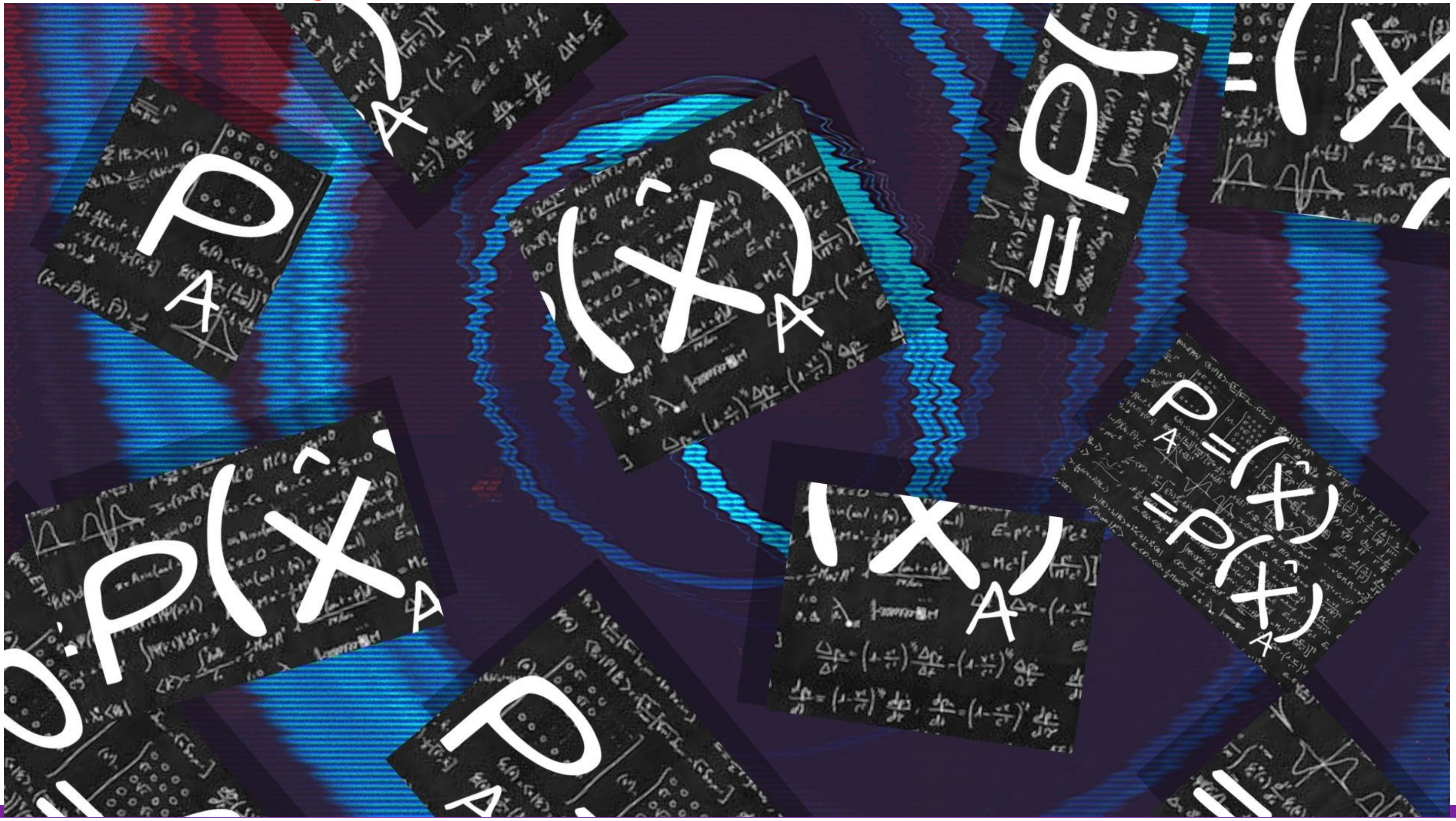
Quantum mechanics

Chapter II Algebraic Formulation of Quantum Mechanics



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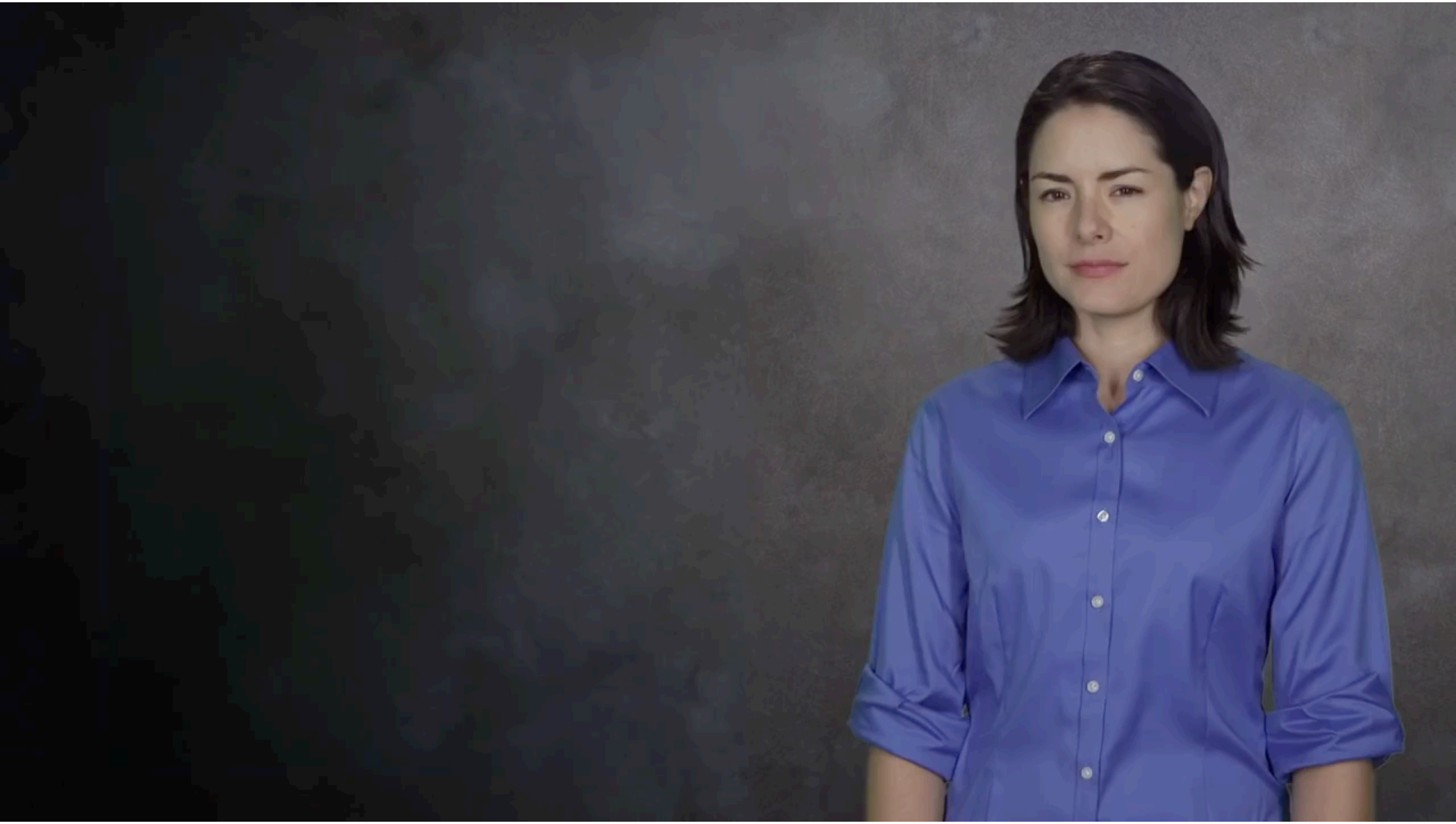

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Let us start by defining a linear vector space and listing out its properties. In general, a linear vector space consists of a set of elements ψ, φ, χ,… (called vectors) and a set of numbers a, b, c, . . . (called scalars), a set of rules each for the addition and multiplication of vectors.

Definition: A linear vector space V is a set of elements ψ, φ, χ,… called vectors, for which the following properties hold:

1. V is closed under addition. This means that if two vectors ψ and φ belong to V then their sum, written as $\psi + \varphi$, also belongs to V .

2. A vector ψ can be multiplied by a scalar a to yield a new, well-defined vector $a\psi$ that belongs to V ,

3. The addition of vectors is commutative, that is, $\psi+\varphi=\varphi+\psi$.

4. The addition of vectors is associative, that is, $\psi+(\varphi+\chi)=(\psi+\varphi)+\chi$.

5. There exists a unique element called 0 that satisfies $\psi+0=\psi$ for every element $\psi\in V$.

6. There exists an identity element, E, in V such that $E\psi=\psi$ for every element $\psi\in V$.

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7. The multiplication of a vector by scalars is associative, that is, $(ab)\psi = a(b\psi)$.

8. The multiplication of a vector by a scalar is linear, that is, $a(\psi+\varphi) = a\psi + a\varphi$, $\psi(a+b) = a\psi + b\psi$.

9. For each ψ in V , there exists a unique additive inverse $(-\psi)$ such that $\psi+(-\psi) = 0$.

If the vectors and the scalars associated with a given vector space are real, we say that we are working with a real vector space. On the other hand, if the vectors and the scalars are complex, then we say that we are working with a complex vector space.

