of the ~~a~~ motion of the above particle is not free but acted upon by a potential $V(r)$, then the time dependent Schrödinger equation for three dimension takes the form

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r},t) \longrightarrow (iv)$$

In a Compact form we rewrite the above equation as

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \hat{H}\psi(\vec{r},t)$$

where $\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})$ is the three dimensional Hamiltonian.

$\boxed{\text{Operators}}$

An operator may be defined as one which operating on a function and transforms it into a new function. If an operator $\hat{A}$ operating on a new function $f(x)$ and transforms it into a new function $g(x)$.

$$\hat{A} f(x) = g(x) \longrightarrow (i)$$

where the function $f(x)$ is called operand.

If for the above example

$$g(x) = \hat{A}(5x^2+8) = 10x^2+16$$

then we can say that the operator $\hat{A}$ multiplies the function $f(x) = 5x^2+8$ by 2 to give $g(x) = 10x^2+16$

the operator $\hat{A}$ here is a multiplication operator.

If $g(x) = \hat{A}(5x^2+8) = 10x$

then the operator $\hat{A}$ differentiates the function $f(x) = (5x^2+8)$ to give $g(x) = 10x$. The operator $\hat{A}$ in this case is a differentiator.

* Any physical quantity that can be measured experimentally is called physical observable or observable or dynamical variable. Position, momentum, energy all are dynamical variables and in quantum mechanics the all variables are represented ~~by~~ each by an operator.

Linear operator :-

An operator $\hat{A}$ is said to be linear if it satisfies the relation

(i) $\hat{A}[c_1 f_1(x) + c_2 f_2(x)] = c_1 \hat{A} f_1(x) + c_2 \hat{A} f_2(x)$

Where f_1 and f_2 are two arbitrary function of x and c_1, c_2 are constants.

If the differentiator operator $\frac{d}{dx}$ obey the following relation then it is said to be a linear operator

$$g(x) = \frac{d}{dx}[c_1 f_1(x) + c_2 f_2(x)]$$

$$= c_1 \frac{d}{dx} f_1 + c_2 \frac{d}{dx} f_2$$

(ii) If $\hat{A}$ is linear operator, c is a constant and $f(x)$ is a function of x, then

$$\hat{A}\{c f(x)\} = c\hat{A} f(x)$$

i.e. $\hat{A} c = c\hat{A}$ [the operator $\hat{A}$ commutes with an arbitrary constant c]

* The operator that squares a function is not however a linear operator.

$$\hat{A}[c_1 f_1(x) + c_2 f_2(x)] = [c_1 f_1(x) + c_2 f_2(x)]^2$$

$$= c_1^2 f_1^2 + c_2^2 f_2^2 + 2c_1c_2 f_1 f_2$$

But the operator to be linear

$$\hat{A}[c_1 f_1(x) + c_2 f_2(x)] = c_1 \hat{A} f_1(x) + c_2 \hat{A} f_2(x)$$

$$= c_1 f_1^2 + c_2 f_2^2$$

$$\neq c_1 f_1^2 + c_2 f_2^2 + 2c_1c_2 f_1 f_2$$

****** In quantum mechanics all operators are linear. The sums and products of two linear operators are also linear. The sum of two linear operators commute but their product may or may not commute.

Among the linear operators, we may have

(a) multiplying functions which when operates on a function, the function simply gets multiplied by the operator to give a new function. Examples are x, x^2, e^x, $\sin x$ etc.

For instance

$$\hat{x} f(x) = x \cdot f(x)$$

$$(e^x) f(x) = e^x \cdot f(x)$$

This type of operators are Called 'C' numbers.

(b) Differential operators such as $\frac{d}{dx}$, $\frac{d^2}{dx^2}$ etc belong to a class known as 'q' numbers. When these operate on a function a new function is obtained.

(c) Mixture of above two types of operators is also possible. For example $\left(x^2 + \frac{d}{dx}\right)$. When operation on e^{ax} i.e

$$\left(x^2 + \frac{d}{dx}\right) e^{ax} = x^2 e^{ax} + a e^{ax}$$

$$= (x^2 + a) e^{ax}$$

this new function is obtained.

* Basic definitions and properties of lineae operators:-

(i) The sum and the difference of two different operators $\hat{A}$ and $\hat{B}$ are ~~diffen~~ defind by

$$(\hat{A} \pm \hat{B}) f(x) = \hat{A} f(x) \pm \hat{B} f(x)$$

The addition is Commutative: $\hat{A} + \hat{B} = \hat{B} + \hat{A}$

The addition is also associative $(\hat{A} + \hat{B}) + \hat{C} = \hat{A} + (\hat{B} + \hat{C})$

(ii) The product of two operators is defined by

$$\hat{A}\hat{B} f(x) = \hat{A}[\hat{B} f(x)] = \hat{A} \phi(x) = g(x)$$

which means that $f(x)$ is first operated by $\hat{B}$ to obtain another function $\phi(x)$. Then $\phi(x)$ is operated on by $\hat{A}$ to get the final function $g(x)$.

