Chapter 5

Dirac's bra and ket notation

We introduce the Dirac bra-ket notation for inner products and for the action of operators. Kets represent vectors in the vector space V. Bras are linear functionals on V, thus elements of the dual space V^*. The working rules for operations with bras follow from this identification. When using bras and kets it is useful to distinguish two cases. In the first case the labels in the kets and bras are themselves vectors. This case is most analogous to the mathematical formalism. In the second case the labels are attributes of vectors, and the bra-ket notation affords some extra flexibility. In bra-ket notation operators are sums of products of kets and bras, in that order. Operators are changed into their adjoints as they move in or out of bras. We use bras and kets to study position and momentum states, wavefunctions, and certain matrix elements.

Dirac invented an alternative notation for inner products that leads to the concepts of bras and kets. Dirac's notation is sometimes more efficient than the conventional mathematical notation we developed in the last two chapters. It is also widely used.

In this chapter we discuss Dirac's notation and spend some time rewriting some of our earlier results using bras and kets. This will afford you an extra opportunity to appreciate the various concepts by looking at them from a slightly different angle. Operators can also be written in terms of bras and kets, using their matrix representation. With this chapter we are providing a detailed explanation for some of the rules we followed in Chapter two, where spin states were written as kets.

A classic application of the bra-ket notation is to systems with a non-denumerable basis of states, such as positions states $|x\rangle$ and momentum states $|p\rangle$ of a particle moving in one dimension.

5.1 From inner products to bra-kets

It all begins by writing the inner product differently. The first step in the Dirac notation is to turn inner products into so called "bra-ket" pairs as follows

$$\langle\, u\,, v\,\rangle \quad \longrightarrow \quad \langle u|\, v\rangle\,. \tag{5.1.1}$$

Instead of the inner product comma we simply put a vertical bar! The object to the right of the arrow is called a bra-ket. Since things look a bit different in this notation let us re-write a few of the properties of inner products in bra-ket notation.

We now say, for example, that $\langle v|v\rangle \geq 0$ for all v, while $\langle v|v\rangle = 0$ if and only if $v = 0$. The conjugate exchange symmetry becomes $\langle u|v\rangle = \langle v|u\rangle^*$. Additivity and homogeneity on the second entry is written as

$$\langle u|c_1 v_1 + c_2 v_2\rangle \;=\; c_1\langle u|v_1\rangle + c_2\langle u|v_2\rangle\,, \quad c_1, c_2 \in \mathbb{C}\,, \tag{5.1.2}$$

while conjugate homogeneity (4.1.16) on the first entry is summarized by

$$\langle c_1 u_1 + c_2 u_2|v\rangle \;=\; c_1^*\,\langle u_1|v\rangle + c_2^*\,\langle u_2|v\rangle\,. \tag{5.1.3}$$

Two vectors u and v are orthogonal if $\langle u|v\rangle = 0$ and the norm $|v|$ of a vector is $|v|^2 \;=\; \langle v|v\rangle$.

The Schwarz inequality, for any pair u and v of vectors reads $|\langle u|v\rangle| \leq |u|\,|v|$.

A set of basis vectors $\{e_i\}$ labelled by the integers $i = 1, \ldots, n$ is orthonormal (recall (4.2.20)) if

$$\langle e_i|e_j\rangle \;=\; \delta_{ij}\,, \tag{5.1.4}$$

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

$$v \;=\; \sum_i \alpha_i\, e_i\,, \tag{5.1.5}$$

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

$$\langle e_k|v\rangle \;=\; \Big\langle e_k\Big|\sum_i \alpha_i e_i\Big\rangle \;=\; \sum_i \alpha_i \big\langle e_k\big|e_i\big\rangle \;=\; \alpha_k\,. \tag{5.1.6}$$

We can therefore write

$$v \;=\; \sum_i e_i\,\langle e_i|v\rangle\;, \tag{5.1.7}$$

just as we did before in (4.2.25).

5.2 Bras and kets

The next step is to isolate bras and kets. To do this we reinterpret the bra-ket form of the inner product. We want to "split" the bra-ket into two ingredients, a bra and a ket:

$$\langle u|v\rangle \quad \to \quad \langle u| \;\; |v\rangle \,. \tag{5.2.1}$$

Here the symbol $|v\rangle$ is called a **ket** and the symbol $\langle u|$ is called a **bra**. The bra-ket is recovered when the space between the bra and the ket collapses.

