A short introduction to quantum mechanics VI: position basis and the Dirac delta function

The position operator is very different in nature than the energy operator. The value of a position of an object can take a continuous value. For example, it can be 0.4567 meter or -3.112938475$\cdots$ meter. Therefore, the position operator admits continuous eigenvalues. Given this, let $|x>$ denote the eigenvector of the position matrix corresponding to eigenvalue x. In other words,

$$\hat{x}|x>= x|x> \tag{1}$$

where $\hat{x}$ is the position operator and x the eigenvalue. Using this notation, the completeness relation can be written as follows

$$1 = \int_{-\infty}^{\infty} dx|x>< x| \tag{2}$$

as briefly mentioned in my article on Dirac's bra-ket notation. The integration range is from negative infinity to positive infinity since the position can take any value between these two numbers. Using this relation, for an arbitrary state vector $|\beta>$, we have:

$$|\beta>= \int_{-\infty}^{\infty} dx < x|\beta>|x> \tag{3}$$

If we define $\beta(x) \equiv< x|\beta>$, we have:

$$|\beta>= \int_{-\infty}^{\infty} dx\beta(x)|x> \tag{4}$$

In other words, $\beta(x)$ is the coefficient of the basis $|x>$ for the vector $|\beta>$.

This should be familiar from the discussion at the very end of our fourth quantum mechanics article. Namely,

$$|\psi>= \sum_i < E_i|\psi>|E_i>= \sum_i \psi(E_i)|E_i> \tag{5}$$

where $\psi(E_i)$ is the coefficient of the basis $|E_i>$ for the vector $|\psi>$.

Similarly, for a ket-vector $<\alpha|$, we have:

$$< \alpha| = \int_{-\infty}^{\infty} dx < \alpha|x >< x| = \int_{-\infty}^{\infty} dx\alpha^*(x) < x| \tag{6}$$

where we have used that $< \alpha|x >=< x|\alpha >^*= \alpha^*(x)$

Now, let's calculate the dot-product between α and β:

$$< \alpha|\beta >= \int_{-\infty}^{\infty} dx < \alpha|x >< x|\beta >= \int_{-\infty}^{\infty} dx\alpha^*(x)\beta(x) \tag{7}$$

This equation should remind you of the discussion from our fourth article on quantum mechanics. Namely, I explained that when $|A >= \sum_i a_i|i >$, and when $|B >= \sum_i b_i|i >$ where $|i >$ is an orthonormal basis, we have $< A|B >= \sum_i a_i^* b_i$.

In order to calculate the probability of finding the particle between position x_a and position x_b, remind yourself of our first article on quantum mechanics. There, I explained that the probability of observing a given eigenvalue is the ratio of the square of the coefficient of the corresponding eigenvector to the sum of the squares of the coefficients of all the eigenvectors. Precisely speaking, as our fourth article suggests, what matters is not the square of the coefficient, but the square of the magnitude of the coefficient. The association can be expressed in the following mathematical formula:

$$P_i = \frac{|c_i|^2}{\sum_j |c_j|^2} = \frac{c_i c_i^*}{\sum_j c_j c_j^*} \tag{8}$$

when the state vector is given by $\sum_j c_j|j >$. In the case that the state vector is normalized, P_i is simply given by $|c_i|^2$, since the denominator is 1 in the above equation.

In the case of the position operator, the probability can be expressed as

$$P = \int_{x_a}^{x_b} dx\phi^*(x)\phi(x) \tag{9}$$

where we have assumed that $|\phi >$ is the normalized state vector of the particle being considered (i.e. $< \phi|\phi >= \int_{-\infty}^{\infty} \phi^*(x)\phi(x)$=1). Notice here that the probability is being represented by "summing" over all the squares of "coefficients" between x_a and x_b. In other words, the probability of finding the particle between x and $x + dx$ is given by $\phi^*(x)\phi(x)dx$. Notice also that upon this view, our normalization condition for $\phi(x)$ can be interpreted that the probability of finding a particle at the position between negative infinity and positive infinity is given by 1. In other words, the probability of finding a particle at anywhere is 1. This interpretation of the normalization of the state vector (that the probability sums up to 1) will play an important role when I discuss the unitarity of the time evolution operator in a later article.

Now, let's change gears and explain Dirac delta function. What would be the wave function $\phi(x)$ that corresponds to $|x_0 >$? Certainly, if you measure the position of the object that corresponds to this state vector, you will get x_0 with 100% certainty, and you will get other values with 0% certainty. Therefore, it is clear that $\phi(x)$ is zero unless $x = x_0$. With this intuition in our mind, let's calculate $\phi(x)$ mathematically.

$$|x_0 >= \int_{-\infty}^{\infty} < x|x_0 > |x > dx \tag{10}$$

In other words, $\phi(x) =< x|x_0 >$. However, as we know that the position operator is a Hermitian matrix, which in turn implies that the eigenvectors are orthogonal to each other unless they have the same eigenvalues, it is easy to see that $< x|x_0 >= 0$ unless $x = x_0$ (i.e. $x - x_0 = 0$). Thus, we recover our earlier argument. Notice also that $< x|x_0 >$ is a function of $(x - x_0)$ only. Therefore, for a certain function $\delta(x - x_0)$, we can write as follows:

$$< x|x_0 >= \delta(x - x_0) \tag{11}$$

This function is called Dirac delta function. Now, let's determine its value when $x - x_0 = 0$. To this end, let's return to (10). We have:

$$|x_0 >= \int_{-\infty}^{\infty} \delta(x - x_0)|x > dx \tag{12}$$

Since $\delta(x - x_0) = 0$ if $x \neq x_0$, the only contribution to the integral comes when $x = x_0$. Therefore, the right-hand side of the above equation becomes $c|x_0 >$ for some c. However, from the left-hand side, it is apparent that c should be 1. Also, notice the following for infinitesimal ϵ

$$\begin{aligned} |x_0 > &= \int_{x=x_0-\epsilon}^{x=x_0+\epsilon} \delta(x - x_0)|x > dx \\ &= \int_{x=x_0-\epsilon}^{x=x_0+\epsilon} \delta(x - x_0)|x_0 > dx \end{aligned} \tag{13}$$

