UNIT 7 OBSERVABLES AND OPERATORS

Structure

7.1 INTRODUCTION

In the block introduction we had said that quantum mechanics developed along two tracks. In Units 4 to *6* we have presented one of these. You have learnt about the wave-particle duality in Unit 4. In the previous unit, you have studied how Erwin Schrodinger discovered the wave equation for matter waves, which is now called the Schrödinger equation. You have also learnt that in quantum mechanics any state of a system is represented by a wave function ψ which can be obtained by solving the Schrödinger equation. You have studied the probabilistic interpretation of ψ given by Max Born, that the de-Broglie Schrödinger waves are waves of probability which also satisfy the uncertainty relation. Thus Units 4 to 6 present the *wave mechanics version* of quantum mechanics. You should,, of course, realise that the existence of ψ and the Schrödinger equation which form the basis of wave mechanics are postulates. Thus quantum mechanics is based on certain postulates which are not proved but are like axioms of geometry.

In this unit, we will introduce the other track of the development of quantum mechanics which is known as *matrix mechanics* and was developed by Werner Heisenberg, Max Born and P. Jordan in the years 1925 and 1926. In this approach, *only physically observable quantities appear.* Each physical quantity is associated with an 'operator' which can be represented by a matrix. What is an operator? You will find' an answer to this question in the next section. You will learn the method of converting a classical function into a quantum mechanical operator. This method is also one of the postulates of quantum mechanics. The essential difference between classical mechanics and matrix mechanics version of quantum mechanics is this: quantum mechanical operators obey non-commutative algebra. We will explain what this means in Sec. 7.2.2 and briefly discuss commutator algebra along with some of its applications.

The two tracks (Schrodinger's wave mechanics and Heisenberg's matrix mechanics) were integrated by Paul A.M. Dirac who invented an abstract formalism for quantum mechanics in 1930. In the remaining unit we shall present some basic concepts of this unified formulation of quantum mechanics given by Dirac (see Fig. 7.1). One of the basic postulates in this formalism connects the measured value of a dynamical variable with its theoretical value obtained with the help of the wave function ψ. We introduce it in Sec. 7.2.2. Thus we shall be able to relate quantum mechanical operators to physically observable quantities.

In certain circumstances, it is possible that when an operator operates on a wave function, the result may be a multiple of the same wave function. This gives rise to what we call the eigenvalue-eigenfunction equation which you will study in Sec. 7.3. Finally, you will learn about the Ehrenfest theorem which shows the similarity as well as one of the basic differences between classical and quantum mechanics.

The concepts presented in this unit may appear too mathematical and abstract to you in the first reading. However, the formalism presented here is a very powerful and elegant way of working with quantum mechanical systems.

Objectives

After studying this unit you should be able to

- express a classical dynamical variable as a quantum mechanical operator,
- define the hermitian operator and the parity operator and apply their properties to quantum mechanical systems,
- compute the expectation value of an operator,
- derive elementary results of commutator algebra,
- calculate the eigenvalues and eigenfunctions of a given operator,
- derive and interpret Ehrenfest theorem.

7.2 QUANTUM MECHANICAL OPERATORS

What is a quantum mechanical '*operator*'? Let us begin with an analogy to explain this idea. When you exercise, your muscles build up by the action of the exercise: Exercise changes the muscles. The action of quantum mechanical operators on functions is a bit like that of exercise on muscles: they change the functions. You know from classical mechanics that the dynamical state of a system is determined at each instant of time by the knowledge of certain physical quantities, such as the position, velocity, linear momentum, angular momentum, energy etc. of the particles constituting the system. These physical quantities are also called dynamical variables.

Fig. 7.1 : Paul A.M. Dirac, English physicist. He was one of the pioneers of quantum mechanics. He also formulated the relativistic wave equation of quantum mechanics which predicted the existence of positron. He was awarded the Nobel Prize in 1933.

The dynamical variables associated with a system can be measured and provide information about the system at a particular point in space-time. In quantum mechanics, all *dynamical* variables are represented by operators because they bring about changes in the wave functions upon which they act.

All measurable attributes of a quantum mechanical system are called observables, and yet another postulate of quantum mechanics states that

Every physical observable is associated with **an** operator which acts on the wave function,

Pustulate 4 :
Description of physical quantities

Most of these dynamical variables or observables are functions of position *(x)*, linear momentum (p) and time (r) variables. Thus, if we can represent x and p by operators we shall be able to express most of the remaining dynamical variables as operators. A method to convert these variables into quantum mechanical operators is postulated in quantum mechanics as follows:

(i)
$$\boxed{x_{op}\,\psi = x\,\psi} \qquad (7.1)$$

i.e., when operator x_{op} operates upon ψ, the result is simply the multiplication of ψ by the variable x. In other words, the operator corresponding to the dynamical variable x is x itself.

(ii)
$$(p_x)_{op}\,\psi = -i\hbar\,\frac{\partial\psi}{\partial x} \qquad (7.2a)$$

Thus, the momentum operator acting on the wave function results in its differentiation with respect to the conjugate position coordinate x and the result is multiplied by $-i\hbar$. Thus, the operator sf p_x is $-i\hbar\partial/\partial x$.

$$\boxed{(p_x)_{op} = -i\hbar\,\frac{\partial}{\partial x}} \qquad (7.2b)$$

Remember that Eqs. (7.1) and (7.2b) are postulated, i.e., they can't be proved. The position and momentum operators are used in the construction of operators of other dynamical variables such as angular momentum, energy etc. How do we do this? For this, we take the classical expression for any operator D in terms of x and p_x and use Eqs. (7.1 and 7.2b) to obtain its operator form $D_{op}(x, -i\hbar\partial/\partial x, t)$. Notice that the time variable has been retained as itself in the operator formalism. In quantum mechanics, time is not treated as an operator. It is a dynamical variable.

