NON-DENUMERABLE BASIS: POSITION AND MOMENTUM STATES

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References: References: edX online course MIT 8.05 Section 5.6.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 1.10; Exercises 1.10.1 - 1.10.3.

Although we've looked at position and momentum operators in quantum mechanics before, it's worth another look at the ways that Zwiebach and Shankar introduce them.

First, we'll have a look at Shankar's treatment. He begins by considering a string fixed at each end, at positions $x=0$ and $x=L$, then asks how we could convey the shape of the string to an observer who cannot see the string directly. We could note the position at some fixed finite number of points between 0 and L, but then the remote observer would have only a partial knowledge of the string's shape; the locations of those portions of the string between the points at which it was measured are still unknown, although the observer could probably get a reasonable picture by interpolating between these points.

We can increase the number of points at which the position is measured to get a better picture, but to convey the exact shape of the string, we need to measure its position at an infinite number of points. This is possible (in principle) but leads to a problem with the definition of the inner product. For two vectors defined on a finite vector space with an orthonormal basis, the inner product is given by the usual formula for the dot product:

$$\langle f\,|g\rangle = \sum_{i=1}^{n} f_i g_i \tag{1}$$

$$\langle f\,|f\rangle = \sum_{i=1}^{n} f_i^2 \tag{2}$$

where f_i and g_i are the components of f and g in the orthonormal basis. If we're taking f to be the displacement of a string and we try to increase the accuracy of the picture by increasing the number n of points at which measurements are taken, then the value of $\langle f\,|f\rangle$ continues to increase as n increases (provided that $f\neq 0$ everywhere). As $n\to\infty$ then $\langle f\,|f\rangle\to\infty$ as well, even though the system we're measuring (a string of finite length with finite displacement) is certainly not infinite in any practical sense.

Shankar proposes getting around this problem by simply redefining the inner product for a *finite* vector space to be

$$\langle f\,|g\rangle = \sum_{i=1}^{n} f(x_i)\,g(x_i)\,\Delta \tag{3}$$

where $\Delta \equiv L/(n+1)$. That is, Δ now becomes the distance between adjacent points at which measurements are taken. If we let $n \to \infty$ this leads to the definition of the inner product as an integral

$$\langle f\,|g\rangle = \int_0^L f(x)\,g(x)\;dx \tag{4}$$

$$\langle f\,|f\rangle = \int_0^L f^2(x)\;dx \tag{5}$$

This looks familiar enough, if you've done any work with inner products in quantum mechanics, but there is a subtle point which Shankar overlooks. In going from 1 to 3, we have introduced a factor Δ which, in the string example at least, has the dimensions of length, so the physical interpretation of these two equations is different. The units of $\langle f\,|g\rangle$ appear to be different in the two cases. Now in quantum theory, inner products of the continuous type usually involve the wave function multiplied by its complex conjugate, with possibly another operator thrown in if we're trying to find the expectation value of some observable. The square modulus of the wave function, $|\Psi|^2$, is taken to be a probability density, so it has units of inverse length (in one dimension) or inverse volume (in three dimensions), which makes the integral work out properly.

Admittedly, when we're using f to represent the displacement of a string, it's not obvious what meaning the inner product of f with anything else would actually have, so maybe the point isn't worth worrying about. However, it does seem to be something that it would be worth Shankar including a comment about.

From this point, Shankar continues by saying that this infinite dimensional vector space is spanned by basis vectors $|x\rangle$, with one basis vector for each value of x. We require this basis to be orthogonal, which means that we must have, if $x \neq x'$

$$\left\langle x\,|x'\right\rangle = 0 \tag{6}$$

We then generalize the identity operator to be

$$I=\int|x\rangle\langle x|\,dx \tag{7}$$

which leads to

$$\langle x|f\rangle=\int\left\langle x\left|x'\right.\right\rangle\left\langle x'|f\right\rangle dx' \tag{8}$$

The bra-ket $\langle x|f\rangle$ is the projection of the vector $|f\rangle$ onto the $|x\rangle$ basis vector, so it is just $f(x)$. This means

$$f(x)=\int\left\langle x\left|x'\right.\right\rangle f\left(x'\right)dx' \tag{9}$$

which leads to the definition of the Dirac delta function as the normalization of $\langle x|x'\rangle$:

$$\left\langle x\left|x'\right.\right\rangle=\delta\left(x-x'\right) \tag{10}$$

Shankar then describes some properties of the delta function and its derivative, most of which we've already covered. For example, we've seen these two results for the delta function:

$$\delta(ax) = \frac{\delta(x)}{|a|} \tag{11}$$

$$\frac{d\theta(x-x')}{dx} = \delta\left(x-x'\right) \tag{12}$$

where θ is the step function

$$\theta\left(x-x'\right)\equiv\begin{cases}0 & x\le x'\\ 1 & x>x'\end{cases} \tag{13}$$

One other result is that for a function $f(x)$ with zeroes at a number of points x_i, we have

$$\delta(f(x))=\sum_i\frac{\delta(x_i-x)}{|df/dx_i|} \tag{14}$$

To see this, consider one of the x_i where $f(x_i)=0$. Expanding in a Taylor series about this point, we have

$$f(x_i+(x-x_i)) = f(x_i)+(x-x_i)\frac{df}{dx_i}+\ldots \tag{15}$$

$$= 0+(x-x_i)\frac{df}{dx_i} \tag{16}$$

From 11 we have

$$\delta\left(\left(x-x_i\right)\frac{df}{dx_i}\right)=\frac{\delta\left(x_i-x\right)}{\left|df/dx_i\right|} \tag{17}$$

The behaviour is the same at all points x_i and since $\delta\left(x_i-x\right)=0$ at all other $x_j\neq x_i$ where $f\left(x_j\right)=0$, we can just add the delta functions for each zero of f.