Linear independence of vectors: Consider a set of n vectors, $\{\phi_1, \phi_2, \phi_3, \dots, \phi_n\}$, and their linear combination $a_1\phi_1 + a_2\phi_2 + a_3\phi_3 + \dots + a_n\phi_n$, where a_j= 1,2,3,…,n are all constants. The vectors of this set are said to be linearly independent if the equation

$$a_1\phi_1 + a_2\phi_2 + a_3\phi_3 + \dots + a_n\phi_n = 0$$

Consider hold only if $a_1 = a_2 = \dots = a_n = 0$. If this condition is not met, we say that the set is linearly dependent.

Note that if a set of vectors is linearly dependent, one of the vectors can be expressed as a linear combination of the others. For instance, assume that

$$a\psi + b\phi + \ldots + c\chi = 0,$$

where not all of the scalars are zero. Then one of the vectors can be expressed in terms of the other vectors as follows. Let a be non-zero. Then, we have

$$\psi = p\,\phi + \ldots + q\,\chi,$$

and

$$p = -\frac{b}{a}, \ldots, q = -\frac{c}{a}.$$

A linear vector space, V , is said to have dimension n, if the maximum number of linearly independent vectors in V equals n.

If this number n is finite, the linear vector space is called finite. On the other hand, if it is possible to find any number (as large as possible) of linearly independent vectors in it, then it is called infinite.

Basis: Any set of n linearly independent vectors, $\{\phi_i\}$, i = 1, 2, 3,...,n, belonging to the n-dimensional linear vector space, V , is called its basis. The elements, ϕ_1 , ϕ_2 , ϕ_3 , . . ., of this set are called the basis vectors.

Moreover, a basis is said to be complete if it spans the entire space; that is, there is no need to introduce any additional basis vector.

It also means that every vector ψ of a linear vector space V, with a complete basis, can be written as a unique linear combination of the basis vectors:

$$\psi = c_1\phi_1 + c_2\phi_1 + c_3\phi_3 + ... + c_n\phi_n,$$

where the expansion coefficients c_i, i = 1, 2, 3, . . . , n are called the components of the vector ψ in the basis $\{\phi_i\}$.

In quantum mechanics, the linear vector spaces are, as a rule, infinite-dimensional. The so-called Hilbert space plays an exceptional role among all the infinite-dimensional linear vector spaces.

A Hilbert space is equipped with an inner product that is essentially positive and allows to introduce metric relationship among various quantities.

In this sense, a Hilbert space is a natural generalization of Euclidean spaces to infinite-dimensional spaces.

Hilbert Space

A Hilbert space H is a collection of vectors, ψ, φ, χ,… and scalars, a, b, c,… that satisfies the following properties.

1. H is an infinite-dimensional linear vector space, that is, it has infinite dimensions and possesses all the properties of a linear vector space discussed earlier.

2. There exists in H a real inner product which is finite and satisfies all the aforementioned properties.

3. H is separable. $\|\psi - \psi_n\| < \varepsilon.$

4. H is complete. $\lim_{n,m\to\infty} \|\psi_n - \psi_m\| = 0,$ $\lim_{n\to\infty} \|\psi - \psi_n\| = 0.$

Square-Integrable Functions

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A In the case of function spaces, a "vector" element is given by a *complex function* and the *scalar product* by *integrals*. That is, the scalar product of two functions $\psi(x)$ and $\phi(x)$ is given by

$$(\psi, \phi) = \int \psi^*(x)\phi(x)\, dx.$$

If this integral *diverges*, the scalar product *does not exist*. As a result, if we want the function space to possess a scalar product, we must select only those functions for which (ψ,ϕ) is *finite*. In particular, a function $\psi(x)$ is said to be *square integrable* if the scalar product of ψ with itself,

$$(\psi, \psi) = \int |\psi(x)|^2\, dx,$$

is finite

We have already stated that vector spaces in quantum mechanics are complex. Therefore, we assume the elements of our n-dimensional linear vector space to be complex. We also assume the vector space to have a fixed basis $\{\phi_i\}$, i= 1, 2, 3,...,n.

Dirac notation: We introduce the notation $|\psi\rangle$ for a vector ψ belonging to an n-dimensional linear vector space V, and we call it a ket vector or simply a ket.

In fixed basis $\{\phi_i\}$, i = 1, 2, 3,..., n, a ket will be characterized by its complex components ψ_i, i = 1, 2, 3,...,n.

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It is convenient to arrange these components in to a column vector and write a ket as a column vector:

$$|\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \cdot \\ \cdot \\ \cdot \\ \psi_n \end{pmatrix}.$$

Dual vector: The familiar notion of a "scalar product" is incorporated by introducing a dual vector, written as $\langle\psi|$, for each of the vectors, $|\psi\rangle$, of V.

In Dirac's language, it is called a bra vector. The bra $\langle\psi|$ dual to a ket $|\psi\rangle$ is constructed by transposing the ket (that is, we write it as a row vector) followed by complex conjugation. In other words:

$$\text{If} \quad |\psi\rangle = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \cdot \\ \cdot \\ \cdot \\ \psi_n \end{pmatrix}, \quad \text{then} \quad \langle\psi| = \begin{pmatrix} \psi_1^* & \psi_2^* & \psi_3^* & \cdot & \cdot & \cdot & \psi_n^* \end{pmatrix}.$$

This method of complex conjugation is known as hermitian conjugation or dagger † operation: $\langle\psi| = (|\psi\rangle)^\dagger$.

There is a one-to-one correspondence between bras (constructed in this manner) and kets, that is, for a given ket $|\psi\rangle$, there is a unique bra $\langle\psi|$. In addition, the following relations hold good:

(a) If $|\lambda\rangle = \alpha|\mu\rangle$, then $\langle\lambda| = \alpha^*\langle\mu|$.

(b) If $|\lambda\rangle = |\alpha\mu\rangle + \beta|\nu\rangle$, then $\langle\lambda| = \alpha^*\langle\mu| + \beta^*\langle\nu|$.

The set of bras, dual to the kets of V , also forms a linear vector space, which is called the dual (to V)vector space. It is denoted as V*.

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The inner (or, scalar) product: The inner product (also called the scalar product) of two vectors $|\psi\rangle$ and $|\phi\rangle$ (written as $\langle\phi|\psi\rangle$) is defined by the following expression:

$$\langle \phi | \psi \rangle = \begin{pmatrix} \phi_1^* & \phi_2^* & \phi_3^* & . & . & . & \phi_n^* \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ . \\ . \\ . \\ \psi_n \end{pmatrix}$$

$$= (\phi_1^* \psi_1 + \phi_2^* \psi_2 + \phi_3^* \psi_3 + ... + \phi_n^* \psi_n) = \sum_{i=1}^{n} \phi_i^* \psi_i.$$

We call $\langle\phi|\psi\rangle$ a 'bracket'.

$$\langle \phi \mid \psi \rangle = \int \phi^*(\vec{r}, t) \psi(\vec{r}, t) \, d^3 r.$$

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Properties of the inner product:

$$\langle\lambda|\psi\rangle = \langle\psi|\lambda\rangle^* = \langle\psi|\alpha\mu\rangle^* = (\alpha\langle\psi|\mu\rangle)^* = \alpha^*\langle\psi|\mu\rangle^* = \alpha^*\langle\mu|\psi\rangle.$$

$$\langle\psi|\left(\alpha|\phi\rangle + \beta|\omega\rangle\right) = \alpha\langle\psi|\phi\rangle + \beta\langle\phi|\omega\rangle,$$

$$\left(\langle\alpha\psi| + \langle\beta\omega|\right)|\phi\rangle = \alpha^*\langle\psi|\phi\rangle + \beta^*\langle\omega|\phi\rangle,$$

$$\langle\psi|\psi\rangle \geq 0.$$

If the inner product between two vectors is zero, $\langle\phi|\psi\rangle = 0$, we say that the vectors are orthogonal.

Norm of a vector: The square root of the inner product of a vector with itself is called the norm, and is written as:

$$\|\psi\| = \sqrt{\langle\psi|\psi\rangle}.$$

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A vector $|\psi\rangle$ is said to be normalized if its norm is equal to 1:

$$\|\psi\| = \sqrt{\langle\psi|\psi\rangle} = 1.$$

Orthonormal and complete basis: An orthonormal basis consists of the basis vectors $\{|\phi_i\rangle\}$, i = 1, 2, 3, . . . , n, which have a unit norm and are pairwise orthogonal:

$$\langle\phi_i|\phi_j\rangle = \delta_{ij}, \qquad \|\phi_i\| = \sqrt{\langle\phi_i|\phi_i\rangle} = 1,$$

Let us first assume the basis to be discrete. An arbitrary vector, $|\psi\rangle$, belonging to the linear vector space can be expanded in this basis as

$$|\psi\rangle = \sum_i c_i\,|\phi_i\rangle,$$

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where the expansion coefficients $c_i = \langle \phi_i | \psi \rangle$ are called the components of the vector ψ in the basis $\{|\phi_i\rangle\}$. Note that if $|\psi\rangle$ is normalized to unity, i.e., $\langle \psi | \psi \rangle = 1$ then

$$\langle \psi | \psi \rangle = \sum_i \sum_j \langle \phi_i | c_i^* c_j | \phi_j \rangle = \sum_i \sum_j c_i^* c_j \langle \phi_i | \phi_j \rangle$$

$$= \sum_i \sum_j c_i^* c_j \delta_{ij} = \sum_i |c_i|^2 = 1.$$

and

$$\sum_i |c_i|^2 = \sum_i c^* c_i = \sum_i \langle \psi | \phi_i \rangle \langle \phi_i | \psi \rangle = \langle \psi \left(\sum_i |\phi_i\rangle \langle \phi_i| \right) \psi \rangle = 1.$$

