DIFFERENTIAL OPERATORS - MATRIX ELEMENTS AND HERMITICITY

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References: Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 1.10.

Here, we'll revisit the differential operator on a continuous vector space which we looked at earlier in its role as the momentum operator. This time around, we'll use the bra-ket notation and vector space results to analyze it, hopefully putting it on a slightly more mathematical foundation.

We define the differential operator D acting on a vector $|f\rangle$ in a continuous vector space as having the action

$$D|f\rangle=\left|\frac{df}{dx}\right\rangle \tag{1}$$

This notation means that D operating on $|f\rangle$ produces the vector (ket) $\left|\frac{df}{dx}\right\rangle$ corresponding to the function whose form in the $|x\rangle$ basis is $\frac{df(x)}{dx}$. That is, the projection of $\left|\frac{df}{dx}\right\rangle$ onto the basis vector $|x\rangle$ is

$$\frac{df(x)}{dx}=\left\langle x\left|\frac{df}{dx}\right.\right\rangle=\langle x|D|f\rangle \tag{2}$$

By a similar argument to that which we used to deduce the matrix element $\langle x|x'\rangle$, we can work out the matrix elements of D in the $|x\rangle$ basis. Inserting the unit operator, we have

$$\langle x|D|f\rangle = \int dx'\left\langle x|D|x'\right\rangle\left\langle x'|f\right\rangle \tag{3}$$

$$= \int dx'\left\langle x|D|x'\right\rangle f\left(x'\right) \tag{4}$$

We need this to be equal to $\frac{df}{dx}$. To get this, we can introduce the derivative of the delta function, except this time the delta function is a function of $x-x'$ rather than just x on its own. To see the effect of this derivative, consider the integral

$$\int dx'\frac{d\delta\left(x-x'\right)}{dx}f\left(x'\right)=\frac{d}{dx}\int dx'\delta\left(x-x'\right)f\left(x'\right)=\frac{df(x)}{dx} \tag{5}$$

In the second step, we could take the derivative outside the integral since x is a constant with respect to the integration. Comparing this with 4 we see that

$$\left\langle x\left|D\right|x'\right\rangle \equiv D_{xx'}=\frac{d\delta\left(x-x'\right)}{dx}=\delta'\left(x-x'\right) \tag{6}$$

Here the prime in δ' means derivative with respect to x, not x'. [Note that this is *not* the same formula as that quoted in the earlier post, where we had $f\left(x\right)\delta'\left(x\right)=-f'\left(x\right)\delta\left(x\right)$ because in that formula it was the same variable x that was involved in the derivative of the delta function and in the integral.]

The operator D is not hermitian as it stands. Since the delta function is real, we have, looking at $D_{xx'}^{\dagger}=D_{x'x}^{*}$ in bra-ket notation, we see that

$$D_{x'x}^{\dagger}=\left\langle x'\left|D^{*}\right|x\right\rangle =\delta'\left(x'-x\right)=-\delta'\left(x-x'\right)\neq D_{xx'} \tag{7}$$

Thus D is anti-hermitian. It is easy to fix this and create a hermitian operator by multiplying by an imaginary number, such as $-i$ (this choice is, of course, to make the new operator consistent with the momentum operator). Calling this new operator $K\equiv-iD$ we have

$$K_{x'x}^{\dagger}=\left\langle x'\left|K^{*}\right|x\right\rangle =i\delta'\left(x'-x\right)=-i\delta'\left(x-x'\right)=K_{xx'} \tag{8}$$

A curious fact about K (and thus about the momentum operator as well) is that it is not automatically hermitian even with this correction. We've seen that it satisfies the hermiticity property with respect to its matrix elements in the position basis, but to be fully hermitian, it must satisfy

$$\left\langle g\left|K\right|f\right\rangle =\left\langle f\left|K\right|g\right\rangle ^{*} \tag{9}$$

for any two vectors $\left|f\right\rangle$ and $\left|g\right\rangle$. Suppose we are interested in x over some range $\left[a,b\right]$. Then by inserting a couple of identity operators, we have

$$\begin{aligned}
\left\langle g\left|K\right|f\right\rangle &=\int_{a}^{b}\int_{a}^{b}\left\langle g\left|x\right.\right\rangle \left\langle x\left|K\right|x'\right\rangle \left\langle x'\left|f\right.\right\rangle dx\,dx' &\quad(10)\\
&=-i\int_{a}^{b}g^{*}\left(x\right)\frac{df}{dx}dx &\quad(11)\\
&=-i\,g^{*}\left(x\right)f\left(x\right)\Big|_{a}^{b}+i\int_{a}^{b}f\left(x\right)\frac{dg^{*}}{dx}dx &\quad(12)\\
&=-i\,g^{*}\left(x\right)f\left(x\right)\Big|_{a}^{b}+\left\langle f\left|K\right|g\right\rangle ^{*} &\quad(13)
\end{aligned}$$

The result is hermitian only if the first term in the last line is zero, which happens only for certain choices of f and g. If the limits are infinite, so we're integrating over all space, and the system is bounded so that both f and g go to zero at infinity, then we're OK, and K is hermitian. Another option is if g and f are periodic and the range of integration is equal to an integral multiple of the period, then g^*f has the same value at each end and the term becomes zero.

However, as we've seen, in quantum mechanics there are cases where we deal with functions such as e^{ikx} (for k real) that oscillate indefinitely, no matter how large x is (see the free particle, for example). There isn't any mathematically airtight way around such cases (as far as I know), but a hand-wavy way of defining a limit for such oscillating functions is to consider their average behaviour as $x \to \pm\infty$. The average defined by Shankar is given as

$$\lim_{x\to\infty} e^{ikx}e^{-ik'x} = \lim_{\substack{L\to\infty \\ \Delta\to\infty}} \frac{1}{\Delta}\int_{L}^{L+\Delta} e^{i(k-k')x}dx \tag{14}$$

This is interpreted as looking at the function very far out on the x axis (at position L), and then considering a very long interval Δ starting at point L. Since the integral of $e^{i(k-k')x}$ over one period is zero (it's just a combination of sine and cosine functions), the integral is always bounded between 0 and the area under half a cycle, as successive half-cycles cancel each other. Dividing by Δ, which is monotonically increasing, ensures that the limit is zero.

This isn't an ideal solution, but it's just one of many cases where an infinitely oscillating function is called upon to do seemingly impossible things. The theory seems to hang together fairly well in any case.

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