SQ11. Aim: ① knowing what a linear operator is

and

② Knowing how to construct a commutator

(a). It is very important for you to know what a linear operator is because there are many linear operator in quantum mechanics.

Definition of a linear operator:

If $\hat{O}$ is a linear operator, then it acts on a linear combination of functions $(c_1 f_1(x) + c_2 f_2(x) + \cdots + c_n f_n(x))$

to yield $c_1 \hat{O} f_1(x) + c_2 \hat{O} f_2(x) + \cdots + c_n \hat{O} f_n(x)$. That is

☆ $$\boxed{\hat{O}(c_1 f_1(x) + c_2 f_2(x) + \cdots + c_n f_n(x)) = c_1 \hat{O} f_1(x) + c_2 \hat{O} f_2(x) + \cdots + c_n \hat{O} f_n(x)}$$

It seems that the definition is too abstract. Examples are given to demonstrate the linearity property.

① differentiation operator $\hat{D} = \frac{d}{dx}$ is a linear operator.

$\boxed{c_1 f_1(x) + c_2 f_2(x)}$ is given.

Step 1 To test for the linearity, we put the operator in front of the linear combination of functions.

$$\hat{D}\,[c_1 f_1(x) + c_2 f_2(x)]$$

Step 2 Simiplify it.

$$\hat{D}\,[c_1 f(x) + c_2 f_2(x)] = \frac{d}{dx}[c_1 f_1(x) + c_2 f_2(x)]$$

$= c_1 \frac{d}{dx} f_1(x) + c_2 \frac{d}{dx} f_2(x)$

$= c_1 \hat{D} f_1(x) + c_2 \hat{D} f_2(x).$

$\boxed{\text{Step 3.}}$ Check it with definition. ☆.

$$\hat{D}\,[c_1 f_1(x) + c_2 f_2(x)] = c_1 \hat{D} f_1(x) + c_2 \hat{D} f_2(x).$$

∴ satisfies ☆. It is a linear operator indeed.

② Integration operator $\hat{I}(\cdots) = \int_a^b (\cdots)\,dx$ is a linear operator.

A linear combination is given: $c_1 f_1(x) + c_2 f_2(x)$

$\boxed{\text{Step 1}}$ put $\hat{I}$ in the front.

$\hat{I}(c_1 f_1(x) + c_2 f_2(x))$.

$\boxed{\text{Step 2}}$ Simplify it.

$\hat{I}(c_1 f_1(x) + c_2 f_2(x))$

$= \int_a^b (c_1 f_1(x) + c_2 f_2(x))\,dx$

$= c_1 \int_a^b f_1(x)\,dx + c_2 \int_a^b f_2(x)\,dx.$

$= c_1 \hat{I}(f_1(x)) + c_2 \hat{I}(f_2(x)).$

$\boxed{\text{Step 3}}$ Check with the definition ☆.

$\hat{I}(c_1 f_1(x) + c_2 f_2(x)) = c_1 \hat{I}(f_1(x)) + c_2 \hat{I}(f_2(x)).$

It is a linear operator.

∴ After knowing these examples, it's time we tackle the sample question.

Define $\hat{A} = \frac{\hbar}{i} \frac{d}{dx}$ and $\hat{B} = x^2$.

There are two operators. One is $\hat{A}^2 = \hat{A}\hat{A}$, the other $[\hat{A}(\cdots)]^2$. (P.3)

I want to show that $\hat{A}^2$ is a linear operator, while $[\hat{A}\ \ ]^2$ isn't.

Proof: $c_1 f_1(x) + c_2 f_2(x)$ is given.

$\boxed{\text{Step 1}}$ put the operator in the front

$$\hat{A}^2(c_1 f_1(x) + c_2 f_2(x))$$

$\boxed{\text{Step 2}}$ Simpify it.

$$\hat{A}^2(c_1 f_1(x) + c_2 f_2(x))$$
$$= \left(\frac{\hbar}{i}\frac{d}{dx}\right)\left(\frac{\hbar}{i}\frac{d}{dx}\right)(c_1 f_1(x) + c_2 f_2(x))$$
$$= \left(\frac{\hbar}{i}\frac{d}{dx}\right)\left(c_1\left(\frac{\hbar}{i}\frac{d}{dx} f_1(x)\right) + c_2\left(\frac{\hbar}{i}\frac{d}{dx} f_2(x)\right)\right).$$
$$= c_1\left(\frac{\hbar}{i}\frac{d}{dx}\right)\left(\frac{\hbar}{i}\frac{d}{dx} f_1(x)\right) + c_2\left(\frac{\hbar}{i}\frac{d}{dx}\right)\left(\frac{\hbar}{i}\frac{d}{dx} f_2(x)\right)$$
$$= c_1 \hat{A}\hat{A} f_1 + c_2 \hat{A}\hat{A} f_2$$
$$= c_1 \hat{A}^2 f_1 + c_2 \hat{A}^2 f_2.$$