Turning now to Zwiebach's treatment, he begins with the basis states $|x\rangle$ and position operator $\hat{x}$ with the eigenvalue equation

$$\hat{x}\left|x\right\rangle=x\left|x\right\rangle \tag{18}$$

and simply *defines* the inner product between two position states to be

$$\left\langle x\left|y\right.\right\rangle=\delta\left(x-y\right) \tag{19}$$

With this definition, 9 follows immediately. We can therefore write a quantum state $|\psi\rangle$ as

$$\left|\psi\right\rangle=I\left|\psi\right\rangle=\int\left|x\right\rangle\left\langle x\left|\psi\right.\right\rangle dx=\int\left|x\right\rangle\psi\left(x\right)dx \tag{20}$$

That is, the vector $|\psi\rangle$ is the integral of its projections $\psi\left(x\right)$ onto the basis vectors $|x\rangle$.

The position operator $\hat{x}$ is hermitian as can be seen from

$$\begin{aligned}\left\langle x_1\left|\hat{x}^{\dagger}\right|x_2\right\rangle &= \left\langle x_2\left|\hat{x}\right|x_1\right\rangle^* && (21)\\ &= x_1\left\langle x_2\left|x_1\right.\right\rangle^* && (22)\\ &= x_1\delta\left(x_2-x_1\right)^* && (23)\\ &= x_1\delta\left(x_2-x_1\right) && (24)\\ &= x_2\delta\left(x_2-x_1\right) && (25)\\ &= \left\langle x_1\left|\hat{x}\right|x_2\right\rangle && (26)\end{aligned}$$

The fourth line follows because the delta function is real, and the fifth follows because $\delta\left(x_2-x_1\right)$ is non-zero only when $x_1=x_2$.

Zwiebach then introduces the momentum eigenstates $|p\rangle$ which are analogous to the position states $|x\rangle$, in that

$$\left\langle p'\left|p\right.\right\rangle = \delta\left(p' - p\right) \tag{27}$$

$$I = \int dp \left|p\right\rangle \left\langle p\right| \tag{28}$$

$$\hat{p}\left|p\right\rangle = p\left|p\right\rangle \tag{29}$$

$$\tilde{\psi}\left(p\right) = \left\langle p\left|\psi\right.\right\rangle \tag{30}$$

By the same calculation as for $|x\rangle$, we see that $\hat{p}$ is hermitian.

To get a relation between the $|x\rangle$ and $|p\rangle$ bases, we require that $\langle x|p\rangle$ is the wave function for a particle with momentum p in the x basis, which we've seen is

$$\psi\left(x\right) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \tag{31}$$

Zwiebach then shows that this is consistent with the equation

$$\left\langle x\left|\hat{p}\right|\psi\right\rangle = \frac{h}{i}\frac{d}{dx}\left\langle x\left|\psi\right.\right\rangle = \frac{h}{i}\frac{d\psi\left(x\right)}{dx} \tag{32}$$

We can get a similar relation by switching x and p:

$$\left\langle p\left|\hat{x}\right|\psi\right\rangle = \int dx \left\langle p\left|x\right.\right\rangle \left\langle x\left|\hat{x}\right|\psi\right\rangle \tag{33}$$

$$= \int dx \left\langle x\left|p\right.\right\rangle^{*} x \left\langle x\left|\psi\right.\right\rangle \tag{34}$$

From 31 we see

$$\left\langle x\left|p\right.\right\rangle^{*} = \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \tag{35}$$

$$\left\langle x\left|p\right.\right\rangle^{*} x = i\hbar\frac{d}{dp}\left\langle x\left|p\right.\right\rangle^{*} \tag{36}$$

$$\int dx \left\langle x\left|p\right.\right\rangle^{*} x \left\langle x\left|\psi\right.\right\rangle = i\hbar\int dx\ \frac{d}{dp}\left\langle x\left|p\right.\right\rangle^{*}\left\langle x\left|\psi\right.\right\rangle \tag{37}$$

$$= i\hbar\frac{d}{dp}\int dx\ \left\langle x\left|p\right.\right\rangle^{*}\left\langle x\left|\psi\right.\right\rangle \tag{38}$$

$$= i\hbar\frac{d}{dp}\int dx\ \left\langle p\left|x\right.\right\rangle\left\langle x\left|\psi\right.\right\rangle \tag{39}$$

$$= i\hbar\frac{d\tilde{\psi}\left(p\right)}{dp} \tag{40}$$

In the fourth line, we took the $\frac{d}{dp}$ outside the integral since p occurs in only one term, and in the last line we used 7. Thus we have

$$\left\langle p\left|\hat{x}\right|\psi\right\rangle = i\hbar\frac{d\tilde{\psi}(p)}{dp} \tag{41}$$

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