Commutation relations

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Using the Mathematica, we derive the formula of the commutation relations related to the momentum and position operators. We use two types of differential operators;

(i) $p \to \frac{\hbar}{i}\frac{\partial}{\partial x}$, (ii) $x \to i\hbar\frac{\partial}{\partial p}$.

The detail of the formula will be discussed later.

1. Commutation relations between $\hat{p}$ and $\hat{x}$

We start with the commutation relation

$$[\hat{x}, \hat{p}] = i\hbar\hat{1}.$$

Then we have

$$[\hat{x}, \hat{p}^2] = \hat{p}[\hat{x}, \hat{p}] + [\hat{x}, \hat{p}]\hat{p} = 2i\hbar\hat{p}.$$

Here we use the formula;

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}],$$

$$[\hat{A}, \hat{B}^2] = [\hat{A}, \hat{B}]\hat{B} + \hat{B}[\hat{A}, \hat{B}],$$

$$[\hat{x}, \hat{p}^3] = [\hat{x}, \hat{p}\hat{p}^2] = [\hat{x}, \hat{p}]\hat{p}^2 + \hat{p}[\hat{x}, \hat{p}^2] = i\hbar\hat{p}\hat{p}^2 + \hat{p}(2i\hbar\hat{p}) = 3i\hbar\hat{p}^2.$$

or

$$[\hat{x}, \hat{p}^3] = \hat{p}^2[\hat{x}, \hat{p}] + \hat{p}[\hat{x}, \hat{p}]\hat{p} + [\hat{x}, \hat{p}]\hat{p}^2 = 3i\hbar\hat{p}^2.$$

Here we use

$$[\hat{A}, \hat{B}^3] = [\hat{A}, \hat{B}]\hat{B}^2 + \hat{B}[\hat{A}, \hat{B}]\hat{B} + \hat{B}^2[\hat{A}, \hat{B}].$$

More generally, let us show that

$$[\hat{x}, \hat{p}^n] = i\hbar n\hat{p}^{n-1}.$$

If we assume that this equation is verified, we obtain

$$[\hat{x}, \hat{p}^{n+1}] = [\hat{x}, \hat{p}\hat{p}^n] = [\hat{x}, \hat{p}]\hat{p}^n + \hat{p}[\hat{x}, \hat{p}^n] = i\hbar\hat{p}^n + \hat{p}i\hbar n\hat{p}^{n-1} = i\hbar(n+1)\hat{p}^n .$$

Suppose that $f(\hat{p})$ is described by a series expansion,

$$f(\hat{p}) = \sum_n a_n \hat{p}^n .$$

Then we have

$$[\hat{x}, f(\hat{p})] = [\hat{x}, \sum_n a_n \hat{p}^n] = \sum_n a_n [\hat{x}, \hat{p}^n] = i\hbar \sum_n n a_n \hat{p}^{n-1} ,$$

or

$$[\hat{x}, f(\hat{p})] = i\hbar f'(\hat{p}) .$$

(b)
Similarly

$$[\hat{p}, \hat{x}^2] = \hat{x}[\hat{p}, \hat{x}] + [\hat{p}, \hat{x}]\hat{x} = 2\frac{\hbar}{i}\hat{x} ,$$

$$[\hat{p}, \hat{x}^3] = \hat{x}^2[\hat{p}, \hat{x}] + \hat{x}[\hat{p}, \hat{x}]\hat{x} + [\hat{p}, \hat{x}]\hat{x}^2 = 3\frac{\hbar}{i}\hat{x}^2 ,$$

$$[\hat{p}, \hat{x}^n] = \frac{\hbar}{i} n\hat{x}^{n-1} ,$$

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

(c) More general cases ((Messiah))

$$\begin{aligned}
[\hat{x}, \hat{p}^2 f(\hat{x})] &= [\hat{x}, \hat{p}^2] f(\hat{x}) + \hat{p}^2[\hat{x}, f(\hat{x})] \\
&= [\hat{x}, \hat{p}^2] f(\hat{x}) \\
&= i\hbar 2\hat{p} f(\hat{x})
\end{aligned}$$

