Quantum Mechanics in Medicine

Presented by

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The Properties of Operators

1- linear operator

i. $\hat{A}(\psi_1 + \psi_2) = \hat{A}\psi_1 + \hat{A}\psi_2$

ii. $\hat{A}(a\psi) = a\hat{A}\psi$ $\quad a$ is constant

2- Commutation

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

If the operator $\hat{C} = 0$ or $[\hat{A}, \hat{B}] = 0$ then $\hat{C}$ is called Commutator operator, and $\hat{A}, \hat{B}$ are called Commute operators

If $\hat{C} \neq 0 \quad \Rightarrow [\hat{A}, \hat{B}] \neq 0$

$$\hat{A}\hat{B} - \hat{B}\hat{A} \neq 0$$

$\hat{A}\hat{B} \neq \hat{B}\hat{A}$ Not commutator operator

3- Unit operator

If the operator $\hat{C} = 1$ then $\hat{C}$ is called Unit operator.

<u>Example 8:</u> Prove that the operator $\hat{C} = \left[\frac{\partial}{\partial x}, x\right]$ is Unit operator.

Solution:

If the operator $\hat{C} = 1$ then $\hat{C}$ is called Unit operator

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

$$= \hat{A}\hat{B} - \hat{B}\hat{A}$$

$$\hat{C} = [\frac{\partial}{\partial x}, x] = \frac{\partial}{\partial x}x - x\frac{\partial}{\partial x}$$

$$\hat{C}\psi(x) = \left\{\frac{\partial}{\partial x}x - x\frac{\partial}{\partial x}\right\}\psi(x)$$

$$= \frac{\partial}{\partial x}x(\psi(x)) - x\frac{\partial}{\partial x}(\psi(x))$$

$$= \psi(x) + x\frac{\partial\psi(x)}{\partial x} - x\frac{\partial\psi(x)}{\partial x}$$

$$\hat{C}\psi(x) = \psi(x)$$

$$\hat{C} = 1$$

H.W.

Prove that $\hat{C} = [x , \frac{\partial}{\partial x}] = -1$

Example: Show that $[\hat{x}, \hat{p}_x] = i\hbar$

Solution:

$$\hat{c} = [\hat{x}, \hat{p}_x]$$

$$\hat{c} = \hat{x}\,\hat{p}_x - \hat{p}_x\hat{x}$$

$$\hat{c} = \hat{x}(-i\hbar\frac{\partial}{\partial x}) + i\hbar\frac{\partial}{\partial x}(\hat{x})$$

$$\hat{c}\,\psi(x) = \left\{\hat{x}(-i\hbar\frac{\partial}{\partial x}) + i\hbar\frac{\partial}{\partial x}(\hat{x})\right\}\psi(x)$$

$$\hat{c}\,\psi(x) = \hat{x}(-i\hbar\frac{\partial\psi(x)}{\partial x}) + i\hbar\frac{\partial}{\partial x}\hat{x}\,\psi(x)$$

$$\hat{c}\psi(x) = x\left(-i\hbar\frac{\partial\psi(x)}{\partial x}\right) + i\hbar\frac{\partial}{\partial x}\left(x\psi(x)\right)$$

$$\hat{c}\psi(x) = -i\hbar x\frac{\partial\psi(x)}{\partial x} + i\hbar\psi(x) + i\hbar x\frac{\partial\psi(x)}{\partial x}$$

$$\hat{c}\psi(x) = i\hbar\psi(x)$$

$i\hbar$ is the eigen value to the operator $\hat{c}$

Example 10: Show that $[\hat{H}, \hat{x}] = \frac{-i\hbar}{m}\hat{p}_x$

$[\hat{H} , \hat{x}] = \hat{H}\,\hat{x} - \hat{x}\,\hat{H}$ Where $\hat{H} = \frac{-\hbar^2}{2m}\nabla^2 + V(x,y,z)$ and