To understand this method further, consider the example of the kinetic energy of a free particle of mass m executing one-dimensional motion given by $p_x^2/2m$. The quantum mechanical operator of the kinetic energy is obtained by replacing p_x by $(p_x)_{op}$. Then using Eq. (7.2b) we get

$$(\text{K.E.})_{op} = \frac{(p_x^2)_{op}}{2m} = \frac{1}{2m}\left(-i\hbar\right)^2 \frac{\partial^2}{\partial x^2} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \tag{7.3a}$$

Furthermore, if its potential energy is given by the function $V(x)$, then its potential energy operator will also be $V(x)$ since x_{op} is x itself:

$$[V(x)]_{op} = V(x) \tag{7.3b}$$

Now do you notice that the sum $\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)_{op}$ is nothing but the quantum mechanical operator of the Hamiltonian which appears in the Schrodinger equation?

Thus, we obtain the Hamiltonian operator:

$$(H)_{op} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \tag{7.4}$$

In this manner, you can convert most of the dynamical variables into quantum mechanical operators. An important quantum mechanical operator that you will encounter in our subsequent discussions is the **parity operator.** We will introduce it here.

The Parity Operator

Parity is a simple but very useful concept in quantum mechanics. Consider a wave function $\psi(x)$. If on changing x to $-x$, the following relationship is obtained

$$\psi(-x) = \pm\,\psi(x) \tag{7.5}$$

then we say that the function $\psi(x)$ has a definite parity. If $\psi(-x) = +\,\psi(x)$, then $\psi(x)$ is of **even** parity. On the other hand, for $\psi(-x) = -\,\psi(x)$, the parity of $\psi(x)$ is said to be **odd.** All functions which do not obey (7.5) are said to have mixed parity. The parity operation is equivalent to transforming a right-handed system of coordinates into a left-handed one. Do you recall where you have first encountered this operation? It was introduced in Unit 1 of the elective PHE-04 (Mathematical Methods in Physics-I) where you have studied about this operation in relation to vectors. The parity operator is defined by

$$P\,\psi(x, t) = \psi(-x, t) \tag{7.6a}$$

and

$$P A\left[x, -i\hbar\frac{\partial}{\partial x}, t\right] = A\left(-x, i\hbar\frac{\partial}{\partial x}, t\right) \tag{7.6b}$$

You can readily see that the parity operator is a space inversion operator, **i.e.**, under its operation $x \rightarrow -x$. Thus if $\psi(x)$ describes the state of a system, P $\psi(x)$ describes its mirror image.

We have discussed a method to obtain quantum mechanical operators from the corresponding classical expression by changing x by x, t by t and p_x by $-i\hbar\frac{\partial}{\partial x}$. However, there is no classical expression, in terms of x and p_x which changes the sign of the argument of a function by its operation. Hence, we say that the parity operator has no classical analog.

You should now carry out a couple of quick exercises to fix all the ideas presented so far in your mind.

SAQ 1

Spend 10 min

(a) Express the variables p_y and p_z in operator form.

(b) Write the three components of the angular momentum L in terms of x, y, z and p_x, p_y and p_z and thus obtain quantum mechanical operators for L_x, L_y and L_z.

You have just studied that in quantum mechanics, the measurable classical dynamical variables like position, momentum etc. are represented by operators. These operators act on a wave function and change it in some way. We have summarised the results obtained so far for ready reference.

Dynamical Variables and Corresponding Operators

Dynamical Variable	*Operator*
Position coordinate x	x
x component of momentum p_x	$-i\hbar \frac{\partial}{\partial x}$
Kinetic energy $T = \frac{p_x^2}{2m}$	$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$
Potential energy $V(x, t)$	$V(x, t)$
Total energy $\frac{p_x^2}{2m} + V(x, t)$	Hamiltonian $H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$
Angular Momentum	
L_x	$yp_z - zp_y$
L_y	$zp_x - xp_z$
L_z	$xp_y - yp_x$

Let us now discuss some important properties of these operators.

7.2.1 Properties of Operators

Firstly, operators in quantum mechanics are generally linear operators. What is a linear operator? By definition, a linear operator satisfies the following properties:

$$D_{op}(\phi + \psi) = D_{op}\phi + D_{op}\psi \quad (7.7a)$$

$$D_{op}\, c\phi = c\, D_{op}\, \phi \quad (7.7b)$$

where c is an arbitrary complex number. In general, we can combine Eqs. (7.7a and b) and write for a linear operator:

$$D_{op}(\lambda\phi + \mu\psi) = \lambda(D_{op}\phi) + \mu(D_{op}\psi) \quad (7.8)$$

where λ and μ are complex numbers. It is easy to see that both x and p_x satisfy Eqs. (7.7). You may like to check it out.

Spend 5 min

SAQ 2

Show that x and p_x satisfy the criterion of linearity.

Secondly, in general, quantum mechanical operators do not necessarily commute. What do we mean by this? To understand it, recall that in classical mechanics, we define angular momentum L as **r × p** and not as **p × r,** which is equal to − L. Putting this result in a mathematical language we can say that **r** and p **do not commute under the operation of vector product.** A similar situation exists for quantum mechanical operators. If two operators A and B operate one after the other on a function ψ, then their order of operation is important. In general, $BA\psi$ is not equal to $AB\psi$ for any arbitrary ψ, i.e.

$$\left[AB - BA \right] \psi \neq 0 \tag{7.9a}$$

The expression AB − BA is denoted by the **commutator bracket** [A, B]. Thus, we define the **commutator** of two operators as the difference AB − BA and denote it by the symbol [A, B]:

$$\boxed{[A, B] \equiv AB - BA} \tag{7.9b}$$

and, in general,

$$[A, B] \neq 0 \tag{7.9c}$$

In other words, in general, the operators A and B do not commute with one another and the value of the commutation bracket [A, B] is non-zero. What does this result mean? It means that we have to be careful,about the order of operators in considering operator products in quantum mechanics. However, if the commutator of the operators A and B vanishes, A and B commute, i.e., AB = BA. Then we can interchange their order.

