

DIRAC'S BRA AND KET NOTATION

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1 From inner products to bra-kets

Dirac invented a useful alternative notation for inner products that leads to the concepts of bras and kets. The notation is sometimes more efficient than the conventional mathematical notation we have been using. It is also widely although not universally used. It all begins by writing the inner product differently. The rule is to turn inner products into bra-ket pairs as follows

$$\langle u, v \rangle \longrightarrow \langle u|v \rangle. \tag{1.1}$$

Instead of the inner product comma we simply put a vertical bar! We can translate our earlier discussion of inner products trivially. In order to make you familiar with the new look we do it.

We now write $\langle u|v \rangle = \langle v|u \rangle^*$, as well as $\langle v|v \rangle \geq 0$ for all v , while $\langle v|v \rangle = 0$ if and only if $v = 0$. We have linearity in the second argument

$$\langle u|c_1v_1 + c_2v_2 \rangle = c_1\langle u|v_1 \rangle + c_2\langle u|v_2 \rangle, \tag{1.2}$$

for complex constants c_1 and c_2 , but antilinearity in the first argument

$$\langle c_1u_1 + c_2u_2|v \rangle = c_1^*\langle u_1|v \rangle + c_2^*\langle u_2|v \rangle. \tag{1.3}$$

Two vectors u and v for which $\langle u|v \rangle = 0$ are orthogonal. For the norm: $|v|^2 = \langle v|v \rangle$. The Schwarz inequality, for any pair u and v of vectors reads $|\langle u|v \rangle| \leq |u| |v|$.

For a given physical situation, the inner product must be defined and should satisfy the axioms. Let us consider two examples:

1. Let $a = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$ and $b = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$ be two vectors in a complex dimensional vector space of dimension two. We then define

$$\langle a|b \rangle \equiv a_1^* b_1 + a_2^* b_2. \quad (1.4)$$

You should confirm the axioms are satisfied.

2. Consider the complex vector space of complex function $f(x) \in \mathbb{C}$ with $x \in [0, L]$. Given two such functions $f(x), g(x)$ we define

$$\langle f|g \rangle \equiv \int_0^L f^*(x)g(x)dx. \quad (1.5)$$

The verification of the axioms is again quite straightforward.

A set of basis vectors $\{e_i\}$ labelled by the integers $i = 1, \dots, n$ satisfying

$$\langle e_i|e_j \rangle = \delta_{ij}, \quad (1.6)$$

is orthonormal. An arbitrary vector can be written as a linear superposition of basis states:

$$v = \sum_i \alpha_i e_i, \quad (1.7)$$

We then see that the coefficients are determined by the inner product

$$\langle e_k|v \rangle = \langle e_k|\sum_i \alpha_i e_i \rangle = \sum_i \alpha_i \langle e_k|e_i \rangle = \alpha_k. \quad (1.8)$$

We can therefore write

$$v = \sum_i e_i \langle e_i|v \rangle. \quad (1.9)$$

To obtain now bras and kets, we reinterpret the inner product. We want to “split” the inner product into two ingredients

$$\langle u|v \rangle \rightarrow \langle u| \ |v \rangle. \quad (1.10)$$

Here $|v\rangle$ is called a **ket** and $\langle u|$ is called a **bra**. We will view the ket $|v\rangle$ just as another way to represent the vector v . This is a small subtlety with the notation: we think of $v \in V$ as a vector and also $|v\rangle \in V$ as a vector. It is as if we added some decoration $| \rangle$ around the vector v to make it clear by inspection that it is a vector, perhaps like the usual top arrows that are added in some cases. The label in the ket is a vector and the ket itself is that vector!

Bras are somewhat different objects. We say that bras belong to the space V^* dual to V . Elements of V^* are linear maps from V to \mathbb{C} . In conventional mathematical notation one has a $v \in V$ and a linear function $\phi \in V^*$ such that $\phi(v)$, which denotes the action of the function of the vector v , is a number. In the bracket notation we have the replacements

$$\begin{aligned} v &\rightarrow |v\rangle, \\ \phi &\rightarrow \langle u|, \\ \phi_u(v) &\rightarrow \langle u|v \rangle, \end{aligned} \quad (1.11)$$

where we used the notation in (6.6). Our bras are labelled by vectors: the object inside the $\langle |$ is a vector. But bras are *not* vectors. If kets are viewed as column vectors, then bras are viewed as row vectors. In this way a bra to the left of a ket makes sense: matrix multiplication of a row vector times a column vector gives a number. Indeed, for vectors

$$a = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}, \quad b = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} \quad (1.12)$$

we had

$$\langle a|b \rangle = a_1^* b_1 + a_2^* b_2 + \dots a_n^* b_n \quad (1.13)$$

Now we think of this as

$$\langle a| = (a_1^*, a_2^*, \dots, a_n^*), \quad |b \rangle = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} \quad (1.14)$$

and matrix multiplication gives us the desired answer

$$\langle a|b \rangle = (a_1^*, a_2^*, \dots, a_n^*) \cdot \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} = a_1^* b_1 + a_2^* b_2 + \dots a_n^* b_n. \quad (1.15)$$

