



On the coordinate representation in the Dirac bra–ket notation

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Abstract In this paper we discuss some traps which can occur in using Dirac bra–ket notation in the coordinate (or momentum) representation. Furthermore, we demonstrate that in order to avoid some misconceptions, it is necessary to distinguish the two operators. First, the ordinary derivative d/dx , is just the usual partial differentiation which acts on the scalar function; and should not be considered as an operator which can act on the vectors in the Hilbert space. Second, the unbounded operator D_x , which is usually mixed up with the former. Our discussion indicates that the action of these two operators is the same on the bra $\langle x|$, but on the ket $|x\rangle$ it really leads to different results.

1 Introduction

Today, Dirac bra–ket notation is widely used in the literature of quantum mechanics. Anyone who ponders this notation will find that this mathematical formulation of quantum mechanics should not be thought of as being merely notation but, instead, as a major conceptual revolution [1]. However, using this notation can sometimes become confusing. For example, when dealing with antilinear operators, we must be careful in their use. As emphasized by Sakurai, Dirac bra–ket notation was invented to handle linear operators, not antilinear operators [2]. This subject is discussed in detail in Ref. [3]. In general, there are debates in Ref. [4]. Furthermore, challenges of this notation are pursued in pedagogical papers [5–7].

The eigenkets $|x\rangle$ of the position operator X satisfy

$$X|x\rangle = x|x\rangle, \quad (1)$$

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where the value of x runs over all possible values of the position of the particle, that is, from $-\infty$ to $+\infty$. It should be noted that $|x\rangle$ is not in the Hilbert space because its norm is infinite. However, the vectors of the Hilbert space can be expanded in terms of the generalized kets $|x\rangle$.

The main problem starts when we want to know the action of the position operator on the derivative of $|x\rangle$, namely

$$X \frac{d}{dx} |x\rangle = ? \quad (2)$$

First, we should emphasize that $\frac{d}{dx}$ is not a good designation for an operator acting on vectors in the Hilbert space. Instead, we can assign D_x as an operator in Hilbert space, defined by $(D_x f)(x) = f'(x)$, where $f'(x)$ denotes the derivative of the function $f(x)$. We endeavor to show that the distinction between these two operators is necessary, and that with this mathematical accuracy, some misconceptions and misleading notations will be eliminated.

In some quantum mechanics literature, misleading notations are seen, such as $[x, \frac{d}{dx}]f(x)$ and $[x, \frac{d}{dx}]|x\rangle$. We make a distinction between the position operator X and the real number x . Also, $f(x)$ is a number; in fact, f is a smooth and differentiable function and $f(x)$ is the value of the function f at the point x , so that $f(x)$ is a point (like x) itself. We begin with the following postulate, which plays a fundamental role in this paper.

Postulate 1. The action of the ordinary derivative d/dx on something independent of x is zero. It can be a function, vector, covector, etc.

From Ref. [2], in position space the wave function is represented by the action of the bra position on the ket state, that is, $\psi(x) = \langle x|\psi\rangle$. Obviously, $\psi(x)$ depends on x , while the abstract state $|\psi\rangle$ itself does not depend on x . Otherwise,

one could ask what is the value of $|\psi\rangle$ when x is, say, 8 or any other numbers?

Let $\psi(x) = N \exp[-a(x-b)^2]$, where a , b , and N are constants with $a > 0$. Obviously, the function $\psi(x)$ is not a constant function of x , but the abstract state $|\psi\rangle$ itself does not depend on x . In fact,

$$|\psi\rangle = \int_{-\infty}^{\infty} dy |y\rangle \langle y|\psi\rangle = \int_{-\infty}^{\infty} dy \psi(y) |y\rangle, \quad (3)$$

In Eq. (3), $|y\rangle$ is the normalized eigenvector of the position operator X with eigenvalue y , and there is no x appearing in this expression. Note that if $a \rightarrow \infty$, the wave function ψ tends to an eigenvector of the position operator X with eigenvalue b , i.e. $\lim_{a \rightarrow \infty} \psi = N'|b\rangle$, where N' is another normalization factor. Clearly, b does not depend on x either; therefore, $\frac{da}{dx} = \frac{db}{dx} = \frac{dN}{dx} = \dots = \frac{d\psi}{dx} = 0$.