We will view the ket $|v\rangle$ as another way to write the vector v. There is a bit of redundancy in this notation that may be confusing: both $v \in V$ and $|v\rangle \in V$. Both are vectors in V but sometimes the ket $|v\rangle$ is called a 'state' in V. The enclosing symbol $|\;\rangle$ is a decoration added to the vector v without changing its meaning, perhaps like the familiar arrows that are added on top of a symbol to denote a vector. The label in the ket is a vector and the ket itself is that vector!

When the label of the ket is a vector the bra-ket notation is a direct rewriting of the mathematical notation. Sometimes, however, the label of the ket is not a vector. The label could be the value of some quantity that characterizes the 'state'. In such cases the notation affords some extra flexibility. We used such labeling, for example, when we wrote $|+\rangle$ and $|-\rangle$ for the spin states that point along the plus z direction and along the minus z direction, respectively. We will encounter similar situations in this chapter.

$$\boxed{\begin{array}{c}\text{Sometimes the label inside a ket is the vector itself,}\\ \text{other times it is a quantity that characterizes the vector.}\end{array}} \tag{5.2.2}$$

Let T be an operator in a vector space V. We wrote Tv as the vector obtained by the action of T on the vector v. Now the same action would be written as $T|v\rangle$. With kets labeled by vectors we can simply identify

$$|Tv\rangle \;\equiv\; T|v\rangle \,. \tag{5.2.3}$$

When kets are labeled by vectors operators go in or out of the ket without change! If the ket labels are not vectors the above identification is not possible. Imagine a non-degenerate system where we label the states (or vectors) by their energies, as in $|E_i\rangle$, where E_i is the value of the energy for the i-th level. Acting with the momentum operator $\hat{p}$ on the state is denoted as $\hat{p}|E_i\rangle$. It would be meaningless, however, to rewrite this as $|\hat{p}E_i\rangle$, since E_i is not a vector, it is an energy.

Bras are rather different from kets although we also label them by vectors. Bras are linear functionals on the vector space V. We defined linear functionals in section 4.3: they are linear maps ϕ from V to the numbers: $\phi(v) \in \mathbb{F}$. The set of all linear functionals on V is in fact a new vector space over $\mathbb{F}$, the vector space V^* **dual to** V. The vector space structure of V^* follows from the natural definitions of sums of linear functionals and multiplication of linear functionals by numbers:

1. For $\phi_1, \phi_2 \in V^*$, we define the sum $\phi_1 + \phi_2 \in V^*$ by :

$$(\phi_1 + \phi_2)v \equiv \phi_1(v) + \phi_2(v)\,. \tag{5.2.4}$$

2. For $\phi \in V^*$ and $a \in \mathbb{F}$ we define $a\phi \in V^*$ by

$$(a\phi)(v) = a\phi(v)\,. \tag{5.2.5}$$

We proved before that for any linear functional $\phi \in V^*$ there is a unique vector $u \in V$ such that $\phi(v) = \langle u, v\rangle$. We made it more explicit by labeling the linear functional by u (see (4.3.6)) :

$$\phi_u(v) \;=\; \langle u\,, v\rangle\,. \tag{5.2.6}$$

Since the elements of V^* are characterized uniquely by vectors, the vector space V^* has the same dimensionality as V.

A bra is also labeled by a vector. The bra $\langle u|$ can also be viewed as a linear functional because it has a natural action on vectors. The bra $\langle u|$ acting on the vector $|v\rangle$ is defined to give the bra-ket number $\langle u|v\rangle$:

$$\langle u| \;:\; |v\rangle \;\to\; \langle u|v\rangle\,. \tag{5.2.7}$$

Compare this with

$$\phi_u \;:\; v \;\to\; \langle u, v\rangle\,. \tag{5.2.8}$$

Since $\langle u, v\rangle = \langle u|v\rangle$ the last two equations mean that we can identify

$$\boxed{\;\phi_u \;\Longleftrightarrow\; \langle u|\,.\;} \tag{5.2.9}$$

This identification will allow us to figure out how to manipulate bras.