Note that the bra labeled by the vector a is obtained by forming the row vector and complex conjugating the entries. More abstractly the bra $\langle u|$ labeled by the vector u is defined by its action on arbitrary vectors $|v \rangle$ as follows

$$\langle u| : |v \rangle \rightarrow \langle u|v \rangle. \quad (1.16)$$

As required by the definition, any linear map from V to \mathbb{C} defines a bra, and the corresponding underlying vector. For example let v be a generic vector:

$$v = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}, \quad (1.17)$$

A linear map $f(v)$ that acting on a vector v gives a number is an expression of the form

$$f(v) = \alpha_1^* v_1 + \alpha_2^* v_2 + \dots \alpha_n^* v_n. \quad (1.18)$$

It is a linear function of the components of the vector. The linear function is specified by the numbers α_i , and for convenience (and without loss of generality) we used their complex conjugates. Note that we need exactly n constants, so they can be used to assemble a row vector or a bra

$$\langle \alpha| = (\alpha_1^*, \alpha_2^*, \dots, \alpha_n^*) \quad (1.19)$$

and the associated vector or ket

$$|\alpha\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_n \end{pmatrix} \quad (1.20)$$

Note that, by construction

$$f(v) = \langle \alpha | v \rangle. \quad (1.21)$$

This illustrates the point that (i) bras represent dual objects that act on vectors and (ii) bras are labelled by vectors.

Bras can be added and can be multiplied by complex numbers and there is a zero bra defined to give zero acting on any vector, so V^* is also a complex vector space. As a bra, the linear superposition

$$\langle \omega | \equiv \alpha \langle a | + \beta \langle b | \in V^*, \quad \alpha, \beta \in \mathbb{C}, \quad (1.22)$$

is defined to act on a vector (ket) $|c\rangle$ to give the number

$$\alpha \langle a | c \rangle + \beta \langle b | c \rangle. \quad (1.23)$$

For any vector $|v\rangle \in V$ there is a *unique* bra $\langle v | \in V^*$. If there would be another bra $\langle v' |$ it would have to act on arbitrary vectors $|w\rangle$ just like $\langle v |$:

$$\langle v' | w \rangle = \langle v | w \rangle \quad \rightarrow \quad \langle w | v \rangle - \langle w | v' \rangle = 0 \quad \rightarrow \quad \langle w | v - v' \rangle = 0. \quad (1.24)$$

In the first step we used complex conjugation and in the second step linearity. Now the vector $v - v'$ must have zero inner product with *any* vector w , so $v - v' = 0$ and $v = v'$.

We can now reconsider equation (1.3) and write an extra right-hand side

$$\langle \alpha_1 a_1 + \alpha_2 a_2 | b \rangle = \alpha_1^* \langle a_1 | b \rangle + \alpha_2^* \langle a_2 | b \rangle = (\alpha_1^* \langle a_1 | + \alpha_2^* \langle a_2 |) | b \rangle \quad (1.25)$$

so that we conclude that the rules to pass from kets to bras include

$$|v\rangle = \alpha_1 |a_1\rangle + \alpha_2 |a_2\rangle \quad \longleftrightarrow \quad \langle v | = \alpha_1^* \langle a_1 | + \alpha_2^* \langle a_2 |. \quad (1.26)$$