Postulate 2. The action of the ordinary derivative $\frac{d}{dx}$ on a ket vector such as $|x\rangle$ can be defined as

$$\frac{d}{dx} |x\rangle \equiv \lim_{h \rightarrow 0} \frac{|x+h\rangle - |x\rangle}{h}, \quad (4)$$

and for the bra position vector,

$$\frac{d}{dx} \langle x| \equiv \lim_{h \rightarrow 0} \frac{\langle x+h| - \langle x|}{h}, \quad (5)$$

where h is a constant number.

Now we can clarify the assignment in Eq. (2):

$$\begin{aligned} X \frac{d}{dx} |x\rangle &= X \lim_{h \rightarrow 0} \frac{|x+h\rangle - |x\rangle}{h} \\ &= \lim_{h \rightarrow 0} \frac{(x+h)|x+h\rangle - x|x\rangle}{h} \\ &= \frac{d}{dx} (X |x\rangle) = |x\rangle + x \frac{d}{dx} |x\rangle. \end{aligned} \quad (6)$$

It is obvious from Eq. (6) that $[\frac{d}{dx}, X]|x\rangle = |x\rangle \neq 0$. On the other hand, the last of the equations of (6) can also be obtained in an alternative way, as described in Appendix A.

Also, we can write

$$\begin{aligned} \frac{d}{dx} [f(x)] &= \left(\frac{d}{dx} \langle x|f \rangle \right) f(x) \\ &= \left(\frac{d}{dx} \langle x| \right) |f\rangle + \langle x| \left(\frac{d}{dx} |f\rangle \right). \end{aligned} \quad (7)$$

We should not simply move $\frac{d}{dx}$ through $\langle x|$, as $\langle x|$ depends on x and the first term in above relation is not zero. Clearly, in Eq. (7), the second term vanishes. So

$$f'(x) = \left(\frac{d}{dx} \langle x| \right) |f\rangle, \quad (8)$$

and this can be seen directly with respect to the postulate

$$\begin{aligned} \left\langle \frac{d}{dx} x \middle| f \right\rangle &= \lim_{h \rightarrow 0} \frac{\langle x+h|f\rangle - \langle x|f\rangle}{h} \\ &= \lim_{h \rightarrow 0} \frac{f(x+h) - f(x)}{h} = f'(x). \end{aligned} \quad (9)$$

Now, with the help of this postulate, we identify the distinction between two operators in a precise way.

2 Difference between D_x and d/dx

In this section, we indicate that $\frac{d}{dx}$ is only the usual partial differentiation which acts on functions, and not an operator on the vectors of the Hilbert space. A discussion about this distinction between the two operators can be found in Ref. [8].

At first, we can indicate the distinction between the two operators by the statement $\langle x|\hat{A}|\psi\rangle = A\langle x|\psi\rangle$, where $|\psi\rangle$ is an arbitrary state. In this relation \hat{A} acts on kets while A acts on functions [9]. We do not use the hat symbol for operators in this paper.

For simplicity, we use the symbol d_x instead of $\frac{d}{dx}$. Assume that another operator D_x is defined by

$$\langle x|D_x|u\rangle = (d_x u)(x). \quad (10)$$

Eq. (10) represents the action of the operator D_x on the function u , and d_x means differentiation with respect to the variable x . To any vector $|u\rangle$ in the Hilbert space corresponds a function $u(x) = \langle x|u\rangle$, so one can write

$$\begin{aligned} \langle x|D_x|u\rangle &= \lim_{h \rightarrow 0} \frac{u(x+h) - u(x)}{h} \\ &= \lim_{h \rightarrow 0} \frac{\langle x+h|u\rangle - \langle x|u\rangle}{h} \\ &= \left(\lim_{h \rightarrow 0} \frac{\langle x+h| - \langle x|}{h} \right) |u\rangle. \end{aligned} \quad (11)$$

From the above equation we can conclude

$$\langle x|D_x = \lim_{h \rightarrow 0} \frac{\langle x+h| - \langle x|}{h}. \quad (12)$$

