



Quantum Mechanics in Medicine

Presented by

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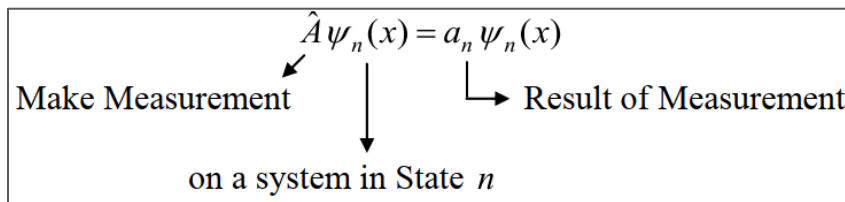
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Third-year students

chapter two: Exercises and examples (Part 1)

Physical Operator

Dynamical Variable	In Classical Mechanics	In Quantum Mechanics- 3D	In Quantum Mechanics- 1D
Position	$\vec{r}, \quad x, y, z$	$\hat{\mathbf{r}}$	$\hat{x}, \quad \hat{y}, \quad \hat{z}$
Momentum	$\vec{p} = m\vec{v},$ $p_x = m\dot{x}$	$\hat{\mathbf{p}} = -i\hbar\nabla$	$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$
Kinetic energy	$T = \frac{p^2}{2m}$	$\hat{T} = \frac{\hat{\mathbf{p}}^2}{2m} = \frac{-\hbar^2}{2m} \nabla^2$	$\hat{T}_x = \frac{\hat{p}_x^2}{2m} = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$
Total energy	$E = T + V$	$\hat{E} = i\hbar \frac{\partial}{\partial t}$	
Hamilton	$H = T + V$	$\hat{H} = \frac{-\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, t)$	$\hat{H}_x = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x, t)$



a_n : eigen value of the operator $\hat{A}$

$\Psi(x)$: eigen function of the operator $\hat{A}$

Eigen value equation

Example 1: By using the eigen value equation show that the function $\Psi(x) = e^{-4x}$ is an eigen function of the operator $\hat{A} = \frac{\partial}{\partial x}$

Solution:

$$\hat{A}\Psi(x) = \frac{\partial}{\partial x}(e^{-4x})$$

$$= -4e^{-4x}$$

$$\hat{A}\Psi(x) = a\Psi(x)$$

Then,

$a = -4$ is the eigen value to the operator $\hat{A} = \frac{\partial}{\partial x}$

$\Psi(x) = e^{-4x}$ is the eigen function to the operator $\hat{A}$

Example 2: By using the eigen value equation show that the function $\Psi(x) = \cos(4x)$ is an eigen function of the operator $-\frac{\partial^2}{\partial x^2}$

$$\hat{A}\Psi(x) = -\frac{\partial^2}{\partial x^2} \cos(4x)$$

$$\hat{A}\Psi(x) = -\frac{\partial}{\partial x} \left(\frac{\partial}{\partial x} \cos(4x) \right) = 4 \frac{\partial}{\partial x} \sin(4x) = 16 \cos(4x)$$

$a = 16$ is the eigen value to the operator $\hat{A} = -\frac{\partial^2}{\partial x^2}$

$\Psi(x) = \cos(4x)$ is the eigen function to the operator $\frac{\partial^2}{\partial x^2}$

Example 3: Prove that, the function $\Psi(x) = Ae^{-\alpha x}$ is an eigen function of the operator $\hat{F}$

$$\hat{F} = \frac{d^2}{dx^2} + \frac{2}{x} \frac{d}{dx} + \frac{2\alpha}{x}$$

Where A, α are constant

Solution:

$$\hat{F}\psi = \frac{d^2}{dx^2} (Ae^{-\alpha x}) + \frac{2}{x} \frac{d}{dx} (Ae^{-\alpha x}) + \frac{2\alpha}{x} (Ae^{-\alpha x})$$

$$\hat{F}\psi = \alpha^2 (Ae^{-\alpha x}) - \frac{2\alpha}{x} (Ae^{-\alpha x}) + \frac{2\alpha}{x} (Ae^{-\alpha x})$$

$$\hat{F}\psi = \alpha^2 (Ae^{-\alpha x})$$

$$\hat{F}\psi = \alpha^2 \psi \quad \therefore Ae^{-\alpha x} \text{ is an eigen function of the operator } \hat{F}$$