Once we choose a basis, a vector can be represented by a column vector, as discussed in (3.5.61). If kets are viewed as column vectors, then **bras should be viewed as row vectors**. In this way a bra to the left of a ket in the bra-ket makes sense: matrix multiplication of a row vector times a column vector gives a number. Indeed, for vectors

$$u = \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix}\,, \quad v = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}\,, \tag{5.2.10}$$

we had with the canonical inner product:

$$\langle u|v\rangle \;=\; u_1^* v_1 + \ldots + u_n^* v_n\,. \tag{5.2.11}$$

Now we think of this as having a bra and a ket:

$$\langle u| = \left(u_1^*, \ldots, u_n^*\right), \quad |v\rangle = \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix}, \tag{5.2.12}$$

and matrix multiplication gives us the desired bra-ket:

$$\langle u|v\rangle \;=\; \left(u_1^*, \ldots, u_n^*\right) \cdot \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} \;=\; u_1^* v_1 + \ldots + u_n^* v_n \,. \tag{5.2.13}$$

The row representative of the bra $\langle u|$ was obtained by transposition and complex conjugation of the column vector representative of $|u\rangle$.

The key properties needed to manipulate bras follow from the properties of linear functionals and the identification (5.2.9). For our linear functionals you can quickly verify that for $u_1, u_2 \in V$ and $a \in \mathbb{F}$,

$$\begin{aligned} \phi_{u_1+u_2} \;&=\; \phi_{u_1} + \phi_{u_2}\,, \\ \phi_{au} \;&=\; a^*\, \phi_u\,. \end{aligned} \tag{5.2.14}$$

With the noted identification with bras, these become

$$\boxed{\begin{aligned} \langle u_1 + u_2| \;&=\; \langle u_1| + \langle u_2|\,, \\ \langle au| \;&=\; a^*\, \langle u|\,. \end{aligned}} \tag{5.2.15}$$

If $\phi_u = \phi_{u'}$ then $u = u'$. Thus we have $\langle u| = \langle u'|$ then $u = u'$.

A rule to pass from general kets to general bras is useful. We can obtain such rule by considering the ket

$$|v\rangle = |\alpha_1 u_1 + \alpha_2 u_2\rangle \;=\; \alpha_1 |u_1\rangle + \alpha_2 |u_2\rangle\,. \tag{5.2.16}$$

Then

$$\langle v| \;=\; \langle \alpha_1 u_1 + \alpha_2 u_2| \;=\; \alpha_1^* \langle u_1| + \alpha_2^* \langle u_2|\,, \tag{5.2.17}$$

using the relations in (5.2.15). We have thus shown that the rule to pass from kets to bras, and viceversa, is

$$\boxed{|v\rangle = \alpha_1 |u_1\rangle + \alpha_2 |u_2\rangle \quad \longleftrightarrow \quad \langle v| = \alpha_1^*\, \langle u_1| + \alpha_2^*\, \langle u_2|\,.} \tag{5.2.18}$$

As we mentioned earlier we sometimes write kets with labels other than vectors. Let us reconsider the basis vectors $\{e_i\}$ discussed in (5.1.4). The ket $|e_i\rangle$ is simply called $|i\rangle$ and the orthonormal condition reads

$$\langle i\,|\,j\rangle \;=\; \delta_{ij}\,. \tag{5.2.19}$$

The expansion (5.1.5) of a vector now reads

$$|v\rangle \;=\; \sum_i |\,i\rangle\,\alpha_i\,, \tag{5.2.20}$$

As in (5.1.6) the expansion coefficients are $\alpha_i \;=\; \langle i\,|\,v\rangle$ so that

$$\boxed{\;|v\rangle \;=\; \sum_i |i\rangle\langle i\,|\,v\rangle\,.\;} \tag{5.2.21}$$

We placed the numerical component $\langle i\,|\,v\rangle$ to the right of the ket $|\,i\rangle$. This is useful as we will soon find that the sum $\sum_i |\,i\rangle\langle\,i|$ has a special meaning.

5.3 Operators and projectors revisited

Let T be an operator in a vector space V. This means that it acts on kets to give kets. As we explained before we denote by $T|v\rangle$ the vector obtained by acting with T on the vector v. Our identification of vectors with kets implies that

$$|T\,v\rangle \;\equiv\; T|v\rangle\,. \tag{5.3.1}$$

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

$$T : V^* \to V^*\,, \tag{5.3.2}$$

We write this as

$$\langle u| \;\to\; \langle u|T \in V^*\,. \tag{5.3.3}$$

The object $\langle u|T$ is *defined* to be the bra (or linear functional) that acting on the ket $|v\rangle$ gives the number $\langle u|T|v\rangle$. Since any linear functional is represented by a vector, we could ask: What is the vector that represents $\langle u|T$? We will answer this question in the next section.

