Commutators

Unlike numbers, operators do not necessarily commute, i.e for two operators A and B in general

$$AB \neq BA$$

It is convenient to introduce the commutator, which is defined as

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

It provides a measure of how badly the two operators fail to commute. Notice that the commutator is an operator itself.

When we investigate any actions of operators it is important to keep in mind that they act on some functions (or vectors). Hence when we 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:

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

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

This result is known as canonical commutation relation

Quantum harmonic oscillator – solution with the operator method

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

(hat is sometimes used to emphasize that an 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

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

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

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

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

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

Let us also define $\hat{N} = \hat{a}^+\hat{a}$

If ψ_n is an eigenfunction of $\hat{N}$ with eigenvalue n

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

then

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

Notice that $n \geq 0$:

$$n = \int \psi_n^* \hat{N} \psi_n \, dx = \int (\hat{a}\psi_n)^* (\hat{a}\psi)\, dx = \int |\varphi|^2 dx \geq 0$$

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

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

Now let us look at this:

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

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

Hence <u>$\hat{a}\psi_n$ is an eigenstate of $\hat{N}$ with eigenvalue $n-1$</u>, i.e. $\hat{a}\psi_n = C\psi_{n-1}$, where C 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

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

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 $n-1, n-2, n-3, \ldots$

That cannot continue forever, however. We know that $n > 0$. Thus, there must be a lowest eigenstate ψ_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:

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

Now let us consider the effect of $\hat{a}^+$:

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

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

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

We can conclude that $\hat{N}$ has eigenvalues

$$0, 1, 2, \ldots \infty$$

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

Let us find the explicit form of ψ_0:

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

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

From normalization we obtain $A_0 = \frac{1}{\pi^{1/4}}$

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

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

We can write an alternative formula for Hermite polynomials then:

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