Problem Set 2: Operator Formalism

PYL101 Solutions

1 (iii) $[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$

$$\begin{aligned} \text{RHS} &= \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B} \\ &= \hat{A}(\hat{B}\hat{C} - \hat{C}\hat{B}) + (\hat{A}\hat{C} - \hat{C}\hat{A})\hat{B} \\ &= \underline{\hat{A}\hat{B}}\hat{C} - \cancel{\hat{A}\hat{C}\hat{B}} + \cancel{\hat{A}\hat{C}\hat{B}} - \hat{C}\underline{\hat{A}\hat{B}} \\ &= [\hat{A}\hat{B}, \hat{C}] = \text{LHS} \end{aligned}$$

Proved.

2. $\langle (\Delta A)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2$

$$\Delta A = A - \langle A \rangle$$

$$\Rightarrow (\Delta A)^2 = (A - \langle A \rangle)^2 = A^2 - 2A\langle A \rangle + \langle A \rangle^2$$

$$\begin{aligned} \Rightarrow \langle (\Delta A) \rangle^2 &= \langle A^2 - 2A\langle A \rangle + \langle A \rangle^2 \rangle \\ &= \langle A^2 \rangle - 2\langle A \rangle^2 + \langle A \rangle^2 \\ &= \langle A^2 \rangle - \langle A \rangle^2 \end{aligned}$$

Proved.

3 (ii) Ehrenfest theorem

$$\frac{\partial}{\partial t}\langle p_x \rangle = -\left\langle \frac{\partial V}{\partial x} \right\rangle$$

$$\langle p_x \rangle = \int_{-\infty}^{\infty} dx\, \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right)\psi = -i\hbar \int_{-\infty}^{\infty} dx\, \psi^* \frac{\partial \psi}{\partial x}$$

Taking time derivative

$$\frac{\partial}{\partial t}\langle p_x \rangle = -i\hbar \int_{-\infty}^{\infty} dx \left(\frac{\partial \psi^*}{\partial t} \frac{\partial \psi}{\partial x} + \psi^* \frac{\partial^2 \psi}{\partial t\, \partial x} \right) \longrightarrow (1)$$

Also, from time-dependent Schrödinger equation,

$$i\hbar \frac{\partial \psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \right)\psi \longrightarrow (2)$$

Differentiating (2) w.r.t. x

$$\frac{\partial^2 \psi}{\partial x\, \partial t} = \frac{1}{i\hbar}\left\{ -\frac{\hbar^2}{2m} \frac{\partial^3}{\partial x^3}\psi + \frac{\partial}{\partial x}(V\psi) \right\} \longrightarrow (3)$$

Taking complex conjugate of (2)

$$-i\hbar \frac{\partial \psi^*}{\partial t} = \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V \right)\psi^* \longrightarrow (4)$$

Substituting ③ and ④ in ①:

$$\frac{\partial}{\partial t}\langle p_x\rangle = -i\hbar\int_{-\infty}^{\infty} dx\left(\frac{1}{-i\hbar}\right)\left[\left(-\frac{\hbar^2}{2m}\frac{\partial^2\psi^*}{\partial x^2}+V\psi^*\right)\frac{\partial\psi}{\partial x}-\psi^*\left(-\frac{\hbar^2}{2m}\frac{\partial^3\psi}{\partial x^3}\right.\right.$$
$$\left.\left.+\frac{\partial}{\partial x}(V\psi)\right)\right]$$

$$=\int_{-\infty}^{\infty} dx\left[\left(-\frac{\hbar^2}{2m}\right)\left(\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x}-\psi^*\frac{\partial^3\psi}{\partial x^3}\right)+V\psi^*\frac{\partial\psi}{\partial x}-\psi^*\frac{\partial}{\partial x}(V\psi)\right]$$

Adding and subtracting $\frac{\partial\psi^*}{\partial x}\frac{\partial^2\psi}{\partial x^2}\left(-\frac{\hbar^2}{2m}\right)$:

$$=-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx\left(\frac{\partial^2\psi^*}{\partial x^2}\frac{\partial\psi}{\partial x}+\frac{\partial\psi^*}{\partial x}\frac{\partial^2\psi}{\partial x^2}-\frac{\partial\psi^*}{\partial x}\frac{\partial^2\psi}{\partial x^2}-\psi^*\frac{\partial^3\psi}{\partial x^3}\right)$$
$$+\int_{-\infty}^{\infty} dx\left[\cancel{V\psi^*\frac{\partial\psi}{\partial x}}-\psi^*\frac{\partial V}{\partial x}\psi-\cancel{\psi^* V\frac{\partial\psi}{\partial x}}\right]$$