Completeness condition

$$\sum_i |\phi_i\rangle \langle \phi_i| = \hat{I}.$$

In the case of a continuous basis in which the vector functions depend on a continuous parameter α, the closure relation reads:

$$\int d\alpha\, |\phi(\alpha)\rangle\langle\phi(\alpha)| = \hat{I}.$$

Finally, let us note that in an orthonormal basis $\{\phi_i\}$,i = 1,2,3,...,n, an arbitrary ket, $|\psi\rangle$ (belonging to the vector space) is represented by a column matrix

$$|\psi\rangle = \begin{pmatrix} \langle\phi_1|\psi\rangle \\ \langle\phi_2|\psi\rangle \\ \langle\phi_3|\psi\rangle \\ . \\ . \\ . \\ \langle\phi_n|\psi\rangle \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ . \\ . \\ . \\ c_n \end{pmatrix}.$$

Schwarz inequality

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For any two states $|\psi\rangle$ and $|\phi\rangle$ of the Hilbert space, we can show that

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

If $|\psi\rangle$ and $|\phi\rangle$ are linearly dependent (i.e., proportional: $|\psi\rangle$ =a $|\phi\rangle$, where is a scalar), this relation becomes an equality. The Schwarz inequality is analogous to the following relation of the real Euclidean space

$$|\vec{A}\cdot\vec{B}|^2 \;\le |\,\vec{A}\,|^2\,|\,\vec{B}\,|^2 \;.$$

Triangle inequality

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$$\sqrt{\langle \psi + \phi \mid \psi + \phi \rangle} \le \sqrt{\langle \psi \mid \psi \rangle} + \sqrt{\langle \phi \mid \phi \rangle}.$$

If $|\psi\rangle$ and $|\phi\rangle$ are linearly dependent and if the proportionality scalar is real and positive, the triangle inequality becomes an equality. The counterpart of this inequality in Euclidean space is given by

$$|\vec{A} + \vec{B}| \le |\vec{A}| + |\vec{B}|.$$

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

$$\langle \psi \mid \phi \rangle = 0, \qquad \langle \psi \mid \psi \rangle = 1, \qquad \langle \phi \mid \phi \rangle = 1.$$

Observables and Operators

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The measurable physical characteristics of a system, such as position, momentum, energy etc, are called observables and are represented by operators.

Mathematically, an operator, O, can be defined as a map $O : V \rightarrow V$ that takes a vector, belonging to a vector space V, to another vector also belonging to V.

In general, an operator is characterized by its action on the basis vectors of V and hence, in a chosen basis, it is represented by a matrix.

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The action of an arbitrary operator A on a ket $|\psi\rangle \in$ V is written as:

$$\hat{A}\,|\psi\rangle = |\phi\rangle\,.$$

The product of an operator A and a number (complex) a is an operator aA, which takes a vector $|\psi\rangle \in$ V into the vector a(A$\psi\rangle$) $\in$ V :

$$(a\hat{A})|\psi\rangle = a(\hat{A}|\psi\rangle.$$

The sum, C, of two operators A and B is defined as

$$\hat{C}\,|\psi\rangle = (\hat{A}+\hat{B})\,|\psi\rangle = \hat{A}\,|\psi\rangle + \hat{B}\,|\psi\rangle\,.$$

The operators in quantum mechanics are linear.

$$\hat{A}(\alpha\,|\psi\rangle + \beta\,|\phi\rangle) = \alpha\hat{A}\,|\psi\rangle + \beta\hat{A}\,|\phi\rangle\,.$$

Consider an operator A acting in V

$$|\phi\rangle = \hat{A}|\psi\rangle.$$

Let us introduce an operator $A^{\dagger}$ which acts in dual space V^{*} by taking the bra $\langle\psi|$,

$$\langle\phi| = \langle\psi|\hat{A}^{\dagger}.$$

Therefore,

$$\langle\psi|\hat{A}^{\dagger}|\chi\rangle^{*} = \langle\chi|\hat{A}|\psi\rangle.$$

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

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

Unity operator: it leaves any ket unchanged

$$\hat{I} \mid \psi\rangle = \mid \psi\rangle.$$

The gradient operator:

$$\vec{\nabla}\psi(\vec{r}) = (\partial\psi(\vec{r})/\partial x)\vec{i} + (\partial\psi(\vec{r})/\partial y)\vec{j} + (\partial\psi(\vec{r})/\partial z)\vec{k}.$$

The linear momentum operator:

$$\vec{P}\psi(\vec{r}) = -i\hbar\vec{\nabla}\psi(\vec{r}).$$

The Laplacian operator:

$$\nabla^2\psi(\vec{r}) = \partial^2\psi(\vec{r})/\partial x^2 + \partial^2\psi(\vec{r})/\partial y^2 + \partial^2\psi(\vec{r})/\partial z^2.$$

The parity operator:

$$\hat{\mathcal{P}}\psi(\vec{r}) = \psi(-\vec{r}).$$

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

$$\hat{A}^n \hat{A}^m = \hat{A}^{n+m}$$

and

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

The *expectation* or *mean* value of an operator *A* with respect to a state

$$\langle \hat{A} \rangle = \frac{\langle \psi \mid \hat{A} \mid \psi \rangle}{\langle \psi \mid \psi \rangle}.$$

The Hermitian adjoint, or simply the adjoint, $A^\dagger$, of an operator A is defined by this relation:

$$\langle \psi \mid \hat{A}^\dagger \mid \phi \rangle = \langle \phi \mid \hat{A} \mid \psi \rangle^*.$$

To obtain the Hermitian adjoint of any expression, we must cyclically reverse the order of the factors and make three replacements:

Replace constants by their complex conjugates: $\alpha^\dagger = \alpha^*.$

Replace kets (bras) by the corresponding bras (kets):

$$(\mid \psi \rangle)^\dagger = \langle \psi \mid \text{and} \ (\langle \psi \mid)^\dagger = \mid \psi \rangle.$$

Replace operators by their adjoints.

Hermitian Adjoint

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Following these rules, we can write

$$
\begin{aligned}
(\hat{A}^\dagger)^\dagger &= \hat{A}, \\
(a\hat{A})^\dagger &= a^*\hat{A}^\dagger, \\
(\hat{A}^n)^\dagger &= (\hat{A}^\dagger)^n, \\
(\hat{A}+\hat{B}+\hat{C}+\hat{D})^\dagger &= \hat{A}^\dagger+\hat{B}^\dagger+\hat{C}^\dagger+\hat{D}^\dagger, \\
(\hat{A}\hat{B}\hat{C}\hat{D})^\dagger &= \hat{D}^\dagger\hat{C}^\dagger\hat{B}^\dagger\hat{A}^\dagger, \\
(\hat{A}\hat{B}\hat{C}\hat{D}\mid\psi\rangle)^\dagger &= \langle\psi\mid D^\dagger C^\dagger B^\dagger A^\dagger.
\end{aligned}
$$

The Hermitian adjoint of the outer product is given by

$$
(\mid\psi\rangle\langle\phi\mid)^\dagger = \mid\phi\rangle\langle\psi\mid.
$$

Hermitian Adjoint

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Operators act inside kets and bras, respectively, as follows:

$$|\alpha\hat{A}\psi\rangle = \alpha\hat{A}\,|\,\psi\rangle, \qquad \langle\alpha\hat{A}\psi\,| = \alpha^*\langle\psi\,|\,\hat{A}^\dagger.$$

and

$$\langle\psi\,|\,\hat{A}\,|\,\phi\rangle = \langle\hat{A}^\dagger\psi\,|\,\phi\rangle = \langle\psi\,|\,\hat{A}\phi\rangle.$$

An operator A is said to be *Hermitian* if it is equal to its adjoint $A^\dagger$:

$$\boxed{\hat{A} = \hat{A}^\dagger \quad \text{or} \quad \langle\psi\,|\,\hat{A}\,|\,\phi\rangle = \langle\phi\,|\,\hat{A}\,|\,\psi\rangle^*.}$$

On the other hand, an operator B is said to be *skew-Hermitian* or *anti-Hermitian* if

$$\boxed{\hat{B}^\dagger = -\hat{B} \quad \text{or} \quad \langle\psi\,|\,\hat{B}\,|\,\phi\rangle = -\langle\phi\,|\,\hat{B}\,|\,\psi\rangle^*.}$$

The Projection Operator

An operator P is said to be a projection operator if it is hermitian and equal to its own square

$$\hat{P} = \hat{P}^\dagger, \qquad \hat{P}^2 = \hat{P}.$$

Clearly, the unit operator I satisfies these properties and is an example of a projection operator.

Consider an operator, A, equal to the outer product of a ket and its corresponding bra:

$$\hat{A} = |\phi\rangle\langle\phi|.$$

By definition it acts on a ket $|\psi\rangle$ through the rule

$$\hat{A}|\psi\rangle = (|\phi\rangle\langle\phi|)\,|\psi\rangle = |\phi\rangle\,\langle\phi|\psi\rangle.$$

The claim is that if $|\phi\rangle$ is normalized to unity, the operator A is a projection operator.

Consider the sum of two projection operators P_1 and P_2.

$$\hat{P}^\dagger = (\hat{P}_1\hat{P}_2)^\dagger = \hat{P}_2^\dagger\hat{P}_1^\dagger = \hat{P}_2\hat{P}_1,$$

$$\hat{P}^2 = (\hat{P}_1\hat{P}_2)^2 = \hat{P}_1\hat{P}_2\hat{P}_1\hat{P}_2 = \hat{P}_1(\hat{P}_2\hat{P}_1)\hat{P}_2.$$

It is quite clear from the aforementioned equations that P will satisfy the required properties for being a projection operator only if P_1 and P_2 commute. It is also clear that, if P_1 and P_2 commute, P does satisfy the required properties for being a projection operator.

