University of Tissemsilt
Faculty of Sciences and Technology
Department of Sciences of Matter (SM)

Chapter 4 : The Mathematical Structure of Quantum Mechanics

The vectors

Classical Physics

$$\vec{V}, \vec{A}, \vec{B}$$

Quantum Mechanics

$$|\phi\rangle, \ |V\rangle, \ |\psi\rangle$$

These objects are called "kets", and this type of notation is known as Dirac notation.

Linear Vector Spaces

A linear vector space $\boldsymbol{V}$ is a set of elements $|a\rangle$, $|b\rangle$, $|c\rangle$ called vectors, or kets, for which the following hold:

- $\boldsymbol{V}$ is closed under addition. This means that if two vectors $|a\rangle$, $|b\rangle$ belong to $\boldsymbol{V}$, then so does their sum $|a\rangle + |b\rangle$
- A vector $|a\rangle$ can be multiplied by a scalar α to yield a new, well-defined vector $\alpha|a\rangle$ that belongs to $\boldsymbol{V}$
- Vector addition is commutative: $|a\rangle + |b\rangle = |b\rangle + |a\rangle$
- Vector addition is associative: $|a\rangle + (|b\rangle + |c\rangle) = (|a\rangle + |b\rangle) + |c\rangle$

- There exists a unique element called 0 that satisfies $|a\rangle + 0 = |a\rangle$ for every $|a\rangle$ in ***V***

- There exists an identity element in *V* such that $I|a\rangle = |a\rangle$ for every vector in ***V***

- Scalar multiplication is associative: $(\alpha\beta)|\,|a\rangle = \alpha(\beta\,|a\rangle)$

- Scalar multiplication is linear:

$$\alpha(|\,|a\rangle + |b\rangle) = \alpha\,|a\rangle + \alpha\,|b\rangle\,, \quad (\alpha + \beta)\,|a\rangle = \alpha\,|a\rangle + \beta\,|a\rangle$$

- For each $|a\rangle$ in ***V***, there exists a unique additive inverse $|-a\rangle$ such that

$$|a\rangle + |-a\rangle = 0$$

What is the "Ket« or the Vector

The "Ket" is a column matrix $(n \times 1)$

$$|\psi\rangle = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix}$$

$$|\psi\rangle = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix}, \quad |\phi\rangle = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}$$

$$|\psi\rangle + |\phi\rangle = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} + \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} z_1 + w_1 \\ z_2 + w_2 \\ \vdots \\ z_n + w_n \end{bmatrix}$$

$$\alpha|\psi\rangle = \alpha \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} = \begin{bmatrix} \alpha z_1 \\ \alpha z_2 \\ \vdots \\ \alpha z_n \end{bmatrix}$$

Dual Vector

In the language of kets, the dual vector is called a "bra". Using Dirac notation, the dual of a vector $|\psi\rangle$ is written as $\langle\psi|$

$$|\psi\rangle = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} \Rightarrow \langle\psi| = [z_1^*, z_2^*, \ldots, z_n^*]$$

The scalar product

Dirac denoted the scalar (inner) product by the symbol $\langle \quad | \quad \rangle$, which he called a "bra-ket". For instance, the scalar product (ϕ, ψ) is denoted by the bra-ket $\langle \phi | \psi \rangle$:

$$(\phi, \psi) \rightarrow \langle \phi | \psi \rangle$$

given two vectors of complex numbers $|\psi\rangle$, $|\phi\rangle$ such that: $|\psi\rangle = \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix}, |\phi\rangle = \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix}$

the scalar product between these two vectors is defined by:

$$\langle \phi | \psi \rangle = (w_1^* w_2^* \ldots w_n^*) \begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} = w_1^*(z_1) + w_2^*(z_2) + \cdots + w_n^*(z_n) = \sum_{i=1}^{n} w_i^* z_i$$