$$\begin{aligned}
[\hat{x}, \hat{p} f(\hat{x})\hat{p}] &= [\hat{x}, \hat{p}] f(\hat{x})\hat{p} + \hat{p}[\hat{x}, f(\hat{x})\hat{p}] \\
&= [\hat{x}, \hat{p}] f(\hat{x})\hat{p} + \hat{p}([\hat{x}, f(\hat{x})]\hat{p} + f(\hat{x})[\hat{x}, \hat{p}] \\
&= [\hat{x}, \hat{p}] f(\hat{x})\hat{p} + \hat{p} f(\hat{x})[\hat{x}, \hat{p}] \\
&= i\hbar[f(\hat{x})\hat{p} + \hat{p} f(\hat{x})]
\end{aligned}$$

$$[\hat{x}, f(\hat{x})\hat{p}^2] = [\hat{x}, f(\hat{x})]\hat{p}^2 + f(\hat{x})[\hat{x}, \hat{p}^2]$$
$$= f(\hat{x})[\hat{x}, \hat{p}^2]$$
$$= 2i\hbar f(\hat{x})\hat{p}$$

(d)
In the same way

$$[\hat{p}, \hat{p}^2 f(\hat{x})] = [\hat{p}, \hat{p}^2] f(\hat{x}) + \hat{p}^2[\hat{p}, f(\hat{x})]$$
$$= \hat{p}^2[\hat{p}, f(\hat{x})]$$
$$= \frac{\hbar}{i}\hat{p}^2 f'(\hat{x})$$

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

$$[\hat{p}, f(\hat{x})\hat{p}^2] = [\hat{p}, f(\hat{x})\hat{p}]\hat{p} + f(\hat{x})\hat{p}[\hat{p}, \hat{p}]$$
$$= [\hat{p}, f(\hat{x})\hat{p}]\hat{p}$$
$$= ([\hat{p}, f(\hat{x})]\hat{p} + f(\hat{x})[\hat{p}, \hat{p}])\hat{p}$$
$$= [\hat{p}, f(\hat{x})]\hat{p}^2$$
$$= \frac{\hbar}{i} f'(\hat{x})]\hat{p}^2$$

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2. Commutation relations of operators

The commutator of two operators $\hat{A}$ and $\hat{B}$:

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

These two operators $\hat{A}$ and $\hat{B}$ commutes when $[\hat{A}, \hat{B}] = 0$.

$$[\hat{A}, \hat{A}] = \hat{0},$$

$$[\hat{A}, f(\hat{A})] = \hat{0},$$

$$[\hat{A}, c] = \hat{0}, \qquad (c\text{: number})$$

$$[\hat{A}, c\hat{B}] = c[\hat{A}, \hat{B}],$$

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

$$[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}],$$

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}],$$

$$[\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}],$$

$$[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = \hat{0},$$

$$[\hat{A}, \hat{B}^2] = [\hat{A}, \hat{B}]\hat{B} + \hat{B}[\hat{A}, \hat{B}],$$

$$[\hat{A}, \hat{B}^3] = [\hat{A}, \hat{B}]\hat{B}^2 + \hat{B}[\hat{A}, \hat{B}]\hat{B} + \hat{B}^2[\hat{A}, \hat{B}],$$

$$[\hat{A}, \hat{B}^4] = [\hat{A}, \hat{B}]\hat{B}^3 + \hat{B}[\hat{A}, \hat{B}]\hat{B}^2 + \hat{B}^2[\hat{A}, \hat{B}]\hat{B} + \hat{B}^3[\hat{A}, \hat{B}],$$

$$[\hat{A}, \hat{B}^5] = [\hat{A}, \hat{B}]\hat{B}^5 + \hat{B}[\hat{A}, \hat{B}]\hat{B}^4 + \hat{B}^2[\hat{A}, \hat{B}]\hat{B}^3 + \hat{B}^3[\hat{A}, \hat{B}]\hat{B}^2 + \hat{B}^4[\hat{A}, \hat{B}]\hat{B} + \hat{B}^5[\hat{A}, \hat{B}].$$