$\boxed{\text{Step 1}}$

$$[\hat{A}\ \ (c_1 f_1(x) + c_2 f_2(x))]^2.$$

$\boxed{\text{Step 2}}$

$$[\hat{A}(c_1 f_1(x) + c_2 f_2(x))]^2$$
$$= \left[\left(\frac{\hbar}{i}\frac{d}{dx}\right)(c_1 f_1(x) + c_2 f_2(x))\right]^2.$$
$$= \left[c_1\left(\frac{\hbar}{i}\frac{d}{dx} f_1(x)\right) + c_2\left(\frac{\hbar}{i}\frac{d}{dx} f_2(x)\right)\right]^2$$
$$= c_1^2\left(\frac{\hbar}{i}\frac{d}{dx} f_1(x)\right)^2 + c_2^2\left(\frac{\hbar}{i}\frac{d}{dx} f_2(x)\right)^2 + 2c_1c_2\left(\frac{\hbar}{i}\frac{d}{dx} f_1(x)\right)\left(\frac{\hbar}{i}\frac{d}{dx} f_2(x)\right)$$
$$= c_1^2[\hat{A} f_1(x)]^2 + c_2^2[\hat{A} f_2(x)]^2 + 2c_1c_2(\hat{A} f_1(x))(\hat{A} f_2(x))$$

$\boxed{\text{Step 3.}}$

Check them with the definition.

$\hat{A}^2(c_1 f_1(x) + c_2 f_2(x)) = c_1 \hat{A}^2 f_1(x) + c_2 \hat{A}^2 f_2(x)$

$\therefore \hat{A}^2$ is a linear operator.

$[\hat{A} \quad (c_1 f_1(x) + c_2 f_1(x))]^2$

$= c_1^2 [\hat{A} f_1(x)]^2 + c_2^2 [\hat{A} f_2(x)]^2 + 2 c_1 c_2 (\hat{A} f_1(x))(\hat{A} f_2(x))$

$\neq c_1 [\hat{A} f_1(x)]^2 + c_2 [\hat{A} f_2(x)]^2$

$\therefore [\hat{A} \quad]^2$ is not a linear operator.

Also, $\hat{A}^2 f(x)$ and $[\hat{A} f(x)]^2$ are different.

For $\hat{A}^2 f(x)$,

We have $\hat{A}^2 f(x) = \left(\frac{\hbar}{i}\frac{d}{dx}\right)\left(\frac{\hbar}{i}\frac{d}{dx}\right) f(x)$

$= \left(\frac{\hbar}{i}\frac{d}{dx}\right)\left(\frac{\hbar}{i}\frac{df}{dx}\right)$

$= -\hbar^2 \frac{d^2 f}{dx^2}$.

For $[\hat{A} f(x)]^2 = \left(\frac{\hbar}{i}\frac{df}{dx}\right)^2 = -\hbar^2 \left(\frac{df}{dx}\right)^2$.

In general, $\frac{d^2 f}{dx^2} \neq \left(\frac{df}{dx}\right)^2$.

$\therefore [\hat{A} f(x)]^2 \neq \hat{A}^2 f(x)$.

(b) In this question, we want to calculate the commutator $[\hat{A}, \hat{B}]$.

To calculate $[\hat{A}, \hat{B}]$, we need to use an auxiliary function $f(x)$.