Properties of kets, bras, and bra-kets

To every *ket* $|\,\psi\rangle$, there corresponds a unique *bra* $\langle\psi\,|$ and vice versa:

$$|\,\psi\rangle \quad \longleftrightarrow \quad \langle\psi\,|$$

There is a one-to-one correspondence between bras and kets:

$$a\,|\,\psi\rangle + b\,|\,\phi\rangle \quad \longleftrightarrow \quad a^*\langle\psi\,| + b^*\langle\phi\,|,$$

where a and b are complex numbers. The following is a common notation:

$$|\,a\psi\rangle = a\,|\,\psi\rangle, \qquad \langle a\psi\,| = a^*\langle\psi\,|$$

$\langle\psi \mid \phi\rangle$ is not the same thing as $\langle\phi \mid \psi\rangle$: $\langle\phi \mid \psi\rangle^* = \langle\psi \mid \phi\rangle$

$$\langle\psi \mid a_1\psi_1 + a_2\psi_2\rangle = a_1\langle\psi \mid \psi_1\rangle + a_2\langle\psi \mid \psi_2\rangle$$

$$\langle a_1\phi_1 + a_2\phi_2 \mid \psi\rangle = a_1^*\langle\phi_1 \mid \psi\rangle + a_2^*\langle\phi_2 \mid \psi\rangle$$

$$\langle a_1\phi_1 + a_2\phi_2 \mid b_1\psi_1 + b_2\psi_2\rangle = \begin{array}{l} a_1^* b_1\langle\phi_1 \mid \psi_1\rangle + a_1^* b_2\langle\phi_1 \mid \psi_2\rangle \\ + a_2^* b_1\langle\phi_2 \mid \psi_1\rangle + a_2^* b_2\langle\phi_2 \mid \psi_2\rangle \end{array}$$

Schwarz inequality: For any two states $\mid \psi\rangle$ and $\mid \phi\rangle$ of the Hilbert space, we can show that

$$|\langle\psi \mid \phi\rangle|^2 \le \langle\psi \mid \psi\rangle\langle\phi \mid \phi\rangle$$

Triangle inequality: $\sqrt{\langle\psi + \phi \mid \psi + \phi\rangle} \le \sqrt{\langle\psi \mid \psi\rangle} + \sqrt{\langle\phi \mid \phi\rangle}$

Orthogonal states: Two *kets*, $\mid \psi\rangle$ and $\mid \phi\rangle$, are said to be orthogonal if they have a vanishing scalar product:

$$\langle\psi \mid \phi\rangle = 0$$

Orthonormal states:

Two *kets*, $|\,\psi\rangle$ and $|\,\phi\rangle$, are said to be orthonormal if they are orthogonal and if each one of them has a unit norm:

$$\langle\psi\,|\,\phi\rangle = 0, \qquad \langle\psi\,|\,\psi\rangle = 1, \qquad \langle\phi\,|\,\phi\rangle = 1$$

Activity 01

Consider the following two kets:

$$| \psi \rangle = \begin{pmatrix} -3i \\ 2+i \\ 4 \end{pmatrix}, \qquad | \phi \rangle = \begin{pmatrix} 2 \\ -i \\ 2-3i \end{pmatrix}$$

(a) Find the bra $\langle \phi |$.

(b) Evaluate the scalar product $\langle \phi | \psi \rangle$.

(c) Examine why the products $| \psi \rangle | \phi \rangle$ and $\langle \phi | \langle \psi |$ do not make sense.

Activity 02

Two vectors in a three-dimensional complex vector space are defined by:

$$|A\rangle = \begin{pmatrix} 2 \\ -7i \\ 1 \end{pmatrix}, |B\rangle = \begin{pmatrix} 1+3i \\ 4 \\ 8 \end{pmatrix}$$

Let $a = 6 + 5i$

(a) Compute $a\,|A\rangle$, $a\,|B\rangle$, and $a(|A\rangle + |B\rangle)$. Show that $a(|A\rangle + |B\rangle) = a\,|A\rangle + a\,|B\rangle$.

(b) Find the inner products $\langle A|B\rangle$, $\langle B|A\rangle$.