When $[\hat{B}, [\hat{A}, \hat{B}]] = \hat{0}$,

$$[\hat{A}, \hat{B}^n] = n\hat{B}^{n-1}[\hat{A}, \hat{B}].$$

3. Baker-Hausdorff Lemma

This theorem is named for Henry Frederick Baker, John Edward Campbell, and Felix Hausdorff. It was first noted in print by Campbell (1897); elaborated by Henri Poincaré (1899) and Baker (1902); and systematized geometrically, and linked to the Jacobi identity by Hausdorff (1906).[1]

http://en.wikipedia.org/wiki/Baker%E2%80%93Campbell%E2%80%93Hausdorff_formula

The operator:

$$f(x) = \exp(\hat{A}x)\hat{B}\exp(-\hat{A}x),$$

can be expanded as

$$f(x) = \exp(\hat{A}x)\hat{B}\exp(-\hat{A}x) = \hat{B} + \frac{x}{1!}[\hat{A},\hat{B}] + \frac{x^2}{2!}[\hat{A},[\hat{A},\hat{B}]] + \frac{x^3}{3!}[\hat{A},[\hat{A},[\hat{A},\hat{B}]]] + ...$$

We can prove this by using a Taylor expansion of $f(x)$ as

$$f(x) = f(0) + \frac{x}{1!}f^{(1)}(0) + \frac{x^2}{2!}f^{(2)}(0) + \frac{x^3}{3!}f^{(3)}(0) + ...,$$

$$f'(x) = \hat{A}\exp(\hat{A}x)\hat{B}\exp(-\hat{A}x) - \exp(\hat{A}x)\hat{B}\exp(-\hat{A}x)\hat{A} = [\hat{A}, f(x)],$$

$$f''(x) = [\hat{A}, f'(x)],$$

$$f^{(3)}(x) = [\hat{A}, f^{(2)}(x)].$$

In general,

$$f^{(n)}(x) = [\hat{A}, f^{(n-1)}(x)].$$

From these relations we have

$$f(0) = \hat{B},$$

$$f'(0) = [\hat{A}, f(0)] = [\hat{A},\hat{B}],$$

$$f''(0) = [\hat{A}, f'(0)] = [\hat{A},[\hat{A},\hat{B}]],$$

$$f^{(3)}(0) = [\hat{A}, f^{(3)}(0)] = [\hat{A},[\hat{A},[\hat{A},\hat{B}]]],$$

$$f^{(4)}(0) = [\hat{A}, f^{(3)}(0)] = [\hat{A},[\hat{A},[\hat{A},[\hat{A},\hat{B}]]]],$$

……………………………………………………………….

Therefore, we get

$$f(x) = \hat{B} + \frac{x}{1!}[\hat{A},\hat{B}] + \frac{x^2}{2!}[\hat{A},[\hat{A},\hat{B}]] + \frac{x^3}{3!}[\hat{A},[\hat{A},[\hat{A},\hat{B}]]] + \frac{x^4}{4!}[\hat{A},[\hat{A},[\hat{A},[\hat{A},\hat{B}]]]] + ...$$

When

$$[\hat{A},[\hat{A},\hat{B}]] = 0,$$

$$f(x) = \hat{B} + x[\hat{A},\hat{B}].$$

((Theorem))

When $[\hat{A},[\hat{A},\hat{B}]] = \hat{0}$,

$$f(x) = \exp(\hat{A}x)\hat{B}\exp(-\hat{A}x) = \hat{B} + \frac{x}{1!}[\hat{A},\hat{B}].$$

4. Baker-Campbell-Hausdorff (BCH) theorem

If the commutator of two operators $\hat{A}$ and $\hat{B}$ commutes with each of them ($\hat{A}$ and $\hat{B}$)

$$[\hat{A},[\hat{A},\hat{B}]] = \hat{0},$$

$$[\hat{B},[\hat{A},\hat{B}]] = \hat{0}.$$

One has an identity

$$\exp(\hat{A}+\hat{B}) = \exp(\hat{A})\exp(\hat{B})\exp(-\frac{1}{2}[\hat{A},\hat{B}]). \qquad \text{(BCH theorem)}$$

((**Proof by Glauber**)) Glauber (Messiah, Quantum Mechanics p.422)

$$f(x) = \exp(\hat{A}x)\exp(\hat{B}x),$$

$$\frac{df(x)}{dx} = \hat{A}\exp(\hat{A}x)\exp(\hat{B}x) + \exp(\hat{A}x)\hat{B}\exp(\hat{B}x)$$

$$= (\hat{A} + \exp(\hat{A}x)\hat{B}\exp(-\hat{A}x))\exp(\hat{A}x)\exp(\hat{B}x)$$

$$= (\hat{A} + \exp(\hat{A}x)\hat{B}\exp(-\hat{A}x))f(x)$$

Since

$$[\hat{A},[\hat{A},\hat{B}]] = \hat{0},$$

$$[\hat{B},[\hat{A},\hat{B}]] = \hat{0},$$

$$\exp(\hat{A}x)\hat{B}\exp(-\hat{A}x) = \hat{B} + [\hat{A},\hat{B}]x. \qquad \text{(BCH Theorem)}$$

