Operators

operator is defined as "An operator Â is a mathematical entity that transforms a function ψ into another function ϕ" e.g.

$$\hat{A}\psi = \phi \qquad (19)$$

Operator Â may be $\frac{d}{dx}$ this means the first derived differential of wave function

$$= \left(\frac{d}{dx}\right)\psi = \frac{d\psi}{dx} = \Phi \qquad (20)\,\hat{A}$$

On the other hand mathematical entity like $\sqrt{\;}$ $or\,(\;)^2 or\, etc$ not operators

A- Liner Operator: liner operator is obey this condition

$$\hat{A}\,(a\,\Psi) = a\,(\hat{A}\,\Psi) \qquad (21)$$

$$\hat{A}\,(\Psi_1 + \Psi_2) = \hat{A}\,\Psi_1 + \hat{A}\,\Psi_2 \qquad (22)$$

Where a is constant for example $\frac{d}{dx}$, and $\hat{x}$ is liner operator

$$\hat{x}(a\psi) = a(\hat{x}\psi) = a\,x\psi \qquad (23)$$

$$\hat{x}(\psi_1 + \psi_2) = \hat{x}\psi_1 + \hat{x}\psi_2 = x\psi_1 + x\psi_2 \qquad (24)$$

$$\frac{\hat{d}}{dx}(a\psi) = a\frac{\hat{d}}{dx}\psi = a\frac{d\psi}{dx} \qquad (25)$$

$$\frac{\hat{d}}{dx}(\psi_1 + \psi_2) = \frac{\hat{d}}{dx}\psi_1 + \frac{\hat{d}}{dx}\psi_2 = \frac{d\psi_1}{dx} + \frac{d\psi_2}{dx} \qquad (26)$$

but $\hat{A} = \sqrt{\;}$, $()^*, ()^2$ *and* exp are not liner operator for example

$$\sqrt{\hat{a}\psi} \neq a\sqrt{\psi} \qquad (27)$$

$$\sqrt{\psi_1+\psi_2} \neq \sqrt{\psi_1} + \sqrt{\psi_2} \qquad (28)$$

$$\left(\hat{a}\psi\right)^2 \neq a\ \psi^2 \qquad (29)$$

$$(\psi_1+\psi_2)^2 \neq \psi_1^2+\psi_2^2 \qquad (30)$$

$$e^{x+y} \neq e^x+e^y \qquad (31)$$

$$e^{cx} \neq ce^x \qquad (32)$$

B- the sum and difference of two operators: if we have an two operator $\hat{A}$ *and* $\hat{B}$ working on an function ψ as

C- $\left(\hat{A}+\hat{B}\right)\psi = \hat{A}\psi + \hat{B}\psi$ and

$\left(\hat{A}-\hat{B}\right)\psi = \hat{A}\psi - \hat{B}\psi$ (33) for example

$$\left(\frac{d}{dx}+\frac{d}{dy}\right)\psi = \frac{d\psi}{dx}+\frac{d\psi}{dy} \quad \text{and} \quad \left(\hat{x}+\frac{\hat{d}}{dx}\right)\psi = x\psi+\frac{d\psi}{dx}$$

D- operators multiplication: in this case

$$\left(\hat{A}\,\hat{B}\right)\psi = \hat{A}\left(\hat{B}\right)\psi \quad \text{and} \quad \left(\hat{A}\,\hat{B}\right)\psi \neq \hat{B}\left(\hat{A}\right)\psi \qquad (34)$$

This means that you should be calculated the effect of operator $\hat{B}$ on the function ψ and then study the effect of operator $\hat{A}$ on the product and not versa.