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$[\hat{H} , \hat{x}]\psi = (\hat{H}\,\hat{x} - \hat{x}\,\hat{H})\,\psi$$

$$\left[\hat{H},\hat{x}\right]\psi=\left\{\left(\frac{-\hbar^2}{2m}\nabla^2+V(x,y,z)\right)x-x\left(\frac{-\hbar^2}{2m}\nabla^2+V(x,y,z)\right)\right\}\psi$$

$$=-\frac{\hbar^2}{2m}\nabla^2 x\psi+V(x,y,z)\,x\psi+x\frac{\hbar^2}{2m}\nabla^2\psi-xV(x,y,z)\psi$$

$$=-\frac{\hbar^2}{2m}\nabla^2 x\psi+x\frac{\hbar^2}{2m}\nabla^2\psi$$

By using,

$$\boldsymbol{\nabla}=\hat{\imath}\frac{\partial}{\partial x}+\hat{\jmath}\frac{\partial}{\partial y}+\hat{k}\frac{\partial}{\partial z}$$

$$\nabla^2 x\psi=\boldsymbol{\nabla}\cdot(\boldsymbol{\nabla}x\psi)=\boldsymbol{\nabla}\cdot(x\boldsymbol{\nabla}\psi+\hat{\imath}\psi)=x\nabla^2\psi+\hat{\imath}\frac{\partial\psi}{\partial x}+\hat{\imath}\frac{\partial\psi}{\partial x}=x\nabla^2\psi+\hat{\imath}2\frac{\partial\psi}{\partial x}$$

$$\left[\hat{H},\hat{x}\right]\psi=\frac{\hbar^2}{2m}\left(-x\,\nabla^2\psi-2\frac{\partial\psi}{\partial x}+x\,\nabla^2\psi\right)$$

$$\left[\hat{H},\hat{x}\right]=-\frac{\hbar^2}{m}\frac{\partial\psi}{\partial x}=\frac{-i\hbar}{m}\left(-i\hbar\frac{\partial\psi}{\partial x}\right)=\frac{-i\hbar}{m}\hat{p}_x$$

4- Variance

The deviation in the measured of the operator $\hat{A}$ from its expected value $\langle A\rangle$

$\Delta A=\sqrt{\langle(A-\langle A\rangle)^2\rangle}$

Prove that $\Delta A=\sqrt{\langle(A-\langle A\rangle)^2\rangle}=\sqrt{\langle A^2\rangle-\langle A\rangle^2}$

$$(\Delta A)^2=\langle(A-\langle A\rangle)^2\rangle=\int\psi^*(A-\langle A\rangle)^2\psi\,dr$$

$$=\int\psi^*(A^2-2A\langle A\rangle+\langle A\rangle^2)\psi\,dr$$

$$=\int\psi^*A^2\psi\,dr-\int\psi^*2A\langle A\rangle\psi\,dr+\int\psi^*\langle A\rangle^2\psi\,dr$$

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

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

So that $\Delta A=\sqrt{\langle A^2\rangle-\langle A\rangle^2}$

1- The variance in position

$$(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2$$

$$\langle x^2\rangle = \int \psi^* \hat{x}^2 \psi \, dx$$

$$\langle x\rangle^2 = (\int \psi^* \hat{x}\, \psi \, dx)^2$$

2- The variance in momentum

$$(\Delta p_x)^2 = \langle p_x^2\rangle - \langle p_x\rangle^2$$

$$\langle p_x^2\rangle = \int \psi^* p_x^2 \psi \, dx$$

$$\langle p_x\rangle^2 = (\int \psi^* p_x \psi \, dx)^2$$

Or

$$\Delta x = \left\langle (x - \langle x\rangle)^2 \right\rangle^{1/2}, \ \Delta p = \left\langle (p - \langle p\rangle)^2 \right\rangle^{1/2}$$

<u>Example 11</u>: Consider a particle of mass *m*, in the quantum state $\psi(x,t) = Ae^{-a(mx^2 - it)/\hbar}$

Where *a*, *A* are constant. Prove that, $\Delta x \Delta p_x \geq \frac{\hbar}{2}$

Solution:

First, Normalize the wave function,

$$\int_{-\infty}^{\infty} \psi^*(x,t)\, \psi(x,t)\, dx = 1$$

$$\int_{-\infty}^{\infty} \left(A^* e^{-a(mx^2 + it)/\hbar}\right) \left(Ae^{-a(mx^2 - it)/\hbar}\right) dx = 1$$

$$|A|^2 \int_{-\infty}^{\infty} \left(e^{\frac{-2amx^2}{\hbar}}\right) dx = 2|A|^2 \int_{0}^{\infty} \left(e^{\frac{-2amx^2}{\hbar}}\right) dx = 1$$

Let $\alpha = \frac{2am}{\hbar}$

$$2|A|^2 \int_0^{\infty} \left(e^{-\alpha x^2}\right) dx = 1$$

Usefull integral $\displaystyle \int_0^{\infty} x^n e^{-\alpha x^2} dx = \frac{1}{2\, \alpha^{\frac{n+1}{2}}} \Gamma\left(\frac{n+1}{2}\right)$ $\qquad \Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$

$$\therefore \int_0^{\infty} \left(e^{-\alpha x^2}\right) dx = \frac{1}{2}\sqrt{\frac{\pi}{\alpha}}$$