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The *commutator* of two operators A and B, denoted by $[A, B]$, is defined by

$$[\hat{A},\ \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A},$$

and the anticommutator {A, B} is defined by

$$\{\hat{A},\ \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}.$$

Two operators are said to commute if their commutator is equal to zero and hence $AB=BA$. Any operator commutes with itself:

$$[\hat{A},\ \hat{A}] = 0.$$

Note that if two operators are Hermitian and their product is also Hermitian, these operators commute

$$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger = \hat{B}\hat{A},$$

We can establish the following properties about the commutator.

Antisymmetry: $$[\hat{A},\ \hat{B}] = -[\hat{B},\ \hat{A}]$$

Linearity: $$[\hat{A},\ \hat{B} + \hat{C} + \hat{D} + \cdots] = [\hat{A},\ \hat{B}] + [\hat{A},\ \hat{C}] + [\hat{A},\ \hat{D}] + \cdots$$

Hermitian conjugate of a commutator: $$[\hat{A},\ \hat{B}]^\dagger = [\hat{B}^\dagger,\ \hat{A}^\dagger]$$

Distributivity:

$$[\hat{A},\ \hat{B}\hat{C}] = [\hat{A},\ \hat{B}]\hat{C} + \hat{B}[\hat{A},\ \hat{C}]$$

$$[\hat{A}\hat{B},\ \hat{C}] = \hat{A}[\hat{B},\ \hat{C}] + [\hat{A},\ \hat{C}]\hat{B}$$

Jacobi identity: $$[\hat{A}, [\hat{B},\ \hat{C}]] + [\hat{B},\ [\hat{C},\ \hat{A}]] + [\hat{C},\ [\hat{A},\ \hat{B}]] = 0$$

Operators commute with scalars: $$[\hat{A},\ b] = 0$$

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An interesting application of the commutator algebra is to derive a general relation giving the uncertainties product of two operators, A and B.

Let A and B denote the expectation values of two Hermitian operators A and B with respect to a normalized state vector

$$\langle \hat{A} \rangle = \langle \psi \mid \hat{A} \mid \psi \rangle \qquad \langle \hat{B} \rangle = \langle \psi \mid \hat{B} \mid \psi \rangle.$$

Introducing the operators

$$\Delta \hat{A} = \hat{A} - \langle \hat{A} \rangle, \qquad \Delta \hat{B} = \hat{B} - \langle \hat{B} \rangle,$$

and

$$(\Delta \hat{A})^2 = \hat{A}^2 - 2\hat{A}\langle \hat{A} \rangle + \langle \hat{A} \rangle^2 \qquad (\Delta \hat{B})^2 = \hat{B}^2 - 2\hat{B}\langle \hat{B} \rangle + \langle \hat{B} \rangle^2,$$

Therefore

$$\langle \psi \mid (\Delta \hat{A})^2 \mid \psi \rangle = \langle (\Delta \hat{A})^2 \rangle = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2, \qquad \langle (\Delta \hat{B})^2 \rangle = \langle \hat{B}^2 \rangle - \langle \hat{B} \rangle^2,$$

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where,

$$\langle \hat{A}^2 \rangle = \langle \psi \mid \hat{A}^2 \mid \psi \rangle \qquad \langle \hat{B}^2 \rangle = \langle \psi \mid \hat{B}^2 \mid \psi \rangle .$$

The uncertainties ΔA and ΔB are defined by

$$\Delta A = \sqrt{\langle (\Delta \hat{A})^2 \rangle} = \sqrt{\langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2}, \qquad \Delta B = \sqrt{\langle (\Delta \hat{B})^2 \rangle} = \sqrt{\langle \hat{B}^2 \rangle - \langle \hat{B} \rangle^2}.$$

Let us write the action of the ΔA operators on any state as follows:

$$\mid \chi \rangle = \Delta \hat{A} \mid \psi \rangle = \left(\hat{A} - \langle \hat{A} \rangle \right) \mid \psi \rangle, \qquad \mid \phi \rangle = \Delta \hat{B} \mid \psi \rangle = \left(\hat{B} - \langle \hat{B} \rangle \right) \mid \psi \rangle.$$

The Schwarz inequality for these states

$$\langle \chi \mid \chi \rangle \langle \phi \mid \phi \rangle \geq |\langle \chi \mid \phi \rangle|^2 .$$

Uncertainty Relation

Since operators A and B are Hermitian, ΔA and ΔB must also be Hermitian:

$$\Delta\hat{A}^{\dagger} = \hat{A}^{\dagger} - \langle\hat{A}\rangle = \hat{A} - \langle\hat{A}\rangle = \Delta\hat{A}$$

$$\Delta\hat{B}^{\dagger} = \hat{B} - \langle\hat{B}\rangle = \Delta\hat{B}.$$

Thus, we can show the following three relations:

$$\langle\chi \mid \chi\rangle = \langle\psi \mid (\Delta\hat{A})^2 \mid \psi\rangle,$$

$$\langle\phi \mid \phi\rangle = \langle\psi \mid (\Delta\hat{B})^2 \mid \psi\rangle,$$

$$\langle\chi \mid \phi\rangle = \langle\psi \mid \Delta\hat{A}\Delta\hat{B} \mid \psi\rangle.$$

The Schwarz inequality leads

$$\langle(\Delta\hat{A})^2\rangle\langle(\Delta\hat{B})^2\rangle \geq \left|\langle\Delta\hat{A}\Delta\hat{B}\rangle\right|^2.$$

Notice that the last term ΔAΔB of this equation can be written as

$$\Delta\hat{A}\Delta\hat{B}=\frac{1}{2}[\Delta\hat{A},\ \Delta\hat{B}]+\frac{1}{2}\{\Delta\hat{A},\ \Delta\hat{B}\}=\frac{1}{2}[\hat{A},\ \hat{B}]+\frac{1}{2}\{\Delta\hat{A},\ \Delta\hat{B}\},$$

Since [A B] is anti-Hermitian and [ΔA ΔB] is Hermitian and since the expectation value of a Hermitian operator is real and that the expectation value of an anti-Hermitian operator is imaginary. Therefore

$$\left|\langle\Delta\hat{A}\Delta\hat{B}\rangle\right|^2=\frac{1}{4}\left|\langle[\hat{A},\ \hat{B}]\rangle\right|^2+\frac{1}{4}\left|\langle\{\Delta\hat{A},\ \Delta\hat{B}\}\rangle\right|^2.$$

Since the last term is a positive real number, we can infer the following relation:

$$\left|\langle \Delta\hat{A}\Delta\hat{B}\rangle\right|^2 \geq \frac{1}{4}\left|\langle[\hat{A},\ \hat{B}]\rangle\right|^2.$$

Finally

$$\boxed{\Delta A \Delta B \geq \frac{1}{2}\left|\langle[\hat{A},\ \hat{B}]\rangle\right|.}$$

This uncertainty relation plays an important role in the formalism of quantum mechanics for position and momentum operators

$$\boxed{\Delta x \Delta p_x \geq \frac{\hbar}{2}, \qquad \Delta y \Delta p_y \geq \frac{\hbar}{2}, \qquad \Delta z \Delta p_z \geq \frac{\hbar}{2}.}$$

Since

$$\boxed{[\hat{X},\ \hat{P}_x] = i\hbar\hat{I}, \qquad [\hat{Y},\ \hat{P}_y] = i\hbar\hat{I}, \qquad [\hat{Z},\ \hat{P}_z] = i\hbar\hat{I},}$$

Functions of Operators

Let $F(A)$ be a function of an operator A. If A is a linear operator, we can Taylor expand $F(A)$ in a power series of A:

$$F(\hat{A}) = \sum_{n=0}^{\infty} a_n \hat{A}^n,$$

where a_n is just an expansion coefficient. As an illustration of an operator function, consider exp(aA) where a is a scalar which can be complex or real. We can expand it as follows:

$$e^{a\hat{A}} = \sum_{n=0}^{\infty} \frac{a^n}{n!} \hat{A}^n = \hat{I} + a\hat{A} + \frac{a^2}{2!}\hat{A}^2 + \frac{a^3}{3!}\hat{A}^3 + \cdots.$$

If A commutes with another operator B, then B commutes with any operator function that depends on A:

$$[\hat{A},\ \hat{B}] = 0 \quad \Longrightarrow \quad [\hat{B},\ F(\hat{A})] = 0;$$

in particular, $F(A)$ commutes with A and with any other function, $G(A)$, of A:

$$[\hat{A},\ F(\hat{A})] = 0, \qquad [\hat{A}^n,\ F(\hat{A})] = 0, \qquad [F(\hat{A}),\ G(\hat{A})] = 0.$$

The adjoint of $F(A)$ is given by

$$[F(\hat{A})]^\dagger = F^*(\hat{A}^\dagger).$$

Note that if A is Hermitian, $F(A)$ is not necessarily Hermitian; $F(A)$ will be Hermitian only if F is a real function and A is Hermitian.

Inverse and Unitary Operators

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Inverse of an operator: Assuming it exists the inverse A^{-1} of a linear operator A is defined by the relation

$$\hat{A}^{-1}\hat{A} = \hat{A}\hat{A}^{-1} = \hat{I},$$

where I is the unit operator, the operator that leaves any state unchanged.