[∵ V is scalar]

$$=-\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} dx\,\frac{\partial}{\partial x}\left(\frac{\partial\psi^*}{\partial x}\frac{\partial\psi}{\partial x}-\psi^*\frac{\partial^2\psi}{\partial x^2}\right)+\int_{-\infty}^{\infty} dx\,\psi^*\left(-\frac{\partial V}{\partial x}\right)\psi$$

$$=-\frac{\hbar^2}{2m}\left[\frac{\partial\psi^*}{\partial x}\cancelto{0}{\frac{\partial\psi}{\partial x}}-\psi^*\cancelto{0}{\frac{\partial^2\psi}{\partial x^2}}\right]_{-\infty}^{\infty}+\int_{-\infty}^{\infty} dx\,\psi^*\left(-\frac{\partial V}{\partial x}\right)\psi$$

For any well-behaved practically feasible wavefunction,
as $x\to\infty,-\infty$,
$\psi,\ \frac{\partial\psi}{\partial x}\to 0$ [$\psi\to 0$ for normalizability; $\frac{\partial\psi}{\partial x}\to 0$ assuming $\frac{\partial\psi}{\partial x}$ is continuous]

∴ The first integral reduces to zero.

$$\Rightarrow \frac{\partial}{\partial t}\langle p_x\rangle=\int_{-\infty}^{\infty} dx\,\psi^*\left(-\frac{\partial V}{\partial x}\right)\psi$$

$$\Rightarrow \boxed{\frac{\partial\langle p_x\rangle}{\partial t}=\left\langle-\frac{\partial V}{\partial x}\right\rangle}$$

Proved.

4. We will use the general form of position-momentum uncertainty principle:

$$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle \geqslant \frac{\hbar^2}{4} + \langle \Delta x \Delta p + \Delta p \Delta x\rangle^2$$

For the above inequality to become an equality, two conditions have to be satisfied:

① $\hat{\Delta P}\,\psi = c\,\hat{\Delta X}\,\psi$ (where c is a scalar)

② $\langle \Delta x \Delta p + \Delta p \Delta x\rangle = 0$ for minima

Now, $(\hat{P} - \langle P\rangle)\psi = c(\hat{X} - \langle X\rangle)\psi$

$$\Rightarrow \hat{P}\psi = \langle P\rangle\psi + c(\hat{X} - \langle X\rangle)\psi$$

$$\Rightarrow -i\hbar\frac{\partial\psi}{\partial x} = \{\langle P\rangle + c(\hat{X} - \langle X\rangle)\}\psi$$

$[\because \hat{X}\psi = x\psi]$

$$\Rightarrow \frac{1}{\psi}\frac{\partial\psi}{\partial x} = \frac{i}{\hbar}\{\langle P\rangle + c(x - \langle X\rangle)\}$$

$$\boxed{\psi = \psi_0 \exp\left(\frac{i\langle P\rangle x}{\hbar}\right)\exp\left(\frac{ic\,(x - \langle X\rangle)^2}{2\hbar}\right)} \longrightarrow ①$$

Also, $(\hat{P} - \langle P\rangle)\psi = c(\hat{X} - \langle X\rangle)\psi \longrightarrow ②$

Taking complex conjugate of ②:

$$\psi^*(\hat{P} - \langle P\rangle) = c^*\psi^*(\hat{X} - \langle X\rangle) \longrightarrow ③$$

From second condition:

$$\langle \Delta x \Delta p + \Delta p \Delta x\rangle = 0$$

$$\Rightarrow \int_{-\infty}^{\infty} dx\, \psi^*[(\hat{X} - \langle X\rangle)(\hat{P} - \langle P\rangle) + (\hat{P} - \langle P\rangle)(\hat{X} - \langle X\rangle)]\psi = 0$$

$$\Rightarrow \int_{-\infty}^{\infty} dx\left[\psi^*(\hat{X} - \langle X\rangle)(\hat{P} - \langle P\rangle)\psi + \psi^*(\hat{P} - \langle P\rangle)(\hat{X} - \langle X\rangle)\psi\right] = 0$$

Using ② and ③

$$\Rightarrow \int_{-\infty}^{\infty} dx\left[c\psi^*(\hat{X} - \langle X\rangle)^2\psi + c^*\psi^*(\hat{X} - \langle X\rangle)^2\psi\right] = 0$$

$$\Rightarrow (c + c^*)\langle(\hat{X} - \langle X\rangle)^2\rangle = 0$$

$\Rightarrow c = -c^* \Rightarrow c$ is purely imaginary $\Rightarrow c = i|c| \longrightarrow ④$

Substituting ④ in ①:

$$\psi = \psi_0 \exp\left(\frac{i\langle P\rangle x}{\hbar}\right)\exp\left(-\frac{|c|\,(x - \langle X\rangle)^2}{2\hbar}\right)$$ which is a Gaussian waveform.