Then

$$\frac{df(x)}{dx} = (\hat{A} + \hat{B} + [\hat{A},\hat{B}]x)f(x)$$

with $f(x=0) = \hat{1}$.

Since the operators $\hat{A} + \hat{B}$ and $[\hat{A},\hat{B}]$ commute, they can be considered as quantities of ordinary algebra

$$\int \frac{1}{f}df = \int (\hat{A} + \hat{B} + [\hat{A},\hat{B}]x)dx,$$

or

$$\ln(f) = (\hat{A} + \hat{B})x + \frac{x^2}{2}[\hat{A},\hat{B}],$$

or

$$f(x) = \exp[(\hat{A} + \hat{B})x]\exp(\frac{x^2}{2}[\hat{A},\hat{B}]).$$

5. Example

Creation operator $\hat{a}^+$ and annihilation operator $\hat{a}$

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

$$\hat{D}_\alpha = \alpha\hat{a}^+ - \alpha^*\hat{a} \,,$$

where α is a complex number.

$$\hat{A} = \alpha\hat{a}^+ \,, \qquad \hat{B} = -\alpha^*\hat{a} \,,$$

$$[\hat{A}, \hat{B}] = [\alpha\hat{a}^+, -\alpha^*\hat{a}] = |\alpha|^2 [\hat{a}, \hat{a}^+] = |\alpha|^2 \,,$$

$$[\hat{A}, [\hat{A}, \hat{B}]] = \hat{0} \text{ and } [\hat{B}, [\hat{A}, \hat{B}]] = \hat{0} \,.$$

Then we have

$$\exp(\hat{D}_\alpha) = \exp(\alpha\hat{a}^+ - \alpha^*\hat{a}) = \exp(\alpha\hat{a}^+)\exp(-\alpha^*\hat{a})\exp(-\frac{1}{2}|\alpha|^2) \,.$$

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6. Commutation relations in the position basis and momentum basis

(a) Momentum operator in the position basis

We start with

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x) \,.$$

Then we have

$$\langle x|\hat{p}^2|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\hat{p}|\psi\rangle = \left(\frac{\hbar}{i}\right)^2 \frac{\partial^2}{\partial x^2}\psi(x) \,,$$

$$\begin{aligned}
\langle x|\hat{x}\hat{p} - \hat{p}\hat{x}|\psi\rangle &= x\langle x|\hat{p}|\psi\rangle - \frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\hat{x}|\psi\rangle \\
&= x\frac{\hbar}{i}\frac{\partial}{\partial x}\langle x|\psi\rangle - \frac{\hbar}{i}\frac{\partial}{\partial x}x\langle x|\psi\rangle \\
&= x\frac{\hbar}{i}\frac{\partial}{\partial x}\psi(x) - \frac{\hbar}{i}\frac{\partial}{\partial x}[x\psi(x)] \\
&= i\hbar\psi(x)
\end{aligned}$$

In general,

$$\langle x|[\hat{x}^n,\hat{p}^m]|\psi\rangle = \langle x|(\hat{x}^n\hat{p}^m - \hat{p}^m\hat{x}^n)|\psi\rangle$$

$$= x^n\left(\frac{\hbar}{i}\right)^m \frac{\partial^m}{\partial x^m}\psi(x) - \left(\frac{\hbar}{i}\right)^m \frac{\partial^m}{\partial x^m}[x^n\psi(x)]$$

(b) Position operator in the momentum basis

We start with

$$\langle p|\hat{x}|\psi\rangle = i\hbar\frac{\partial}{\partial p}\langle p|\psi\rangle = i\hbar\frac{\partial}{\partial p}\psi(p).$$