Therefore Eq. (12) gives the result

$$\langle x|D_x = \frac{d}{dx} \langle x|. \quad (13)$$

Now, one might be tempted to write this result as

$$D_x = \frac{d}{dx}. \quad (14)$$

We do not like this! And we think this is one of the misleading notations that happen in quantum mechanics literatures. Indeed, consider

$$\langle x|y \rangle = \delta(x - y), \quad (15)$$

then, using Eq. (10), it is shown that

$$\langle x|D_x|y \rangle = (d_{x1}\delta)(x - y). \quad (16)$$

where d_1 means differentiation with respect to the first variable, i.e. x . The reason we have used d_{x1} instead of d_x is that now there are two variables, x and y . The relation $\langle x|y \rangle = \delta(x - y)$ confirms Eq. (16), which can be written as follows:

$$\langle x|D_x|y \rangle = -(d_{x2}\delta)(x - y). \quad (17)$$

where d_{x2} denotes differentiation with respect to the second variable, i.e. y . So,

$$\begin{aligned} \langle x|D_x|y \rangle &= \lim_{h \rightarrow 0} \frac{\Delta(x, y - h) - \Delta(x, y)}{h} \\ &= \lim_{h \rightarrow 0} \frac{\langle x|y - h \rangle - \langle x|y \rangle}{h} \\ &= \langle x| \lim_{h \rightarrow 0} \frac{|y - h \rangle - |y \rangle}{h}. \end{aligned} \quad (18)$$

In the equation above, Δ is a two-variable function.

Now, we can conclude

$$D_x|x \rangle = -\frac{d}{dx}|x \rangle. \quad (19)$$

It is shown that Eq. (19) is not the same as Eq. (13). Also, it is simple to show that $[X, D_x]|x \rangle = -|x \rangle$. From Eq. (19), we immediately infer that, on the basis position vector $|x \rangle$, the action of the momentum operator becomes

$$P|x \rangle = -i\hbar D_x|x \rangle = i\hbar \frac{d|x \rangle}{dx}. \quad (20)$$

We can use the function notation

$$(Pf)(x) = -i\hbar f'(x), \quad (21)$$

where $f'(x)$ designates differentiation of $f(x)$. For the position operator X , with eigenvalue x , and using the definition Eq. (1), we obtain $[X, P]|x \rangle = i\hbar|x \rangle$, that is, the canonical commutation relation $[X, P] = i\hbar$.

In Ref. [2], considering the momentum operator as the generator of translations, the action of the momentum operator on an arbitrary vector independent of x , such as $|\alpha \rangle$, gives $P|\alpha \rangle = -i\hbar \int dx' |x' \rangle \frac{\partial}{\partial x'} \langle x'|\alpha \rangle$, and obviously choosing $|\alpha \rangle \equiv |x \rangle$ we immediately arrive at Eq. (20). From the formula for $P|\alpha \rangle$ we can write $\langle x'|P|\alpha \rangle = -i\hbar \frac{\partial}{\partial x'} \langle x'|\alpha \rangle$, so $\langle x'|P = -i\hbar \frac{\partial}{\partial x'} \langle x'|$. It is simple to show that $\left(\frac{\partial}{\partial x'} \langle x'| \right)^\dagger = \frac{\partial}{\partial x'} |x' \rangle$, and then the matrix elements of the momentum in the position representation are $\langle x'|P|x'' \rangle = -i\hbar \frac{\partial}{\partial x'} \langle x'|x'' \rangle = i\hbar \frac{\partial}{\partial x''} \langle x'|x'' \rangle = i\hbar \left(\frac{\partial}{\partial x''} \langle x'| \right) |x'' \rangle = i\hbar \langle x'| \frac{\partial}{\partial x''} |x'' \rangle$, since $\frac{\partial}{\partial x''} \langle x'| = 0$. Thus, we again arrive at the same Eq. (20), i.e. $P|x'' \rangle = i\hbar \frac{\partial}{\partial x''} |x'' \rangle$. Employing the operator D_x , we can deduce generalized momentum operators, and there is a detailed discussion of these operators in Ref. [10] and the references therein.