For simplicity of notation we sometimes write kets with labels simpler than vectors. Let us reconsider the basis vectors $\{e_i\}$ discussed in (1.6). The ket $|e_i\rangle$ is simply called $|i\rangle$ and the orthonormal condition reads

$$\langle i | j \rangle = \delta_{ij}. \quad (1.27)$$

The expansion (1.7) of a vector now reads

$$|v\rangle = \sum_i |i\rangle \alpha_i, \quad (1.28)$$

As in (1.8) the expansion coefficients are $\alpha_k = \langle k | v \rangle$ so that

$$|v\rangle = \sum_i |i\rangle \langle i | v \rangle. \quad (1.29)$$

2 Operators revisited

Let T be an operator in a vector space V . This means that acting on vectors on V it gives vectors on V , something we write as

$$\Omega : V \rightarrow V. \quad (2.30)$$

We denote by $\Omega|a\rangle$ the vector obtained by acting with Ω on the vector $|a\rangle$:

$$|a\rangle \in V \rightarrow \Omega|a\rangle \in V. \quad (2.31)$$

The operator Ω is linear if additionally we have

$$\Omega(|a\rangle + |b\rangle) = \Omega|a\rangle + \Omega|b\rangle, \quad \text{and} \quad \Omega(\alpha|a\rangle) = \alpha\Omega|a\rangle. \quad (2.32)$$

When kets are labeled by vectors we sometimes write

$$|\Omega a\rangle \equiv \Omega|a\rangle, \quad (2.33)$$

It is useful to note that a linear operator on V is also a linear operator on V^*

$$\Omega : V^* \rightarrow V^*, \quad (2.34)$$

We write this as

$$\langle a| \rightarrow \langle a|\Omega \in V^*. \quad (2.35)$$

The object $\langle a|\Omega$ is defined to be the bra that acting on the ket $|b\rangle$ gives the number $\langle a|\Omega|b\rangle$.

We can write operators in terms of bras and kets, written in a suitable order. As an example of an operator consider a bra $\langle a|$ and a ket $|b\rangle$. We claim that the object

$$\Omega = |a\rangle\langle b|, \quad (2.36)$$

is naturally viewed as a linear operator on V and on V^* . Indeed, acting on a vector we let it act as the bra-ket notation suggests:

$$\Omega|v\rangle \equiv |a\rangle\langle b|v\rangle \sim |a\rangle, \quad \text{since } \langle b|v\rangle \text{ is a number.} \quad (2.37)$$

Acting on a bra it gives a bra:

$$\langle w|\Omega \equiv \langle w|a\rangle\langle b| \sim \langle b|, \quad \text{since } \langle w|a\rangle \text{ is a number.} \quad (2.38)$$

Let us now review the description of operators as matrices. The choice of basis is ours to make. For simplicity, however, we will usually consider orthonormal bases.

Consider therefore, two vectors expanded in an orthonormal basis $\{|i\rangle\}$:

$$|a\rangle = \sum_n |n\rangle a_n, \quad |b\rangle = \sum_n |n\rangle b_n. \quad (2.39)$$

Assume $|b\rangle$ is obtained by the action of Ω on $|a\rangle$:

$$\Omega|a\rangle = |b\rangle \quad \rightarrow \quad \sum_n \Omega|n\rangle a_n = \sum_n |n\rangle b_n. \quad (2.40)$$

Acting on both sides of this vector equation with the bra $\langle m|$ we find

$$\sum_n \langle m|\Omega|n\rangle a_n = \sum_n \langle m|n\rangle b_n = b_m \quad (2.41)$$

We now define the ‘matrix elements’

$$\boxed{\Omega_{mn} \equiv \langle m|\Omega|n\rangle.} \quad (2.42)$$

so that the above equation reads

$$\sum_n \Omega_{mn} a_n = b_m, \quad (2.43)$$

which is the matrix version of the original relation $\Omega|a\rangle = |b\rangle$. The chosen basis has allowed us to view the linear operator Ω as a matrix, also denoted as Ω , with matrix components Ω_{mn} :

$$\Omega \longleftrightarrow \begin{pmatrix} \Omega_{11} & \Omega_{12} & \dots & \dots & \Omega_{1N} \\ \Omega_{21} & \Omega_{22} & \dots & \dots & \Omega_{2N} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \Omega_{N1} & \Omega_{N2} & \dots & \dots & \Omega_{NN} \end{pmatrix}, \quad \text{with } \Omega_{ij} = \langle i|\Omega|j\rangle. \quad (2.44)$$

There is one additional claim. The operator itself can be written in terms of the matrix elements and basis bras and kets. We claim that

$$\boxed{\Omega = \sum_{m,n} |m\rangle \Omega_{mn} \langle n|.} \quad (2.45)$$

We can verify that this is correct by computing the matrix elements using it:

$$\langle m'|\Omega|n'\rangle = \sum_{m,n} \Omega_{mn} \langle m'|m\rangle \langle n|n'\rangle = \sum_{m,n} \Omega_{mn} \delta_{m'm} \delta_{nn'} = \Omega_{m'n'}, \quad (2.46)$$

as expected from the definition (2.42).