We can actually write operators using bras and kets, written in a suitable order. As an example, consider a bra $\langle u|$ and a ket $|w\rangle$, with $u, w \in V$. We claim that the object

$$S \;=\; |u\rangle\langle w|\,, \tag{5.3.4}$$

is naturally viewed as a linear operator on V. While surprising, this could have been anticipated: the matrix product of a column vector (the ket) times a row vector (the bra), in that order, gives a matrix. Indeed, acting with S on a vector we let it act as the bra-ket notation suggests:

$$S|v\rangle \;\equiv\; |u\rangle\,\langle w|v\rangle \sim |u\rangle\,, \quad \text{since } \langle w|v\rangle \text{ is a number.} \tag{5.3.5}$$

Acting on a bra it gives a bra:

$$\langle v|S \equiv \langle v|u\rangle \langle w| \sim \langle w|, \quad \text{since } \langle v|u\rangle \text{ is a number.} \tag{5.3.6}$$

Let us now review the description of operators as matrices. For simplicity we will usually consider orthonormal bases and we recall that in this case matrix elements of an operator are easily read from an inner product, as given in (4.4.48):

$$T_{ij} = \langle e_i, Te_j\rangle . \tag{5.3.7}$$

In bra-ket notation this reads

$$T_{ij} = \langle e_i|Te_j\rangle = \langle e_i|T|e_j\rangle . \tag{5.3.8}$$

Labelling the kets with the subscripts on the basis vectors we write

$$\boxed{T_{ij} = \langle i\,|T|j\rangle .} \tag{5.3.9}$$

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

$$\boxed{T = \sum_{i,j} |i\,\rangle\, T_{ij}\, \langle\, j| .} \tag{5.3.10}$$

We can verify that this is correct by computing the matrix elements of this T:

$$\begin{aligned}\langle i'|T|j'\rangle &= \sum_{i,j} \langle i'|\big(|i\,\rangle\, T_{ij}\, \langle\, j|\big)|j'\rangle = \sum_{i,j} \langle i'|\, i\,\rangle\, T_{ij}\, \langle\, j|j'\rangle \\ &= \sum_{i,j} \delta_{ii'}\, T_{ij}\, \delta_{jj'} = T_{i'j'} ,\end{aligned} \tag{5.3.11}$$

consistent with (5.3.9). The above boxed result means that $|\,i\rangle\langle j|$ is represented by a matrix with all zeroes except for a 1 at the (i,j) position.

Let us now reconsider projector operators. Choose one element $|m\rangle$ from the orthonormal basis to form an operator P_m defined by

$$P_m \equiv |m\rangle\langle m| . \tag{5.3.12}$$

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

$$P_m|v\rangle = |m\rangle\langle m|v\rangle \sim |m\rangle . \tag{5.3.13}$$

It follows that P_m is a projector to the one-dimensional subspace spanned by $|m\rangle$. It is in fact manifestly an orthogonal projector because any vector $|v\rangle$ killed by P must satisfy

$\langle m|v\rangle = 0$ and is therefore orthogonal to $|m\rangle$. In the chosen basis, P_m is represented by a matrix all of whose elements are zero, except for the (m, m) element $(P_m)_{mm}$ which is one:

$$P_m \;=\; \text{diag}\,(0, \ldots, 1, \ldots, 0)\,. \tag{5.3.14}$$

As it befits a projector $P_m P_m = P_m$:

$$P_m P_m \;=\; \big(|m\rangle\langle m|\big)\big(|m\rangle\langle m|\big) \;=\; |m\rangle\,\langle m|m\rangle\,\langle m| \;=\; |m\rangle\langle m|\,, \tag{5.3.15}$$

since $\langle m|m\rangle = 1$. The operator P_m is a *rank one* projection operator since it projects to a one-dimensional subspace of V, the subspace generated by $|m\rangle$. The rank of the projector is also equal to the trace of its matrix representation, which for P_m is equal to one.