A generalized delta function can be defined as $\langle x|y \rangle = \frac{\delta(x - y)}{\sqrt{g(y)}}$ [11]. For brevity, we choose $f(y) = \frac{1}{\sqrt{g(y)}}$. Thus, with respect to our discussion, we can write

$$\begin{aligned} \langle x|D_x|y \rangle &= -f(y) \frac{\partial}{\partial y} \delta(x - y) \\ &= \langle x| \left[-f(y) \frac{\partial}{\partial y} \left(\frac{|y \rangle}{f(y)} \right) \right]. \end{aligned} \quad (22)$$

As shown in Ref. [11], using $f(x)$ or $f(y)$ has no effect on the result. Applying D_x on the position state we obtain

$$|D_x|x\rangle = -f(x) \frac{d}{dy} \left(\frac{|x\rangle}{f(x)} \right). \quad (23)$$

Obviously, D_x is not an anti-Hermitian operator. According to Eq. (23), the adjoint of D_x takes the form

$$\langle x|D_x^\dagger = -\frac{d\langle x|}{dx} + \left(\frac{f'(x)}{f(x)} \right) \langle x|. \quad (24)$$

In this equation, we have used exactly the definition of the adjoint of a linear operator [12]. From Eq. (13), we know that $\langle x|D_x = \frac{d\langle x|}{dx}$, and hence we can write

$$D_x^\dagger = -D_x + \frac{f'(x)}{f(x)}, \quad (25)$$

where X is the position operator. Now, we can build an anti-Hermitian operator from D_x , which is obviously not anti-Hermitian. Suppose an operator O in which

$$O = \frac{1}{2} (D_x - D_x^\dagger). \quad (26)$$

Using Eq. (23) and taking into account the anti-Hermiticity of O , we obtain

$$\langle x|O = \frac{d\langle x|}{dx} - \frac{f'(x)}{2f(x)} \langle x|. \quad (27)$$

Now, by considering $f = \frac{1}{\sqrt{g}}$, Eq. (27) takes the form

$$\langle x|O = \frac{1}{\sqrt{g(x)}} \frac{d}{dx} \left(\langle x|\sqrt{g(x)} \right). \quad (28)$$

Therefore, the generalized momentum operator P is related to O via $P = -i\hbar O$. In Eq. (28), $g(x)$ is the metric of the generalized space under consideration.

Finally, we intend to examine the distinction between the two operators on the integral operator. Let us consider I as the integral operator, $I|x\rangle = \int_{-\infty}^x |y\rangle dy$, which is reminiscent of the inverse momentum operator (see Ref. [13] and references therein).

Now, we need to use the fundamental theorem of calculus. So we have

$$\frac{d}{dx} \left(\int_{-\infty}^x |y\rangle dy \right) = |x\rangle, \quad (29)$$

and, by inserting D_x into the integral operator and using Eq. (19), we can obtain

$$D_x \left(\int_{-\infty}^x |y\rangle dy \right) = \int_{-\infty}^x D_x |y\rangle dy = -|x\rangle. \quad (30)$$

As can be seen, the results of the two cases are not the same. Note that Eq. (19) was used to obtain Eq. (30).

Here, in order to show the distinction more thoroughly, suppose $F(x) = \int_b^x |y\rangle dy$. Again, the fundamental theorem of calculus implies that $\frac{d}{dx} F(x) = |x\rangle$, but in the latter case we have $D_x F(x) = -(|x\rangle - |b\rangle)$. Thus, as can be seen, apart from the minus sign in Eq. (19), an additional term arises as well.

3 Conclusion

Eq. (19) shows a correct representation of the action of a differential operator in Hilbert space on the vector $|x\rangle$. From this result, the correct form of the action of the momentum operator on $|x\rangle$ is also obtained, $P|x\rangle = -i\hbar \frac{d}{dx} |x\rangle$.

We should stress the difference between the two operators. The operator $\frac{d}{dx}$ acts on anything that depends on x , whether it is a scalar, vector, etc., whereas D_x is an unbounded operator which acts on vectors and covectors in Hilbert space. Furthermore, statements such as $[x, \frac{d}{dx}] f(x)$ and $[x, \frac{d}{dx}] |x\rangle$ are misleading and should be avoided when dealing with Hilbert-space operators. It should also be noted that $[X, \frac{d}{dx}] = 0$, but $[X, D_x] = -1$, and in general $\frac{d}{dx} (x|x\rangle) = |x\rangle + x \frac{d}{dx} |x\rangle$, while $D_x (x|x\rangle) = x D_x |x\rangle = -x \frac{d|x\rangle}{dx}$, since D_x is a linear operator and Eq. (19) is used.