Then we have

$$\langle p|\hat{x}^2|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial p}\langle p|\hat{x}|\psi\rangle = \left(\frac{\hbar}{i}\right)^2\frac{\partial^2}{\partial p^2}\psi(p),$$

$$\langle p|[\hat{x}^n,\hat{p}^m]|\psi\rangle = \langle p|\hat{x}^n\hat{p}^m - \hat{p}^m\hat{x}^n|\psi\rangle$$

$$= (i\hbar)^n\frac{\partial^n}{\partial p^n}[p^m\psi(p)] - (i\hbar)^n p^m\frac{\partial^m}{\partial p^m}\psi(p)$$

7. Schrödinger equation in the position basis

Suppose that the Hamiltonian $\hat{H}$ is given by

$$\hat{H} = \frac{1}{2m}\hat{p}^2 + V(\hat{x}).$$

Eigenvalue problem for the stationary energy eigen state is described by

$$\hat{H}|\psi\rangle = E|\psi\rangle.$$

In the $|x\rangle$ representation, the above equation can be written by the Schrodinger equation for the wave function $\psi(x) = \langle x|\psi\rangle$,

$$\langle x|\hat{H}|\psi\rangle = \langle x|\frac{1}{2m}\hat{p}^2 + V(\hat{x})|\psi\rangle = E\langle x|\psi\rangle,$$

or

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\langle x|\psi\rangle + V(x)\langle x|\psi\rangle = E\langle x|\psi\rangle,$$

or simply

$$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)]\psi(x)=E\psi(x). \qquad \text{(Schrodinger equation)}$$

8. Wave function in the momentum basis

Next we consider the special case: Schrödinger equation in the free particles. The Hamiltonian of the free particle is given by

$$\hat{H}_0=\frac{1}{2m}\hat{p}^2.$$

$|p\rangle$ is the eigenstate of with the energy eigenvalue

$$E=\frac{p^2}{2m}.$$

Note that

$$\hat{H}_0|p\rangle=\frac{1}{2m}\hat{p}^2|p\rangle=\frac{1}{2m}p^2|p\rangle.$$

In the $|x\rangle$ representation,

$$\begin{aligned}\langle x|\hat{H}|p\rangle&=\langle x|\frac{1}{2m}\hat{p}^2|p\rangle\\&=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\langle x|p\rangle\\&=E\langle x|p\rangle\\&=\frac{p^2}{2m}\langle x|p\rangle\end{aligned}$$

or

$$(\frac{\partial^2}{\partial x^2}+k^2)\langle x|k\rangle=0,$$

where

$$E = \frac{p^2}{2m}, \qquad p = \hbar k, \qquad |p\rangle = \frac{1}{\sqrt{\hbar}}|k\rangle .$$

and the wave function is actually the transformation function,

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}\exp(\frac{ipx}{\hbar}), \qquad \text{or} \qquad \langle x|k\rangle = \frac{1}{\sqrt{2\pi}}\exp(ikx) .$$

9. Commutation relations (formula)

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

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

$$[\hat{x}, \exp(\frac{ia}{\hbar}\hat{p})] = -a\exp(\frac{ia}{\hbar}\hat{p}),$$

$$[\hat{x}, \hat{p}^2 f(\hat{p})] = 2i\hbar\hat{p}f(\hat{p}) + i\hbar\hat{p}^2 f'(\hat{p}),$$

$$[\hat{x}, \hat{p}^2 f(\hat{q})] = 2i\hbar\hat{p}f(\hat{x}),$$

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

$$[\hat{x}, f(\hat{x})\hat{p}^2] = 2i\hbar f(\hat{x})\hat{p},$$

$$[\hat{p}, \hat{p}^2 f(\hat{q})] = -i\hbar\hat{p}^2 f'(\hat{q}),$$

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

$$[\hat{p}, f(\hat{x})\hat{p}^2] = -i\hbar f'(\hat{x})\hat{p}^2,$$

$$[\hat{p}^2, \hat{x}^2] = -4i\hbar\hat{x}\hat{p} - 2\hbar^2\hat{1},$$

$$[\hat{p}^3, \hat{x}^3] = -18\hbar^2\hat{x}\hat{p} - 9i\hbar\hat{x}^2\hat{p}^2 + 6i\hbar^3\hat{1}.$$

8. Mathematica (1): momentum operator

By using the Mathematica, we calculate the commutation relation

$$
\begin{aligned}
f(n,m) &= \langle x|\hat{x}^n \hat{p}^m - \hat{p}^m \hat{x}^n|\psi\rangle \\
&= x^n p^m[\psi(x)] - p^m[x^m\psi(x)] \\
&= x^n \left(\frac{\hbar}{i}\right)^m \frac{\partial^m}{\partial x^m}\psi(x) - \left(\frac{\hbar}{i}\right)\frac{\partial^m}{\partial x^m}[x^n\psi(x)]
\end{aligned}
$$

with

$$p = \frac{\hbar}{i}\frac{\partial}{\partial x},$$

where $\psi(x) = \langle x|\psi\rangle$ is an arbitrary function of *x*.