2.1 Projection Operators

Consider the familiar orthonormal basis $\{|i\rangle\}$ of V and choose one element $|m\rangle$ from the basis to form an operator P_m defined by

$$P_m \equiv |m\rangle \langle m|. \quad (2.47)$$

This operator maps any vector $|v\rangle \in V$ to a vector along $|m\rangle$. Indeed, acting on $|v\rangle$ it gives

$$P_m|v\rangle = |m\rangle \langle m|v\rangle \sim |m\rangle. \quad (2.48)$$

Comparing the above expression for P_m with (2.45) we see that in the chosen basis, P_n is represented by a matrix all of whose elements are zero, except for the (n, n) element $(P_n)_{nn}$ which is one:

$$P_n \longleftrightarrow \begin{pmatrix} 0 & 0 & \dots & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & 0 \\ 0 & 0 & \dots & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & 0 \\ 0 & 0 & \dots & 0 & \dots & 0 \end{pmatrix}. \quad (2.49)$$

A hermitian operator P is said to be a *projection* operator if it satisfies the operator equation $PP = P$. This means that acting twice with a projection operator on a vector gives the same as acting once. The operator P_m is a projection operator since

$$P_m P_m = (|m\rangle\langle m|)(|m\rangle\langle m|) = |m\rangle\langle m|m\rangle\langle m| = |m\rangle\langle m|, \quad (2.50)$$

since $\langle m|m\rangle = 1$. The operator P_m is said to be a *rank one* projection operator since it projects to a one-dimensional subspace of V , the subspace generated by $|m\rangle$.

Using the basis vector $|m\rangle$ with $m \neq n$ we can define

$$P_{m,n} \equiv |m\rangle\langle m| + |n\rangle\langle n|. \quad (2.51)$$

Acting on any vector $|v\rangle \in V$, this operator gives us a vector in the subspace spanned by $|m\rangle$ and $|n\rangle$:

$$P_{m,n}|v\rangle = |m\rangle\langle m|v\rangle + |n\rangle\langle n|v\rangle. \quad (2.52)$$

Using the orthogonality of $|m\rangle$ and $|n\rangle$ we quickly find that $P_{m,n}P_{m,n} = P_{m,n}$ and therefore $P_{m,n}$ is a projector. It is a rank two projector, since it projects to a two-dimensional subspace of V , the subspace spanned by $|m\rangle$ and $|n\rangle$. Similarly, we can construct a rank three projector by adding an extra term $|k\rangle\langle k|$ with $k \neq m$ and $k \neq n$. If we include all basis vectors we would have the operator

$$P_{1,\dots,N} \equiv |1\rangle\langle 1| + |2\rangle\langle 2| + \dots + |N\rangle\langle N|. \quad (2.53)$$

As a matrix $P_{1,\dots,N}$ has a one on every element of the diagonal and a zero everywhere else. This is therefore the unit matrix, which represents the identity operator. Indeed we anticipated this in (1.29), and we thus write

$$\mathbf{1} = \sum_i |i\rangle\langle i|. \quad (2.54)$$

This is the completeness relation for the chosen orthonormal basis. This equation is sometimes called the ‘resolution’ of the identity.

Example. For the spin one-half system the unit operator can be written as a sum of two terms since the vector space is two dimensional. Using the orthonormal basis vectors $|+\rangle$ and $|-\rangle$ for spins along the positive and negative z directions, respectively, we have

$$\mathbf{1} = |+\rangle\langle +| + |-\rangle\langle -|. \quad (2.55)$$

Example. We can use the completeness relation to show that our formula (2.42) for matrix elements is consistent with matrix multiplication. Indeed for the product $\Omega_1\Omega_2$ of two operators we write

$$\begin{aligned} (\Omega_1\Omega_2)_{mn} &= \langle m|\Omega_1\Omega_2|n\rangle = \langle m|\Omega_1 \mathbf{1} \Omega_2|n\rangle \\ &= \langle m|\Omega_1 \left(\sum_{k=1}^N |k\rangle\langle k| \right) \Omega_2|n\rangle = \sum_{k=1}^N \langle m|\Omega_1|k\rangle\langle k|\Omega_2|n\rangle = \sum_{k=1}^N (\Omega_1)_{mk}(\Omega_2)_{kn}. \end{aligned} \quad (2.56)$$

This is the expected rule for the multiplication of the matrices corresponding to Ω_1 and Ω_2 .