$\boxed{\text{Step 1.}}$ Calculate $\hat{A}\hat{B}f(x)$.

$$\hat{A}\hat{B}f(x) = \left(\frac{\hbar}{i}\frac{d}{dx}\right)(x^2 f)$$
$$= \left(\frac{\hbar}{i}\right)\left(2xf + x^2\frac{df}{dx}\right).$$

$\boxed{\text{Step 2.}}$ Calculate $\hat{B}\hat{A}f(x)$

$$\hat{B}\hat{A}f(x) = (x^2)\left(\frac{\hbar}{i}\frac{df}{dx}\right) = \left(\frac{\hbar}{i}\right)\left(x^2\frac{df}{dx}\right).$$

$\boxed{\text{Step 3.}}$ Calculate $\hat{A}\hat{B}f(x) - \hat{B}\hat{A}f(x)$

$$= \left(\frac{\hbar}{i}\right)\left(2xf + x^2\frac{df}{dx}\right) - \left(\frac{\hbar}{i}\right)\left(x^2\frac{df}{dx}\right)$$
$$= 2x\left(\frac{\hbar}{i}\right)f = -i\hbar(2x)f$$

$\boxed{\text{Step 4.}}$ Using the definition $[\hat{A},\hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$.

$$[\hat{A},\hat{B}]f(x) = \hat{A}\hat{B}f(x) - \hat{B}\hat{A}f(x)$$
$$= -i\hbar(2x)f(x).$$
$$\therefore [\hat{A},\hat{B}] = -i\hbar(2x).$$

A Common Mistake:

Some students forgot to include the a xiliary function $f(x)$. when calculating commutator.

For example, "$\hat{A}\hat{B} = \frac{\hbar}{i}\frac{d}{dx}(x^2) = \frac{2\hbar}{i}x$"

"$\hat{B}\hat{A} = x^2\frac{\hbar}{i}\frac{d}{dx}$".

"$\therefore \hat{A}\hat{B} - \hat{B}\hat{A} = \frac{2\hbar}{i}x - x^2\frac{\hbar}{i}\frac{d}{dx}$".

These steps are wrong.

which is different from $-i\hbar(2x)$.

Whenever you calculate the commutator, you have to use an auxiliary function.

SQ12) (a) $-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + \frac{1}{2}m\omega^2x^2\psi(x,t) = i\hbar\frac{\partial\psi}{\partial t}(x,t)$

(b)

$$-\frac{\hbar^2}{2m}\psi''(x) + \frac{1}{2}m\omega^2x^2\psi(x) = E\psi(x)$$

(c) $\psi(x) = A^{\frac{1}{2}}x\,e^{-\frac{m\omega x^2}{2\hbar}}$

$$\psi'(x) = A^{\frac{1}{2}}\left[e^{-\frac{m\omega x^2}{2\hbar}} - \frac{m\omega x^2}{\hbar}e^{-\frac{m\omega x^2}{2\hbar}}\right]$$

$$\psi''(x) = A^{\frac{1}{2}}\left[-\frac{m\omega x}{\hbar}e^{-\frac{m\omega x^2}{2\hbar}} - \frac{2m\omega x}{\hbar}e^{-\frac{m\omega x^2}{2\hbar}} + \frac{m^2\omega^2x^3}{\hbar^2}e^{-\frac{m\omega x^2}{2\hbar}}\right]$$

$$= A^{\frac{1}{2}}\left[\frac{m^2\omega^2x^3}{\hbar^2}e^{-\frac{m\omega x^2}{2\hbar}} - \frac{3m\omega x}{\hbar}e^{-\frac{m\omega x^2}{2\hbar}}\right]$$

$$= A^{\frac{1}{2}}\frac{m\omega x}{\hbar^2}\left(m\omega x^2 - 3\hbar\right)e^{-\frac{m\omega x^2}{2\hbar}}$$

$$L.H.S. = -\frac{\hbar^2}{2m}\psi''(x) + \frac{1}{2}m\omega^2x^2\psi(x)$$

$$= A^{\frac{1}{2}}e^{-\frac{m\omega x^2}{2\hbar}}x\left[-\frac{\omega}{2}(m\omega x^2 - 3\hbar)\right] + A^{\frac{1}{2}}e^{-\frac{m\omega x^2}{2\hbar}}x\left(\frac{m\omega^2x^2}{2}\right)]$$

$$= A^{\frac{1}{2}}e^{-\frac{m\omega x^2}{2\hbar}}x\left[\frac{3\hbar\omega}{2}\right]$$

$$= \frac{3\hbar\omega}{2}\psi(x) = C\psi(x)$$, where C is a constant

If this is true, then $E = C = \frac{3\hbar\omega}{2}$

* The second harmonic normalized wave function is $\psi_1 = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}}\sqrt{2}\,x\,e^{-x^2/2}$, $\alpha = \frac{m\omega}{\hbar}$, $y = \sqrt{\alpha}x$

which is in the same form but different pre factor.