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

$$P_{m,n} \;\equiv\; |m\rangle\langle m| + |n\rangle\langle n|\,. \tag{5.3.16}$$

It should be clear to you that this is a projector to the two-dimensional subspace spanned by $|m\rangle$ and $|n\rangle$. It should also be clear that it is an orthogonal projector of rank two. You should also verify that $P_{m,n}P_{m,n} = P_{m,n}$. Similarly, we can construct a rank three projector by adding an extra term $|k\rangle\langle k|$ with $k \neq m, n$. If we include *all* basis vectors of a vector space of dimension N we would have the operator

$$P_{1,\ldots,N} \;\equiv\; |1\rangle\langle 1| + \ldots + |N\rangle\langle N|\,. \tag{5.3.17}$$

As a matrix $P_{1,\ldots,N}$ 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. We thus have the surprising relation

$$\boxed{\;\mathbf{1} \;=\; \sum_i |i\,\rangle\,\langle i\,|\,.\;} \tag{5.3.18}$$

This equation is sometimes called a 'resolution' of the identity: it decomposes the identity operator as a sum of projectors to one-dimensional orthogonal subspaces. The fact that the above right-hand side is the identity is hinted at in (5.2.21):

$$|v\rangle \;=\; \sum_i |i\rangle\langle i\,|\,v\rangle\,, \tag{5.3.19}$$

that on the light of the above resolution looks like $|v\rangle = \mathbf{1}|v\rangle$, which is certainly consistent. Since the expansion of any $|v\rangle$ is possible because the $|\,i\rangle$ states form a basis, equation(5.3.18) is a completeness relation for the chosen orthonormal basis.

Example 1. 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

$$\mathbf{1} \;=\; |+\rangle\langle +| \;\;+\;\; |-\rangle\langle -|\,. \tag{5.3.20}$$

Example 2. We can use the completeness relation to show that our formula (5.3.9) for matrix elements is consistent with matrix multiplication. Indeed for the product T_1T_2 of two operators we write

$$\begin{aligned}(T_1T_2)_{mn} = \ \langle m|T_1T_2|n\rangle \ &= \ \langle m|T_1\,\mathbf{1}\,T_2|n\rangle \ = \ \langle m|T_1\Big(\sum_{k=1}^{N}|k\rangle\langle k|\Big)T_2|n\rangle \\ = \ \sum_{k=1}^{N}\langle m|T_1|k\rangle\langle k|T_2|n\rangle \ &= \ \sum_{k=1}^{N}(T_1)_{mk}(T_2)_{kn}\,.\end{aligned} \tag{5.3.21}$$

This is the expected result for the product of T_1 and T_2.

5.4 Adjoint of a linear operator

We defined the linear operator $T^\dagger$ associated with T in (4.3.16). In bra-ket language this key relation is written as

$$\langle T^\dagger v|u\rangle \ = \ \langle v|Tu\rangle\,. \tag{5.4.1}$$

It is convenient to rewrite this as an equality that gives the matrix elements of $T^\dagger$ when those of T are known. Flipping the order on the left-hand side we get

$$\langle u|T^\dagger v\rangle^* \ = \ \langle v|Tu\rangle \quad \to \quad \langle u|T^\dagger|v\rangle^* \ = \ \langle v|T|u\rangle\,. \tag{5.4.2}$$

Complex conjugating the final relation we get the desired relation between matrix elements:

$$\boxed{\langle u|T^\dagger|v\rangle \ = \ \langle v|T|u\rangle^*\,, \quad \forall u, v \in V\,.} \tag{5.4.3}$$

The right-hand side above can be written as $\langle v|Tu\rangle^* = \langle Tu|v\rangle$. Comparing with the left-hand side, we can take away the ket to learn that

$$\boxed{\langle u|T^\dagger \ = \ \langle Tu|\,.} \tag{5.4.4}$$

The linear operator T 'exits' the bra as its adjoint! With the substitution $T \to T^\dagger$ this equation also implies that

$$\langle u|T \ = \ \langle T^\dagger u|\,, \tag{5.4.5}$$

showing that a linear operator 'enters' the bra as its adjoint. This last equation also shows that the vector that represents the bra $\langle u|T$ is $T^\dagger u$. We raised this question below eqn. (5.3.3).

Since $\langle Tu|$ is the bra associated with $|Tu\rangle$ the above relation says that

$$\boxed{\langle u|T^\dagger \ \text{ is the bra associated with } \ T|u\rangle\,.} \tag{5.4.6}$$

The matrix elements of $T^\dagger$ are simply related to those of T in an orthonormal basis. Taking u, v to be orthonormal basis vectors in equation (5.4.3) we find

$$\langle i|T^\dagger|j\rangle \;=\; \langle j|T|i\rangle^* \quad\rightarrow\quad (T^\dagger)_{ij} \;=\; (T_{ji})^*\,. \tag{5.4.7}$$

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

Exercise. Show that $(T_1T_2)^\dagger = \; T_2^\dagger T_1^\dagger$ by taking matrix elements.