Quotient of two operators: Dividing an operator A by another operator B (provided that the inverse B^{-1} exists) is equivalent to multiplying A by B^{-1}:

$$\frac{\hat{A}}{\hat{B}} = \hat{A}\hat{B}^{-1}.$$

The side on which the quotient is taken matters:

$$\frac{\hat{A}}{\hat{B}} = \hat{A}\frac{\hat{I}}{\hat{B}} = \hat{A}\hat{B}^{-1} \quad \text{and} \quad \frac{\hat{I}}{\hat{B}}\hat{A} = \hat{B}^{-1}\hat{A}.$$

Inverse and Unitary Operators

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We may mention here the following properties about the inverse of operators:

$$\left(\hat{A}\hat{B}\hat{C}\hat{D}\right)^{-1} = \hat{D}^{-1}\hat{C}^{-1}\hat{B}^{-1}\hat{A}^{-1}, \qquad \left(\hat{A}^n\right)^{-1} = \left(\hat{A}^{-1}\right)^n.$$

Unitary operators: A linear operator U is said to be unitary if its inverse U^{-1} is equal to its adjoint $U^{\dagger}$:

$$\hat{U}^{\dagger} = \hat{U}^{-1} \qquad \text{or} \qquad \hat{U}\hat{U}^{\dagger} = \hat{U}^{\dagger}\hat{U} = \hat{I}.$$

The product of two unitary operators is also unitary, since

$$(\hat{U}\hat{V})(\hat{U}\hat{V})^{\dagger} = (\hat{U}\hat{V})(\hat{V}^{\dagger}\hat{U}^{\dagger}) = \hat{U}(\hat{V}\hat{V}^{\dagger})\hat{U}^{\dagger} = \hat{U}\hat{U}^{\dagger} = \hat{I},$$

This result can be generalized to any number of operators; the product of a number of unitary operators is also unitary, since

$$\begin{aligned}(\hat{A}\hat{B}\hat{C}\hat{D}\cdots)(\hat{A}\hat{B}\hat{C}\hat{D}\cdots)^{\dagger} &= \hat{A}\hat{B}\hat{C}\hat{D}(\cdots)\hat{D}^{\dagger}\hat{C}^{\dagger}\hat{B}^{\dagger}\hat{A}^{\dagger} = \hat{A}\hat{B}\hat{C}(\hat{D}\hat{D}^{\dagger})\hat{C}^{\dagger}\hat{B}^{\dagger}\hat{A}^{\dagger} \\ &= \hat{A}\hat{B}(\hat{C}\hat{C}^{\dagger})\hat{B}^{\dagger}\hat{A}^{\dagger} = \hat{A}(\hat{B}\hat{B}^{\dagger})\hat{A}^{\dagger} \\ &= \hat{A}\hat{A}^{\dagger} = \hat{I},\end{aligned}$$

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

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

where a is a complex number, called an *eigenvalue* of A. This equation is known as the *eigenvalue equation*, or *eigenvalue problem*, of the operator A. Its solutions yield the eigenvalues and eigenvectors of A.

A simple example is the eigenvalue problem for the unity operator I:

$$\hat{I} \mid \psi\rangle = \mid \psi\rangle.$$

This means that all vectors are eigenvectors of I with one eigenvalue, 1. Note that

$$\hat{A} \mid \psi\rangle = a \mid \psi\rangle \Longrightarrow \hat{A}^n \mid \psi\rangle = a^n \mid \psi\rangle \quad \text{and} \quad F(\hat{A}) \mid \psi\rangle = F(a) \mid \psi\rangle.$$

For instance, we have

$$\hat{A} \mid \psi\rangle = a \mid \psi\rangle \quad \Longrightarrow \quad e^{i\hat{A}} \mid \psi\rangle = e^{ia} \mid \psi\rangle.$$

For a Hermitian operator, all of its eigenvalues are real and the eigenvectors corresponding to different eigenvalues are orthogonal.

If $\hat{A}^\dagger = \hat{A}, \quad \hat{A} \mid \phi_n\rangle = a_n \mid \phi_n\rangle \quad \Longrightarrow \quad a_n = \text{real number, and } \langle\phi_m \mid \phi_n\rangle = \delta_{mn}.$

Since $\quad \hat{A} \mid \phi_n\rangle = a_n \mid \phi_n\rangle \quad \Longrightarrow \quad \langle\phi_m \mid \hat{A} \mid \phi_n\rangle = a_n\langle\phi_m \mid \phi_n\rangle,$

$$\langle\phi_m \mid \hat{A}^\dagger = a_m^*\langle\phi_m \mid \quad \Longrightarrow \quad \langle\phi_m \mid \hat{A}^\dagger \mid \phi_n\rangle = a_m^*\langle\phi_m \mid \phi_n\rangle.$$

$$(a_n - a_m^*)\langle\phi_m \mid \phi_n\rangle = 0.$$

The eigenstates of a Hermitian operator define a complete set of mutually orthonormal basis states. The operator is diagonal in this eigenbasis with its diagonal elements equal to the eigenvalues. This basis set is unique if the operator has no degenerate eigenvalues and not unique (in fact it is infinite) if there is any degeneracy.

If two Hermitian operators, A and B, commute and if A has no degenerate eigenvalue, then each eigenvector of A is also an eigenvector of B. In addition, we can construct a common orthonormal basis that is made of the joint eigenvectors of A and B.

The eigenvalues of an anti-Hermitian operator are either purely imaginary or equal to zero.

The eigenvalues of a unitary operator are complex numbers of moduli equal to one; the eigenvectors of a unitary operator that has no degenerate eigenvalues are mutually orthogonal.

We can write

$$(\langle\phi_m \mid \hat{U}^\dagger)(\hat{U} \mid \phi_n\rangle) = a_m^* a_n \langle\phi_m \mid \phi_n\rangle.$$

Since $U^\dagger U=I$ this equation can be rewritten as

$$(a_m^* a_n - 1)\langle\phi_m \mid \phi_n\rangle = 0,$$

Consider a discrete, complete, and orthonormal basis which is made of an infinite set of kets ϕ_1, ϕ_2, ϕ_3,…,ϕ_n and denote it by $\{|\phi_n\rangle\}$. Let us now examine how to represent the vector within the context of the basis $\{|\phi_n\rangle\}$. The completeness property of this basis enables us to expand any state vector $|\psi\rangle$ in terms of $|\phi_n\rangle$

$$|\psi\rangle = \hat{I}|\psi\rangle = \left(\sum_{n=1}^{\infty}|\phi_n\rangle\langle\phi_n|\right)|\psi\rangle = \sum_{n=1}^{\infty} a_n|\phi_n\rangle,$$

So, within the basis $\{|\phi_n\rangle\}$, the ket is represented by the set of its components, a_1, a_2, a_3, along ϕ_1, ϕ_2, ϕ_3,…, respectively.

Hence $|\psi\rangle$ can be represented by a *column* vector which has a countably infinite number of components:

$$| \psi \rangle \longrightarrow \begin{pmatrix} \langle \phi_1 \mid \psi \rangle \\ \langle \phi_2 \mid \psi \rangle \\ \vdots \\ \langle \phi_n \mid \psi \rangle \\ \vdots \end{pmatrix} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \\ \vdots \end{pmatrix}.$$

The bra $\langle\psi|$ can be represented by a *row* vector:

$$\begin{aligned} \langle \psi \mid \longrightarrow & \; (\langle \psi \mid \phi_1 \rangle \; \langle \psi \mid \phi_2 \rangle \; \cdots \; \langle \psi \mid \phi_n \rangle \; \cdots) \\ = & \; (\langle \phi_1 \mid \psi \rangle^* \; \langle \phi_2 \mid \psi \rangle^* \; \cdots \; \langle \phi_n \mid \psi \rangle^* \; \cdots) \\ = & \; (a_1^* \; a_2^* \; \cdots \; a_n^* \; \cdots). \end{aligned}$$

Using this representation, we see that a bra-ket is a complex number equal to the matrix product

$$\langle\psi \mid \phi\rangle = (a_1^* \;\; a_2^* \;\; \cdots \;\; a_n^* \;\; \cdots)\begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \\ \vdots \end{pmatrix} = \sum_n a_n^* b_n,$$

where $b_n = \langle\phi_n|\phi\rangle$. We see that, within this representation, the matrices representing and are Hermitian adjoints of each other.

Matrix Representation of Operators

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For each linear operator A, we can write

$$\hat{A} = \hat{I}\hat{A}\hat{I} = \left(\sum_{n=1}^{\infty} | \phi_n\rangle\langle\phi_n |\right)\hat{A}\left(\sum_{m=1}^{\infty} | \phi_m\rangle\langle\phi_m |\right) = \sum_{nm} A_{nm} | \phi_n\rangle\langle\phi_m |,$$

where A_{nm} is the nm matrix element of the operator A:

$$A_{nm} = \langle\phi_n | \hat{A} | \phi_m\rangle.$$

We see that the operator A is represented, within the basis $\{|\phi_n\rangle\}$, by a *square* matrix A

$$A = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

For instance, the *unit* operator I is represented by the unit matrix; when the unit matrix is multiplied with another matrix, it leaves that unchanged:

$$I = \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ 0 & 0 & 1 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

In summary, kets are represented by column vectors, bras by row vectors, and operators by square matrices.

Let us see how do we get the hermitian conjugate of an operator in practice. Let the matrix A = (A_{ij}), where i stands for the number of rows and j for the number of columns, represent an operator A in a linear vector space.

The first step is to find the matrix A^T which is transposed of the matrix A.

$$A^T = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}^T = \begin{pmatrix} A_{11} & A_{21} & A_{31} \\ A_{12} & A_{22} & A_{32} \\ A_{13} & A_{23} & A_{33} \end{pmatrix}.$$

The second and the final step is to find the matrix complex conjugate to the matrix A.