Then

$$|A|^2 \sqrt{\frac{\pi}{\alpha}} = 1$$

$|A|^2 = \sqrt{\frac{\alpha}{\pi}}$ *and the normalize constant is* $|A| = \left(\frac{2am}{\pi\hbar}\right)^{\frac{1}{4}}$

$\langle x\rangle = \int_{-\infty}^{\infty} \psi^*(x,t)\hat{x}\, \psi(x,t)\, dx = \int_{-\infty}^{\infty}\left(|A|e^{-a(mx^2+it)/\hbar}\right)x\left(|A|e^{-a(mx^2-it)/\hbar}\right) dx$

$\langle x\rangle = |A|^2 \int_{-\infty}^{\infty}\left(e^{\frac{-2amx^2}{\hbar}}\right)x\ \ dx = 0$ (Integral of odd function)

$\langle x\rangle = 0$

$\langle x^2\rangle = \int_{-\infty}^{\infty} \psi^*(x,t)x^2\, \psi(x,t)\, dx = \int_{-\infty}^{\infty}\left(|A|e^{-a(mx^2+it)/\hbar}\right)x^2\left(|A|e^{-a(mx^2-it)/\hbar}\right) dx$

$\langle x^2\rangle = |A|^2 \int_{-\infty}^{\infty}\left(e^{-\alpha x^2}\right)x^2\ \ dx = 2|A|^2\int_{0}^{\infty}\left(e^{-\alpha x^2}\right)x^2\ \ dx$

From table of integrals $\int_{0}^{\infty}\left(e^{-\alpha x^2}\right)x^2\ \ dx = \frac{1}{4\alpha}\sqrt{\frac{\pi}{\alpha}}$

$\langle x^2\rangle = |A|^2\frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}} = \sqrt{\frac{\alpha}{\pi}}\,\frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}} = \frac{1}{2\alpha} = \frac{\hbar}{4am}$

$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} = \sqrt{\frac{\hbar}{4am} - 0} = \sqrt{\frac{\hbar}{4am}}$

$\langle p_x\rangle = m\frac{d}{dt}\langle x\rangle = 0$ *(becouse* $\langle x\rangle = 0$)

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

$= -\hbar^2\int_{-\infty}^{\infty} \psi^*(x,t)\frac{\partial^2}{\partial x^2}\psi(x,t)\, dx = -\hbar^2\int_{-\infty}^{\infty}\left(|A|e^{-\frac{a(mx^2+it)}{\hbar}}\right)\frac{\partial^2}{\partial x^2}\left(|A|e^{-\frac{a(mx^2-it)}{\hbar}}\right) dx$

$= -\hbar^2\sqrt{\frac{\alpha}{\pi}}\int_{-\infty}^{\infty}\left(e^{-\frac{\alpha x^2}{2}-i\frac{at}{\hbar}}\right)\frac{\partial^2}{\partial x^2}\left(e^{-\frac{\alpha x^2}{2}+i\frac{at}{\hbar}}\right) dx$

$= -\hbar^2\sqrt{\frac{\alpha}{\pi}}\int_{-\infty}^{\infty}\left(e^{-\frac{\alpha x^2}{2}-i\frac{at}{\hbar}}\right)\frac{d}{dx}\left(\frac{d}{dx}e^{-\frac{\alpha x^2}{2}+i\frac{at}{\hbar}}\right) dx$

$= -\hbar^2\sqrt{\frac{\alpha}{\pi}}\int_{-\infty}^{\infty}\left(e^{-\frac{\alpha x^2}{2}-i\frac{at}{\hbar}}\right)\frac{d}{dx}\left(-\alpha x\, e^{-\frac{\alpha x^2}{2}+i\frac{at}{\hbar}}\right) dx$

$= -\hbar^2\sqrt{\frac{\alpha}{\pi}}\int_{-\infty}^{\infty}\left(e^{-\frac{\alpha x^2}{2}-i\frac{at}{\hbar}}\right)((\alpha x)^2 - \alpha)e^{-\frac{\alpha x^2}{2}+i\frac{at}{\hbar}}\, dx$

$$= -2\hbar^2\alpha\sqrt{\frac{\alpha}{\pi}}\left[\int_0^{\infty} \alpha x^2\, e^{-\alpha x^2}\ dx - \int_0^{\infty} e^{-\alpha x^2}\ dx\right]$$