The multiplication is associative

$$\hat{A}(\hat{B}\hat{C}) = (\hat{A}\hat{B})\hat{C}$$

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

(iii) The square of an operator is defined as the self product of the operator.

So, $\hat{A}^2 = \hat{A}\cdot\hat{A}$

i.e $\hat{A}\hat{A}f(x) = \hat{A}^2 f(x)$

If the same operator applies a number of times in succession, then the operator is to be written with power.

$$\hat{A}\hat{A}\hat{A}\hat{A}\cdots\hat{A}f(x) = \hat{A}^n f(x).$$

Commutators

If $\hat{A}$ and $\hat{B}$ are two linear operators, then the commutator or the commutator bracket of two operators ~~may Sepamble~~ symbolized by

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

again $[\hat{A},\hat{B}] = -(\hat{B}\hat{A} - \hat{A}\hat{B})$
$= -[\hat{B},\hat{A}]$

If $\hat{A}\hat{B} = \hat{B}\hat{A}$, i.e $[\hat{A},\hat{B}] = 0$, then the operator $\hat{A}$ is said to commute with $\hat{B}$.

If $\hat{A}\hat{B} \neq \hat{B}\hat{A}$ i.e $[\hat{A},\hat{B}] \neq 0$, then there operators is said to not commute with $\hat{B}$.

If however $\hat{A}\hat{B} + \hat{B}\hat{A} = 0$, then the operators $\hat{A}$ and $\hat{B}$ are said to anti commute and symbolized by $\{\hat{A}, \hat{B}\}$.

* The powers of the same operator commute.

$$[\hat{A}^m, \hat{A}^n] = \hat{A}^m . \hat{A}^n - \hat{A}^n . \hat{A}^m$$
$$= \hat{A}^{m+n} - \hat{A}^{m+n}$$
$$= 0$$

* Commutator of an operator with its self inverse commute

$$[\hat{A}, \hat{A}^{-1}] = \hat{A}\hat{A}^{-1} - \hat{A}^{-1}\hat{A} = 0$$
$$[\because \hat{A}\hat{A}^{-1} = \hat{A}^{-1}\hat{A} = 1]$$

* Commutators of $\frac{d}{dx}, x$

$$\left[\frac{d}{dx}, \hat{x}\right] f(x) = \left[\frac{d}{dx}\hat{x} - \hat{x}\frac{d}{dx}\right] f(x)$$
$$= \frac{d}{dx}\{\hat{x} f(x)\} - \hat{x}\frac{d}{dx} f(x)$$
$$= f(x) + \hat{x}\frac{df}{dx} - \hat{x}\frac{df}{dx}$$
$$= f(x)$$
$$\therefore \left[\frac{d}{dx}, \hat{x}\right] = 1.$$

so, $\frac{d}{dx}, f(x)$ do not commute with each other.

Again by definition $\left[\hat{x}, \frac{d}{dx}\right] = -\left[\frac{d}{dx}, \hat{x}\right]$
$$= -1$$

The above equation is an example

of an operator equation. The right ~~side~~ hand side (-1) is also an operator - the negative of a unit operator, also called the identity operator, 1.

$\boxed{\text{Operators for momentum and energy}}$

The operators for momentum and energy of a free particle may be obtained from one dimensional time independent Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}(x,t) \longrightarrow (i)$$

or, $$\left(i\hbar\frac{\partial}{\partial t}\right)\psi(x,t) = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial x}\right)\psi(x,t) \longrightarrow (ii)$$

For a free particle, the classical expression for energy is given by

$$E = \frac{p_x^2}{2m} \longrightarrow (iii)$$

Comparing (ii) and (iii), it may be concluded that the dynamical variables energy E and momentum $\vec{p}$ can be represented by the differential operators

$$\hat{E} \longrightarrow i\hbar\frac{\partial}{\partial t} \text{ and } \hat{p}_x = -i\hbar\frac{\partial}{\partial x}$$

respectively, operating on the wave function $\psi(x,t)$.

$$\therefore\ p_x \to \hat{p}_x = -i\hbar\frac{\partial}{\partial x}\ ;\ E \to \hat{E} = i\hbar\frac{\partial}{\partial t}$$

for three dimension

$$E \rightarrow \hat{E} = i\hbar \frac{\partial}{\partial t} \; ; \quad \vec{p} \rightarrow \hat{\vec{p}} = -i\hbar \vec{\nabla}$$

multiplying operators may be represented as

$$x \rightarrow \hat{x}, \; y \rightarrow \hat{y}, \; z \rightarrow \hat{z}, \; t \rightarrow \hat{t}, \; \vec{r} \rightarrow \hat{\vec{r}}$$

■ Other dynamical variables

The operators corresponding to other dynamical variables, which are functions of the co-ordinate x and momentum p_x, may be obtained by substituting for these corresponding quantum mechanical operators in classical expressions.