To understand these concepts better, let us take a concrete example of operators. Let us examine whether the operators x and p_x commute with one another. For this purpose we evaluate

$$[x, p_x]\, \psi = x \left(-i\hbar \frac{\partial \psi}{\partial x} \right) + i\hbar \frac{\partial}{\partial x} (x\, \psi) = i\hbar\, \psi$$

Since ψ is arbitrary we obtain

$$\boxed{[x, p_x] = i\hbar} \tag{7.10}$$

Thus we have found that x and p_x operators do not commute with one another and the value of the commutation bracket is $i\hbar$. This result also tells us that we have to take care of the order of these operators when we apply them on a system. For instance, if the momentum operator acts first on a system followed by the position operator, it yields a certain result. The result is different if the position operator operates first and is followed by the momentum operator. This result has an interesting fallout. Sometimes, you may come across a situation where the product of x and p occurs in a classical dynamical variable. Now in quantum mechanics, the order of operators matters. So in which order do we put x and p? In such a case, we simply symmetrize the product, i.e., we replace the variable xp_x by the operator $\frac{1}{2}(xp_x + p_x x)$:

$$xp_x \to \frac{1}{2}(xp_x + p_x x)$$

You should note that x and p_x are what are termed in classical mechanics as ***canonically conjugate variables.*** In classical mechanics we do not have an equation like Eq. (7.10), since x and p_x are dynamical variables which have complex numerical values. So they occur interchangeably in classical expressions of physical quantities. You should feel completely at home with these concepts before proceeding further. So work out this exercise.

SAQ 3

Spend 5 min

(a) Show that x_{op} commutes with $(p_y)_{op}$ and $(p_z)_{op}$.

(b) Determine $[y, p_y]$ and $[z, p_z]$.

Thus you have found that the quantum mechanical operators corresponding to classical canonically conjugate position and momentum variables do not commute with one another: x does not commute with p_x, y does not commute with p_y and z does not commute with p_z. The value of the commutation bracket is $i\hbar$ in each case. Because of this non-commutability we are required to write xp_x (yp_y or zp_z) in a symmetric form while converting a dynamical variable D containing such terms into its quantum mechanical operator. Let us now make use of the definition of $[A, B]$ given by Eq. (7.9b) to derive some interesting basic results of commutator algebra.

Basic Commutator Algebra

1. The following results satisfied by operators are useful and readily proved

$$[A, B] = - [B, A] \tag{7.11a}$$

$$[A, B+C] = [A, B] + [A, C] \tag{7.11b}$$

$$[AB, C] = A[B, C] + [A, C]B \tag{7.11c}$$

and

$$[A, BC] = B[A, C] + [A, B]C \tag{7.11d}$$

You should quickly verify Eqs. (7.11a) to (7.11d) before studying further.

2. Any operator always commutes with its own power, i.e.,

$$[A^n, A] = 0,\ n = 1, 2, 3 \ldots. \tag{7.12}$$

It follows from Eqs. (7.11) and (7.12) that if $f(x)$ is an operator which can be expanded in the powers of x then

$$[f(x), p_x] = i\hbar \frac{\partial}{\partial x}(f(x)) \tag{7.13}$$

Similarly, if $f(p_x)$ can be expanded in the powers of p_x we have

$$[x, f(p_x)] = i\hbar \frac{\partial f(p_x)}{\partial p_x} \tag{7.14}$$

You may like to prove Eqs. (7.13) and (7.14) before studying further.

SAQ 4

Spend 10 min

(a) Prove Eqs. (7.13) and (7.14).

(b) Show that the parity operator commutes with

$$A(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + ax^2 + bx^4$$

Now, since ***observables are measurable attributes of any physical system, they are real quantities.*** Therefore, they should be represented by operators which, when operating on a physical system, yield real values of the observables. In quantum mechanics, all observables are represented by such operators, which are called **hermitian operators.** Let us now study briefly about them.

Hermitian Operators

A hermitian operator is defined as follows:

$$\int \phi^* (D_{op}\psi)\, d\tau = \int (D_{op}\phi)^* \, \psi \, d\tau \qquad (7.15a)$$

For a one-dimensional system the volume element $d\tau$ is simply dx and the limit of integration is from $-\infty$ to $+\infty$. However, for a three dimensional systems $d\tau$ is the volume element $dx\, dy\, dz$ and all the three variables cover the whole space, **i.e., the** variables vary from $-\infty$ to $+\infty$.

Integrals like Eq. (7.15a) will occur quite often in this course. Hence we adopt a short hand notation and take

$$\int \phi^* (D_{op}\psi)\, d\tau = (\phi, D\psi) \qquad (7.15b)$$

and

$$\int (D_{op}\phi)^* \, \psi d\tau = (D\phi, \psi) \qquad (7.15c)$$

Henceforth, we shall use the same symbol D for the dynamical variable and also for its operator if there is no confusion. The integral $(\phi, D\psi)$ is also known **as inner product** or **scalar product** of 4 with $D\psi$. For $\phi = \psi$ and D = I, the identity operator, the integral (ψ, ψ) is known as the **norm of the wave function** ψ**.** You should notice that for a *normalised* ψ the *norm* is *equal* to unity. The norm of a wave function representing a state of a system is always positive. It can be zero only when $\psi = 0$, **i.e.,** that state of the system does not exist.