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix}^* = \begin{pmatrix} A_{11}^* & A_{12}^* & A_{13}^* \\ A_{21}^* & A_{22}^* & A_{23}^* \\ A_{31}^* & A_{32}^* & A_{33}^* \end{pmatrix}.$$

Thus, for any operator F, the corresponding **hermitian conjugate** operator, $F^\dagger$, is given by

$$F^\dagger = \begin{pmatrix} F_{11}^* & F_{21}^* & F_{31}^* \\ F_{12}^* & F_{22}^* & F_{32}^* \\ F_{13}^* & F_{23}^* & F_{33}^* \end{pmatrix}.$$

Trace of an operator

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The trace Tr(A) of an operator A is given, within an orthonormal basis $\{|\phi_n\rangle\}$, by the expression

$$\mathrm{Tr}(\hat{A}) = \sum_n \langle \phi_n \mid \hat{A} \mid \phi_n \rangle = \sum_n A_{nn};$$

we will see later that the trace of an operator does not depend on the basis. The trace of a matrix is equal to the sum of its diagonal elements:

$$\mathrm{Tr}\begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} = A_{11} + A_{22} + A_{33} + \cdots.$$

We can ascertain that

$$\mathrm{Tr}(\hat{A}^{\dagger}) = (\mathrm{Tr}(\hat{A}))^*,$$

$$\mathrm{Tr}(\alpha\hat{A} + \beta\hat{B} + \gamma\hat{C} + \cdots) = \alpha\mathrm{Tr}(\hat{A}) + \beta\mathrm{Tr}(\hat{B}) + \gamma\mathrm{Tr}(\hat{C}) + \cdots,$$

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Matrix representation of

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

can be written as

$$\left(\sum_n |\,\phi_n\rangle\langle\phi_n\,|\right)|\,\phi\rangle = \left(\sum_n |\,\phi_n\rangle\langle\phi_n\,|\right)\hat{A}\left(\sum_m |\,\phi_m\rangle\langle\phi_m\,|\right)|\,\psi\rangle,$$

therefore

$$\sum_n b_n\,|\,\phi_n\rangle = \sum_{nm} a_m\,|\,\phi_n\rangle\langle\phi_n\,|\,\hat{A}\,|\,\phi_m\rangle = \sum_{nm} a_m A_{nm}\,|\,\phi_n\rangle,$$

where $b_n = \langle\phi_n\,|\,\phi\rangle$, $A_{nm} = \langle\phi_n\,|\,\hat{A}\,|\,\phi_m\rangle$, and $a_m = \langle\phi_m\,|\,\psi\rangle$.

Hence

$$\begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix}.$$

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Matrix representation of

$$\langle \phi \mid \hat{A} \mid \psi \rangle$$

we have

$$\begin{aligned}\langle \phi \mid \hat{A} \mid \psi \rangle &= \langle \phi \mid \hat{I}\hat{A}\hat{I} \mid \psi \rangle = \langle \phi \mid \left(\sum_{n=1}^{\infty} \mid \phi_n \rangle \langle \phi_n \mid \right) \hat{A} \left(\sum_{m=1}^{\infty} \mid \phi_m \rangle \langle \phi_m \mid \right) \mid \psi \rangle \\ &= \sum_{nm} \langle \phi \mid \phi_n \rangle \langle \phi_n \mid \hat{A} \mid \phi_m \rangle \langle \phi_m \mid \psi \rangle \\ &= \sum_{nm} b_n^* A_{nm} a_m .\end{aligned}$$

This is a complex number; its matrix representation goes as follows:

$$\langle \phi \mid \hat{A} \mid \psi \rangle \longrightarrow (b_1^* \quad b_2^* \quad b_3^* \quad \cdots) \begin{pmatrix} A_{11} & A_{12} & A_{13} & \cdots \\ A_{21} & A_{22} & A_{23} & \cdots \\ A_{31} & A_{32} & A_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix}.$$

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Properties of a Matrix A

Real if $A = A^*$ or $A_{mn} = A^*_{mn}$

Imaginary if $A = -A^*$ or $A_{mn} = -A^*_{mn}$

Symmetric if $A = A^T$ or $A_{mn} = A_{nm}$

Antisymmetric if $A = -A^T$ or $A_{mn} = -A_{nm}$ with $A_{mm} = 0$

Hermitian if $A = A^\dagger$ or $A_{mn} = A^*_{nm}$

Anti-Hermitian if $A = -A^\dagger$ or $A_{mn} = -A^*_{nm}$

Orthogonal if $A^T = A^{-1}$ or $AA^T = I$ or $(AA^T)_{mn} = \delta_{mn}$

Unitary if $A^\dagger = A^{-1}$ or $AA^\dagger = I$ or $(AA^\dagger)_{mn} = \delta_{mn}$

Unitary Transformations

One can choose one or the other set of basis vectors in the Hilbert space H of states of a quantum mechanical system to represent the state vectors and the operators belonging to H .

Therefore, it is important to ascertain that the change in basis is done in such a way that the basic physical consequences remain unchanged.

Evidently, for this to be the case, the norm of the state vector in the new basis must not change.

Let $\{|\phi_n\rangle\}$ and $\{|\phi'_n\rangle\}$ be two bases in H . Assume that we change from the so-called original (old) basis $\{|\phi_n\rangle\}$ to the new basis $\{|\phi'_n\rangle\}$. We can expand each ket $|\phi_n\rangle$ of the old basis in terms of the new basis $|\phi'_n\rangle$ as follows:

$$|\phi_n\rangle = \left(\sum_m |\phi'_m\rangle\langle\phi'_m|\right)|\phi_n\rangle = \sum_m U_{mn}|\phi'_m\rangle,$$

where

$$U_{mn} = \langle\phi'_m|\phi_n\rangle.$$

The matrix U , providing the transformation from the old basis $|\phi_n\rangle$ to the new basis $|\phi'_n\rangle$, is given by

$$U = \begin{pmatrix} \langle\phi'_1|\phi_1\rangle & \langle\phi'_1|\phi_2\rangle & \langle\phi'_1|\phi_3\rangle \\ \langle\phi'_2|\phi_1\rangle & \langle\phi'_2|\phi_2\rangle & \langle\phi'_2|\phi_3\rangle \\ \langle\phi'_3|\phi_1\rangle & \langle\phi'_3|\phi_2\rangle & \langle\phi'_3|\phi_3\rangle \end{pmatrix}.$$

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Let us prove that the matrix U is indeed a unitary matrix.

We have

$$\langle \phi_m \mid \hat{U}\hat{U}^\dagger \mid \phi_n \rangle = \langle \phi_m \mid \hat{U} \left(\sum_l \mid \phi_l \rangle \langle \phi_l \mid \right) \hat{U}^\dagger \mid \phi_n \rangle = \sum_l U_{ml} U^*_{nl},$$

where

$$U_{ml} = \langle \phi_m \mid \hat{U} \mid \phi_l \rangle \quad U^*_{nl} = \langle \phi_l \mid \hat{U}^\dagger \mid \phi_n \rangle = \langle \phi_n \mid \hat{U} \mid \phi_l \rangle^*.$$

Therefore

$$\sum_l U_{ml} U^*_{nl} = \sum_l \langle \phi'_m \mid \phi_l \rangle \langle \phi_l \mid \phi'_n \rangle = \langle \phi'_m \mid \phi'_n \rangle = \delta_{mn}.$$

We can infer

$$\langle \phi_m \mid \hat{U}\hat{U}^\dagger \mid \phi_n \rangle = \delta_{mn}, \text{ or } \hat{U}\hat{U}^\dagger = \hat{I}.$$

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The matrix elements A'_{mn} of an operator A in the new basis can be expressed in terms of the old matrix elements,

$$A'_{mn} = \langle \phi'_m \mid \left(\sum_j \mid \phi_j \rangle \langle \phi_j \mid \right) \hat{A} \left(\sum_l \mid \phi_l \rangle \langle \phi_l \mid \right) \mid \phi'_n \rangle = \sum_{jl} U_{mj} A_{jl} U^*_{nl};$$

that is,

$$\hat{A}_{new} = \hat{U} \hat{A}_{old} \hat{U}^\dagger \qquad \text{or} \qquad \hat{A}_{old} = \hat{U}^\dagger \hat{A}_{new} \hat{U}.$$

We may summarize the results of the change of basis in the following relations:

$$\mid \psi_{new} \rangle = \hat{U} \mid \psi_{old} \rangle, \qquad \langle \psi_{new} \mid = \langle \psi_{old} \mid \hat{U}^\dagger, \qquad \hat{A}_{new} = \hat{U} \hat{A}_{old} \hat{U}^\dagger,$$

or,

$$\mid \psi_{old} \rangle = \hat{U}^\dagger \mid \psi_{new} \rangle, \qquad \langle \psi_{old} \mid = \langle \psi_{new} \mid \hat{U}, \qquad \hat{A}_{old} = \hat{U}^\dagger \hat{A}_{new} \hat{U}.$$

Unitary Transformations

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The transformation matrix U is unitary. The components $\langle\phi'_n|\psi\rangle$ of a state vector $|\psi\rangle$ in a new basis $|\phi'_n\rangle$ can be expressed in terms of the components $\langle\phi_n|\psi\rangle$ of $|\psi\rangle$ in an old basis $|\phi_n\rangle$ as follows:

$$\langle\phi'_m \mid \psi\rangle = \langle\phi'_m \mid \hat{I} \mid \psi\rangle = \langle\phi'_m \mid \left(\sum_n \mid \phi_n\rangle\langle\phi_n \mid\right) \mid \psi\rangle = \sum_n U_{mn}\langle\phi_n \mid \psi\rangle.$$

This relation, along with its complex conjugate, can be generalized into

$$\mid \psi_{new}\rangle = \hat{U} \mid \psi_{old}\rangle, \qquad \langle\psi_{new} \mid = \langle\psi_{old} \mid \hat{U}^\dagger.$$

Let us now examine how operators transform when we change from one basis to another.

