11.2: Operator Algebra

Let's start by defining the identity operator, usually denoted by $\hat{E}$ or $\hat{I}$. The identity operator leaves the element on which it operates unchanged: $\hat{E}f(x) = f(x)$. This is analogous to multiplying by the number 1.

We can add operators as follows:

$$(\hat{A}+\hat{B})f = \hat{A}f + \hat{B}f.$$

For example,

$$\left(\hat{x}+\frac{d}{dx}\right)f = \hat{x}f + \frac{df}{dx} = xf + \frac{df}{dx}$$

(remember that $\hat{x}$ means "multiply by x").

The product between two operators is defined as the successive operation of the operators, with the one on the right operating first. For example,

$$\left(\hat{x}\frac{d}{dx}\right)f = \hat{x}\left(\frac{df}{dx}\right) = x\frac{df}{dx}. \tag{11.2.1}$$

We first apply the operator on the right (in this case "take the derivative of the function with respect to x"), and then the operator on the left ("multiply by x whatever you got in the first step"). We can use this definition to calculate the square of an operator. For example, if we define the operator $\hat{A}$ as $\hat{A} = \frac{d}{dx}$, the operator $\hat{A}^2$ is

$$\hat{A}\hat{A} = \frac{d}{dx}\frac{d}{dx} = \frac{d^2}{dx^2}. \tag{11.2.2}$$

Operator multiplication is not, in general, commutative: $\hat{A}\hat{B} \neq \hat{B}\hat{A}$. In other words, in general, the order of the operations matters. Before, we saw that $(\hat{x}\frac{d}{dx})f = x\frac{df}{dx}$. Let's revert the order of the operation: $(\frac{d}{dx}\hat{x})f$. Now, we first multiply the function by x and then take the derivative of the result:

$$\left(\frac{d}{dx}\hat{x}\right)f = \frac{d}{dx}(xf) = x\frac{df}{dx} + f. \tag{11.2.3}$$

In the last step, we calculated the derivative of the product using the differentiation rules we are familiar with.

We just proved that $\hat{x}\frac{d}{dx} \neq \frac{d}{dx}\hat{x}$, or in other words, the order in which we apply these two operators matters (i.e. whether we first take the derivative and then multiply by x, or first multiply by x and then take the derivative). Whether order matters or not has very important consequences in quantum mechanics, so it is useful to define the so-called commutator, defined as

$$[\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}. \tag{11.2.4}$$

For example, the commutator of the operators $\hat{x}$ and $\frac{d}{dx}$, denoted by $[\hat{x}, \frac{d}{dx}]$, is by definition $\hat{x}\frac{d}{dx} - \frac{d}{dx}\hat{x}$. When $[\hat{A},\hat{B}] = 0$, the operators $\hat{A}$ and $\hat{B}$ are said to commute. Therefore, if the operators $\hat{A}$ and $\hat{B}$ commute, then $\hat{A}\hat{B} = \hat{B}\hat{A}$. When the operators $\hat{A}$ and $\hat{B}$ do not commute, $\hat{A}\hat{B} \neq \hat{B}\hat{A}$, and the commutator $[\hat{A},\hat{B}] \neq 0$.

Before we move on, it is important to recognize that the product of two operators is also an operator. For instance, let's consider the product $\frac{d}{dx}\hat{x}$. This is an operator that, when applied to a function f, gives a new function $x\frac{df}{dx} + f$. For example, if $f = \sin(kx)$, $\frac{d}{dx}\hat{x}f = kx\cos(kx) + \sin(kx)$. In addition, notice that the operator $\frac{d}{dx}\hat{x}$ can be expressed as $\hat{E} + \hat{x}\frac{d}{dx}$, where $\hat{E}$ is the identity operator. When the operator $\hat{E} + \hat{x}\frac{d}{dx}$ operates on a function f, the result is the function itself (multiplied by one) plus x times the derivative of the function, which is exactly what we get when we perform $\frac{d}{dx}\hat{x}f$.

$$\underbrace{\frac{d}{dx}\hat{x}}_{\text{an operator}} = \underbrace{\hat{E} + \hat{x}\frac{d}{dx}}_{\text{an operator}}$$

$$\underbrace{\left(\frac{d}{dx}\hat{x}\right)f = \left(\hat{E} + \hat{x}\frac{d}{dx}\right)}_{\text{an operator}}\underbrace{f}_{\text{a function}} = \underbrace{f + x\frac{df}{dx}}_{\text{another function}}$$

