# Commutators

Unlike numbers, operators do not necessarily commute, i.e. for two operators A and B the result of the action AB on a function is generally not the same as that of BA. In other words

$$AB \neq BA$$

In order to have a measure of how badly the two operators fail to commute it is convenient to introduce the commutator, which is defined as

$$[A,B] = AB - BA$$

Note that the commutotor itself is an operator.
When we investigate actions of operators it is important to keep in mind that they act on some functions (or vectors). Hence when we are to evaluate a commutator we should keep in mind some function on the right, which does not need to be explicitly defined.

Let us evaluate the commutator of operators x and p as an example:

$$[x,p]f(x) = x\left(-i\hbar\frac{d}{dx}\right)f(x) - \left(-i\hbar\frac{d}{dx}\right)xf(x) =$$

$$= x\left(-i\hbar\frac{d}{dx}\right)f(x) + i\hbar x\frac{d}{dx}f(x) + i\hbar f(x) = i\hbar f(x)$$

or, if we drop the arbitrary function f(x) we have

$$[x,p] = xp - px = i\hbar$$

This simple result is of fundamental importance and is known as the canonical commutation relation

It should be noted that sometimes a related object is used in quantum mechanics – the anticommutator. It is defined as

$$\{A,B\} = AB + BA \qquad \text{(plus sign)}$$

In some literature brackets with $\mp$ index are used to denote the commutator and anticommutator respectively:

$$[A,B]_\pm = AB \pm BA$$

However in this course we are unlikely to have the need for anticommutators ($[A,B]_+$). Hence, the notation $[A,B]$ should always be understood as commutator.

## Quantum harmonic oscillator – solution using the raising and lowering operators

Here we will learn a neat method of solving the problem of the quantum harmonic oscillator. Beside the elegance the method is important as it lies at the origin of the approach called second quantization, which has numerous applications in quantum many-body systems and quantum field theory.

Let us start with the Hamiltonian.

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2\hat{x}^2}{2}$$

In quantum mechanics the hat symbol (such as in $\hat{x}$) is commonly used to emphasize that the object is an operator).

Let us introduce dimensionless position and momentum

$$\hat{\xi} = \sqrt{\frac{m\omega}{\hbar}}\,\hat{x} \qquad \hat{\pi} = -i\frac{d}{d\xi} = \frac{\hat{p}}{\sqrt{\hbar m\omega}}$$

Then the Hamiltonian becomes:

$$\hat{H} = \frac{\hbar\omega}{2}\left(\hat{\pi}^2 + \hat{\xi}^2\right)$$

We can try to factorize $\hat{\pi}^2 + \hat{\xi}^2$:

$$(\hat{\xi} - i\hat{\pi})(\hat{\xi} + i\hat{\pi}) = \hat{\xi}^2 + \hat{\pi}^2 + i\hat{\xi}\hat{\pi} - i\hat{\pi}\hat{\xi} = \hat{\xi}^2 + \hat{\pi}^2 + i\underbrace{[\hat{\xi},\hat{\pi}]}_{i} =$$

$$= \hat{\pi}^2 + \hat{\xi}^2 - 1$$

Thus.

$$\hat{H} = \frac{\hbar\omega}{2}\left((\hat{\xi} - i\hat{\pi})(\hat{\xi} + i\hat{\pi}) + 1\right)$$

Now let us define

$$\hat{a} = \frac{\hat{\xi} + i\hat{\pi}}{\sqrt{2}} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + \frac{i\hat{p}}{\sqrt{2m\hbar\omega}}$$

$$\hat{a}^+ = \frac{\hat{\xi} - i\hat{\pi}}{\sqrt{2}} = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} - \frac{i\hat{p}}{\sqrt{2m\hbar\omega}}$$

With that the Hamiltonian can be written as

$$\hat{H} = \hbar\omega\left(\hat{a}^+\hat{a} + \frac{1}{2}\right)$$

Operators $\hat{a}$ and $\hat{a}^+$ are commonly called the lowering and raising operators respectively. Quite often they are also called the annihilation and creation operators.

Let us also define the operator

$$\hat{N} = \hat{a}^+ a$$

If $\psi_n$ is an eigenfunction of $\hat{N}$ corresponding to eigenvalue $n$, i.e.

$$\hat{N}\psi_n = n\psi_n$$

then

$$H\psi_n = \hbar\omega\left(n+\tfrac{1}{2}\right)\psi_n$$

Note that $n \geq 0$, because

$$n = \int \psi_n^* \hat{N}\psi_n\, dx = \int \psi_n^* \hat{a}^+\hat{a}\,\psi_n\, dx = \int (\hat{a}\psi_n)^* (\hat{a}\psi_n)\, dx =$$

$$= \int |\varphi|^2 dx \geq 0$$ (here we used the fact that $\int \varphi\,\hat{p}\psi\, dx = \int (\hat{p}\psi)^* \varphi\, dx$)