Example 3. Let $T = |u\rangle\langle w|$, for arbitrary vectors u, w. Write a bra-ket expression for $T^\dagger$.

Solution: Acting with T on $|v\rangle$ and then passing to the associated bras:

$$T|v\rangle \;=\; |u\rangle\,\langle w|v\rangle \quad\rightarrow\quad \langle v|T^\dagger \;=\; \langle v|w\rangle\,\langle u|\,, \tag{5.4.8}$$

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

$$T^\dagger \;=\; |w\rangle\langle u|\,. \tag{5.4.9}$$

This equation allows us to compute in bra-ket language the adjoint of any operator.

5.5 Hermitian and Unitary Operators

Recall that a linear operator T is hermitian is $T^\dagger = T$. In quantum mechanics Hermitian operators are associated with observables. The eigenvalues of a Hermitian operator are the possible measured values of the observables. 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.

It should be clear from our earlier work that

$$\text{For } T = T^\dagger: \quad \langle Tu|v\rangle \;=\; \langle u|Tv\rangle\,, \quad \text{and} \quad \langle v|T|u\rangle^* \;=\; \langle u|T|v\rangle\,, \quad \forall u, v\,. \tag{5.5.1}$$

It follows that the expectation value of a Hermitian operator in *any* state is real. Inside a bra-ket, a hermitian operator moves freely from the bra to the ket and viceversa.

Example 4. For wavefunctions $f(x), g(x) \in \mathbb{C}$ we have the inner product

$$\langle f|g\rangle \;=\; \int_{-\infty}^{\infty} (f(x))^* g(x)dx\,. \tag{5.5.2}$$

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

$$\int_{-\infty}^{\infty} (\Omega f(x))^* g(x)dx \;=\; \int_{-\infty}^{\infty} (f(x))^* \Omega g(x)dx\,. \tag{5.5.3}$$

Verify that the linear operator $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$ is Hermitian when we restrict to functions that vanish at $\pm\infty$ and whose derivatives are not infinite at $\pm\infty$.

An operator U is said to be a unitary operator if $U^\dagger U = UU^\dagger = \mathbf{1}$. You may remember that unitary operators preserve inner products. If you have two vectors u, w their inner product is the same as the inner product of Uu, Uw:

$$\langle Uu|Uw\rangle \;=\; \langle u|U^\dagger|Uw\rangle \;=\; \langle u|U^\dagger U|w\rangle \;=\; \langle u|w\rangle\,. \tag{5.5.4}$$

Another important property of unitary operators is that acting on an orthonormal basis they give another orthonormal basis. If $|e_i\rangle$ are an orthonormal basis then $|f_i\rangle$ defined by

$$|f_i\rangle \equiv U|e_i\rangle\,, \quad \forall\, i \tag{5.5.5}$$

are another orthonormal basis, as you can quickly check. In fact we can write the unitary operator explicitly in terms of the two sets of basis vectors! Here it is:

$$U \;=\; \sum_k |f_k\rangle\langle e_k|\,. \tag{5.5.6}$$

It is clear that this sum acting on $|e_i\rangle$ gives $|f_i\rangle$, as desired. This construction shows that given any two orthonormal bases on the state space, there is a unitary operator that relates them. Example 3 implies that

$$U^\dagger \;=\; \sum_k |e_k\rangle\langle f_k|\,, \tag{5.5.7}$$

and now you can quickly verify that $U^\dagger U = UU^\dagger = \mathbf{1}$.

Exercise: Prove that $\langle e_i|U|e_j\rangle \;=\; \langle f_i|U|f_j\rangle$. This is the by-now familiar property that the matrix elements of a basis-changing operator are the same in both bases. This is almost obvious in the new notation!

5.6 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. Roughly, $|x\rangle$ represents the state of the system where the particle is at the position x. The full state space requires position states $|x\rangle$ for all values of x. Physically, we consider all of these states to be linearly independent: the state of a particle at some point x_0 can't be build by superposition of states where the particle is elsewhere. Since x is a continuous variable the basis states form a non-denumerable infinite set. This is surprising, but does not imply an obstruction. In summary, we have

$$\text{Basis states}: \quad |x\rangle\,, \quad \forall x \in \mathbb{R}\,. \tag{5.6.1}$$

Since we have an infinite number of basis vectors, this state space is an infinite dimensional complex vector space. This should not surprise you. The states of a particle on the real line can be represented by wavefunctions, and the set of possible wavefunctions form an infinite dimensional complex vector space.

