

The Properties of Operators

1- linear operator

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

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

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

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

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

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

3- Unit operator

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

Example 8: 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

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

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

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

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

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

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

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

$$\hat{C} = 1$$

H.W.

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

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

Solution:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

By using,

$$\nabla = \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z}$$

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

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

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

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

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

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

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

2- The variance in momentum

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

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

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

Or

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

Example 11: 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,

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

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

$$|A|^2 \int_{-\infty}^{\infty} \left(e^{\frac{-2amx^2}{\hbar}} \right) dx = 2|A|^2 \int_0^{\infty} \left(e^{\frac{-2amx^2}{\hbar}} \right) dx = 1$$

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

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

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

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

Then

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

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

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

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

$$\langle x \rangle = 0$$

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

$$\langle x^2 \rangle = |A|^2 \int_{-\infty}^{\infty} (e^{-\alpha x^2})x^2 dx = 2|A|^2 \int_0^{\infty} (e^{-\alpha x^2})x^2 dx$$

$$\text{From table of integrals } \int_0^{\infty} (e^{-\alpha x^2})x^2 dx = \frac{1}{4\alpha} \sqrt{\frac{\pi}{\alpha}}$$

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

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

$$\langle p_x \rangle = m \frac{d}{dt} \langle x \rangle = 0 \quad (\text{because } \langle x \rangle = 0)$$

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

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

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

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

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

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

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

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

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

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

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

Hermitian operator

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

Example 12: 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, $a = a^*$

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

Multiply, 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

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

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

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