2.2 Adjoint of a linear operator

A linear operator Ω on V is defined by its action on the vectors in V . We have noted that Ω can also be viewed as a linear operator on the dual space V^* . We defined the linear operator Ω^\dagger associated with Ω . In general Ω^\dagger by

$$\langle \Omega^\dagger u|v\rangle = \langle u|\Omega v\rangle \quad (2.57)$$

Flipping the order on the left-hand side we get

$$\langle v|\Omega^\dagger u\rangle^* = \langle u|\Omega v\rangle \quad (2.58)$$

Complex conjugating, and writing the operators more explicitly

$$\boxed{\langle v|\Omega^\dagger|u\rangle = \langle u|\Omega|v\rangle^*, \quad \forall u, v.} \quad (2.59)$$

Flipping the two sides of (2.57) we also get

$$\langle v|\Omega^\dagger|u\rangle = \langle \Omega v|u\rangle \quad (2.60)$$

from which, taking the ket away, we learn that

$$\boxed{\langle v|\Omega^\dagger \equiv \langle \Omega v|.} \quad (2.61)$$

Another way to state the action of the operator Ω^\dagger is as follows. The linear operator Ω induces a map $|v\rangle \rightarrow |v'\rangle$ of vectors in V and, in fact, is defined by giving a complete list of these maps. The operator Ω^\dagger is defined as the one that induces the maps $\langle v| \rightarrow \langle v'|$ of the *corresponding* bras. Indeed,

$$\begin{aligned} |v'\rangle &= |\Omega v\rangle = \Omega|v\rangle, \\ \langle v'| &= \langle \Omega v| = \langle v|\Omega^\dagger \end{aligned} \quad (2.62)$$

The first line is just definitions. On the second line, the first equality is obtained by taking bras of the first equality on the first line. The second equality is just (2.61). We say it as

$$\boxed{\text{The bra associated with } \Omega|v\rangle \text{ is } \langle v|\Omega^\dagger.} \quad (2.63)$$

To see what hermiticity means at the level of matrix elements, we take u, v to be orthonormal basis vectors in (2.59)

$$\langle i|\Omega^\dagger|j\rangle = \langle j|\Omega|i\rangle^* \rightarrow (\Omega^\dagger)_{ij} = (\Omega_{ji})^*. \quad (2.64)$$

In matrix notation we have $\Omega^\dagger = (\Omega^t)^*$ where the superscript t denotes transposition.

Exercise. Show that $(\Omega_1\Omega_2)^\dagger = \Omega_2^\dagger\Omega_1^\dagger$ by taking matrix elements.

Exercise. Given an operator $\Omega = |a\rangle\langle b|$ for arbitrary vectors a, b , write a bra-ket expression for Ω^\dagger .

Solution: Acting with Ω on $|v\rangle$ and then taking the dual gives

$$\Omega|v\rangle = |a\rangle\langle b|v\rangle \rightarrow \langle v|\Omega^\dagger = \langle v|b\rangle\langle a|, \quad (2.65)$$

Since this equation is valid for any bra $\langle v|$ we read

$$\Omega^\dagger = |b\rangle\langle a|. \quad (2.66)$$

2.3 Hermitian and Unitary Operators

A linear operator Ω is said to be *hermitian* if it is equal to its adjoint:

Hermitian Operator: $\Omega^\dagger = \Omega$.

(2.67)

In quantum mechanics Hermitian operators are associated with observables. The eigenvalues of a Hermitian operator are the possible measured values of the observables. As we will show soon, the eigenvalues of a Hermitian operator are all real. An operator A is said to be *anti-hermitian* if $A^\dagger = -A$.

Exercise: Show that the commutator $[\Omega_1, \Omega_2]$ of two hermitian operators Ω_1 and Ω_2 is anti-hermitian.

There are a couple of equations that rewrite in useful ways the main property of Hermitian operators. Using $\Omega^\dagger = \Omega$ in (2.59) we find

If Ω is a Hermitian Operator: $\langle v|\Omega|u\rangle = \langle u|\Omega|v\rangle^*, \forall u, v$.

(2.68)

It follows that the expectation value of a Hermitian operator in *any* state is real

$$\langle v|\Omega|v\rangle \text{ is real for any hermitian } \Omega. \quad (2.69)$$

Another neat form of the hermiticity condition is derived as follows:

$$\langle \Omega u|v\rangle = \langle u|\Omega^\dagger|v\rangle = \langle u|\Omega|v\rangle = \langle u|\Omega v\rangle, \quad (2.70)$$

so that all in all

Hermitian Operator: $\langle \Omega u|v\rangle = \langle u|\Omega v\rangle$.

(2.71)

In this expression we see that a hermitian operator moves freely from the bra to the ket (and viceversa).