Note here that the label in the ket is not a vector; it is the position on a line. If we did not have the decoration provided by the ket it would be hard to recognize that the object is a state in an infinite dimensional complex vector space. Therefore, the following should be noted

$$\begin{aligned} |ax\rangle \ &\neq a|x\rangle\,, \quad \text{for any real} \ \ a \neq 1\,, \\ |-x\rangle \ &\neq \ -|x\rangle\,, \quad \text{unless } x = 0\,, \\ |x_1 + x_2\rangle \ &\neq |x_1\rangle + |x_2\rangle\,, \end{aligned} \tag{5.6.2}$$

All these equations would hold if the labels inside the kets were vectors. In the first line, roughly, the left hand side is a state with a particle at the position ax while the right hand side is a state with a particle at the position x. Analogous remarks hold for the other lines. Note also that $|0\rangle$, a particle at $x = 0$, not the zero vector on the state space, for which we would probably have to use the symbol 0.

For quantum mechanics of a particle moving in three spatial dimensions, we would 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 the decoration enclosing the vector label plays a crucial role: it reminds us that the state lives in an infinite dimensional complex vector space.

Let us go back to our position basis states for the one-dimensional problem. The inner product must be defined, so we will take

$$\langle x|y\rangle \ \equiv \ \delta(x-y)\,. \tag{5.6.3}$$

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

$$\mathbf{1} \ = \ \int dx\, |x\rangle\langle x|\,. \tag{5.6.4}$$

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

$$|y\rangle \ = \ \int dx\, |x\rangle\langle x|y\rangle \ = \ \int dx\, |x\rangle\, \delta(x-y) \ = \ |y\rangle\,. \tag{5.6.5}$$

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

$$\hat{x}\,|x\rangle \ \equiv \ x\,|x\rangle\,, \tag{5.6.6}$$

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:

$$\langle x_1|\hat{x}^\dagger|x_2\rangle = \langle x_2|\hat{x}|x_1\rangle^* = [x_1\delta(x_1-x_2)]^* = x_2\delta(x_1-x_2) = \langle x_1|\hat{x}|x_2\rangle\,. \tag{5.6.7}$$

We thus conclude that $\hat{x}^\dagger = \hat{x}$ and the bra associated with (5.6.6) is

$$\langle x|\hat{x} = x\langle x|\,. \tag{5.6.8}$$

The wavefunction associated with a state is formed by taking the inner product of a position state with the given state. Given the state $|\psi\rangle$ of a particle, we define the associated position-state wavefunction $\psi(x)$ by

$$\psi(x) \equiv \langle x|\psi\rangle \;\in \mathbb{C}\,. \tag{5.6.9}$$

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

$$|\psi\rangle \;=\; \mathbf{1}|\psi\rangle \;=\; \int dx\,|x\rangle\,\langle x|\psi\rangle \;=\; \int dx\,|x\rangle\,\psi(x)\,. \tag{5.6.10}$$

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

$$\langle\phi|\psi\rangle \;=\; \langle\phi|\mathbf{1}|\psi\rangle \;=\; \int dx\,\langle\phi|x\rangle\,\langle x|\psi\rangle \;=\; \int dx\;\phi^*(x)\psi(x)\,. \tag{5.6.11}$$

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

$$\langle\phi|\hat{x}|\psi\rangle \;=\; \langle\phi|\hat{x}\mathbf{1}|\psi\rangle \;=\; \int dx\,\langle\phi|\hat{x}|x\rangle\,\langle x|\psi\rangle \;=\; \int dx\,\langle\phi|x\rangle\,x\,\langle x|\psi\rangle \;=\; \int dx\;\phi^*(x)\,x\,\psi(x)\,. \tag{5.6.12}$$

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

$$\begin{aligned} &\text{Basis states}: \quad |p\rangle\,, \quad \forall p\in\mathbb{R}\,. \\ &\langle p'|p\rangle \;=\; \delta(p-p')\,, \\ &\mathbf{1} \;=\; \int dp\,|p\rangle\langle p|\,, \\ &\hat{p}\,|p\rangle \;=\; p\,|p\rangle \end{aligned} \tag{5.6.13}$$

Just as for coordinate space we also have

$$\hat{p}^\dagger = \hat{p}\,, \quad \text{and} \qquad \langle p|\hat{p} = p\langle p|\,. \tag{5.6.14}$$