Example 4: Verify the following operator equation $\left(\frac{d}{dy} - y\right) \left(\frac{d}{dy} + y\right) = \left(\frac{d^2}{dy^2} - y^2 + 1\right)$

$$\left(\frac{d}{dy} - y\right) \left(\frac{d}{dy} + y\right) \psi(y) = \left(\frac{d}{dy} - y\right) \left\{ \left(\frac{d}{dy} + y\right) \psi(y) \right\}$$

$$= \left(\frac{d}{dy} - y\right) \left\{ \frac{d\psi(y)}{dy} + y\psi(y) \right\}$$

$$= \frac{d}{dy} \left\{ \frac{d\psi(y)}{dy} + y\psi(y) \right\} - y \left\{ \frac{d\psi(y)}{dy} + y\psi(y) \right\}$$

$$\begin{aligned}
&= \left\{ \frac{d^2\psi(y)}{dy^2} + \frac{d}{dy}(y\psi(y)) \right\} - \left\{ y \frac{d\psi(y)}{dy} + y^2\psi(y) \right\} \\
&= \frac{d^2\psi(y)}{dy^2} + y \frac{d\psi(y)}{dy} + \psi(y) - y \frac{d\psi(y)}{dy} - y^2\psi(y) \\
&= \frac{d^2\psi(y)}{dy^2} + \psi(y) - y^2\psi(y) \\
&= \left(\frac{d^2}{dy^2} + 1 - y^2 \right) \psi(y) \\
&\therefore \left(\frac{d}{dy} - y \right) \left(\frac{d}{dy} + y \right) = \left(\frac{d^2}{dy^2} - y^2 + 1 \right)
\end{aligned}$$

Normalization and expectation value

Example 5: Suppose that a particle moves in x direction for the interval $(0 \leq x \leq 0.3)$, Calculate the normalization constant for the wave function $\psi(x) = Ae^{3ix}$

The normalization condition is,

$$\begin{aligned}
\int \psi^*(x)\psi(x)dx &= 1 \\
\int_0^{0.3} A^*e^{-3ix}Ae^{3ix}dx &= 1 \\
|A|^2 \int_0^{0.3} dx &= 1 \\
|A|^2(0.3) &= 1 \\
|A| &= \frac{1}{\sqrt{0.3}} \\
\psi(x) &= \frac{1}{\sqrt{0.3}}e^{3ix}
\end{aligned}$$

Example 5: If $\psi(x, t) = A(ax - x^2)$ is a normalized wave function in the period $0 \leq x \leq a$ find:

- 1- The normalization constant
- 2- The expectation value of the position in x-direction $\langle x \rangle$

Solution

$$\int |\psi(x)|^2 dx = 1$$

$$\int_0^a |A|^2 (ax - x^2)^2 dx = 1$$

$$|A|^2 \int_0^a (a^2 x^2 - 2ax^3 + x^4) dx = 1$$

$$|A|^2 \left[a^2 \frac{x^3}{3} - 2a \frac{x^4}{4} + \frac{x^5}{5} \right]_0^a = 1$$

$$|A|^2 \left[\frac{a^5}{3} - \frac{a^5}{2} + \frac{a^5}{5} \right] = 1$$

$$|A|^2 \frac{a^5}{30} = 1 \quad A = \sqrt{\frac{30}{a^5}}$$

$$\psi(x) = \sqrt{\frac{a^5}{30}} (ax - x^2)$$

(2)

$$\langle x \rangle = \int_0^a \psi^* \hat{x} \psi dx = \int_0^a \left(\sqrt{\frac{a^5}{30}} (ax - x^2) \right)^* x \left(\sqrt{\frac{a^5}{30}} (ax - x^2) \right) dx$$