Activity 03

Let two vectors be defined by

$$|A\rangle = \begin{pmatrix} 2 \\ -7i \\ 1 \end{pmatrix}, |B\rangle = \begin{pmatrix} 1+3i \\ 4 \\ 8 \end{pmatrix}$$

Find the norm of each vector.

Activity 04

Show that the vectors

$$|\psi\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, |\phi\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$$

are orthogonal. Is $|\psi\rangle$ normalized?

Basis Vectors

We call a set of vectors $\{|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_n\rangle\}$ a *basis* if the set satisfies three criteria:

1. The set $\{|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_n\rangle\}$ *spans* the vector space V, meaning that every vector $|\psi\rangle$ in V can be written as a unique linear combination of the $\{|\phi_i\rangle\}$.

$$|\psi\rangle = c_1 |\phi_1\rangle + c_2 |\phi_2\rangle + \ldots + c_n |\phi_n\rangle$$

2. The set $\{|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_n\rangle\}$ is linearly independent

3. The closure relation is satisfied.

Linearly Independent

A collection of vectors $\{|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_n\rangle\}$ are *linearly independent* if the equation

$$a_1 |\phi_1\rangle + a_2 |\phi_2\rangle + \ldots + a_n |\phi_n\rangle = 0$$

implies that $a_1 = a_2 = \cdots = a_n = 0$. If this condition is not met we say that the set is *linearly dependent*.

Activity 05

Show that the following vectors are linearly dependent:

$$|a\rangle = \begin{pmatrix} 1 \\ 2 \\ 1 \end{pmatrix} |b\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} |c\rangle = \begin{pmatrix} -1 \\ 0 \\ -1 \end{pmatrix}$$

Activity 06

Is the following set of vectors linearly independent?

$$|a\rangle = \begin{pmatrix} 2 \\ 0 \\ 0 \end{pmatrix}, |b\rangle = \begin{pmatrix} -1 \\ 0 \\ -1 \end{pmatrix}, |c\rangle = \begin{pmatrix} 0 \\ 0 \\ -4 \end{pmatrix}$$

The Closure Relation

An orthonormal set $\{|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_n\rangle\}$ constitutes a basis if and only if the set satisfies the closure relation

$$\sum_{i=1}^{n} |\phi_i\rangle \langle\phi_i| = 1$$

$$|\psi\rangle = c_1 |\phi_1\rangle + c_2 |\phi_2\rangle + \ldots + c_n |\phi_n\rangle \quad \text{with} \quad c_i = \langle\phi_i|\psi\rangle$$

$$|\psi\rangle = \sum_i c_i |\phi_i\rangle \Leftrightarrow |\psi\rangle = \sum_i |\phi_i\rangle \left(\langle\phi_i|\psi\rangle\right) \Leftrightarrow |\psi\rangle = \underbrace{\sum_i |\phi_i\rangle\langle\phi_i|}_{1} \psi\rangle$$

Operators

- Physical Observables – quantities that can be measured like position and momentum – are represented within the mathematical structure of quantum mechanics by operators.
- Mathematically, an operator $\hat{A}$ can be represented by a matrix, it is a mathematical rule or instruction that transforms one vector $|\psi\rangle$ into a new, generally different vector $|\psi'\rangle$. $\hat{A}\,|\psi\rangle = |\psi'\rangle$ or $\langle\psi|\hat{A} = \langle\psi'|$
- the eigenvalues of the matrix tell us that the possible outcomes of measuring a quantity represent the operator,
- while the eigenvectors of the matrix give us a basis that we can use to represent the states.

Products of operators

The product of two operators is generally not commutative: $\hat{A}\hat{B} \neq \hat{B}\hat{A}$

The product of operators is, however, associative: $\hat{A}\hat{B}\hat{C} = \hat{A}(\hat{B}\hat{C}) = (\hat{A}\hat{B})\hat{C}$

We may also write $\hat{A}^n \hat{A}^m = \hat{A}^{n+m}$

When the product $\widehat{A}\,\widehat{B}$ operates on a ket $|\psi\rangle$ (the order of application is important), the operator $\widehat{B}$ acts first on $|\psi\rangle$ and then $\widehat{A}$ acts on the new ket $\widehat{B}\,|\psi\rangle$:

$$\hat{A}\hat{B} \mid \psi\rangle = \hat{A}(\hat{B} \mid \psi\rangle)$$

Similarly, when $\hat{A}\hat{B}\hat{C}\hat{D}$ operates on a ket $\mid \psi\rangle$, $\hat{D}$ acts first, then $\hat{C}$, then $\hat{B}$, and then $\hat{A}$.