(i) Kinetic energy operator :-

For one dimension case

$$E_K = E_K(p_x) = \frac{p_x^2}{2m}$$

$$\therefore \hat{E}_K = \frac{\hat{p}_x^2}{2m} = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2$$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \longrightarrow (iv)$$

For three dimensional case $\hat{E}_K = -\frac{\hbar^2}{2m}\nabla^2$

(ii) Hamiltonian :-

The classical expression of Hamiltonian, which is equal to the total energy of the particle if the potential V is not an explicit function of t.

$$\hat{H}(x, p_x) = \frac{p_x^2}{2m} + V(x) \longrightarrow (v)$$

$$\therefore \hat{H} = \frac{\hat{p}_x^2}{2m} + V(\hat{x})$$

$$\hat{H} = \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)^2 + V(x)$$

$$\therefore \boxed{\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)} \longrightarrow (vi)$$

This is Hamiltonian operator.

for three dimensional case

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) \longrightarrow (vii)$$

Commutator and quantization rule

For one dimensional motion, quantum mechanical operator $\hat{x}$, $\hat{P}_x$ satisfies the following relation

$$[\hat{x}, \hat{P}_x]\psi = (\hat{x}\hat{P}_x - \hat{P}_x\hat{x})\psi = \hat{x}\cancel{(-i\hbar\frac{\partial}{\partial x})}$$

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

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

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

$$= i\hbar\psi$$

dropping ψ from each side

$$[\hat{x}, \hat{P}_x] = i\hbar \longrightarrow (i)$$

The above equation is very significant because it gives us the "basic quantization rule" in quantum mechanics.

We are familiar with Poisson bracket ~~in et~~ of two dynamical variable α, β in classical mechanics

$$\{\alpha, \beta\} = \frac{\partial\alpha}{\partial x}\cdot\frac{\partial\beta}{\partial p} - \frac{\partial\alpha}{\partial p}\cdot\frac{\partial\beta}{\partial x} \longrightarrow (ii)$$

where α, β are functions of independent variables x and p.

Dirac showed that the quantum poisson bracket of any pair of variables (α, β) should be defined as $\alpha\beta - \beta\alpha = i\hbar \{\alpha, \beta\}_q \longrightarrow$ (iii)

where $\hbar = h/2\pi$, h plancks constant and q denotes the quantum Poisson bracket.

If α, β are replaced by x and p respectively then classical Poisson bracket

$$\{x, p\} = \frac{\partial x}{\partial x} \cdot \frac{\partial p}{\partial p} - \frac{\partial x}{\partial p} \cdot \frac{\partial p}{\partial x} = 1 \longrightarrow \text{(iv)}$$

So, by eqn (iii) and (iv) $xp - px = i\hbar \longrightarrow$ (v)

The eqn (v) is identical with eqn (i), if its left hand side is put equal to the commutator bracket of quantum mechanical operators $\hat{x}$ and $\hat{p}$, of the ~~co~~ position and momentum variables respectively.

Comparison of eqn (iv) and (v) leads to the statement of correspondence principle.

<u>Correspondence principle:</u>

If $\hat{\alpha}$ and $\hat{\beta}$ be two classical dynamical variables, then their representative quantum mechanical operators $\hat{\alpha}$ and $\hat{\beta}$ must be so chosen that the product $i\hbar\{\alpha, \beta\}$ of classical Poisson bracket of variables α, β with $i\hbar$ leads to the commutator $[\hat{\alpha}, \hat{\beta}]$ of quantum operators.

Simply $i\hbar\{\alpha, \beta\} = [\hat{\alpha}, \hat{\beta}] \longrightarrow$ (vi)

Problems :-

1. Show that the operators $\frac{\partial}{\partial x}$ and $\partial^2/\partial x^2$ operating on a differentiable function $f(x)$ commute.

(2) Examine whether the following operators are linear or not

(i) $\hat{L} f(x) = f(x) + x^2$

(ii) $\hat{L} f(x) = f(5x^2+1)$

(iii) $\hat{L} f(x) = \left(\frac{df}{dx}\right)^2$

(iv) $\hat{L} f(x) = f(-x)$

(v) $\hat{L} f(x) = f^*(x)$, where $*$ denotes complex conjugate.

(3) Show that if $\hat{\alpha}$ and $\hat{\beta}$ are two linear operators, then their sum $(\hat{\alpha}+\hat{\beta})$ and product $(\hat{\alpha}\hat{\beta})$ are also linear.

(4) Verify that $[AB, C] = [A, C] B + A[B, C]$

where A, B, C are three operators.

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