SQ13)

(a) $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$ Normalization condition

$$\boxed{\frac{d}{da} e^{-ax^2} = -x^2 e^{-ax^2} \Rightarrow x^2 e^{-ax^2} = -\frac{d}{da} e^{-ax^2}}$$

$\int_{-\infty}^{\infty} A x^2 e^{-\frac{m\omega x^2}{\hbar}} dx = 1$, let $a = \frac{m\omega}{\hbar}$

$$\boxed{\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}}$$

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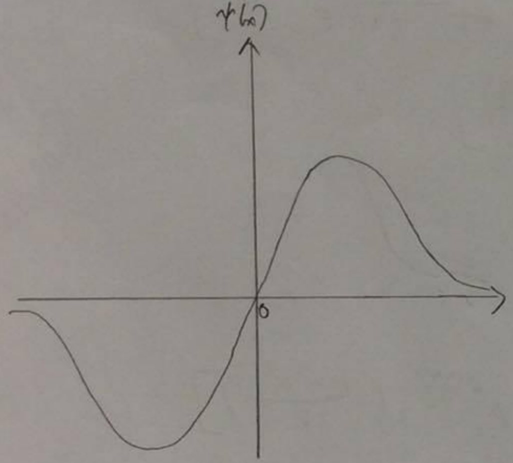
$$A \int_{-\infty}^{\infty} -\frac{d}{da} e^{-ax^2} dx = -A \frac{d}{da} \sqrt{\frac{\pi}{a}}$$

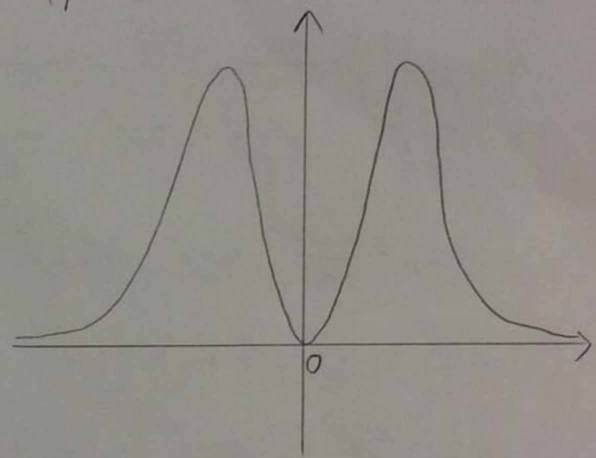
$$= -A\sqrt{\pi}\left(-\frac{1}{2}\right) a^{-\frac{3}{2}}$$

$$= \frac{A\sqrt{\pi}}{2}\left(\frac{m\omega}{\hbar}\right)^{-\frac{3}{2}} = 1$$

$$A = \frac{2}{\sqrt{\pi}}\left(\frac{m\omega}{\hbar}\right)^{\frac{3}{2}}$$

(b) $\psi(x) = A^{\frac{1}{2}} x e^{-\frac{m\omega x^2}{2\hbar}}$ $|\psi(x)|^2 = A x^2 e^{-\frac{m\omega x^2}{\hbar}}$





(c) $\langle x \rangle = \int_{-\infty}^{\infty} x |\psi(x)|^2 dx = \int_{-\infty}^{\infty} A x^3 e^{-\frac{m\omega x^2}{\hbar}} dx = 0$ As this is odd function

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx = \int_{-\infty}^{\infty} A x^4 e^{-\frac{m\omega x^2}{\hbar}} dx$$

$$\boxed{\frac{d^2}{da^2} e^{-ax^2} = x^4 e^{-ax^2}}$$

$$= \frac{d^2}{da^2} A \int_{-\infty}^{\infty} e^{-ax^2} dx$$

$$= A \frac{d^2}{da^2} \sqrt{\frac{\pi}{a}}$$

$$= A\sqrt{\pi}\left(-\frac{1}{2}\right)\left(-\frac{3}{2}\right) a^{-\frac{5}{2}}$$

$$= A\sqrt{\pi}\, \frac{3}{4}\left(\frac{m\omega}{\hbar}\right)^{-\frac{5}{2}}$$

$$(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{2}{\sqrt{\pi}} \sqrt{\pi}\, \frac{3}{4}\left(\frac{m\omega}{\hbar}\right)^{\frac{3}{2}}\left(\frac{m\omega}{\hbar}\right)^{-\frac{5}{2}}$$

$$= \frac{3}{2}\left(\frac{\hbar}{m\omega}\right)$$

(d) The physics will be the same but the coordinate $x' = x - x_0$.