$$= \frac{a^5}{30} \int_0^a (ax - x^2)^2 dx$$

$$\begin{aligned}
 &= \frac{30}{a^5} \int_0^a x (ax - x^2)^2 dx = \frac{30}{a^5} \int_0^a (a^2 x^3 - 2ax^4 + x^5) dx \\
 &= \frac{30}{a^5} \left[a^2 \frac{x^4}{4} - 2a \frac{x^5}{5} + \frac{x^6}{6} \right]_0^a = \frac{30}{a^5} \left[\frac{a^6}{4} - 2 \frac{a^6}{5} + \frac{a^6}{6} \right] = \frac{30}{a^5} \frac{a^6}{60} = \frac{a}{2} \\
 \langle x \rangle &= \frac{a}{2}
 \end{aligned}$$

Example 6: Normalize the wave function $\psi(x, t) = A e^{-\frac{(x-x_0)^2}{2a^2}} e^{-ip_0 x/\hbar}$

$$\psi(x) = A e^{-\frac{(x-x_0)^2}{2a^2}} e^{ip_0 x/\hbar}, \quad \psi^*(x) = A e^{-\frac{(x-x_0)^2}{2a^2}} e^{-ip_0 x/\hbar}$$

$$|\psi(x)|^2 = AA^* e^{-\frac{(x-x_0)^2}{a^2}}$$

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

$$AA^* \int_{-\infty}^{\infty} e^{-\frac{(x-x_0)^2}{a^2}} dx = 1 \quad \text{let } (x - x_0) = z \Rightarrow dx = dz$$

$$AA^* \int_{-\infty}^{\infty} e^{-\frac{z^2}{a^2}} dz = 1$$

$$AA^* \int_{-\infty}^{\infty} e^{-\frac{z^2}{a^2}} dz = 2 \int_0^{\infty} e^{-\frac{z^2}{a^2}} dz = a\sqrt{\pi}$$

Usefull integral $\int_0^{\infty} x^n e^{-ax^2} dx = \frac{1}{2a^{\frac{n+1}{2}}} \Gamma\left(\frac{n+1}{2}\right) \quad \Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$

$$AA^* a\sqrt{\pi} = 1$$

$$AA^* = \frac{1}{a\sqrt{\pi}}$$

If A is real then $A = A^* = \left(\frac{1}{a\sqrt{\pi}}\right)^{\frac{1}{2}}$

Example 7: Suppose that a particle moves in x direction for the period $(0 \leq x \leq 0.5)$, in the wave function $\Psi(x) = Ae^{ix^2}$ find:

1- normalization constant.

2- The expectation value of $\langle x \rangle$, $\langle p_x \rangle$, $\langle T_x \rangle$

$$\int \psi^*(x)\psi(x)dx = 1$$

$$\int_0^{0.5} A^* e^{-ix^2} A e^{ix^2} dx = 1$$

$$|A|^2 \int_0^{0.5} dx = 1$$

$$A = \sqrt{2}$$

$$\langle x \rangle = \int \psi^* x \psi dx = \int_0^{0.5} \sqrt{2} e^{-ix^2} x \sqrt{2} e^{ix^2} dx = 2 \int_0^{0.5} x dx = \frac{1}{4}$$

$$\langle p_x \rangle = \int \psi^* \hat{p}_x \psi dx = \int_0^{0.5} \sqrt{2} e^{-ix^2} \left(-i\hbar \frac{\partial}{\partial x}\right) \sqrt{2} e^{ix^2} dx$$

$$\langle p_x \rangle = -i2\hbar \int_0^{0.5} e^{-ix^2} (2ix) e^{ix^2} dx = 4\hbar \int_0^{0.5} x dx$$

$$\langle p_x \rangle = \frac{\hbar}{2}$$

H.W. Find $\langle T_x \rangle$

H.W. : Suppose that a particle moves in the interval $(0 \leq x \leq 2)$, if the probability density is given by, $|\Psi|^2 = \frac{15}{16} \left(x^2 - \frac{x^4}{4}\right)$, Find the expectation value of the position $\langle x \rangle$.