An operator operates on a function to give another function

Similarly, the commutator between two operators is also an operator:

In general...

$$\underbrace{\left[\hat{A},\hat{B}\right]}_{\text{an operator}} = \hat{A}\hat{B} - \hat{B}\hat{A}$$

$$\underbrace{\left[\hat{A},\hat{B}\right]}_{\text{an operator}}\underbrace{f}_{\text{a function}} = \underbrace{\hat{A}\hat{B}f - \hat{B}\hat{A}f}_{\text{another function}}$$

An operator operates on a function to give another function

Example...

$$\left[\hat{x},\frac{d}{dx}\right] = \hat{x}\frac{d}{dx} - \frac{d}{dx}\hat{x}$$

$$\left[\hat{x},\frac{d}{dx}\right]f = \left(\hat{x}\frac{d}{dx}\right)f - \left(\frac{d}{dx}\hat{x}\right)f$$

$$\underbrace{\left[\hat{x},\frac{d}{dx}\right]}_{\text{an operator}}\underbrace{f}_{\text{a function}} = x\frac{df}{dx} - \left[f + x\frac{df}{dx}\right] = \underbrace{-f}_{\text{another function}}$$

Note that in the example on the right side of the figure we demonstrated that the operator $[\hat{x}, \frac{d}{dx}]$ equals the operator $-\hat{E}$ ("multiply by -1"). In other words, when the commutator $[\hat{x}, \frac{d}{dx}]$ (an operator) operates on a function f, the result is $-f$. Because $[\hat{x}, \frac{d}{dx}] \neq 0$, the operators $\hat{x}$ and $\frac{d}{dx}$ do not commute. This is directly related to the uncertainty principle, which (in its simplest form) states that the more precisely the position of some particle is determined, the less precisely its momentum can be known. We will see the connection between this statement and the commutator in a moment, and you will discuss this in a lot of detail in your future physical chemistry courses.

Example 11.2.1

Find the commutator

$$\left[\hat{x}^2, \frac{d^2}{dx^2}\right]$$

Solution

Remember that the commutator is an operator, so your answer should be an operator as well (that is, it should not contain a function). To 'see' what the commutator does (so we can write the equivalent operator), we apply an arbitrary function:

$$\left[\hat{x}^2, \frac{d^2}{dx^2}\right] f = \hat{x}^2 \frac{d^2}{dx^2} f - \frac{d^2}{dx^2} \hat{x}^2 f$$

Remember that when we have expressions such as $\frac{d^2}{dx^2}\hat{x}^2 f$ we need to go from right to left, that is, we first multiply by x^2 and only then take the second derivative.

$$\frac{d^2}{dx^2}\hat{x}^2 f = \frac{d^2(x^2 f)}{dx^2} = \frac{d\left(2xf + x^2\frac{df}{dx}\right)}{dx} = 2x\frac{df}{dx} + 2f + x^2\frac{d^2 f}{dx^2} + 2x\frac{df}{dx} = 4x\frac{df}{dx} + 2f + x^2\frac{d^2 f}{dx^2}$$

$$\left[\hat{x}^2, \frac{d^2}{dx^2}\right] f = \hat{x}^2\frac{d^2}{dx^2}f - \frac{d^2}{dx^2}\hat{x}^2 f = x^2\frac{d^2 f}{dx^2} - \left(4x\frac{df}{dx} + 2f + x^2\frac{d^2 f}{dx^2}\right) = -4x\frac{df}{dx} - 2f$$

$$\left[\hat{x}^2, \frac{d^2}{dx^2}\right] = -4\hat{x}\frac{d}{dx} - 2\hat{E}$$

Again, your result should be an operator, and therefore should not contain the function f. Because $[\hat{x}^2, \frac{d^2}{dx^2}] \neq 0$, the two operators do not commute.

Common mistakes:

- to write the commutator as $[\hat{x}^2, \frac{d^2}{dx^2}] = -4x\frac{df}{dx} - 2f$
- to use an actual function (e.g. $\sin x$) instead of an arbitrary function f