...the curve is zero.

2.20 OBSERVABLE AND OPERATORS

When studying the state of a system, one typically makes various measurements of its properties, such as mass, volume, position, momentum and energy. Each individual property is called an *observable*. An observable is any property of the system which could be measured. Since quantum mechanics postulates that the state of a system is given by a wave function, how does one determine the value of various observables (say, position or momentum, or energy) from wave functions.

The next postulates of quantum mechanics states that in order to determine the value of an observable you have to perform some mathematical operation on a wave function. This operation is represented by an *operator*.

"An operator represents a mathematical rule that transforms one function into another or one vector into another".

or

"An operator is an instruction to carry out certain operations".

or

"An operator is a symbol or sign that tells us to do something of what follows the symbol".

Consider some examples

(i) In the differential equation $\frac{d}{dx}\sin x = \cos x$. The operator is $\frac{d}{dx}$. It differentiates the function on its right.

(ii) In the equation

$$y = \ln x$$

The ln operator takes the natural logarithm of x, transforming into y.

(iii) In the equation

$$y = x\, f(x)$$

The operator x stands for the rule: multiple by x the function to the right of x. The result is a new function called y.

(iv) In the matrix equation

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ i \end{pmatrix} = \begin{pmatrix} i \\ 1 \end{pmatrix}$$

The matrix operator transforms one vector into another vector.

Evidently an operator is a set of instructions embodied in the definition of the operator and the operations can always be written in the form of an equation

$$\text{(operator) (function)} = \text{(another function)} \tag{2.64}$$

The function on which the operation is carried out is often called an *operand*. The left hand side of Eq.(2.64) does not mean that the function is multiplied by the operator. In a sense an operator therefore does not have any meaning when it stands alone. For example $\sqrt{\ }$ is an operator which is itself does not mean anything, but if a quantity or number put under it, it transforms that quantity into its square root, another quantity. An operator, unless it is otherwise obvious, is hereafter written with a symbol (^) overhead. Thus an operator A is symbolised by $\hat{A}$. Operators are extremely important in quantum mechanics because they provide the means for calculating possible measured values of observable properties of the system. It is the postulate of quantum mechanics that for any observable in classical mechanics, there is a linear quantum mechanical operator. It is further postulated that the possible measured values are the eigen values obtained from SWE. The physical significance of the eigen values of any physical quantity is, that they are the possible results of measurements of physical quantity.

Algebra of Operators

Although operators do not have any physical meaning, they can be added, subtracted, multiplied, and have some other properties.

Addition and Subtraction

The addition or subtraction of operators yields new operators, the sum or the difference of operators being defined by

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

For example, let $\hat{A}$ be $\log_e$ and $\hat{B}$ be $\frac{d}{dx}$, and f(x) be x^2; then

$$(\hat{A} \pm \hat{B})\, f(x) = \left(\log_e \pm \frac{d}{dx}\right) x^2 = \log_e x^2 \pm \frac{d}{dx}(x^2)$$

$$= 2\log_e x \pm 2x = \hat{A}\, f(x) \pm \hat{B}\, f(x)$$

Multiplication

Multiplication of two operators means operation by the two operators one after the other, the order of operation being from right to left; for example, $\hat{A}\hat{B}$ f(x) means that the function f(x) is first operated on by $\hat{B}$ to yield a new function g(x) which is then operated on by $\hat{A}$ to yield the final function h(x).

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

For example, let $\hat{A}$ be $4x^2$, $\hat{B}$ be $\frac{d}{dx}$, and $f(x) = ax^3$, then

$$\hat{A}\hat{B}\, f(x) = 4x^2 \cdot \frac{d}{dx}(ax^3) = 4x^2 \cdot (3ax^2) = 12ax^4$$

The square of an operator means that the same operator is applied successively twice, i.e. $\hat{A}^2 f(x) = \hat{A}\hat{A}\, f(x)$. For example,

let $\quad \hat{A} = \frac{d}{dx}$ and $f(x) = \sin x$, then $\hat{A}^2 f(x) \left(\frac{d}{dx}\right)^2 \sin x$

or $\quad \frac{d^2}{dx}(\sin x) = \frac{d}{dx}\left[\frac{d}{dx}(\sin x)\right] = \frac{d}{dx}(\cos x) = -\sin x$

Commutative Property

When a series of operation is performed on a function successively the result depends on the sequence in which the operation is performed; in other words, in operator algebra it is not necessary that $\hat{A}\hat{B}\, f(x) = \hat{B}\hat{A}\, f(x)$. For example, let $\hat{A}$ denote $\frac{d}{dx}$, $\hat{B}$ stand for $3x^2$, and the function f(x) be sin x; then,

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

$$= 6x \sin x + 3x^2 \cos x$$

and $\quad \hat{B}\hat{A}\, f(x) = 3x^2 \cdot \frac{d}{dx}(\sin x) = 3x^2 \cdot \cos x = 3x^2 \cos x$

If two operators are such that the result of their successive applications is the same irrespective of the order of operations then the two operators are said to be *commutative*. In the above example, the two operators are non commutative. Now

let $\quad \hat{A}$ stand for 3 +, $\hat{B}$ for 4, and f(x) be ax; then,

$$\hat{A}\hat{B}\, f(x) = 3 + 4 + (ax) = 3 + (4 + ax) = 7 + ax$$

$$\hat{B}\hat{A}\, f(x) = 4 + 3 + (ax) = 4 + (3 + ax) = 7 + ax$$

Thus, $\hat{A}$ and $\hat{B}$ commute

Linear Operator

An operator is said to be linear if its application on the sum of two functions gives the result which is equal to the sum of the operation on the two functions separately, i.e. if