As an application of the discussion in this paper, and according to the distinction between these two operators, the generalized translation operator in curved space is obtained [14].

Appendix A

Another way to obtain Eq. (2) is by using the translation operator. Suppose

$$|x\rangle = e^{\frac{-iPx}{\hbar}} |0\rangle, \quad (A.1)$$

where P is the momentum operator and 0 is related to the position $x = 0$. Differentiating both sides of the above equation, we get

$$\frac{d}{dx} |x\rangle = -\frac{iP}{\hbar} |x\rangle, \quad (A.2)$$

that immediately implies Eq. (20).

Now one can write

$$X \frac{d}{dx} |x\rangle = -\frac{i}{\hbar} XP |x\rangle. \quad (\text{A.3})$$

From the canonical commutation relation $[X, P] = i\hbar$, we have

$$X \frac{d}{dx} |x\rangle = -\frac{i}{\hbar} (i\hbar |x\rangle + PX |x\rangle) = -\frac{i}{\hbar} PX |x\rangle. \quad (\text{A.4})$$

For the last term, we should note that P is a linear operator and we can write

$$PX |x\rangle = P x |x\rangle = x P |x\rangle = i\hbar x \frac{d|x\rangle}{dx}. \quad (\text{A.5})$$

Therefore

$$X \frac{d}{dx} |x\rangle = |x\rangle + x \frac{d}{dx} |x\rangle. \quad (\text{A.6})$$

For the commutation relations, consider in general $|\alpha\rangle$, so that $|\alpha\rangle = \int dy f(x, y) |y\rangle$, then it is clear that $X|\alpha\rangle = \int dy f(x, y) y |y\rangle$ and $\frac{d}{dx} |\alpha\rangle = \int dy \left[\frac{\partial}{\partial x} f(x, y) \right] |y\rangle$, so one can write

$$X \frac{d}{dx} |\alpha\rangle = \int dy \frac{\partial f(x, y)}{\partial x} y |y\rangle, \quad (\text{A.7})$$

and

$$\frac{d}{dx} X |\alpha\rangle = \int dy \frac{\partial f(x, y)}{\partial x} y |y\rangle. \quad (\text{A.8})$$

Obviously, the result is

$$\left[X, \frac{d}{dx} \right] = 0. \quad (\text{A.9})$$

Again, using Ref. [2], we have $P|\alpha\rangle = \int dy \left(-i\hbar \frac{\partial}{\partial y} \langle y|\alpha\rangle \right) y |y\rangle$. So

$$\begin{aligned} XP|\alpha\rangle &= \int dy \left(-i\hbar \frac{\partial}{\partial y} \langle y|\alpha\rangle \right) y |y\rangle \\ &= i\hbar \int dy \frac{\partial}{\partial y} (y |y\rangle) \langle \alpha|y\rangle, \end{aligned} \quad (\text{A.10})$$

and

$$\begin{aligned} PX|\alpha\rangle &= \int P y |y\rangle \langle \alpha|y\rangle dy = \int y P |y\rangle \langle \alpha|y\rangle dy \\ &= \int y \langle \alpha|y\rangle dy (-i\hbar) \int \left[\frac{\partial}{\partial z} \langle z|y\rangle \right] |z\rangle dz \\ &= \int y \langle \alpha|y\rangle dy (i\hbar) \int \left[\frac{\partial}{\partial y} \langle z|y\rangle \right] |z\rangle dz \\ &= i\hbar \int \left[\frac{\partial}{\partial y} |y\rangle \right] y \langle \alpha|y\rangle dy. \end{aligned} \quad (\text{A.11})$$

Therefore

$$[X, P] |\alpha\rangle = i\hbar |\alpha\rangle, \quad (\text{A.12})$$

or

$$[X, P] = i\hbar, \quad (\text{A.13})$$

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