Example: For wavefunction $f(x) \in \mathbb{C}$ we have written

$$\langle f|g \rangle = \int_{-\infty}^{\infty} (f(x))^* g(x) dx \quad (2.72)$$

For a Hermitian Ω we have $\langle \Omega f|g \rangle = \langle f|\Omega g \rangle$ or explicitly

$$\int_{-\infty}^{\infty} (\Omega f(x))^* g(x) dx = \int_{-\infty}^{\infty} (f(x))^* \Omega g(x) dx \quad (2.73)$$

Verify that the linear operator $\Omega = \frac{\hbar}{i} \frac{d}{dx}$ is hermitian when we restrict to functions that vanish at $\pm\infty$.

An operator U is said to be a unitary operator if U^\dagger is an inverse for U , that is, $U^\dagger U$ and $U U^\dagger$ are both the identity operator:

$U \text{ is a unitary operator: } U^\dagger U = U U^\dagger = \mathbf{1}$

(2.74)

In finite dimensional vector spaces $U^\dagger U = \mathbf{1}$ implies $U U^\dagger = \mathbf{1}$, but this is not always the case for infinite dimensional vector spaces. A key property of unitary operators is that they preserve the norm of states. Indeed, assume that $|\psi'\rangle$ is obtained by the action of U on $|\psi\rangle$:

$$|\psi'\rangle = U|\psi\rangle \quad (2.75)$$

Taking the dual we have

$$\langle \psi'| = \langle \psi|U^\dagger, \quad (2.76)$$

and therefore

$$\langle \psi'|\psi'\rangle = \langle \psi|U^\dagger U|\psi\rangle = \langle \psi|\psi\rangle, \quad (2.77)$$

showing that $|\psi\rangle$ and $U|\psi\rangle$ are states with the same norm. More generally

$\langle Ua|Ub \rangle = \langle a|U^\dagger U|b \rangle = \langle a|b \rangle.$

(2.78)

Another important property of unitary operators is that acting on an orthonormal basis they give another orthonormal basis. To show this consider the orthonormal basis

$$|a_1\rangle, |a_2\rangle, \dots |a_N\rangle, \quad \langle a_i|a_j \rangle = \delta_{ij} \quad (2.79)$$

Acting with U we get

$$|Ua_1\rangle, |Ua_2\rangle, \dots |Ua_N\rangle, \quad (2.80)$$

To show that this is a basis we must prove that

$$\sum_i \beta_i |Ua_i\rangle = 0 \quad (2.81)$$

implies $\beta_i = 0$ for all i . Indeed, the above gives

$$\sum_i \beta_i |U a_i\rangle = \sum_i \beta_i U |a_i\rangle = U \sum_i \beta_i |a_i\rangle = 0. \quad (2.82)$$

Acting with U^\dagger from the left we find that $\sum_i \beta_i |a_i\rangle = 0$ and, since the $|a_i\rangle$ form a basis, we get $\beta_i = 0$ for all i , as desired. The new basis is orthonormal because

$$\langle U a_i | U a_j \rangle = \langle a_i | U^\dagger U | a_j \rangle = \langle a_i | a_j \rangle = \delta_{ij}. \quad (2.83)$$

It follows from the above that the operator U can be written as

$$U = \sum_{i=1}^N |U a_i\rangle \langle a_i|, \quad (2.84)$$

since

$$U |a_j\rangle = \sum_{i=1}^N |U a_i\rangle \langle a_i | a_j \rangle = |U a_j\rangle. \quad (2.85)$$

In fact for *any* unitary operator U in a vector space V there exist orthonormal bases $\{|a_i\rangle\}$ and $\{|b_i\rangle\}$ such that U can be written as

$$U = \sum_{i=1}^N |b_i\rangle \langle a_i|. \quad (2.86)$$

Indeed, this is just a rewriting of (2.84), with $|a_i\rangle$ any orthonormal basis and $|b_i\rangle = |U a_i\rangle$.

Exercise: Verify that U in (2.86) satisfies $U^\dagger U = U U^\dagger = \mathbf{1}$.

Exercise: Prove that $\langle a_i | U | a_j \rangle = \langle b_i | U | b_j \rangle$.

3 Non-denumerable basis

In this section we describe the use of bras and kets for the position and momentum states of a particle moving on the real line $x \in \mathbb{R}$.