Example 1

If operator $\hat{B} = \frac{d}{dx}$, $\hat{A} = x$ working on ψ calculate $\left(\hat{A}\ \hat{B}\right)\psi$ and $\left(\hat{B}\hat{A}\right)\psi$

Solution

$$\left(\hat{A}\ \hat{B}\right)\psi = \left(x\frac{d}{dx}\right)\psi = x\frac{d\psi}{dx}$$ and

$$\left(\hat{B}\hat{A}\right)\psi = \left(\frac{d}{dx}x\right)\psi = \frac{d}{dx}(x\psi) = x\frac{d\psi}{dx} + \psi$$

i.e. $\left(\hat{A}\ \hat{B}\right) \neq \left(\hat{B}\hat{A}\right)$

E- Hermitian operator: the operator says Hermitian if it obey this conditions

$$\int \psi_1^* \hat{A}\ \psi_2\ d\tau = \int \psi_2 \hat{A}\ \psi_1^* d\tau \quad (36)$$

From equation 36 if the operator working first on function ψ_1 and then multiply by other function ψ_2 or the operator working on function ψ_2 and then multiply ψ_1 the result is the same. Hermitian operator is very important because having only eigenvalue in quantum mechanics such as momentum and energy. The Hermitian operator having exchange properties as

$\hat{B} = \frac{d}{dy}$, $\hat{A} = x$ Work on function ψ then

$$\left(\hat{A}\hat{B}\right)\psi = \left(x\frac{d}{dy}\right)\psi = x\frac{d\psi}{dy}$$

$$\left(\hat{B}\hat{A}\right)\psi = \left(\frac{d}{dy}x\right)\psi = \frac{d}{dy}(x\psi) = x\frac{d\psi}{dy}$$

F-Eigen function and Eigen value:

In general, the function ψ obtained by the application of the operator Â on an arbitrary function ψ, is linearly independent of ψ. However, for some particular function ψ, it is possible that

$$\hat{A}\psi = a\,\psi \qquad (37)$$

Then ψ called eigenfunction and (a) called eigenvalue

Special case: sometimes two or more eigenfunctions have the same eigenvalue. In that situation the eigenvalue is said to be degenerate. When two, three . . . n eigenfunctions have the same eigenvalue, the eigenvalue is doubly, triply . . . n-fold degenerate. When an eigenvalue corresponds only to a single eigenfunction, the eigenvalue is non-degenerate.

Example 2

a) Show that sin (3.63 x) is not an eigenfunction of the operator d/dx.

b) Show that exp (−3.63ix) is an eigenfunction of the operator d/dx. What is its eigenvalue?

c) Show that (1/π) sin (3.63x) is an eigenfunction of the operator $((-h^2/8\pi^2 m)\, d^2/dx^2)$. What is its eigenvalue?

Solution

a) $\frac{d(\sin 3.63x)}{dx} = 3.63\cos 3.63x \neq (cons\tan t)(function)$

b) $\dfrac{d\,e^{-3,63x}}{dx} = -3.63e^{-3.63}x \, and\, eigenvalue is - 3.63i$

c) $\dfrac{-h^2}{8\pi^2 m}\dfrac{d^2}{dx^2}\dfrac{1}{\pi}(\sin 3,63x) = \dfrac{-h^2}{8\pi^2 m}\dfrac{1}{\pi}3.63\dfrac{d}{dx}(\cos 3,63x)$

$= \dfrac{h^2}{8\pi^2 m}(3.63)^2\dfrac{1}{\pi}(\sin 3,63x)\, and\, eigenvalue = \dfrac{h^2}{8\pi^2 m}(3.63)^2$

Example 3

Show that if this function $f(x) = \sin^2 x$ is eigenfunction to any one of both operators

$[\tan x(d^3/dx^3)] or\ [\cos x(d^3/dx^3)]$

Solution

For first operator

$$\cos x\frac{d^3}{dx^3}(\sin^2 x) = \cos x\frac{d^2}{dx^2}(\frac{d}{dx}\sin^2 x)$$