Linear operators

The operators that are most interesting to us are linear operators.

An operator $\hat{A}$ is said to be *linear* if it obeys the distributive law and, like all operators, it commutes with constants.

That is, an operator $\hat{A}$ is linear if, for any vectors $|\psi_1\rangle$ and $|\psi_2\rangle$ and any complex numbers a_1 and a_2, we have

$$\hat{A}\left(a_1 \mid \psi_1\rangle + a_2 \mid \psi_2\rangle\right) = a_1 \hat{A} \mid \psi_1\rangle + a_2 \hat{A} \mid \psi_2\rangle$$

Simple Operators

We now consider some simple operators:

The Identity Operator: The simplest operator of all is the identity operator, which does nothing to a ket $I\,|u\rangle = |u\rangle$

Outer Product: The outer product between a ket and a bra is written as follows

$$|\psi\rangle\,\langle\phi|$$

This expression is an operator.

$$(|\psi\rangle\,\langle\phi|)\,|\chi\rangle = |\psi\rangle\,\langle\phi\,|\chi\,\rangle$$

$$(|\psi\rangle\,\langle\phi|)\,|\chi\rangle = \alpha\,|\psi\rangle$$

Activity 07

The outer product $|\phi\rangle\langle\psi|$ is an operator, and is therefore can be represented by a matrix. Show this for:

$$|\Phi\rangle = \begin{pmatrix} 2 \\ 3i \\ 4 \end{pmatrix} |\Psi\rangle = \begin{pmatrix} -1 \\ 0 \\ i \end{pmatrix}$$

Given that $\langle\Psi|\Psi\rangle = 2$, the action of this operator on a ket

$$(|\Phi\rangle\langle\Psi|)(3|\Psi\rangle) = 3(\langle\Psi|\Psi\rangle)|\Phi\rangle = 3(2)|\Phi\rangle = \begin{pmatrix} 12 \\ 18i \\ 24 \end{pmatrix}$$

Show this with matrix multiplication.

The Representation of an Operator

The representation of an operator is formed by considering its action on a given set of basis vectors.

In a basis that we label $|u_i\rangle$, the components of an operator $\hat{T}$ are found by forming the following inner product: $T_{ij} = \langle u_i|\hat{T}|u_j\rangle$

When the given vector space is n dimensional, the components of the operator can be arranged into an $n \times n$ matrix, where T_{ij} is the element at row i and column j :

$$\hat{T} \to (T_{ij}) = \begin{pmatrix} T_{11} & T_{12} & \dots & T_{1n} \\ T_{21} & T_{22} & \dots & T_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ T_{n1} & T_{n2} & \dots & T_{nn} \end{pmatrix} = \begin{pmatrix} \langle u_1|\hat{T}|u_1\rangle & \langle u_1|\hat{T}|u_2\rangle & \dots & \langle u_1|\hat{T}|u_n\rangle \\ \langle u_2\hat{T}|u_1\rangle & \langle u_2|\hat{T}|u_2\rangle & \dots & \langle u_2|\hat{T}|u_n\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle u_n|\hat{T}|u_1\rangle & \langle u_n|\hat{T}|u_2\rangle & \dots & \langle u_n|\hat{T}|u_n\rangle \end{pmatrix}$$

Activity 08

Suppose that in some orthonormal basis $\{|u_1\rangle, |u_2\rangle, |u_3\rangle\}$ an operator $\hat{A}$ acts as follows:

$$\hat{A}|u_1\rangle = 2|u_1\rangle$$

$$\hat{A}|u_2\rangle = 3|u_1\rangle - i|u_3\rangle$$

$$\hat{A}|u_3\rangle = -|u_2\rangle$$

Write the matrix representation of the operator.

