- Operators

In quantum mechanics, a physical system is not represented by direct numbers as in classical physics, but is described by a mathematical function called the wave function Ψ. To calculate any physical quantity, we do not use direct numbers; instead, we use what are called operators.

An operator is a mathematical process that acts on the wave function and produces a new wave function, meaning it affects the mathematical state of the system.

In quantum mechanics, a measurable quantity (Observable) is defined as a physical property of the system whose value can be measured experimentally, such as position, momentum, or energy, and in quantum mechanics it is represented by a mathematical operator acting on the wave function.

Thus, the main idea can be summarized as follows: operators form the mathematical foundation of quantum mechanics, as they represent measurable physical quantities on one hand, and the mechanism by which the system changes over time on the other. Without operators, it would be impossible to describe the behavior of a quantum system or predict the results of experimental measurements.

في ميكانيكا الكم لا نُمثِّل النظام الفيزيائي بأرقام مباشرة كما في الفيزياء الكلاسيكية، بل نصفه بدالة رياضية تُسمّى الدالة الموجية Ψ. ولكي نحسب أي كمية فيزيائية فإننا لا نستخدم أرقامًا مباشرة، وإنما نستخدم ما يُسمّى بـ المؤثرات. اذن **المؤثر**: هو عملية رياضية تعمل على الدالة الموجية فتُنتج دالة موجية جديدة, اي يؤثر على الحالة الرياضية للنظام. في ميكانيكا الكم تُعرَّف **الكمية القابلة للقياس** : بأنها خاصية فيزيائية للنظام يمكن قياس قيمتها عمليًا، مثل الموضع أو الزخم أو الطاقة، وتمثل في ميكانيكا الكم بمؤثر رياضي على الدالة الموجية إذن يمكن تلخيص الفكرة بأن المؤثرات هي الأساس الرياضي لميكانيكا الكم، فهي تمثل الكميات الفيزيائية القابلة للقياس من جهة، وتمثل آلية تغير النظام مع الزمن من جهة أخرى. ومن دون المؤثرات لا يمكن وصف سلوك النظام الكمومي أو التنبؤ بنتائج القياسات التجريبية.

Description Operator	**Classical Dynamical Variable**	**QM Operator Representation**
Position	X	$\hat{X}$
Potential Energy	V(x)	$\hat{V}_{(x)}$
Momentum	P_x	$-i\hbar\frac{\partial}{\partial x}$
Kinetic Energy	$\frac{P_X^2}{2m}$	$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}$
Total Energy	E_{Total}	$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+\hat{V}_{(x)}$
Angular Momentum (z)	$L_z = x\,P_y - y\,P_x$	$-i\hbar\,(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})$
Number of Particles	N	$\hat{N}$

Eigen Value and Eigen Function

A wave function Ψ, which satisfies all the properties is said to be Eigen function

An operator $\hat{A}$ is a mathematical operator (differentiation, integration, addition, multiplication, division, etc.) which may be applied to a function $\Psi_{(x)}$, called the **operand**: When the operator acts on a general function, it may produce a different function and as a result, changes it into another function $\phi_{(x)}$, this can be represented as:

$$\hat{A}\Psi_{(x)} = \phi_{(x)}$$

If a function is **Eigen function** the result is the same function multiplied by a constant λ, called the **eigenvalue** it is the number that appears when measuring a physical quantity associated with the Eigen function, which represents the actual measurable value of the system.

$\hat{A}\Psi_{(x)} = \lambda\, \Psi_{(x)}$

$\hat{A}$ = Operator

$\Psi_{(x)}$ = operand

$\Psi_{(x)}$= Eigen function

λ = Eigen value

Example:

$-\frac{d^2}{dx^2}\ (\sin 2x)\ = 4(\sin 2x)$

Here $\hat{A} = -\frac{d^2}{dx^2}$ $\quad ,\lambda = 4 \quad ,\Psi_{(x)} = \sin 2x$

H.W: Is wave function $\Psi_{(x)} = \sin(-ar)$ an Eigen function for the operator $\widehat{A} = \frac{d^2}{dx^2}$

-Algebra of Operators

Just like the normal algebra, the resultants like addition or the multiplication of operators also follow certain rules, however, these rules are different from the typical algebra. Some of the most important rules of operator algebra are given below.