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

$$= 2\cos x\frac{d}{dx}(-\sin x.\sin x) + (\cos x\cos x)$$

$$= 2\cos x\frac{d}{dx}(\cos^2 x + \sin^2 x)$$

$$= 2\cos x(-2\cos x\sin x) - 2\cos x(2\sin x\cos x)$$

$$= -4\cos^2 x\sin x\ - 4\cos^2 x\sin x = -8\cos^2 x\sin x$$

This is not eigenfunction

For second operator

$$\tan x\frac{d^3}{dx^3}(\sin^2 x) = \cos x\frac{d^2}{dx^2}(\frac{d}{dx}\sin^2 x)$$

$$= \tan x\frac{d^2}{dx^2}2\sin x\ \cos x = 2\tan x\frac{d}{dx}(\frac{d}{dx}\sin x\ \cos x)$$

$$= 2\tan x \frac{d}{dx}(-\sin x.\sin x) + (\cos x \cos x)$$
$$= 2\tan x \frac{d}{dx}(\cos^2 x - \sin^2 x)$$
$$= 2\tan x(-2\cos x \sin x) - 2\tan x(2\sin x \cos x)$$
$$= -4\frac{\sin x}{\cancel{\cos x}}\cancel{\cos x}\sin x \; - 4\frac{\sin x}{\cancel{\cos x}}\cancel{\cos x}\sin x = -8\sin^2 x$$

This eigenfunction and eigenvalue is -8

Postulation of quantum theory

Postulate 1. The state of a quantum mechanical system is completely specified by a function ψ (r; t) that depends on the coordinates of the particle(s) and on time. This function, called the wave function or state function, has the important property that ψ^* (r; t) ψ (r; t) $d\tau$ is the probability that the particle lies in the volume element $d\tau$ located at r at time t.

The wave function must satisfy certain mathematical conditions because of this probabilistic interpretation. For the case of a single particle, the probability of finding it somewhere is 1, so that we have the normalization condition

$$\int_{-\infty}^{\infty} \psi^*(r,t)\psi(r,t)d\tau = 1$$

It is customary to also normalize many-particle wave functions to 1[2] .The wave function must also be single-valued, continuous, and finite.

Postulate 2. To every observable in classical mechanics there corresponds a linear, Hermitian operator in quantum mechanics.

In this case if you like to write any physical quantity in quantum, first described it by classical physics and then changed into quantum mechanics

For example the kinetic energy, classically

$$K.E_x = \frac{1}{2} mu^2 \qquad (38)$$

$$K.E_x = \frac{m^2u^2}{2m} = \frac{P_x^2}{2m} \qquad (39)$$

But momentum in quantum is

$$P_x = -\frac{ih}{2\pi}\frac{d}{dx} \qquad (40)$$

Then subsisted the value of momentum from eqn.39 in eqn 40 we get

$$K.E = \frac{1}{2m}\left(-\frac{ih}{2\pi}\frac{d}{dx}\right)\left(-\frac{ih}{2\pi}\frac{d}{dx}\right) \qquad (41)$$

$$K.E = \frac{h^2}{4\pi^2 m}\left(\frac{d^2}{dx^2}\right) \qquad (42)$$

See the difference between them

Postulate 3. In any measurement of the observable associated with operator Â, the only values that will ever be observed are the eigenvalue a, which satisfy the eigenvalue equation

$$\hat{A}\psi = a\psi$$

This postulate captures the central point of quantum mechanics the values of dynamical variables can be quantized (although it is still possible to have a continuum of eigenvalues in the case of unbound states). If the system is in an eigenstate of Â with eigenvalue a, then any measurement of the quantity A will yield a.

Postulate 4. If a system is in a state described by a normalized wave function, then the average value of the observable corresponding to Â is given by

$$\prec A \succ = \int_{-\infty}^{\infty} \psi^* \hat{A}(r,t) d\tau$$

Postulate 5. The wavefunction or state function of a system evolves in time according to the time-dependent Schrödinger equation

$$H\psi(q,t) = \frac{h}{2i\pi} \cdot \frac{d}{dt}\psi(q,t) \qquad (43)$$

Postulate 6. The total wavefunction must be antisymmetric with respect to the interchange of all coordinates of one fermion's with those of another. Electronic spin must be included in this set of coordinates.

The Pauli Exclusion Principle is a direct result of this antisymmetry principle. We will later see that Slater determinants provide a convenient means of enforcing this property on electronic wavefunctions