The Trace of an Operator

The trace of an operator $\hat{T}$ is the sum of the diagonal elements of its matrix and is denoted $t_r(\hat{T})$. If

$$\hat{T} = (T_{ij}) = \begin{pmatrix} T_{11} & T_{12} & \dots & T_{1n} \\ T_{21} & T_{22} & \dots & T_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ T_{n1} & T_{n2} & \dots & T_{nn} \end{pmatrix} = \begin{pmatrix} \langle u_1|\hat{T}|u_1\rangle & \langle u_1|\hat{T}|u_2\rangle & \dots & \langle u_1|\hat{T}|u_n\rangle \\ \langle u_2|\hat{T}|u_1\rangle & \langle u_1|\hat{T}|u_2\rangle & \dots & \langle u_2|\hat{T}|u_n\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle u_n|\hat{T}|u_1\rangle & \langle u_n|\hat{T}|u_2\rangle & \dots & \langle u_n|\hat{T}|u_n\rangle \end{pmatrix}$$

then $Tr(\hat{T}) = T_{11} + T_{22} + \ldots + T_{nn} = \sum_{i=1}^{n} T_{ii}$. Alternatively, we can write the trace as:

$$Tr(\hat{T}) = \langle u_1|\hat{T}|u_2\rangle + \langle u_2|\hat{T}|u_2\rangle + \ldots + \langle u_n|\hat{T}|u_n\rangle = \sum_{i=1}^{n} \langle u_i|\hat{T}|u_i\rangle.$$

Activity 09

By using a data from the previous example,

Find $T_r(\hat{A})$ from $\sum_{i=1}^{n}\langle u_i|A|u_j\rangle$ and show that this is equal to the sum of the diagonal elements of the matrix.

Eigenvalues and Eigenvectors of an Operator

- To each physical observable, such as energy or momentum, there exists an operator, which can be represented by a matrix; the eigenvalues of the matrix are the possible results of measurement for that operator.

- Finding the eigenvectors is also important, for they give us a basis for the space and therefore give us a way to represent any state.

A state vector $|\psi\rangle$ is said to be an eigenvector (also called an eigenket or eigenstate) of an operator $\hat{A}$ if the application of $\hat{A}$ to $|\psi\rangle$ gives

$$\hat{A}\,|\psi\rangle = a|\psi\rangle$$

where a is a complex number, called an *eigenvalue* of $\hat{A}$.

This equation is known as the *eigenvalue equation*, or *eigenvalue problem*, of the operator $\hat{A}$. Its solutions yield the eigenvalues and eigenvectors of $\hat{A}$.

A simple example is the eigenvalue problem for the unity operator $\hat{I}$:

$$\hat{I}\,|\psi\rangle = |\psi\rangle$$

This means that all vectors are eigenvectors of $\hat{I}$ with one eigenvalue, 1.

To find the eigenvalues and eigenvectors of a matrix A, we find the *characteristic polynomial* and set it equal to zero.

The polynomial is found by considering the determinant of the following quantity:

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

where I is the identity matrix. The characteristic polynomial is found from $\det(A - \lambda I)$; solving the equation above gives us the eigenvalues λ. We can then use them to find the eigenvectors for the matrix.

Activity 10

Find the characteristic polynomial and eigenvalues for each of the following matrices:

$$A = \begin{pmatrix} 5 & 3 \\ 2 & 10 \end{pmatrix}, \quad B = \begin{pmatrix} 7i & -1 \\ 2 & -6i \end{pmatrix}, \quad C = \begin{pmatrix} 2 & 0 & -1 \\ 0 & 3 & 1 \\ 1 & 0 & 4 \end{pmatrix}$$

Activity 11

In some orthonormal basis an operator $T = |\Phi_1\rangle\langle\Phi_1| + 2|\Phi_1\rangle\langle\Phi_2| + |\Phi_2\rangle\langle\Phi_1|$.

Find the matrix, representing T and find its (normalized) eigenvectors and eigenvalues. This vector space is two-dimensional.