Therefore, we conlcude:

$$\begin{aligned} 1 &= \int_{x=x_0-\epsilon}^{x=x_0+\epsilon} \delta(x - x_0)dx \\ &= \int_{x-x_0=-\epsilon}^{x-x_0=\epsilon} \delta(x - x_0)dx \\ &= \int_{-\epsilon}^{\epsilon} \delta(x)dx \end{aligned} \tag{14}$$

$$1 = \int_{-\infty}^{\infty} \delta(x)dx \tag{15}$$

where we used the change of variable in going from the second line to the third line, and we used that $\delta(x) = 0$ unless $x = 0$ in going from the third line to the fourth line. In conclusion, Dirac delta function is defined by two conditions. First, $\delta(x) = 0$ unless x=0. Second, the formula (15).

Let me also remark that the eigenvector of position operator $|x>$ is not normalized. Otherwise $< x|x >$ would have been 1, which is not the case. If $< x|x >= 1$ (i.e.$\delta(x - x = 0) = 1$ were true, in light of (14), this would imply:

$$
\begin{aligned}
1 &= \int_{-\epsilon}^{\epsilon} 1 dx = 0 \\
&= 2\epsilon \\
&= 0
\end{aligned} \tag{16}
$$

Actually, it is easy to see that (14) implies that $\delta(0) = \infty$, since integrating this on an infinitesimal interval yielded a finite value. In conclusion, the eigenvector of the position operator is not normalized, as eigenvalues are continuous. In fact, enforcing its normalization is not natural.

Finally, let's show you another property of Dirac delta function.

$$
f(x_0) = \int_{-\infty}^{\infty} f(x)\delta(x - x_0)dx \tag{17}
$$

The reasoning is as follows. As $\delta(x - x_0)$ is non-zero only when $x = x_0$, the integration picks up the contribution only when $x = x_0$. So, as before, we get:

$$
\int_{x_0-\epsilon}^{x_0+\epsilon} f(x)\delta(x - x_0)dx \tag{18}
$$

$$
= \int_{x_0-\epsilon}^{x_0+\epsilon} f(x_0)\delta(x - x_0)dx \tag{19}
$$

$$
= f(x_0) \int_{x_0-\epsilon}^{x_0+\epsilon} \delta(x - x_0)dx \tag{20}
$$

$$
= f(x_0) \tag{21}
$$

where in the last step we used (14)

We will revisit Dirac delta function when we talk about the relation between position basis and momentum basis in a later article.

Problem 1. Evaluate the followings:

$$
\int_{-\infty}^{\infty} dx(x^2 + 4x)\delta(x - 4), \qquad \int_{-3}^{3} dx(x^2 - 4x)\delta(x + 4) \tag{22}
$$

Problem 2. Convince yourself of the followings:

$$
\delta(-x) = \delta(x), \qquad \delta(3x) = \frac{1}{3}\delta(x), \qquad \delta(-3x) = \frac{1}{3}\delta(x) \tag{23}
$$

Problem 3. Some books use the following notation: $\delta(x,y) \equiv \delta(x-y)$. Given this, calculate the following:

$$\int_{-\infty}^{\infty} f(y)\delta(x,y)dy \tag{24}$$

Problem 4. Calculate the following:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta(x)\delta(y)\delta(z)dxdydz \tag{25}$$

Some books use the following notation: $\delta^3(\vec{x}) \equiv \delta(x)\delta(y)\delta(z)$.

Problem 5. Calculate the following:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta(x-f(y,z))\delta(y-g(z))\delta(z)dxdydz \tag{26}$$

Problem 6. Remember that we have seen in the last article that $\langle x\rangle = \langle\psi|\hat{x}|\psi\rangle$. To complete the calculation, show the following:

$$\langle\psi|\hat{x}|\psi\rangle = \int_{-\infty}^{\infty} dx\psi^*(x)x\psi(x) \tag{27}$$

where $\psi(x) = \langle x|\psi\rangle$. (Hint[1])

Problem 7. Heaviside step function θ is defined as follows:

$$\theta(x) = \int_{-\infty}^{x} \delta(x)dx \tag{28}$$

Given this, evaluate the followings:

$$\theta(-50), \qquad \theta(-30), \qquad \theta(5), \qquad \theta(0.3) \tag{29}$$

Problem 8. Evaluate the following (Hint[2]):

$$\int_{-\infty}^{\infty} \delta(x^2-4x)(x+2)dx \tag{30}$$

Summary

- $|x\rangle$ is an eigenvector of position operator $\hat{x}$ with eigenvalue x.
- It satisfies the normalization condition $\langle x|x_0\rangle = \delta(x-x_0)$.
- Dirac delta function $\delta(x)$ is 0 for $x \neq 0$, and infinite when $x = 0$. It satisfies $1 = \int_{-\infty}^{\infty}\delta(x)dx$.
- $$f(x_0) = \int_{-\infty}^{\infty} f(x)\delta(x-x_0)dx$$

[1] Remember what we have done in the last article. Use also (1) and (2).

[2] Use $x^2-4x = x(x-4)$, and think about when the Dirac delta function is non-zero. Then, use similar formulas to the ones in Problem 2.