

Commutation relations
Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(Date November 13, 2013)

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;

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

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))

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

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

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

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

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

(d)

In the same way

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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 Theorem (or Baker- Campbell-Hausdorff Theorem)

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

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

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

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

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

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

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

In general,

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

From these relations we have

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

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

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

$$f^{(3)}(0) = [\hat{A}, f^{(2)}(0)] = [\hat{A}, [\hat{A}, [\hat{A}, \hat{B}]]]$$

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

.....

Therefore, we get

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

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-Hausdorff Lemma

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

$$\exp(\hat{A} + \hat{B}) = \exp(\hat{A})\exp(\hat{B})\exp\left(-\frac{1}{2}[\hat{A}, \hat{B}]\right)$$

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

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

$$\begin{aligned}
\frac{df(x)}{dx} &= \hat{A} \exp(\hat{A}x) \exp(\hat{B}x) + \exp(\hat{A}x) \hat{B} \exp(\hat{B}x) \\
&= (\hat{A} + \exp(\hat{A}x) \hat{B} \exp(-\hat{A}x)) \exp(\hat{A}x) \exp(\hat{B}x) \\
&= (\hat{A} + \exp(\hat{A}x) \hat{B} \exp(-\hat{A}x)) f(x)
\end{aligned}$$

Since

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

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

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

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

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

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.

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

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

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

Then we have

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

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,

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

(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

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

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

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

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

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

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

where

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

and the wave function is actually the transformation function,

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

9. Commutation relations (formula)

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

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

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

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

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

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

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

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

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

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

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

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

8. Mathematica (1): momentum operator

By using the Mathematica, we calculate the commutation relation

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

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 :=  $\frac{\hbar}{i}$  D[#, x] &;
f[n_, m_] := Nest[p, xm ψ[x], n] - xm Nest[p, ψ[x], n] // Simplify;

f[1, 1]
- i ħ ψ[x]

f[2, 1]
- 2 ħ2 ψ'[x]

f[3, 1]
3 i ħ3 ψ''[x]

f[4, 1]
4 ħ4 ψ(3)[x]

f[100, 1]
100 ħ100 ψ(99)[x]

f[1, 2]
- 2 i x ħ ψ[x]

f[2, 2]
- 2 ħ2 (ψ[x] + 2 x ψ'[x])

f[3, 2]
6 i ħ3 (ψ'[x] + x ψ''[x])

f[4, 2]
4 ħ4 (3 ψ''[x] + 2 x ψ(3)[x])

f[1, 3]
- 3 i x2 ħ ψ[x]

f[2, 3]
- 6 x ħ2 (ψ[x] + x ψ'[x])

f[3, 3]
3 i ħ3 (2 ψ[x] + 3 x (2 ψ'[x] + x ψ''[x]))

f[4, 3]
12 ħ4 (2 ψ'[x] + x (3 ψ''[x] + x ψ(3)[x]))

```

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]

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

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]

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

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

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

REFERENCES

A. Messiah, *Quantum Mechanics*, vol.I and vol.II (North-Holland, 1961).

J.J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*, second edition (Addison-Wesley, New York, 2011).

Eugen Merzbacher, *Quantum Mechanics*, third edition (John Wiley & Sons, New York, 1998).