7·2. Operators.

An operator is a rule by means of which we can map on elements A of a linear space on elements B of another linear space, such that an equation may be set

$$B = TA.$$

B is range of operator,

A is domain of operator,

T is operator.

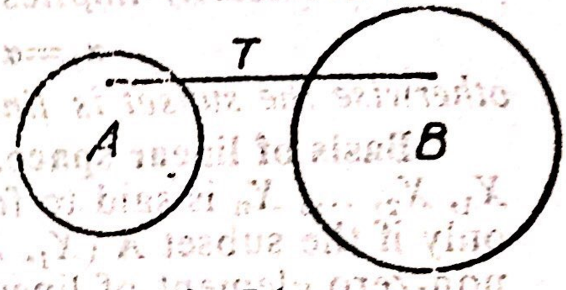

Fig. 7·1.

This is generalization of the idea of a function

$$y = f(x)$$

by means of which one variable x is a mapped on another variable y.

An operator *may also be defined as a mathematical term which is used in operation on function such that it tranforms to another function.*

Thus if T_{op} is some operator applied to function $\psi(x)$, then

$$T_{op}\,\psi(x) = \phi(x)$$

where $\phi(x)$ is the transformed function.

Linear Operators. In quantum mechanics we are concerned almost exclusively with linear operators and throughout the book the term operators will be used to mean **linear operators** unless the contrary is explicitly stated. An operator T is said to be linear operator if it satisfies the following conditions

$$T(u+v) = Tu + Tv$$

and $$Tc = cT$$

where u and v are arbitrary operators and c is an arbitrary constant.

Let us now discuss some examples of linear operators and some of their properties.

Identity operator and null operator. Unit or identity operator is such an operator, in which function remains unchanged after operation.

Here I is identity operator because function A before and after operation is unchanged.

Null or zero operator is such an operator, by which the function becomes zero. Thus if

$O_{op}.A=\bar{0}$ then O_{op} is called **null operator.**

Laws of operator. Let us take F and G as two operators.

$$\left.\begin{array}{ll} \text{I.} & (F+G)A=FA+GA \\ \text{II.} & (FG)\,A=F\,(GA) \\ \text{III.} & FG\neq GF \end{array}\right]$$

Addition is commutative but in general multiplication is non-commutative.

In the special case $FG=GF$.

Then these two operators are said to be **commuting.**

Examples. Let us take two operators α and β, such that

$$\alpha=x,\ \beta=\frac{d}{dx}$$

$$\alpha\beta\,[\psi(x)]=x\frac{d}{dx}[\psi(x)]=x\frac{\partial\psi(x)}{\partial x}$$

and

$$\beta\alpha\,[\psi(x)]=\frac{d}{dx}[x\psi(x)]=x\frac{\partial\psi(x)}{\partial x}+\psi(x).$$

Therefore $\alpha\beta\neq\beta\alpha.$

Hence α and β do not commute.

Multiplication of operators ; Commutators.

Let us consider the multiplication of two operators; the position operator x and momentum operator p.

The momentum operator p is given by

$$p=\frac{\hbar}{i}\frac{\partial}{\partial x}$$

If $\psi(x)$ is any function, then

$$p\psi(x)=\frac{\hbar}{i}\frac{\partial\psi}{\partial x}$$

so that

$$xp\psi(x)=x\frac{\hbar}{i}\frac{\partial\psi}{\partial x} \qquad ...(1)$$

and

$$px\,\psi(x)=\frac{\hbar}{i}\frac{\partial}{\partial x}(x\psi)$$

$$=\frac{\hbar}{i}\psi+\frac{\hbar}{i}x\frac{\partial\psi}{\partial x} \qquad ...(2)$$

It is obvious that (1) and (2) are not the same *i.e.*

$$xp\neq px$$

we have

$$(xp-px)\,\psi=\frac{\hbar}{i}\,x\frac{\partial\psi}{\partial x}-\frac{\hbar}{i}\,\psi-\frac{\hbar}{i}\,x\frac{\partial\psi}{\partial x}$$

i.e. $$(xp-px)\,\psi=i\hbar\psi \qquad \ldots(3)$$

$(xp-px)$ is called the commutator of two operators x and p and is denoted by $[x, p]$.

From eqn. (3) it is clear that the commutator of position operator and momentum operator satisfies the relation

$$[x, p]=i\hbar \qquad \ldots(4)$$

Power of linear operator. Consider F is any linear operator

$$F^2=F.F$$

In general $F^n=F.F...F$ (product up to n)

Polynomial of operator. If F is linear operator and $\alpha_1, \alpha_2 \ldots$ are complex numbers, then

$(\alpha_1 F+\alpha_2 F^2+\ldots)$ is called polynomial.

If F is linear operator, then any power (or polynomial) of F will also be linear operator.

Differential operators. Consider any function $\psi(x)$ like x^3, $\sin x$ and e^{ikx} and differentiate these functions with respect to x.

The expression $[d/dx]\,\psi(x)$ consists of two consituents ; the operator $[d/dx]$ and the operand $\psi(x)$

$$\left[\frac{d}{dx}\right]\psi(x)=\psi'(x) \qquad \ldots(5)$$

$\psi(x)$ being the first derivative of $\psi(x)$ obtained by the rules of differential calculus. Similarly expression $[x]\,\psi(x)$ consists of two constituents the operator $[x]$ and operand $\psi(x)$

$$[x]\,\psi(x)=x\psi\,(x) \qquad \ldots(6)$$

For an ordinary $\psi(x)$, the right side of (6) is the algebraic product of x and $\psi(x)$; and the operator $[c]$ is defined as

$$[c]\,\psi(x)=c\psi\,(x) \qquad \ldots(7)$$

For an arbitrary $\psi(x)$, the right side of (7) is the algebraic product of (ψ), and constant c.