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 (1.6.38) that

$$\langle x|p\rangle \;=\; \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\,. \tag{5.6.15}$$

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

$$\langle p'|p\rangle \;=\; \int dx\langle p'|x\rangle\langle x|p\rangle \;=\; \frac{1}{2\pi\hbar}\int dx e^{i(p-p')x/\hbar} \;=\; \frac{1}{2\pi}\int du\, e^{i(p-p')u}\,, \tag{5.6.16}$$

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 $\delta(p-p')$:

$$\frac{1}{2\pi}\int du\, e^{i(p-p')u} \;=\; \delta(p-p')\,. \tag{5.6.17}$$

This, then gives the correct value for the overlap $\langle p|p'\rangle$, as we claimed. The integral (5.6.17) can be justified using the fact that the functions

$$f_n(x) \equiv \frac{1}{\sqrt{L}}\exp\Bigl(\frac{2\pi i n x}{L}\Bigr)\,, \tag{5.6.18}$$

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

$$\sum_{n\in\mathbb{Z}} f_n^*(x) f_n(x') \;=\; \delta(x-x')\,. \tag{5.6.19}$$

We thus have

$$\sum_{n\in\mathbb{Z}} \frac{1}{L}\exp\Bigl(2\pi i\,\frac{n}{L}(x-x')\Bigr) \;=\; \delta(x-x')\,. \tag{5.6.20}$$

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

$$\sum_{n\in\mathbb{Z}} \frac{1}{L}\exp\Bigl(2\pi i\,\frac{n}{L}(x-x')\Bigr) \;=\; \sum_{u} \frac{\Delta u}{2\pi}\exp\Bigl(i\,u(x-x')\Bigr) \;\to\; \frac{1}{2\pi}\int du e^{iu(x-x')}\,, \tag{5.6.21}$$

and back in (5.6.20) we have justified (5.6.17).

We can now ask: What is $\langle p|\psi\rangle$? The answer is quickly obtained by computation:

$$\langle p|\psi\rangle \;=\; \int dx\langle p|x\rangle\langle x|\psi\rangle \;=\; \frac{1}{\sqrt{2\pi\hbar}}\int dx e^{-ipx/\hbar}\psi(x) \;=\; \tilde{\psi}(p)\,, \tag{5.6.22}$$

which is the Fourier transform of $\psi(x)$, as defined in (1.6.40). Thus the *Fourier transform of $\psi(x)$ is simply the wavefunction in the momentum representation.*

It is often necessary to evaluate $\langle x|\hat{p}|\psi\rangle$. This is, by definition, the wavefuntion of the state $\hat{p}|\psi\rangle$. We would expect it to be simply the familiar action of the momentum operator on the wavefunction for $|\psi\rangle$. There is no need to speculate because we can calculate this matrix element with the rules defined so far. We do it by inserting a complete set of momentum states:

$$\langle x|\,\hat{p}\,|\psi\rangle \;=\; \int dp\,\langle x|p\rangle\langle p|\hat{p}\,|\psi\rangle \;=\; \int dp\,(p\langle x|p\rangle)\langle p|\psi\rangle \tag{5.6.23}$$

Now we notice that

$$p\langle x|p\rangle \;=\; \frac{\hbar}{i}\frac{d}{dx}\langle x|p\rangle \tag{5.6.24}$$

and thus

$$\langle x|\,\hat{p}\,|\psi\rangle \;=\; \int dp\,\Big(\frac{\hbar}{i}\frac{d}{dx}\langle x|p\rangle\Big)\langle p|\psi\rangle\,. \tag{5.6.25}$$

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

$$\langle x|\,\hat{p}\,|\psi\rangle \;=\; \frac{\hbar}{i}\frac{d}{dx}\int dp\,\langle x|p\rangle\langle p|\psi\rangle\,. \tag{5.6.26}$$

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

$$\boxed{\langle x|\,\hat{p}\,|\psi\rangle \;=\; \frac{\hbar}{i}\frac{d}{dx}\,\langle x|\psi\rangle \;=\; \frac{\hbar}{i}\frac{d}{dx}\,\psi(x)\,.} \tag{5.6.27}$$

Exercise. Show that

$$\langle p|\,\hat{x}\,|\psi\rangle \;=\; i\hbar\frac{d}{dp}\tilde{\psi}(p)\,. \tag{5.6.28}$$