((**Mathematica**))

```
Clear["Global`*"]; p := ℏ/ⅈ D[#, x] &;
f[n_, m_] := Nest[p, x^m ψ[x], n] - x^m Nest[p, ψ[x], n] // Simplify;
```

f[1, 1]

$-i \hbar \psi[x]$

f[2, 1]

$-2 \hbar^2 \psi'[x]$

f[3, 1]

$3 i \hbar^3 \psi''[x]$

f[4, 1]

$4 \hbar^4 \psi^{(3)}[x]$

f[100, 1]

$100 \hbar^{100} \psi^{(99)}[x]$

f[1, 2]

$-2 i x \hbar \psi[x]$

f[2, 2]

$-2 \hbar^2 (\psi[x] + 2 x \psi'[x])$

f[3, 2]

$6 i \hbar^3 (\psi'[x] + x \psi''[x])$

f[4, 2]

$4 \hbar^4 \left(3 \psi''[x] + 2 x \psi^{(3)}[x]\right)$

f[1, 3]

$-3 i x^2 \hbar \psi[x]$

f[2, 3]

$-6 x \hbar^2 (\psi[x] + x \psi'[x])$

f[3, 3]

$3 i \hbar^3 (2 \psi[x] + 3 x (2 \psi'[x] + x \psi''[x]))$

f[4, 3]

$12 \hbar^4 \left(2 \psi'[x] + x \left(3 \psi''[x] + x \psi^{(3)}[x]\right)\right)$

10. Mathematica (1): position operator

By using the Mathematica, we calculate the commutation relation

$$f(n,m) = (x^n p^m - p^m x^n)\psi(p) = x^n[p^m\psi(p)] - p^m[x^n\psi(p)],$$

with

$$x = i\hbar\frac{\partial}{\partial p},$$

where $\psi(p)$ is an arbitrary function of *x*.

((**Mathematica**))

Position oprator in quantum mechanics;

```
Clear["Global`*"]; x := ⅈ ℏ D[#, p] &;
f[n_, m_] := Nest[x, p^m ψ[p], n] - p^m Nest[x, ψ[p], n] //
  Simplify;

f[1, 1]

ⅈ ℏ ψ[p]

f[2, 1]

-2 ℏ^2 ψ'[p]

f[3, 1]

-3 ⅈ ℏ^3 ψ''[p]

f[4, 1]

4 ℏ^4 ψ^(3)[p]

f[100, 1]

100 ℏ^100 ψ^(99)[p]

f[1, 2]

2 ⅈ p ℏ ψ[p]
```

```
f[2, 2]
```
$-2\hbar^2 (\psi[p] + 2 p \psi'[p])$

```
f[3, 2]
```
$-6 i \hbar^3 (\psi'[p] + p \psi''[p])$

```
f[4, 2]
```
$4 \hbar^4 \left(3 \psi''[p] + 2 p \psi^{(3)}[p]\right)$

```
f[1, 3]
```
$3 i p^2 \hbar \psi[p]$

```
f[2, 3]
```
$-6 p \hbar^2 (\psi[p] + p \psi'[p])$

```
f[5, 5]
```
$5 i \hbar^5 \left(24 \psi[p] + 5 p \left(24 \psi'[p] + p \left(24 \psi''[p] + 8 p \psi^{(3)}[p] + p^2 \psi^{(4)}[p]\right)\right)\right)$

$x\left[\mathrm{Exp}\left[\frac{i\, p\, a}{\hbar}\right] \psi[p]\right] - \mathrm{Exp}\left[\frac{i\, p\, a}{\hbar}\right] x[\psi[p]]$ // Simplify

$-a\, e^{\frac{i a p}{\hbar}} \psi[p]$

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