To find the eigenvalues of $\hat{N}$ we need the commutator.

$$[\hat{a},\hat{a}^+] = \frac{1}{2}[\hat{\xi}+i\hat{\pi},\hat{\xi}-i\hat{\pi}] = \frac{i}{2}\Big(\underbrace{[\hat{\pi},\hat{\xi}]}_{-i} - \underbrace{[\hat{\xi},\hat{\pi}]}_{i}\Big) = 1$$

Now let us note that

$$\hat{N}\hat{a} = \underbrace{\hat{a}^+\hat{a}}_{\hat{a}\hat{a}^+-1}\hat{a} = (\hat{a}\hat{a}^+ - 1)\hat{a} = \hat{a}(\hat{N}-1)$$

$$\hat{N}\hat{a}\psi_n = \hat{a}(\hat{N}-1)\psi_n = (n-1)\hat{a}\psi_n$$

Therefore, $\hat{a}\psi_n$ is an eigenstate of $\hat{N}$ with eigenvalue $n-1$, i.e. $\hat{a}\psi_n = C_n\psi_{n-1}$, where $C_n$ is some constant

If we require that $\int |\psi_n|^2 dx = 1$ then

$$\int (\hat{a}\psi_n)^*(\hat{a}\psi_n)\, dx = \int \psi_n^* \hat{a}^+\hat{a}\,\psi_n\, dx = \int \psi_n^* \hat{N}\psi_n\, dx = n$$

so that the constant, $C_n = \sqrt{n}$, i.e.

$$\hat{a}\psi_n = \sqrt{n}\,\psi_{n-1}$$ (disregard the arbitrary phase)

Similarly, $\hat{a}^2\psi_n$ is an eigenstate of $\hat{N}$ with eigenvalue $n-2$ and

$$\hat{a}^2\psi_n = \hat{a}\sqrt{n}\,\psi_{n-1} = \sqrt{n(n-1)}\,\psi_{n-2}$$

Therefore, if $n$ is an eigenvalue of $\hat{N}$, so are $n-1$, $n-2$, $n-3$, and so on.

This sequence cannot continue forever, however. We know that $n>0$. Thus, there must be the lowest eigenstate $\psi_0$ such that

$$\hat{a}\psi_0 = 0$$

This is exactly the case if $n$ is an integer.

Using $\hat{a}\psi_n = \sqrt{n}\,\psi_{n-1}$ we obtain:

$$\hat{a}\psi_1 = \sqrt{1}\,\psi_0 \quad , \quad a\psi_0 = 0$$

Now let us see how $\hat{a}^+$ act on $\psi_n$. Note

$$\hat{N}\hat{a}^+ = \hat{a}^+\underbrace{\hat{a}\,\hat{a}^+}_{\hat{a}^+\hat{a}+1} = \hat{a}^+(\hat{a}^+\hat{a}+1) = \hat{a}^+(\hat{N}+1)$$

$$\hat{N}\,\hat{a}^+\psi_n = \hat{a}^+(\hat{N}+1)\psi_n = (n+1)\,\hat{a}^+\psi_n$$

Thus, $\hat{a}^+\psi_n$ is an eigenstate of $\hat{N}$ corresponding to eigenvalue $n+1$.

Based on the above analysis we can conclude that $\hat{N}$ has eigenvalues

$$0, 1, 2, \dots, \infty$$

In general $\psi_n = \dfrac{(a^+)^n}{\sqrt{n!}}\psi_0$

Let us find the explicit form of $\psi_0$:

$$\hat{a}\psi_0 = 0 \qquad \hat{a} = \frac{1}{\sqrt{2}}(\hat{\xi} + i\hat{\pi}) = \frac{1}{\sqrt{2}}\left(\hat{\xi} + \frac{d}{d\xi}\right)$$

$$\left(\xi + \frac{d}{d\xi}\right)\psi_0(\xi) = 0 \qquad \psi_0' = -\xi\psi_0 \Rightarrow \psi_0 = A_0 e^{-\frac{\xi^2}{2}}$$

From the normalization condition we obtain $A_0 = \dfrac{1}{\pi^{1/4}}$

$$\psi_n(\xi) = \frac{1}{\sqrt{2^n n!}}\left(\xi - \frac{d}{d\xi}\right)^n \psi_0(\xi)$$

$$= \frac{1}{\sqrt{2^n n! \, \pi^{1/2}}}\left(\xi - \frac{d}{d\xi}\right)^n e^{-\frac{\xi^2}{2}}$$

Then we can write an alternative formula for the Hermite polynomials

$$H_n(\xi) = e^{\frac{\xi^2}{2}}\left(\xi - \frac{d}{d\xi}\right)^n e^{-\frac{\xi^2}{2}}$$