Inserting the unit operator between A and and multiplying by $<\phi_m|$, we can cast the eigenvalue equation in the form

$$\langle\phi_m \mid \hat{A}\left(\sum_n \mid \phi_n\rangle\langle\phi_n \mid\right) \mid \psi\rangle = a\langle\phi_m \mid \left(\sum_n \mid \phi_n\rangle\langle\phi_n \mid\right) \mid \psi\rangle,$$

or

$$\sum_n A_{mn}\langle\phi_n \mid \psi\rangle = a\sum_n\langle\phi_n \mid \psi\rangle\delta_{nm},$$

which can be rewritten as

$$\sum_n \left[A_{mn} - a\delta_{nm}\right]\langle\phi_n \mid \psi\rangle = 0,$$

with

$$A_{mn} = \langle\phi_m \mid \hat{A} \mid \phi_n\rangle.$$

This system of equations can have nonzero solutions only if its determinant vanishes:

$$\det\left(A_{mn} - a\delta_{nm}\right) = 0.$$

The problem that arises here is that this determinant corresponds to a matrix with an infinite number of columns and rows. To solve above equation, we need to truncate the basis and assume that it contains only N terms,

$$\begin{vmatrix} A_{11} - a & A_{12} & A_{13} & \cdots & A_{1N} \\ A_{21} & A_{22} - a & A_{23} & \cdots & A_{2N} \\ A_{31} & A_{32} & A_{33} - a & \cdots & A_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & A_{N3} & \cdots & A_{NN} - a \end{vmatrix} = 0.$$

This is known as the *secular* or *characteristic equation*. The solutions of this equation yield the N *eigenvalues* a_1, a_2, a_3, , a_N, since it is an Nth order equation in a. The set of these N eigenvalues is called the spectrum of A.

Knowing the set of eigenvalues a_1, a_2, a_3, … , a_N , we can easily determine the corresponding set of *eigenvectors*, ϕ_1, ϕ_2, ϕ_3

If a number of different eigenvectors have the same eigenvalue, this eigenvalue is said to be *degenerate*. The order of degeneracy is determined by the number of linearly independent eigenvectors that have the same eigenvalue.

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In the case where the set of eigenvectors ϕ_n of A is complete and orthonormal, this set can be used as a basis. In this basis the matrix representing the operator A is diagonal,

$$A = \begin{pmatrix} a_1 & 0 & 0 & \cdots \\ 0 & a_2 & 0 & \cdots \\ 0 & 0 & a_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$

the diagonal elements being the eigenvalues a_n of A, since

$$\langle \phi_m \mid \hat{A} \mid \phi_n \rangle = a_n \langle \phi_m \mid \phi_n \rangle = a_n \delta_{mn}.$$

Note that the trace and determinant of a matrix are given, respectively, by the sum and product of the eigenvalues:

$$\mathrm{Tr}(A) = \sum_n a_n = a_1 + a_2 + a_3 + \cdots,$$

$$\det(A) = \prod_n a_n = a_1 a_2 a_3 \cdots.$$

Some theorems pertaining to the eigenvalue problem

1. The eigenvalues of a symmetric matrix are real; the eigenvectors form an orthonormal basis.
2. The eigenvalues of an antisymmetric matrix are purely imaginary or zero.
3. The eigenvalues of a Hermitian matrix are real; the eigenvectors form an orthonormal basis.
4. The eigenvalues of a skew-Hermitian matrix are purely imaginary or zero.
5. The eigenvalues of a unitary matrix have absolute value equal to one.

If the eigenvalues of a square matrix are not degenerate (distinct), the corresponding eigenvectors form a basis (i.e., they form a linearly independent set).

The orthonormality condition of the base *kets* of the continuous basis $|\chi_k\rangle$ is expressed Dirac's *continuous delta* function:

$$\langle \chi_k \mid \chi_{k'} \rangle = \delta(k' - k),$$

where k and k' are continuous parameters and where δ(k,k') is the Dirac delta function which is defined by

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx} dk.$$

As for the completeness condition of this continuous basis, by an integral over the continuous variable

$$\int_{-\infty}^{+\infty} dk \mid \chi_k \rangle \langle \chi_k \mid = \hat{I},$$

Before dealing with the representation of kets, bras, and operators, let us make a short detour to list some of the most important properties of the Dirac delta function

$$\delta(x) = 0, \qquad \text{for} \qquad x \neq 0,$$

$$\int_a^b f(x)\delta(x - x_0)\, dx = \begin{cases} f(x_0) & \text{if} \quad a < x_0 < b, \\ 0 & \text{elsewhere,} \end{cases}$$

$$\int_{-\infty}^{\infty} f(x) \frac{d^n \delta(x-a)}{dx^n}\, dx = (-1)^n \left. \frac{d^n f(x)}{dx^n} \right|_{x=a},$$

$$\delta(\vec{r} - \vec{r}\,') = \delta(x - x')\delta(y - y')\delta(z - z') = \frac{1}{r^2 \sin\theta}\delta(r - r')\delta(\theta - \theta')\delta(\varphi - \varphi').$$

The representation of kets, bras, and operators can be easily inferred from the study that was carried out in the previous section, for the case of a discrete basis.

$$| \psi \rangle \longrightarrow \begin{pmatrix} \vdots \\ \langle \chi_k | \psi \rangle \\ \vdots \end{pmatrix}.$$

Operators are represented by square continuous matrices whose rows and columns have continuous and infinite numbers of components:

$$\hat{A} \longrightarrow \begin{pmatrix} \ddots & \vdots & \ddots \\ \cdots & A(k, k') & \cdots \\ \ddots & \vdots & \ddots \end{pmatrix}.$$

Position Representation

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In the position representation, the basis consists of an infinite set of vectors $|r\rangle$ which are eigenkets to the position operator R:

$$\hat{\vec{R}}\,|\,\vec{r}\rangle = \vec{r}\,|\,\vec{r}\rangle,$$

where r (without a hat), the position vector, is the eigenvalue of the operator R. The orthonormality and completeness conditions are respectively given by

$$\begin{aligned} \langle\vec{r}\,|\,\vec{r}\,'\rangle = \delta(\vec{r}-\vec{r}\,') &= \delta(x-x')\delta(y-y')\delta(z-z'), \\ \int d^3r\,|\,\vec{r}\rangle\langle\vec{r}\,| &= \hat{I}, \end{aligned}$$

since, the three-dimensional delta function is given by

$$\delta(\vec{r}-\vec{r}\,') = \frac{1}{(2\pi)^3}\int d^3k\, e^{i\vec{k}\cdot(\vec{r}-\vec{r}\,')}.$$

So every state vector can be expanded as follows:

$$|\psi\rangle = \int d^3 r\, |\vec{r}\rangle\langle\vec{r}\,|\,\psi\rangle \equiv \int d^3 r\, \psi(\vec{r})\,|\,\vec{r}\rangle,$$

where

$$\langle\vec{r}\,|\,\psi\rangle = \psi(\vec{r}).$$

This is known as the *wave function* for the state vector. The scalar product between two state vectors, can be expressed in this form:

$$\langle\phi\,|\,\psi\rangle = \langle\phi\,|\left(\int d^3 r\, |\vec{r}\rangle\langle\vec{r}\,|\right)|\,\psi\rangle = \int d^3 r\, \phi^*(\vec{r})\psi(\vec{r}).$$

Therefore

$$\langle\vec{r}\,'\,|\,\hat{\vec{R}}^{\,n}\,|\,\vec{r}\rangle = \vec{r}^{\,n}\delta(\vec{r}\,'-\vec{r}).$$

and

$$\begin{aligned}\langle\phi\,|\,\hat{\vec{R}}\,|\,\psi\rangle &= \int d^3 r\, \vec{r}\langle\phi\,|\,\vec{r}\rangle\langle\vec{r}\,|\,\psi\rangle = \left[\int d^3 r\, \vec{r}\langle\psi\,|\,\vec{r}\rangle\langle\vec{r}\,|\,\phi\rangle\right]^* \\ &= \langle\psi\,|\,\hat{\vec{R}}\,|\,\phi\rangle^*.\end{aligned}$$

Momentum Representation

The basis $|p\rangle$ of the momentum representation is obtained from the eigenkets of the momentum operator P:

$$\hat{\vec{P}}\,|\,\vec{p}\rangle = \vec{p}\,|\,\vec{p}\rangle,$$

The orthonormality and completeness conditions of the momentum space basis $|p\rangle$ are given by

$$\langle\vec{p}\,|\,\vec{p}\,'\rangle = \delta(\vec{p}-\vec{p}\,') \qquad \text{and} \qquad \int d^3p\;|\,\vec{p}\rangle\langle\vec{p}\,| = \hat{I}.$$

Expanding the vector state in this basis, we obtain

$$|\,\psi\rangle = \int d^3p\;|\,\vec{p}\rangle\langle\vec{p}\,|\,\psi\rangle = \int d^3p\,\Psi(\vec{p})\,|\,\vec{p}\rangle,$$

where the expansion coefficient $\Psi(p)$ represents the *momentum space wave function*.