To understand these concepts concretely, let us now consider the linear momentum operator **p** and show that it is a hermitian operator. We have $\mathbf{p} = \hat{\mathbf{l}}\, p_x + \hat{\mathbf{m}}\, p_y + \hat{\mathbf{n}}\, p_z$ where $\hat{\mathbf{l}}$, $\hat{\mathbf{m}}$ and $\hat{\mathbf{n}}$ are unit vectors along x, y and z axes, respectively. You have already proved in **SAQ** 2 that

$$p_x (\lambda\phi + \mu\psi) = \lambda(p_x\, \phi) + \mu\, (p_x\psi)$$

This result holds for p_y and p_z as well. Hence, p_x, p_y and p_z are linear operators, Now let us consider the integral

$$I = \int_{-\infty}^{\infty} \phi^* \, (p_{op}\psi)\, dx = -i\hbar \int_{-\infty}^{\infty} \phi^* \frac{\partial \psi}{\partial x}\, dx$$

where p_{op} stands for p_x, p_y or p_z. Integrating by parts we get

$$I = -i\hbar\, [\phi^*\psi]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \left(-i\hbar \frac{\partial \phi}{\partial x}\right)^* \psi\, dx$$

If at least one of the functions is a normalizable wave function then the first term vanishes because the normalizable wave'functions go to zero at $x = \pm\infty$. Thus

$$I = \int_{-\infty}^{\infty} (p_{op}\, \phi)^* \, \psi\, dx \qquad (7.16)$$

implying that p_{op} is a hermitian operator. Thus p_x, p_y, p_z and **p** are all hermitian operators.

The position operator x is obviously linear and hermitian. Hence the angular momentum and Hamiltonian operators are also linear and hennitian,

The operators which satisfy Eq. (7.15a) are also known as self **adjoint** operators. Here it is useful to introduce the *adjoint* or Hermitian conjugate of an operator D, by the relation.

$$\int \phi^* D\psi\, d\tau = \int (D^\dagger\, \phi)^* \psi d\tau \qquad (7.17a)$$

If $D = D^\dagger$ then the operator D is said to be **self adjoint.** You can readily compare Eqs. (7.15a) and (7.17a) and see that for a **hermitian** operator

$$D^\dagger = D \tag{7.17b}$$

Now suppose $D = AB$ then according to Eq. (7.17a)

$$\int \phi^* (AB\psi)d\tau = \int \{(AB)^\dagger \phi\}^* \psi d\tau \tag{7.18a}$$

But we can also write

$$\int \phi^* (AB\psi)d\tau = \int \phi^* \{A(B\psi)\}d\tau$$

Thus, applying Eq. (7.17a) twice we have

$$\int \phi^* (AB\psi)d\tau = \int \{(A^\dagger \phi\}^* (B\psi)d\tau = \int (B^\dagger A^\dagger \phi)^* \psi d\tau \tag{7.18b}$$

Hence, comparing Eqs. (7.18a) and (7.18b), we obtain an important result for **adjoint operators** which applies to **hermitian** operators also:

$$\boxed{(AB)^\dagger = B^\dagger A^\dagger} \tag{7.18c}$$

In quantum mechanics, operators are represented by matrices. In terms of matrix algebra, the matrix representing $D^\dagger$ is obtained by taking the complex conjugate and the transpose of the matrix representing D.

So far, we have introduced you to the concepts of observables and operators. We have said that every observable is associated with an operator. Now you may ask: Exactly what is the connection between observables and operators? That is what we shall discover in the next section.

7.2.2 Expectation Values

Let us consider the measurement of a dynamical variable or the observable D of a system. Keeping the system always in a particular state ψ we measure D repeatedly. In general, each individual measurement will yield a different result. Hence we take the average of these measurements $\langle D\rangle$ as the value of the dynamical variable for that particular state. Since we have always started with the same state ψ, it is reasonable to assume that knowing ψ we should be able to calculate $\langle D\rangle$. Such a relationship between ψ and $\langle D\rangle$ is provided by another postulate of the quantum mechanics. According to this postulate,

Postulate 5: The measurement postulate

> The average of the measured value of D is given by
>
> $$\langle D\rangle = \frac{\int \psi^* D\psi \, d\tau}{\int \psi^* \psi \, d\tau} = \frac{(\psi, D\psi)}{(\psi, \psi)} \tag{7.19}$$
>
> $\langle D\rangle$ is known as the **expectation value** of the operator D.

If $\langle D\rangle$ as obtained from Eq. (7.19) comes out to be real then the dynamical variable D is said to be an **observable.** Hence we can say that

> **An observable is a dynamical variable having a real expectation value.**

Now we can understand the significance of a hermitian operator. **Hermitian operators** have **real expectation values.** To prove this result, we have

$$\langle D\rangle = \frac{\int \psi^* D\psi \, d\tau}{\int \psi^* \psi \, d\tau} = C \int \psi^* (D\psi) \, d\tau \tag{7.20a}$$

where C is some constant representing the normalisation of ψ. The complex conjugate of this equation gives

$$\langle D\rangle^* = C\int \psi\,(D\psi)^*\,d\tau \tag{7.20b}$$

The difference is

$$\langle D\rangle - \langle D\rangle^* = C\int \psi^*\,(D\psi)\,d\tau - C\int \psi\,(D\psi)^*\,d\tau$$

Using Eq. (7.15a) this becomes

$$\langle D\rangle - \langle D\rangle^* = C\int \psi^*\,(D\psi)\,d\tau - C\int \psi^*\,(D\psi)\,d\tau$$

$$= 0$$

or $$\langle D\rangle = \langle D\rangle^* \tag{7.21}$$

which means that (D) is real. Thus, we have proved that ***in quantum mechanics all observables are represented by hennitian operators.***

We will now introduce you to another interesting feature arising out of the discussion so far: Representing the Schriidinger equation as an eigenvalue-eigenfunction equation.