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

or $\quad \hat{A}[Cf(x)] = C \cdot \hat{A}\,f(x)$, where C is constant

Examples

(i) $\frac{d}{dx}$ is a linear operator because $\frac{d}{dx}(ax^m + bx^n) = \frac{d}{dx}(ax^m) + \frac{d}{dx}(bx^n)$

(ii) $\sqrt{\;}$, square root, is not a linear operator because

$$\sqrt{f(x) + g(x)} \neq \sqrt{f(x)} + \sqrt{g(x)}$$

Commutator Operator

For any two operator $\hat{A}$ and $\hat{B}$, the difference $\hat{A}\,\hat{B} - \hat{B}\,\hat{A}$, which is simply denoted by $\hat{A}\,\hat{B} - \hat{B}\,\hat{A}$ or [A, B] is called "commutator operator".

If $\hat{A}$ and $\hat{B}$ commute then [A, B] = 0, where 0 is called the zero operator which means multiplying a function with zero.

In the earlier example, where, $\hat{A} = \frac{d}{dx}$, $\hat{B} = 3x^2$ and f(x) = sin x, the commutator is obtained as follows

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

$$= (6x \sin x + 3x^2 \cos\,) - 3x^2 \cos x$$

$$= 6x \sin x = 6x\,f(x)$$

or $\quad [A, B] = 6x$

The Operator ∇ and ∇^2

So far we have given the examples of simple one-dimensional operators viz. $\frac{d}{dx}$, 4x, etc., which operate on functions of a single variable like f(x) or f(x) + g(x). But there may be two-or three-dimensional operators which operate on function or more than one variable, i.e., f(x, y, z). Thus, the operator $\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}$ when applied to a function f, where f stands for f(x, y, z), gives the results,

$$\left(\frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z}\right) f = \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} + \frac{\partial}{\partial z}$$

A very important differential operator, known as "del" or ∇-operator, or a vector operator, is defined as,

$$\nabla = \vec{i}\,\frac{d}{dx} + \vec{j}\,\frac{d}{dy} + \vec{k}\,\frac{d}{dz}$$

where $\vec{i}$, $\vec{j}$ and $\vec{k}$ are unit vectors along the x, y and z axes. This is a vector operator in the sense that when applied to a scalar function it transforms it into its gradient which is a vector.

The rules for converting a classical function to corresponding quantum mechanical operator are as follows:

1. Quantum mechanical operator corresponding to each Cartesian coordinate is the same as its classical value, for example,

$$\hat{x} = x;, \hat{y} = y \text{ etc.} \tag{2.65}$$

2. Each Cartesian component of linear momentum is replaced by the operator.

$$\hat{p_x} = \frac{h}{2\pi i} \cdot \frac{\delta}{\delta x} = -\frac{ih}{2\pi}\frac{\delta}{\delta x} \tag{2.66}$$

Similarly,

$$\hat{p_y} = \frac{h}{2\pi i} \cdot \frac{\delta}{\delta y} \text{ and } \hat{p_z} = \frac{h}{2\pi i} \cdot \frac{\delta}{\delta z}$$

where $i = \sqrt{-1}$. The quantity $\frac{1}{i}$ is equal to $-i$, become $i(-1) = 1$.

On the basis of these rules operator for other quantities can be determined. Thus the operator for energy is the Hamiltonian ($\hat{H}$) angular momentum is $\hat{L}$. These can be expressed in terms of equations (2.65, 2.66). As we know that the total energy of a conservative system in classical mechanics is represented by H and its value is equal to the kinetic energy (T) and the potential energy (V), i.e.

$$H = T + V$$

The corresponding Hamiltonian operator

$$\hat{H} = \hat{T} + \hat{V} \tag{2.67}$$

Thus the eigenvalue equation for the energy may be written as

$$\hat{H}\Psi = E\Psi$$

Some common quantum-mechanical operators as derived from their classical expressions are shown in Table 2.1

Actually the rules given here relating the operators to classical observable are only one of the many possible ways of constructing a set of rules. We call a given set of rules a particular representation (here the coordinates representation) of quantum mechanics. The other representation is the momentum representation.

Table 2.1 Common Quantum-Mechanical Operators as Derived from their Classical Expressions

Classical Variable	Quantum Mechanical Operator	Operation
Position x	$\hat{x}$ (similarly for the y- and z-direction)	x(multiplication)
Linear momentum p_x(x-direction)	$\hat{p}_x$ (similarly for the y- and z-direction)	$\frac{h}{2\pi i}\left(\frac{\partial}{\partial x}\right)$
Angular momentum L_z (rotation about the z axis)	$\hat{L}_z$	$\frac{h}{2\pi i}\left(\frac{\partial}{\partial \phi}\right)$
Kinetic energy T	$\hat{T}$	$-\frac{h^2}{8\pi^2 m}\nabla^2$
Potential energy $V(x, y, z)$	$\hat{V}(x, y, z)$	$V(x, y, z)$ (multiplication)
Total energy H(Hamiltonain)	$\hat{H} = \hat{T} + \hat{V}$	$-\frac{h^2}{8\pi^2 m}\nabla^2 + \hat{V}$

Example 2.12

Show that if all the eigen functions of two ...