To find the expression for the transformation function $\langle r|p\rangle$, let us establish a connection between the position and momentum representations of the state vector :

$$\langle \vec{r} \mid \psi \rangle = \langle \vec{r} \mid \left(\int d^3p \mid \vec{p}\rangle\langle \vec{p} \mid \right) \mid \psi \rangle = \int d^3p \ \langle \vec{r} \mid \vec{p}\rangle \Psi(\vec{p});$$

that is

$$\psi(\vec{r}) = \int d^3p \, \langle \vec{r} \mid \vec{p}\rangle \Psi(\vec{p}).$$

Similarly, we can write

$$\Psi(\vec{p}) = \langle \vec{p} \mid \psi \rangle = \langle \vec{p} \mid \int d^3r \mid \vec{r}\rangle\langle \vec{r} \mid \psi \rangle = \int d^3r \langle \vec{p} \mid \vec{r}\rangle \psi(\vec{r}).$$

The last two relations imply that $\psi(r)$ and $\Psi(p)$ are to be viewed as Fourier transforms of each other.

In quantum mechanics the Fourier transform of a function $f(r)$ is given by

$$f(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p\, e^{i\vec{p}\cdot\vec{r}/\hbar} g(\vec{p});$$

notice the presence of Planck's constant. Hence the function $\langle r|p\rangle$ is given by

$$\langle \vec{r} \mid \vec{p} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\vec{p}\cdot\vec{r}/\hbar}.$$

This function transforms from the momentum to the position representation. The function corresponding to the inverse transformation is given by

$$\langle \vec{p} \mid \vec{r} \rangle = \langle \vec{r} \mid \vec{p} \rangle^* = \frac{1}{(2\pi\hbar)^{3/2}} e^{-i\vec{p}\cdot\vec{r}/\hbar}.$$

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If the position wave function

$$\psi(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p\, e^{i\vec{p}\cdot\vec{r}/\hbar}\Psi(\vec{p})$$

is normalized, its Fourier transform

$$\Psi(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3r\, e^{-i\vec{p}\cdot\vec{r}/\hbar}\psi(\vec{r})$$

must also be normalized, since

$$\begin{aligned}
\int d^3p\, \Psi^*(\vec{p})\Psi(\vec{p}) &= \int d^3p \Psi^*(\vec{p})\left[\frac{1}{(2\pi\hbar)^{3/2}} \int d^3r\, e^{-i\vec{p}\cdot\vec{r}/\hbar}\psi(\vec{r})\right] \\
&= \int d^3r\, \psi(\vec{r})\left[\frac{1}{(2\pi\hbar)^{3/2}} \int d^3p\, \Psi^*(\vec{p})e^{-i\vec{p}\cdot\vec{r}/\hbar}\right] \\
&= \int d^3r\, \psi(\vec{r})\psi^*(\vec{r}) \\
&= 1.
\end{aligned}$$

The form of the position operator R in the momentum representation can be easily inferred from the representation of P in the position space. In momentum space the position operator can be written as follows:

$$\hat{R}_j = i\hbar \frac{\partial}{\partial p_j} \qquad (j = x, y, z)$$

The commutator $[R_j P_k]$ in the position representation

$$[\hat{R}_j, \hat{P}_k] = i\hbar\delta_{jk}, \qquad [\hat{R}_j, \hat{R}_k] = 0, \qquad [\hat{P}_j, \hat{P}_k] = 0 \qquad (j,\ k = x, y, z).$$

and

$$[\hat{X}^n, \hat{P}_x] = i\hbar n \hat{X}^{n-1}, \qquad [\hat{X}, \hat{P}_x^n] = i\hbar n \hat{P}_x^{n-1}.$$

$$[f(\hat{X}), \hat{P}_x] = i\hbar \frac{df(\hat{X})}{d\hat{X}} \quad \Longrightarrow \quad \left[\hat{\vec{P}},\ F(\hat{\vec{R}})\right] = -i\hbar\vec{\nabla}F(\hat{\vec{R}}),$$

1. Show that the vectors

$$\psi_1 = \begin{pmatrix} 5 \\ 3 \\ 4 \end{pmatrix}, \quad \psi_2 = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}, \quad \psi_3 = \begin{pmatrix} 7 \\ 7 \\ 10 \end{pmatrix}$$

are linearly dependent.

1. Show that the vectors

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are linearly dependent.

Solution

$$a\begin{pmatrix} 5 \\ 3 \\ 4 \end{pmatrix} + b\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} + c\begin{pmatrix} 7 \\ 7 \\ 10 \end{pmatrix} = \begin{pmatrix} 5a+b+7c \\ 3a+2b+7c \\ 4a+3b+10c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

For instance, it is satisfied for $a = 1, b = 2$ and $c = -1$, which shows that ψ_3 is a linear combination of the other two vectors: $\psi_3 = \psi_1 + 2\psi_2$.

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2. Suppose that $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$ constitute an $\langle\phi_i|\phi_j\rangle=\delta_{ij}$. Consider the following kets given in this basis:

$$|\psi\rangle = 3i\,|\phi_1\rangle + 2\,|\phi_2\rangle + i\,|\phi_3\rangle\,,$$

$$|\phi\rangle = 2\,|\phi_1\rangle - 3\,|\phi_2\rangle + 5\,|\phi_3\rangle\,.$$

(a) Find $\langle\psi|$ and $\langle\phi|$.

(b) Compute the inner product $\langle\phi|\psi\rangle$ and show that $\langle\phi|\psi\rangle = \langle\psi|\phi\rangle^*$.

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Solution:

$$\langle\psi| = (3i)^*\,\langle\phi_1| + 2\,\langle\phi_2| + (i)^*\,|\phi_3\rangle = -3i\,\langle\phi_1| + 2\,\langle\phi_2| - i\,\langle\phi_3|$$

$$\langle\phi| = 2\,\langle\phi_1| - 3\,\langle\phi_2| + 4\,\langle\phi_3|\,.$$

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(b)

$$\langle\phi|\psi\rangle = (2\langle\phi_1| - 3\langle\phi_2| + 4\langle\phi_3|)(3i|\phi_1\rangle + 2|\phi_2\rangle + i|\phi_3\rangle)$$

$$= 6i\langle\phi_1|\phi_1\rangle + 4\langle\phi_1|\phi_2\rangle + 2i\langle\phi_1|\phi_3\rangle - 9i\langle\phi_2|\phi_1\rangle - 6\langle\phi_2|\phi_2\rangle - 3i\langle\phi_2|\phi_3\rangle$$

$$+ 12i\langle\phi_3|\phi_1\rangle + 8\langle\phi_3|\phi_2\rangle + 4i\langle\phi_3|\phi_3\rangle$$

$$= 6i - 6 + 4i = -6 + 10i.$$

$$\langle\psi|\phi\rangle = (-3i|\phi_1\rangle + 2|\phi_2\rangle - i|\phi_3\rangle)(2\langle\phi_1| - 3\langle\phi_2| + 4\langle\phi_3|)$$

$$= -6i\langle\phi_1|\phi_1\rangle + 9i\langle\phi_1|\phi_2\rangle - 12i\langle\phi_1|\phi_3\rangle + 4\langle\phi_2|\phi_1\rangle - 6\langle\phi_2|\phi_2\rangle + 8\langle\phi_2|\phi_3\rangle$$

$$- 2i\langle\phi_3|\phi_1\rangle + 3i\langle\phi_3|\phi_2\rangle - 4i\langle\phi_3|\phi_3\rangle$$

$$= -6i - 6 - 4i = -6 - 10i = \langle\phi|\psi\rangle^*.$$

(c)

$$|a\psi\rangle = (2+3i)(3i|\phi_1\rangle + 2|\phi_2\rangle + i|\phi_3\rangle) = 6i|\phi_1\rangle + 4|\phi_2\rangle + 2i|\phi_3\rangle$$

$$-9|\phi_1\rangle + 6i|\phi_2\rangle - 3|\phi_3\rangle = (-9+6i)|\phi_1\rangle + (4+6i)|\phi_2\rangle - (3-2i)|\phi_3\rangle.$$

Exercise

3. Let the Hamiltonian for a system be given by:

$$\hat{H} = \begin{pmatrix} \varepsilon_1 & \varepsilon_2 \\ \varepsilon_2 & \varepsilon_1 \end{pmatrix},$$

Find the eigenvalues and the corresponding eigenvectors of H and, thus, set up the basis in the state space of the system.

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Solution:

$$\det(H - \lambda I) = \det \begin{pmatrix} \varepsilon_1 - \lambda & \varepsilon_2 \\ \varepsilon_2 & \varepsilon_1 - \lambda \end{pmatrix} = 0.$$

The solutions to this equation yield the eigenvalues of H:

$$\lambda_1 = \varepsilon_1 + \varepsilon_2, \;\; \lambda_1 = \varepsilon_1 - \varepsilon_2.$$

Exercise

Let

$$|\alpha_1\rangle = \begin{pmatrix} a \\ b \end{pmatrix}$$

be the eigenvector corresponding to λ_1. We have

$$\begin{pmatrix} \varepsilon_1 & \varepsilon_2 \\ \varepsilon_2 & \varepsilon_1 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = (\varepsilon_1 + \varepsilon_2)\begin{pmatrix} a \\ b \end{pmatrix}.$$

This equation leads to

$$\varepsilon_1 a + \varepsilon_2 b = (\varepsilon_1 + \varepsilon_2)a,$$

$$\varepsilon_2 a + \varepsilon_1 b = (\varepsilon_1 + \varepsilon_2)b,$$

As a result,

$$|\alpha_1\rangle = \begin{pmatrix} a \\ a \end{pmatrix} = a\begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

Therefore,

$$|\alpha_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad |\alpha_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$