7.3 EIGENFUNCTIONS AND EIGENVALUES

So far you have studied that, in general, when an operator D operates upon ψ we get a new function ψ'. However, under special circumstances ψ' may just be a multiple of ψ itself, i.e.,

$$D\psi = d\psi \tag{7.22}$$

where d is a complex number. Under this situation, ψ is said to be an **eigenfunction** of the operator D having d as its **eigenvalue.** Eq. (7.22) is called the **eigenvalue-eigenfunction equation** for **the** operator D. Now recall the time independent Schriidinger equation given in Unit 6:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V\right]\psi = E\psi$$

Do you **recognise** that the left hand side is nothing but the **Hamiltonian** H? We can also write this equation as

$$H\psi = E\psi \tag{7.23}$$

Thus, the time independent **Schrödinger** equation is an eigenvalue eigenfunction equation for the operator H (see Eq. 7.4). It tells us that H operating on a special class of wave functions gives back the same wavefunctions multiplied by the eigenvalue E of H. Since H **is hermitian,** the eigenvalue E is real. This result can be proved for any hennitian operator satisfying an eigenvalue eigenfunction equation as follows:

From Eq. (7.15a) we have

$$(\psi, D\psi) = (D\psi, \psi)$$

Now with the help of Eq. (7.22) we get

$$d\,(\psi, \psi) = d^*\,(\psi, \psi)$$

But for a given state ψ **is** not zero, hence (ψ, ψ) is finite. Thus we obtain

$$d = d^*$$

Hence, **the eigenvalue of a hermitian operator is always real,** In this case the expectation value $\langle D\rangle$ is equal to d **itself,** which is real.

Using the concepts presented so far, we would like to introduce an important class of eigenfunctions namely, eigenfunctions which are **normalised to unity** and satisfy the **orthogonality property.** Such eigenfunctions are called **orthonormal eigenfunctions.** In this connection, we will also introduce another useful concept of the **degeneracy of eigenfunctions.**

Orthonormal Eigenfunctions

Suppose for a system there are more than one eigenfunctions of an operator having the same eigenvalue. Then all such functions are called **degenerate eigenfunctions.** Eigenfunctions of an operator having different eigenvalues are called **non-degenerate eigenfunctions.** Let us now take two non-degenerate eigenfunctions ϕ and ψ of a hermitian operator D, having eigenvalues d_1 and d_2, respectively:

$$D\phi = d_1\phi \quad \text{and} \quad D\psi = d_2\psi$$

Let these eigenfunctions be normalised to unity. Then from Eqs. (7.15a) and *(7.22)* we obtain:

$$\int \phi^* (D\psi)\, d\tau = \int (D\phi)^* \psi d\tau$$

or $$d_2 (\phi, \psi) = d_1(\phi, \psi)$$

or $$(d_2 - d_1) (\phi, \psi) = 0 \tag{7.24}$$

Since $d_1 \neq d_2$ we find that the inner product (4, ψ) of ϕ and ψ in Eq. *(7.24)* is zero. Eigenfunctions having inner product equal to zero are said to be **orthogonal** to each other:

$$(\psi_i, \psi_j) = 0, \quad \text{for} \quad i \neq j \tag{7.25}$$

We can generalise this statement. If $\psi_1, \psi_2, \ldots \psi_n$ are ***non-degenerate eigenfunctions of a hermitian operator, normalised to unity*** then they satisfy the following ***orthonormality condition***

$$(\psi_i, \psi_j) = 0 \quad \text{for } i \neq j \tag{7.26a}$$

$$(\psi_i, \psi_j) = 1 \quad \text{for } i = j \tag{7.26b}$$

Thus, the eigenfunctions are normalised to unity, and all eigenfunctions ψ_i, ψ_j satisfy the orthogonality property (7.26a) for $i \neq j$. We can make use of the Kronecker delta symbol δ_{ij} and write Eqs. (7.26a and *b)* in a compact form:

$$(\psi_i, \psi_j) = \delta_{ij} \tag{7.26}$$

where δ_{ij} is defined as:

$$\delta_{ij} = 0 \quad \text{for} \quad i \neq j$$

$$\delta_{ij} = 1 \quad \text{for} \quad i = j$$

Such eigenfunctions which satisfy Eq. *(7.26)* are called **orthonormal functions** and form an **orthonormal set.**

Using these ideas we can show that if ψ is a non-degenerate eigenfunction of an bperator D and D commutes with another operator B then ψ is also an eigenfunction of B. To prove it let us operate B on Eq. *(7.22)* from *the* left to obtain

$$BD\psi = d(B\psi) \tag{7.27a}$$

since d is a number. Furthermore, B commutes with D, hence, we also have

$$D(B\psi) = B(D\psi) = d(B\psi) \tag{7.27b}$$

The above equation clearly shows that $(B\psi)$ is an **eigenfunction** of D with the same eigenvalue d. Since ψ is not degenerate with $B\psi$, the eigenfunction B y must be a multiple of ψ, i.e.,

$$B\psi = b\psi \qquad (7.28)$$

From Eq. (7.28) we conclude that ψ is also an eigenfunction of the operator B with **the** eigenvalue b. In general, if there are n commuting operators and Ψ is a non-degenerate eigenfunction of any one of them then it is an eigenfunction of the remaining $(n-1)$ operators also. These n operators form ***a* set** of **commuting operators.**

We now proceed to demonstrate that ***if an operator A commutes with the parity operator P, then the non-degenerate eigenfunctions of A have definite parity.***

Let

$$A(x, p_x)\,\psi(x) = \lambda\,\psi(x) \qquad (7.29a)$$

Applying P to Eq. (7.29a) from left and using the condition $[P, A] = 0$ we get

$$A(x, p_x)\left\{P\,\psi(x)\right\} = \lambda\left\{P\,\psi(x)\right\} \qquad (7.29b)$$

