

This paper deals with commutators, using functions of operators. It is based on “Commutation relations for functions of operators”, Mark K. Transtrum and Jean-Francois S. Van Huele.

The original paper can be found at:

<https://scholarsarchive.byu.edu/cgi/viewcontent.cgi?article=1371&context=facpub>

Hope I can help you with learning quantum mechanics.

List of often used operators:

| Symbol | Name | Effect |
|-----------------------------------|---|---|
| \hat{x} | Position operator | Multiplication by x |
| | The position operator can be expressed in terms of lowering operator \hat{a} and raising operator \hat{a}^\dagger : | $\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} (\hat{a} + \hat{a}^\dagger)$ |
| \hat{x}^2 | Position operator squared | Multiplication by x^2 |
| \hat{x}^n | Position operator to n -th power | Multiplication by x^n |
| \hat{p} | Momentum operator | $-i\hbar \frac{\partial}{\partial x}$ |
| | The momentum operator can be expressed in terms of lowering operator \hat{a} and raising operator \hat{a}^\dagger : | $\hat{p} = \sqrt{\frac{m\omega\hbar}{2}} (\hat{a}^\dagger - \hat{a})$ |
| \hat{p}^2 | Momentum operator squared | $-\hbar^2 \frac{\partial^2}{\partial x^2}$ |
| \hat{p}^n | Momentum operator to n -th power | $(-i)^n \hbar^n \frac{\partial^2}{\partial x^2}$ <p>Note: $(-i)^1 = -i, (-i)^2 = -1$ $(-i)^3 = i, (-i)^4 = +1$ $(-i)^5 = -i, \dots$</p> |
| $\hat{T} := \frac{\hat{p}^2}{2m}$ | Kinetic energy | $-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$ |
| $\hat{V}(x)$ | Potential energy | Multiplication by $V(x)$ |
| \hat{H} | Hamiltonian, total energy, kinetic plus potential energy | $-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$ |
| \hat{a} | Lowering operator | Reduces the n -th state wave function of the harmonic oscillator by one: $\hat{a}\psi_n = \sqrt{n} \psi_{n-1}$ |
| | The lowering operator can be expressed in terms of \hat{x} and \hat{p} : | $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + i \frac{1}{m\omega} \hat{p} \right)$ |
| \hat{a}^\dagger | Raising operator | Increments the n -th state wave function of the harmonic oscillator by one: $\hat{a}^\dagger \psi_n = \sqrt{n+1} \psi_{n+1}$ |
| | The raising operator can be expressed in terms of \hat{x} and \hat{p} : | $\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} - i \frac{1}{m\omega} \hat{p} \right)$ |
| \hat{N} | Number operator: $\hat{N} = \hat{a}^\dagger \hat{a}$ | Gives back the n -th state wave function of the harmonic oscillator multiplied by n : $\hat{N}\psi_n = n \psi_n$ |

Note: The ground state wave function of the harmonic oscillator:

$$\psi_0 = N_0 e^{-\frac{m\omega x^2}{2\hbar}}$$

 Note: N_0, N_1, N_2, \dots are normalizing constants.

Commuting Operators describe quantities that can simultaneously be measured exactly.

Operators that do not commute describe quantities that cannot be measured simultaneously exact.

In one-dimensional problems the position operator \hat{x} and the momentum operator \hat{p} are an example.

We have the commutation relation:

$$[\hat{x}, \hat{p}_x] = (\hat{x}\hat{p}_x - \hat{p}_x\hat{x}) = i\hbar$$

The position operator \hat{x} is realized by multiplying with x , the momentum operator \hat{p}_x by applying the partial derivation $-i\hbar \frac{\partial}{\partial x}$.

For 3-dimensional spatial systems the commutation relations are generalized to:

$$[\hat{x}_i, \hat{p}_j] = \delta_{ij}i\hbar$$

Note: δ_{ij} is the Kronecker delta.

Independent dimensions are simultaneously measurable because $\delta_{ij} = 0$ for $i \neq j$.

If we do not have the plain operators \hat{x} and \hat{p} , but reasonable functions of them, then the commutators change.

If we have $[\hat{x}, \hat{p}] = i\hbar$, then we get:

$$[\hat{x}, f(\hat{p})] = i\hbar \frac{df(\hat{p})}{d\hat{p}}$$

$$[\hat{p}, f(\hat{x})] = -i\hbar \frac{df(\hat{x})}{d\hat{x}}$$

In general:

If:

$$[\hat{x}_1, \hat{x}_2] = c$$

Then:

$$[\hat{x}_1, f(\hat{x}_2)] = c \frac{df(\hat{x}_2)}{d\hat{x}_2}$$

Note: c is a constant.

Note: $f(\hat{x}_2)$ must be an analytic function that allows Taylor expansion, so it must be infinitely differentiable.

Examples with lowering and raising operators.

$$[\hat{a}, \hat{a}^\dagger] = \hat{1}$$

Note: $\hat{1}$ often written as 1 is the unit operator.

$$[\hat{N}, \hat{a}] = -\hat{a}$$

$$[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger$$

$$[\hat{a}, (\hat{a}^\dagger)^k] = k(\hat{a}^\dagger)^{k-1}$$

$$[\hat{a}^\dagger, (\hat{a})^k] = -k(\hat{a})^{k-1}$$

$$[\hat{N}, (\hat{a})^k] = -k(\hat{a})^k$$

$$[\hat{N}, (\hat{a}^\dagger)^k] = k(\hat{a}^\dagger)^k$$

Linear example

We shift the operator \hat{x}_2 by a linear function:

$$f(\hat{x}_2) = a \cdot \hat{x}_2 + \hat{b}$$

Note: a is a real number, \hat{b} an appropriate operator.

By assumption $[\hat{x}_1, \hat{x}_2] = c$ we get:

$$[\hat{x}_1, f(\hat{x}_2)] = c \frac{df(\hat{x}_2)}{d\hat{x}_2} = c \cdot a$$

Power example

We shift the second operator to its second power:

$$f(\hat{x}_2) = (\hat{x}_2)^2 = \hat{x}_2 \cdot \hat{x}_2$$

By assumption $[\hat{x}_1, \hat{x}_2] = c$ we get:

$$[\hat{x}_1, f(\hat{x}_2)] = c \cdot \frac{df(\hat{x}_2)}{d\hat{x}_2} = c \cdot \frac{d}{d\hat{x}_2} (\hat{x}_2)^2 = c \cdot 2 \cdot \hat{x}_2$$

The general case $[f(\hat{x}_1), g(\hat{x}_2)]$ leads to complex results – please look at the original paper if you need to deal with.

Mixed example

By assumption $[\hat{x}_1, \hat{x}_2] = c$ we get:

$$[(\hat{x}_1)^2, f(\hat{x}_2)] = 2 \cdot c \cdot \hat{x}_1 \frac{df(\hat{x}_2)}{d\hat{x}_2} - c^2 \cdot \frac{d^2 f(\hat{x}_2)}{d\hat{x}_2^2}$$

This can be generalized to any power of (\hat{x}_1) :

$$[(\hat{x}_1)^n, f(\hat{x}_2)] = \sum_{k=1}^n (-1)^{k+1} \cdot \binom{n}{k} \cdot c^k \cdot \hat{x}_1^{n-k} \cdot \frac{d^k f(\hat{x}_2)}{d\hat{x}_2^k}$$