1. **Addition and subtraction of operators:**

   Let A and B as two different operators, f as the function that has to be used as the operand. Then, the addition and subtraction of these two operators must be carried out in the manner discussed below.

$$(\hat{A}+\hat{B})f = \hat{A}f + \hat{B}f$$

And

$$(\hat{A}-\hat{B})f = \hat{A}f - \hat{B}f$$

2. Linear Operator:

An operator Â is said to be a linear operator if its application on the sum of two functions f and g gives the same result as the sum of its individual operations. Mathematically, it can be shown as given below

$$\hat{A}(f+g) = \hat{A}f + \hat{A}g$$

For example, consider the differential operator A; with f and g as the functions which have to be used as the operand.

$$\hat{A} = \frac{d}{dx}; \; f = 2x^2; \; g = 3x^2$$

Or

$$\hat{A}(f+g) = \frac{d}{dx}(2x^2+3x^2) = \frac{d}{dx}(5x^2) = 10x \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ (1)$$

Or

$$\hat{A}f+\hat{A}g = \frac{d}{dx}(2x^2) + \frac{d}{dx}(3x^2) = 4x+6x = 10x \qquad \ldots\ldots\ldots\ldots\ldots\ldots\ (2)$$

Hence, from equation (1) and equation (2), it is clear that the differential operator is clearly linear in nature. On the other hand, the “square root” operator is not linear as it does not give the same result when operated individually.

3. Multiplication of operators:

If A and B as two different operators; and f as the function that has to be used as operand. Then, the multiplication of these two operators must be carried out in the manner discussed below.

$$\hat{A}\hat{B}f = f''$$

The interpretation of the above equation is that: first we need to operate B on f, which would give us another function f', which in turn is further used as the operand for operator giving the final result f''. In other words, we can say that when multiplication of two or more operators is used, we should follow from left to right. Moreover, the square or cube of a particular operator must be considered as double or triple multiplication of the operator itself; mathematically, it can be shown as given below.

$$\hat{A}^2 f = \hat{A}\hat{A}f$$

At this point it also very important to discuss one of the most fundamental properties of operator multiplication, the commutation relation or the commutation rule. Consider two operators, A and B which can be operated over the function f.

$$\hat{A}=\frac{d}{dx}, \hat{B}= X, f = X^3$$

$$\hat{A}\hat{B}f = \frac{d}{dx} X\,(X^3) = \frac{d}{dx} X^4 = 4\,X^3$$

And

$$\hat{B}\hat{A}f = X\frac{d}{dx}(X^3) = x(3\,X^2) = 3\,X^3$$

From this equation, it's clear that in this case

$$\hat{A}\hat{B}f \neq \hat{B}\hat{A}f$$

These operators are said to be **non-commutating** with the commutator given below:

$$\hat{A}\hat{B} - \hat{B}\hat{A} = 4x^3 - 3x^3$$

However, the two operators are said to be **commute** if their result is the same even after reverting their order of application. Mathematically, it can be stated as given by equation

$$\hat{A}\hat{B}f = \hat{B}\hat{A}\,f$$

Summarizing the commutation rule, it can be concluded that

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = 0 \rightarrow Commutating$$

And

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \neq 0 \rightarrow Non\text{-}commutating$$

H.W: For each pair of operators given below, determine whether they commute or do not commute**.** Calculate the commutator

1- $\hat{A} = \frac{d}{dx}$, $\hat{B} = X$, $F_{(x)} = x^2$

2- $\hat{A} = X$, $\hat{B} = X^2$, $F_{(x)} = x^3$

3- $\hat{A} = \frac{d}{dx}$, $\hat{B} = \frac{d^2}{dx^2}$, $F_{(x)} = x^3$

4- $\hat{A} = X$, $\hat{B} = 3X$, $F_{(x)} = x^2$