Thus we notice that both $\psi(x)$ and $P\psi(x)$ are eigenfunctions of A with the same eigenvalue. Since $\psi(x)$ is non-degenerate, the two functions $\psi(x)$ and $P\psi(x)$ can differ at the most by a ccnstant. Hence

$$P\,\psi(x) = p\,\psi(x) \qquad (7.30a)$$

Thus $\psi(x)$ is an eigenfunction of the parity operator with p as the eigenvalue. Applying once again the parity operator we get

$$P^2\psi(x) = p\,P\psi(x) = p^2\psi(x) \qquad (7.30b)$$

But $\psi(x)$ and $P^2\psi(x)$ are identically the same. Hence $p^2 = 1$, i.e., $p = \pm 1$. Thus, $\psi(x)$ are of definite parity. For degenerate eigenfunctions it is possible to take linear combinations of $\psi(x)$ and $\psi(-x)$ to obtain eigenfunctions of definite parity. Equation (7.30b) also gives us the **eigenvalues of the parity operator;** these **are ± 1.**

We shall use the parity operators in the next block to obtain eigenfunctions and. eigenvalues of some simple systems,

We end this discussion with an exercise for you.

Spend 10 min

SAQ 5

Show that the functions exp $(-x^2/2)$ and x exp $(-x^2/2)$ are eigenfunctions of the operator $(-d^2/dx^2 + x^2)$. Calculate the eigenvalues and show that the two functions are orthogonal to each other.

In the last section of this unit, it would not be out of place to establish a correspondence between the quantum mechanical and .Classical concepts. Remember that in quantum mechanics we have operators and in classical mechanics there are only dynamical variables which may be complex numbers. Thus we have to consider the expectation values of operators. Now, according to the correspoqdence principle we expect that the motion of a quantum object, represented by ψ, should agree with that of a classical particle whenever the distances and momenta become so large that we can ignore the uncertainty principle. When we try to explore this point, we arrive at the **Ehrenfest theorem.**

7.4 EHRENPEST THEOREM

Let us consider the rate of change of an observable D, which does not depend explicitly on time. From Eq. (7.19) we obtain for a normalized wave function ψ

$$\frac{d\langle D\rangle}{dt} = \left(\frac{\partial\psi}{\partial t}, D\psi\right) + \left(\psi, D\frac{\partial\psi}{\partial t}\right) \quad (7.31)$$

Now we use time dependent Schrödinger equation in Eq. (7.31) to replace $\frac{\partial\psi}{at}$ by $\frac{1}{iA}H\psi$. Thus

$$\frac{d\langle D\rangle}{dt} = -\frac{1}{i\hbar}(H\psi, D\psi) + \frac{1}{i\hbar}(\psi, DH\psi)$$

or

$$\frac{d\langle D\rangle}{dt} = \frac{l}{i\hbar}\left[\int\psi^* DH\psi\, d\tau - \int\psi^* HD\psi\, d\tau\right], \text{ since } H \text{ is hermitian } H^\dagger = H.$$

or

$$\frac{d\langle D\rangle}{dt} = \left(\psi, \frac{1}{i\hbar}[D, H]\psi\right) \quad (7.32a)$$

or

$$\frac{d\langle D\rangle}{dt} = \frac{1}{i\hbar}\langle[D, H]\rangle \quad (7.32b)$$

Let us now take D to be ,position operator then

$$[D, H] = [x, H] = \frac{1}{2m}[x, p_x^2] = i\hbar\frac{p_x}{m}. \quad (7.33)$$

Putting Eq. (7.33) into Eq. (7.32b) we obtain

$$\frac{d\langle x\rangle}{dt} = \frac{1}{m}\langle p_x\rangle \quad (7.34)$$

Furthermore, let us take D to be the linear momentum operator, In this case

$$\frac{d\langle p_x\rangle}{dt} = \left\langle -\frac{\partial V}{\partial x}\right\rangle \quad (7.35)$$

You should note that Eqs. (7.34) and (7.35) are very similar to the equations which define linear momentum and force in classical mechanics. However, the basic difference between the two mechanics is that x, p_x and $\frac{\partial V}{\partial x}$ of classical mechanics a n *replaced* by *their average values in quantum mechanics.* For *a* macroscopic system there is hardly any difference between x, p_x and $\partial V/\partial x$ and their average values. However, for microscopic systems they are quite different. As a matter of fact you have seen that for a microscopic system the precise values of x and p_x do not exist simultaneously but their average values $\langle x\rangle$ and $\langle p_x\rangle$ can be obtained.

Eqs. (7.34) and (7.35) constitute the Ehrenfest theorem which shows the correspondence as well as a basic difference between classical and quantum mechanics, You may like to apply these ideas and make use of Eq. (7.32b) to arrive at an interesting result.

Spend 5 min

SAQ 6

Show that when an operator commutes with the Hamiltonian, the expectation value of the observable associated with it is a constant of motion. Hence prove that the linear momentum of a system is conserved when no net force fields acts on the system.

Let us now summarise what you have studied in this unit.

7.5 SUMMARY

- In this unit you have learned about two more postulates of the quantum mechanics, in addition to the postulates given in the previous unit. According to the first of these postulates, **every observable is associated with an operator.** The operators corresponding to the dynamical variables x and p_x are x and $-i\hbar \frac{\partial}{\partial x}$
- To construct an operator of any other dynamical variable we write that function in terms of x, p_x (in a symmetric form) and then replace p_x by $-i\hbar\,\partial/\partial x$.
- Most of the operators relevant to quantum mechanics are **linear** and **hermitian,** i.e.,

$$D\,(a\psi + b\,\phi) = aD\,\psi + bD\,\phi$$

$$(\psi,\, D\,\phi) = (D\psi,\, \phi)$$

- According to another postulate of quantum mechanics the **expectation value** of a dynamical variable D, is equal to the average value of D, obtained by the repeated measurement of D for that system in the same state. A ***dynamical variable having real expectation value is said to be an* observable.**
- For quantum mechanical operators in general $AB\psi \neq BA\psi$ and the value of the commutation bracket **[A, B] = AB – BA** is non-zero.
- If the operation of D on ψ produces a multiple of ψ say $d\psi$ then ψ is said to be an **eigenfunction** of D having **eigenvalue** d. ***The eigenvalues of a hermitian operator are real.***
- The rate of change of average $\langle x \rangle$ and $\langle p_x \rangle$ for a system of mass m and potential energy $V(x)$ are equal to $\langle p_x \rangle / m$ and $\langle -\partial V/\partial x \rangle$, respectively. These relations are called **Ehrenfest theorems** and are very similar to those obtained in classical mechanics with the difference that in classical mechanics we consider x, p_x and $\partial V/\partial x$ themselves instead of their averages.