Let us begin with position. We will introduce position states $|x\rangle$ where the label x in the ket is the value of the position. Since x is a continuous variable and we position states $|x\rangle$ for all values of x to form a basis, we are dealing with an infinite basis that is not possible to label as $|1\rangle, |2\rangle, \dots$, it is a non-denumerable basis. So we have

$$\text{Basis states : } |x\rangle, \quad \forall x \in \mathbb{R}. \quad (3.87)$$

Basis states with different values of x are different vectors in the state space (a complex vector space, as always in quantum mechanics). Note here that the label on the ket is not a vector! So $|ax\rangle \neq a|x\rangle$, for any real $a \neq 1$. In particular $| -x \rangle \neq |x\rangle$ unless $x = 0$. For quantum mechanics in three dimensions, we have position states $|\vec{x}\rangle$. Here the label is a vector in a three-dimensional real vector space (our space!) while the ket is a vector in the infinite dimensional complex vector space of states of the theory.

Again something like $|\vec{x}_1 + \vec{x}_2\rangle$ has nothing to do with $|\vec{x}_1\rangle + |\vec{x}_2\rangle$. The $|\ \rangle$ enclosing the label of the position eigenstates plays a crucial role: it helps us see that object lives in an infinite dimensional complex vector space.

The inner product must be defined, so we will take

$$\langle x|y\rangle = \delta(x - y). \quad (3.88)$$

It follows that position states with different positions are orthogonal to each other. The norm of a position state is infinite: $\langle x|x\rangle = \delta(0) = \infty$, so these are not allowed states of particles. We visualize the state $|x\rangle$ as the state of a particle perfectly localized at x , but this is an idealization. We can easily construct normalizable states using superpositions of position states. We also have a completeness relation

$$\mathbf{1} = \int dx |x\rangle\langle x|. \quad (3.89)$$

This is consistent with our inner product above. Letting the above equation act on $|y\rangle$ we find an equality:

$$|y\rangle = \int dx |x\rangle\langle x|y\rangle = \int dx |x\rangle\delta(x - y) = |y\rangle. \quad (3.90)$$

The position operator \hat{x} is defined by its action on the position states. Not surprisingly we let

$$\hat{x}|x\rangle = x|x\rangle, \quad (3.91)$$

thus declaring that $|x\rangle$ are \hat{x} eigenstates with eigenvalue equal to the position x . We can also show that \hat{x} is a Hermitian operator by checking that \hat{x}^\dagger and \hat{x} have the same matrix elements:

$$\langle x_1|\hat{x}^\dagger|x_2\rangle = \langle x_2|\hat{x}|x_1\rangle^* = [x_1\delta(x_1 - x_2)]^* = x_2\delta(x_1 - x_2) = \langle x_1|\hat{x}|x_2\rangle. \quad (3.92)$$

We thus conclude that $\hat{x}^\dagger = \hat{x}$ and the bra associated with (3.91) is

$$\langle x|\hat{x} = x\langle x|. \quad (3.93)$$

Given the state $|\psi\rangle$ of a particle, we define the associated position-state wavefunction $\psi(x)$ by

$$\psi(x) \equiv \langle x|\psi\rangle \in \mathbb{C}. \quad (3.94)$$

This is sensible: $\langle x|\psi\rangle$ is a number that depends on the value of x , thus a function of x . We can now do a number of basic computations. First we write any state as a superposition of position eigenstates, by inserting $\mathbf{1}$ as in the completeness relation

$$|\psi\rangle = \mathbf{1}|\psi\rangle = \int dx |x\rangle\langle x|\psi\rangle = \int dx |x\rangle\psi(x). \quad (3.95)$$

As expected, $\psi(x)$ is the component of ψ along the state $|x\rangle$. Overlap of states can also be written in position space:

$$\langle\phi|\psi\rangle = \int dx \langle\phi|x\rangle\langle x|\psi\rangle = \int dx \phi^*(x)\psi(x). \quad (3.96)$$

Matrix elements involving \hat{x} are also easily evaluated

$$\langle \phi | \hat{x} | \psi \rangle = \langle \phi | \hat{x} \mathbf{1} | \psi \rangle = \int dx \langle \phi | \hat{x} | x \rangle \langle x | \psi \rangle = \int dx \langle \phi | x \rangle x \langle x | \psi \rangle = \int dx \phi^*(x) x \psi(x). \quad (3.97)$$

We now introduce momentum states $|p\rangle$ that are eigenstates of the momentum operator \hat{p} in complete analogy to the position states

$$\begin{aligned} \text{Basis states : } & |p\rangle, \quad \forall p \in \mathbb{R}. \\ \langle p' | p \rangle &= \delta(p - p'), \\ \mathbf{1} &= \int dp |p\rangle \langle p|, \\ \hat{p} |p\rangle &= p |p\rangle \end{aligned} \quad (3.98)$$