We shall use further these operators $[d/dx]$, $[x]$ and $[c]$ as simply d/dx, x and c. These operators are called differential operators.

$$\left(\frac{d}{dx}\right)\psi(x)-x\psi(x)=\left(\frac{d}{dx}+x\right)\psi(x). \qquad \ldots(8)$$

$$\frac{d}{dx}\,[x\psi(x)]=x\left(\frac{d}{dx}\right)\psi(x)+\psi(x)$$

or $$\frac{d}{dx}\,x\psi(x)=x\,\frac{d}{dx}\,\psi(x)+\psi(x) \qquad \ldots(9)$$

so that $$\frac{d}{dx}\,x\psi(x)\neq x\,\frac{d}{dx}\,\psi(x)$$

unless $\psi(x)=0$.

Inverse operator. Consider A is one linear space and B is another linear space and T is any linear operator, such that

$$B=TA$$

and
$$A=T^{-1}B \qquad ...(11)$$

If T is linear operator, then T^{-1} is inverse operator.

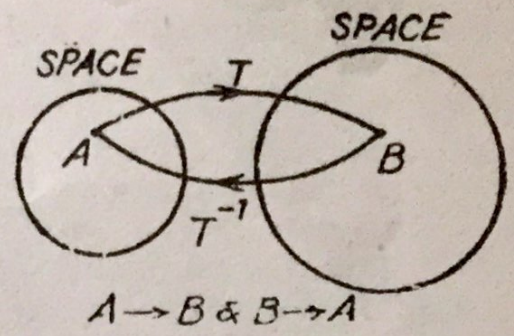

Fig. 7·2

Theorem. If T^{-1} exists then $TA=\bar{0}$ implies that $A=\bar{0}$, where $\bar{0}$ is null or zero operaror.

Let
$$TA'=B$$
and
$$TA''=B.$$
Then
$$T(A'-A'')=\bar{0}$$
$$A'=A''.$$

Therefore $TA=B$ is unique correspondence.

Singular and non-singular operators. If the two operators A and B have the following relation

$$AB=BA=I,$$

where I is identity operator.

Then A and B are reciprocal to each other, *i.e.*,

$$A^{-1}=B,\ B^{-1}=A.$$

An **operator** *for which a reciprocal exists is called* **non-singular.** For a non-singular operator if the relation $\phi=A\psi$ holds good *i.e.*, operator A has reciprocal, then ψ can be obtained by the help of A^{-1}.

$$\psi=A^{-1}\phi.$$

And if for non-zero ψ, $A\psi=0$ exists, then A operator has no reciprocal *i.e.*, A is singular. *Therefore an operator which has reciprocal, is called singular operator.*

7·3. Eigen functions and eigen values.

If a wave function is well behaved function and satisfies the continuity conditions and boundary conditions, then by result of operation with an operator P, we get the same function as :

$$P\,\psi(x)=\lambda\,\psi(x) \qquad ...(1)$$

where λ is complex number, $\psi(x)$ is called eigen function and λ is called eigen value of operater P.

Let us take a well behaved function sin $2x$. If it is operated by an operator $-\left(\frac{d^2}{dx^2}\right)$ the result is :

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

On comparison with general equation (1), we get

$$p=\frac{d^2}{dx^2}$$

$$\lambda=4$$

$$\psi(x)=\sin 2p.$$

So, the number 4 is the eigen value of the operator $-d^2/dx^2$ and sin $2x$ is the function of the operator.

7·4. The operator formalism in qnantum mechanics.

The expectation values of position and momentum is given by the following relations.

$$\langle x\rangle=\frac{\int \psi^* x\psi\, dx}{\int \psi^*\psi\, dx},\ \langle p\rangle=\frac{\int \psi^*\left(\frac{\hbar}{i}\frac{d}{dx}\right)\psi\, dx}{\int \psi^*\psi\, dx} \quad ...(1)$$

Here $\frac{\hbar}{i}\frac{d}{dx}$ is momentum operator,

i.e. $$p_{op}\rightarrow\left(\frac{\hbar}{i}\frac{d}{dx}\right).$$

The Schroedinger equation for a particle is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V\psi=E\psi. \quad ...(2)$$

We know that it can be obtained by the energy expression

$$\frac{p^2}{2m}+V=E$$

By replacing $p\rightarrow p_{op}=\frac{\hbar}{i}\frac{d}{dx}$, we get the equation

$$H_{op}\psi=\psi \quad ...(3)$$

in which $$H_{op}=\frac{p^2_{op}}{2m}+V. \quad ...(4)$$

As $$H=\frac{p^2}{2m}+V.$$

And $$H_{op}\rightarrow\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+V(x, y, z)$$

in three demensions.

The one dimension H_{op}, Hamitonian opertor is given by

$$H_{op}\rightarrow\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x).$$

These observations suggest classical dynamical quantity of the system has its correspondence in the quantum mechanical theory. So classical dynamical variable and quantum mechanical operator are linked together.