7.6 TERMINAL QUESTIONS

Spend 45 min

1. A state of a particle of mass m is given by $e^{-\alpha x^2}$. Normalise the wave function **and** calculate the expectation value of the kinetic energy of the particle.

2. If for two operators **A** and **B**

$$[A, B] = 1$$

then show that $[A^2, B^2] = 2\,(AB + BA)$.

3. If two non-commuting operators **A** and **B** commute with their commutator **[A, B],** show that

$$[A, B^n] = n\, B^{n-1}\, [A, B]$$

where n is an integer. Hence obtain the value of $[e^x, p_x]$.

4. If for a quantum mechanical system

$$(p_x^2/2m + V(x))\,\psi(x) = E\,\psi(x)$$

show that $\langle \text{K.E.} \rangle = \frac{1}{2}\langle x\,\partial V/\partial x \rangle$.

The expression is known as **Virial** theorem.

Hint: Start with $\langle [xp_x, H] \rangle = 0$.

5. a) Determine whether the parity operator P is hermitian or not.

   b) Show that all operators which are invariant under space inversion commute with the parity operator.

6. The Hamiltonian of a system is given by

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

and $\psi_1(x)$ and $\psi_2(x)$ are two degenerate energy eigenfunctions of the system. Show that

$$(\psi_1, (xp_x + p_x x)\,\psi_2) = 0$$

Hint: Start with $(\psi_1, [H, x^2]\,\psi_2) = 0$.

7. Show that $[L_z, L_x] = i\hbar L_y$. Hence prove that if ϕ is an eigenfunction of L_z,

$$\langle L_y \rangle = \langle L_x \rangle = 0.$$

8. Suppose $\psi(x) = \sum_i c_i\,\phi_i(x)$

where $\phi_i(x)$ are eigenfunctions of a hermitian operator D with eigenvalues d_i and $(\phi_i, \phi_j) = \delta_{ij}$ then show that

$$(\psi, D\psi) = \sum_i d_i |c_i|^2$$

7.7 SOLUTIONS AND ANSWERS

Self-Assessment Questions

1. a)

$$p_y = -i\hbar\frac{\partial}{\partial y}$$

$$p_z = -i\hbar\frac{\partial}{\partial z}$$

b)

$$L_x = yp_z - zp_y = -i\hbar\, y\frac{\partial}{\partial z} + i\hbar\, z\frac{\partial}{\partial y}$$

$$L_y = zp_x - xp_z = -i\hbar\, z\frac{\partial}{\partial x} + i\hbar\, x\frac{\partial}{\partial z}$$

$$L_z = xp_y - yp_x = -i\hbar\, x\frac{\partial}{\partial y} + i\hbar\, y\frac{\partial}{\partial x}$$

2. $x\,[a\psi + b\phi] = ax\,\psi + bx\,\phi$

$$p_x\,[a\psi + b\phi] = -i\hbar\frac{\partial}{\partial x}[a\psi + b\phi]$$

$$= -i\hbar\, a \frac{\partial \psi}{\partial x} - i\hbar\, b \frac{\partial \psi}{\partial x}$$

$$= a\, p_x \psi + b\, p_x\, \phi$$

Therefore, x and p_x are linear.

3. (a) $[x, p_y] = [xp_y - p_y x]$

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

$$= -i\hbar x \frac{\partial \psi}{\partial y} + i\hbar x \frac{\partial \psi}{\partial y}$$ ($\because$ x and y are independent)

$$= 0$$

Since ψ is arbitrary,

$$xp_y - p_y x = 0$$

Thus operators x and p_y commute.

Similarly, we can show that x commutes with p_z.

(b) $[y, p_y] = i\hbar$

$[z, p_z] = i\hbar$

Proof is similar to that of $[x, p_x] = i\hbar$

4. (a) Since f (x) can be expanded in powers of x, we may write

$$[f(x), p_x] = [\sum_{n=0}^{\infty} x^n, p_x]$$

$$= [x + x^2 + \ldots + x^n + \ldots, p_x]$$

$$= [x, p_x] + [x^2, p_x] + \ldots + [x^n, p_x] + \ldots$$

Now using Eq. (7.11c) we can write

$$[x^2, p_x] = x\,[x, p_x] + [x, p_x]x$$

$$= 2\, i\hbar\, x$$

and

$$[x^3, p_x] = x\,[x^2, p_x] + [x, p_x]x^2$$

$$= x\,[2\, i\hbar x] + i\hbar x^2$$

$$= 3\, i\hbar\, x^2$$

Similarly,

$$[x^n, p_x] = nx^{n-1} i\hbar$$

Thus, we have

$$[f(x), p_x]$$

$$= i\hbar\,[1 + 2x + 3x^2 + \ldots + nx^{n-1} + \ldots]$$

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

You can prove Eq. (7.14) in the same way.

b) Now $A(x) = -\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx^2} + ax^2 + bx^4$

Since $A(-x) = A(x)$ hence $PA(x)\,\psi(x) = A(-x)\,\psi(-x) = A(x)\,P\,\psi(x)$. Since $\psi(x)$ is arbitrary, $A(x)$ commutes with P.