Just as for coordinate space we also have

$$\hat{p}^\dagger = \hat{p}, \quad \text{and} \quad \langle p | \hat{p} = p \langle p|. \quad (3.99)$$

In order to relate the two bases we need the value of the overlap $\langle x | p \rangle$. Since we interpret this as the wavefunction for a particle with momentum p we have from (6.39) of Chapter 1 that

$$\langle x | p \rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}. \quad (3.100)$$

The normalization was adjusted properly to be compatible with the completeness relations. Indeed, for example, consider the $\langle p' | p \rangle$ overlap and use the completeness in x to evaluate it

$$\langle p' | p \rangle = \int dx \langle p' | x \rangle \langle x | p \rangle = \frac{1}{2\pi\hbar} \int dx e^{i(p-p')x/\hbar} = \frac{1}{2\pi} \int du e^{i(p-p')u}, \quad (3.101)$$

where we let $u = x/\hbar$ in the last step. We claim that the last integral is precisely the integral representation of the delta function $\delta(p - p')$:

$$\frac{1}{2\pi} \int du e^{i(p-p')u} = \delta(p - p'). \quad (3.102)$$

This, then gives the correct value for the overlap $\langle p | p' \rangle$, as we claimed. The integral (3.102) can be justified using the fact that the functions

$$f_n(x) \equiv \frac{1}{\sqrt{L}} \exp\left(\frac{2\pi i n x}{L}\right), \quad (3.103)$$

form a complete orthonormal set of functions over the interval $x \in [-L/2, L/2]$. Completeness then means that

$$\sum_{n \in \mathbb{Z}} f_n^*(x) f_n(x') = \delta(x - x'). \quad (3.104)$$

We thus have

$$\sum_{n \in \mathbb{Z}} \frac{1}{L} \exp\left(2\pi i \frac{n}{L}(x - x')\right) = \delta(x - x'). \quad (3.105)$$

In the limit as L goes to infinity the above sum can be written as an integral since the exponential is a very slowly varying function of $n \in \mathbb{Z}$. Since $\Delta n = 1$ with $u = 2\pi n/L$ we have $\Delta u = 2\pi/L \ll 1$ and then

$$\sum_{n \in \mathbb{Z}} \frac{1}{L} \exp\left(2\pi i \frac{n}{L}(x - x')\right) = \sum_u \frac{\Delta u}{2\pi} \exp\left(i u(x - x')\right) \rightarrow \frac{1}{2\pi} \int du e^{iu(x-x')}, \quad (3.106)$$

and back in (3.105) we have justified (3.102).

We can now ask: What is $\langle p|\psi\rangle$? We compute

$$\langle p|\psi\rangle = \int dx \langle p|x\rangle \langle x|\psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int dx e^{-ipx/\hbar} \psi(x) = \tilde{\psi}(p), \quad (3.107)$$

which is the Fourier transform of $\psi(x)$, as defined in (6.41) of Chapter 1. Thus the Fourier transform of $\psi(x)$ is the wavefunction in the momentum representation.

It is useful to know how to evaluate $\langle x|\hat{p}|\psi\rangle$. We do it by inserting a complete set of momentum states:

$$\langle x|\hat{p}|\psi\rangle = \int dp \langle x|p\rangle \langle p|\hat{p}|\psi\rangle = \int dp (p\langle x|p\rangle) \langle p|\psi\rangle \quad (3.108)$$

Now we notice that

$$p\langle x|p\rangle = \frac{\hbar}{i} \frac{d}{dx} \langle x|p\rangle \quad (3.109)$$

and thus

$$\langle x|\hat{p}|\psi\rangle = \int dp \left(\frac{\hbar}{i} \frac{d}{dx} \langle x|p\rangle\right) \langle p|\psi\rangle. \quad (3.110)$$

The derivative can be moved out of the integral, since no other part of the integrand depends on x :

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i} \frac{d}{dx} \int dp \langle x|p\rangle \langle p|\psi\rangle \quad (3.111)$$

The completeness sum is now trivial and can be discarded to obtain

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i} \frac{d}{dx} \langle x|\psi\rangle = \frac{\hbar}{i} \frac{d}{dx} \psi(x). \quad (3.112)$$

Exercise. Show that

$$\langle p|\hat{x}|\psi\rangle = i\hbar \frac{d}{dp} \tilde{\psi}(p). \quad (3.113)$$

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8.05 Quantum Physics II

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