From $\Gamma -$ integrals $\int_0^{\infty} e^{-\alpha x^2} x^2\ dx = \frac{1}{4\alpha}\sqrt{\frac{\pi}{\alpha}}$ and $\int_0^{\infty}\left(e^{-\alpha x^2}\right)\ dx = \frac{1}{2}\sqrt{\frac{\pi}{\alpha}}$

$$\langle p_x^2\rangle = -2\hbar^2\alpha\sqrt{\frac{\alpha}{\pi}}\left[\frac{1}{4}\sqrt{\frac{\pi}{\alpha}} - \frac{1}{2}\sqrt{\frac{\pi}{\alpha}}\right] = -2\hbar^2\alpha\left[\frac{1}{4} - \frac{1}{2}\right] = \hbar am$$

$$\Delta p_x = \sqrt{\langle p_x^2\rangle - \langle p_x\rangle^2} = \sqrt{\hbar am}$$

$$\Delta p_x \Delta x = \sqrt{\hbar am}\ \sqrt{\frac{\hbar}{4am}} = \frac{\hbar}{2}$$

Hermitian operator

If the operator $\hat{A}$ satisfy the condition $\int \boldsymbol{\psi^* \hat{A} \psi\ dr} = \int \left(\boldsymbol{\hat{A}\psi}\right)^* \boldsymbol{\psi\ dr}$ is called Hermitian operator.

<u>**Example 12**</u>**:** Prove that p_x is Hermitian operator?

Operator $\hat{p}_x$ is said to be Hermitian when satisfying the relation:

$$\int \psi^* \hat{p}_x \psi\ dx = \int (\hat{p}_x \psi)^* \psi\ dx$$

$$\int_{-\infty}^{\infty} \psi^* \hat{p}_x \psi\ dx \int_{-\infty}^{\infty} \psi^* \left(-i\hbar\frac{\partial}{\partial x}\right)\psi\ dx = -i\hbar\int_{-\infty}^{\infty} \psi^* \left(\frac{\partial}{\partial x}\right)\psi\ dx$$

using integration by parts method, let $\psi^* = u$, $\frac{\partial \psi}{\partial x} dx = dv$

$$\int_{-\infty}^{\infty} u\, dv = uv\big|_{-\infty}^{+\infty} - \int_{-\infty}^{\infty} v\, du$$

Then, $v = \psi$, $du = \frac{\partial \psi^*}{\partial x} dx$

$$-i\hbar\int_{-\infty}^{\infty} \psi^* \left(\frac{\partial}{\partial x}\right)\psi\ dx = -i\hbar\psi^*\psi\big|_{-\infty}^{+\infty} + i\hbar\int_{-\infty}^{\infty} \psi\frac{\partial \psi^*}{\partial x}\ dx$$

$$= 0 + \int_{-\infty}^{\infty} \psi\left(i\hbar\frac{\partial}{\partial x}\psi^*\right)\ dx = \int_{-\infty}^{\infty} \psi\left(-i\hbar\frac{\partial}{\partial x}\psi\right)^*\ dx = \int_{-\infty}^{\infty} \psi(\hat{p}_x\psi)^*\ dx$$

So that $\hat{p}_x$ is a Hermitian operator.

H.W.: Is the operator $\frac{\partial}{\partial x}$ Hermitian operator

Example 13: Prove that the eigen value correspond to any Hermitian operator are real quantities

So, we need to prove the eigen value a equal its conjugate, $a = a^*$

$\hat{A}\psi = a\psi \quad and\ \hat{A}^*\psi^* = a^*\psi^*$

Multibly, from the left, the first equation by ψ^*, and the second equation by ψ and integrated them for the all space.

Assume, ψ is a normalized wave function

$$\int \psi^*(\hat{A}\psi)\, dr = \int \psi^*(a\psi)\, dr = a \int \psi^*\psi\, dr = a \qquad (1)$$

$$\int \psi(\hat{A}\psi)^* dr = \int \psi(a^*\psi^*) dr = a^* \int \psi\psi^*\, dr = a^* \qquad (2)$$

By subtracting equations (1), (2)

$$\int \psi^*(\hat{A}\psi)\, dr - \int \psi(\hat{A}\psi)^* dr = a - a^*$$

Since $\hat{A}$ Hermitian operator then $\int \psi^*(\hat{A}\psi)\, dr = \int \psi(\hat{A}\psi)^* dr$

And $a = a^*$ That's mean the eigen value are real quantities