is automatically normal, since if $A^{\dagger} = A$, then:

$$AA^{\dagger} = A^2 = A^{\dagger}A$$

The Spectral Decomposition Theorem

Theorem (Spectral Decomposition)

An operator is **normal** *if and only if it is* **diagonalizable***.*

Remarkable Result

This representation theorem provides a complete characterization of normal operators in terms of diagonalizability.

Spectral Decomposition Formula

Theorem

If A is a normal operator, then it can be written in the form:

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

where:

- *λ_i are the eigenvalues of A*
- *$\{|i\rangle\}$ form an orthonormal basis of eigenvectors*
- *$A|i\rangle = \lambda_i |i\rangle$ for each i*

Significance of the Theorem

- **Characterization**: Provides necessary and sufficient conditions for diagonalizability
- **Computational Power**: Simplifies many operator calculations
- **Functional Calculus**: Enables defining functions of operators:

$$f(A) = \sum_i f(\lambda_i) \left| i \right\rangle \left\langle i \right|$$

- **Quantum Mechanics**: Fundamental for observable measurements and time evolution

Applications in Quantum Mechanics

- **Observables**: All quantum observables are Hermitian (hence normal)
- **Measurement**: Projective measurements use spectral decomposition:

$$M_m = \sum_{i:\lambda_i = m} |i\rangle \langle i|$$

- **Density Operators**: Can be diagonalized (spectral theorem)
- **Time Evolution**: Unitary operators are normal

Summary

- Normal operators: $AA^\dagger = A^\dagger A$
- Includes all Hermitian and unitary operators
- Spectral decomposition: Normal $\Leftrightarrow$ Diagonalizable
- Powerful representation: $A = \sum_i \lambda_i |i\rangle \langle i|$
- Fundamental for quantum mechanics and operator theory

Definition of Unitary Operators

Definition

A matrix U is said to be **unitary** if:

$$U^\dagger U = I$$

Similarly, an operator U is unitary if $U^\dagger U = I$.

Matrix Representation

An operator is unitary if and only if **each** of its matrix representations is unitary.

Properties of Unitary Operators

Theorem

If U is unitary, then it also satisfies:

$$UU^\dagger = I$$

Corollary

Unitary operators are **normal***:*

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

and therefore have a **spectral decomposition***.*

Constructing Unitary Operators from Bases

Theorem

If $\{|v_i\rangle\}$ and $\{|w_i\rangle\}$ are any two orthonormal bases, then the operator:

$$U \equiv \sum_i |w_i\rangle \langle v_i|$$

is a unitary operator.

Physical Significance in Quantum Mechanics

- **Time Evolution**: Quantum dynamics is described by unitary operators
- **Symmetry Operations**: Rotations, translations, and other symmetries
- **Quantum Gates**: All quantum computations are unitary transformations
- **State Changes**: Unitary operators describe reversible state transformations

Summary: Key Properties

- $U^\dagger U = UU^\dagger = I$
- Preserve inner products: $\langle Uv | Uw | Uv | Uw \rangle = \langle v | w | v | w \rangle$
- Preserve norms: $\| U \, |v\rangle \| = \| \, |v\rangle \|$
- Have complete orthonormal sets of eigenvectors
  item Eigenvalues lie on the unit circle in complex plane
- Can be constructed from any two orthonormal bases

Examples of Unitary Operators

Example (Pauli Matrices)

The Pauli matrices are both Hermitian and unitary:

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

Example (Rotation Operators)

$$R_x(\theta) = e^{-i\theta\sigma_x/2} = \cos(\theta/2)I - i\sin(\theta/2)\sigma_x$$

Activity: Verify $R_x(\theta) = e^{-i\theta\sigma_x/2}$

Identity to verify

$$R_x(\theta) = e^{-i\theta\sigma_x/2} = \cos(\theta/2)I - i\sin(\theta/2)\sigma_x$$

1. First, verify that $\sigma_x^2 = I$
2. Use the exponential Taylor series expansion
3. Separate into even and odd terms
4. Identify cosine and sine series

Python + QM in the Cloud

- We will use **Python** to explore to see the examples of today.
- Environment: **Anaconda Cloud** at `https://anaconda.com/app`
  1. Launch a **Jupyter Notebook** session in the cloud.
  2. Create a new project.
  3. From the course **Canvas Files section**, download the provided Jupyter notebook.
  4. Upload it into your Anaconda project.

Proofs

You can find the proofs here

The Spectral Decomposition Theorem

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where:

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- $A|i\rangle = \lambda_i |i\rangle$ *for each* i

Proof Outline ($\Rightarrow$)

Normal $\Rightarrow$ Diagonalizable

1. Use the fact that normal operators have a complete set of orthonormal eigenvectors
2. Show that the operator can be expressed in its eigenbasis
3. Construct the spectral decomposition explicitly

Proof Outline ($\Leftarrow$)

Diagonalizable $\Rightarrow$ Normal

1. Assume $A = \sum_i \lambda_i |i\rangle \langle i|$ (diagonalizable)
2. Compute $A^\dagger = \sum_i \lambda_i^* |i\rangle \langle i|$
3. Show that $AA^\dagger = A^\dagger A$ by direct computation:

$$AA^\dagger = \sum_i |\lambda_i|^2 |i\rangle \langle i| = A^\dagger A$$

Outer Product Representation

Theorem

Any unitary operator U can be written in the elegant outer product form:

$$U = \sum_i |w_i\rangle \langle v_i|$$

where $\{|v_i\rangle\}$ is any orthonormal basis and $|w_i\rangle \equiv U |v_i\rangle$.

Proof of Outer Product Representation

Proof.

1. Let $\{|v_i\rangle\}$ be any orthonormal basis
2. Define $|w_i\rangle \equiv U|v_i\rangle$
3. Since U preserves inner products, $\{|w_i\rangle\}$ is also an orthonormal basis
4. Check the action on basis vectors:

$$U|v_j\rangle = |w_j\rangle = \left(\sum_i |w_i\rangle\langle v_i|\right)|v_j\rangle$$

5. Therefore, $U = \sum_i |w_i\rangle\langle v_i|$

$\square$

Constructing Unitary Operators from Bases

Theorem

If $\{|v_i\rangle\}$ and $\{|w_i\rangle\}$ are any two orthonormal bases, then the operator:

$$U \equiv \sum_i |w_i\rangle \langle v_i|$$

is a unitary operator.

Proof: Constructed Operator is Unitary

Proof.

Check $U^\dagger U = I$:

$$U^\dagger U = \left(\sum_j |v_j\rangle \langle w_j|\right)\left(\sum_i |w_i\rangle \langle v_i|\right) = \sum_{i,j} |v_j\rangle \underbrace{\langle w_j|w_i|w_j|w_i\rangle}_{\delta_{ji}} \langle v_i|$$

$$= \sum_i |v_i\rangle \langle v_i| = I$$

Similarly, $UU^\dagger = I$. □