5. We have to show that

$$\left(-\frac{d^2}{dx^2}+x^2\right) f_i = \lambda_i f_i$$

and calculate λ where

(i) $f_1 = \exp\left(-\frac{x^2}{2}\right)$

and

(ii) $f_2 = x \exp\left(-\frac{x^2}{2}\right)$

(i) $\left(-\frac{d^2}{dx^2}+x^2\right)\exp\left(-\frac{x^2}{2}\right)$

$$= -x^2\exp\left(\frac{-x^2}{2}\right) + x^2\exp\left(\frac{-x^2}{2}\right) + e^{-x^2/2}$$

$$= e^{-x^2/2} \text{ implying } \lambda_1 = 1.$$

(i) $\left(-\frac{d^2}{dx^2}+x^2\right)\left(x\, e^{-x^2/2}\right)$

$$= [3x\, e^{-x^2/2} - x^3 e^{-x^2/2} + x^3 e^{-x^2/2}]$$

$$= 3x\, e^{-x^2/2} \text{ implying } \lambda_2 = 3.$$

Terminal Questions

1. The normalisation condition is $N^2 \int_{-\infty}^{\infty} e^{-2\alpha x^2}\, dx = 1$

or

$$N^2 (\pi/2\alpha)^{1/2} = 1 \quad \text{or} \quad N = (2\alpha/\pi)^{1/4} \quad \left[\because \int_{-\infty}^{\infty} e^{-2\alpha x^2}\, dx = \left(\frac{\pi}{2\alpha}\right)^{1/2}\right]$$

$$\{\text{K.E.}\} = \langle p^2/2m\rangle = (2\alpha/\pi)^{1/2}\left(e^{-\alpha x^2}, -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} e^{-\alpha x^2}\right)$$

$$= -\frac{\hbar^2}{2m}(2\alpha/\pi)^{1/2}\left(e^{-\alpha x^2}, -2\alpha(1-2\alpha x^2)\, e^{-\alpha x^2}\right)$$

$$= -\frac{\hbar^2}{2m}\left(\frac{2\alpha}{\pi}\right)^{1/2}\left[-2\alpha\left(\frac{\pi}{2\alpha}\right)^{1/2} + \frac{4\alpha^2}{4\alpha}\left(\frac{\pi}{2\alpha}\right)^{1/2}\right]$$

$$\left[\because \int_{-\infty}^{\infty} e^{-2\alpha x^2}\, dx = \left(\frac{\pi}{2\alpha}\right)^{1/2} \text{ and } \int_{-\infty}^{\infty} x^2\, e^{-2\alpha x^2}\, dx = \frac{1}{2}\left(\frac{\pi}{8\alpha^3}\right)^{1/2}\right]$$

or $\langle \text{K.E}\rangle = \frac{1}{2}\alpha\hbar^2/m.$

2. $[A^2, B^2] = A\,[A, B^2] + [A, B^2]A$ (Using Eq. 7.11c)

$$= A\,\{B[A,B] + [A,B]\,B\} + \{B[A,B] + [A,B]\,B\}\,A$$

$$= AB + AB + BA + BA \qquad \because [A,B] = 1$$

$$= 2(AB + BA)$$

3. Let $[A, B^n] = n\, B^{n-1}[A, B]$ (1)

Hence from Eq. (7.11d)

$$[A, B^{n+1}] = B[A, B^n] + [A, B]\, B^n$$

$= n B^{n} [A,B] + [A,B] B^{n}$ (Using Eq. 7.14)

$= (n+1) B^{n} [A,B].$ (2)

Hence if (1) is true for n it is also true for $n+1$. Since (1) is certainly true for $n = 1$ hence it is also true for n = 2. Thus Eq. (1) is true for any n.

$$\text{Now } e^{x} = \sum_{n=0}^{\infty} x^{n}/n!$$

$$\therefore \quad [e^{x}, p_x] = \sum_{n=0}^{\infty} \frac{1}{n!} [x^{n}, p_x]$$

$$= \sum_{n=1}^{\infty} \frac{1}{(n-1)!} x^{n-1} [x, p_x]$$

$$= i\hbar \sum_{n=1}^{\infty} \frac{x^{n-1}}{(n-1)!} = i\hbar\, e^{x}.$$

4. We have $(\psi, [xp_x, H]\, \psi) = E\,(\psi, xp_x\, \psi) - E\,(\psi, xp_x\, \psi) = 0.$ (1)

Now $[xp_x, H] = [xp_x, p_x^2/2m + V(x)]$

$$= \frac{1}{2m} [xp_x, p_x^2] + [xp_x, V(x)]$$

From Eqs. (7.11b, 7.11c and 7.11d)

$$[xp_x, H] = \frac{1}{2m} [x, p_x^2]\, p_x + x\, [p_x, V(x)] \quad (\because [p_x, p_x^n] = 0,\ [x, V(x)] = 0$$

$$= \frac{1}{2m} [x, p_x]\, 2p_x^2 + x\, [p_x, x]\, (\partial V/\partial x)$$

$$= i\hbar\, p_x^2/m - i\hbar\, x \frac{\partial V}{\partial x}$$

$\because$ Using (1) we get $\langle K.E \rangle = 1/2\, \langle x\, \partial V/\partial x \rangle$.

5. a) We have

$$\int_{-\infty}^{\infty} \psi^*(x)\, P\, \psi(x)\, dx = \int_{-\infty}^{\infty} \psi^*(x)\, \psi(-x) dx = -\int_{\infty}^{-\infty} \psi^*(-x')\, \psi(x') dx'$$

where $x' = -x$

$$= \int_{-\infty}^{\infty} \{P\psi(x')\}^*\, \psi(x')\, dx'$$

Hence P is a Hermitian operator.

b) $PA(x, p_x)\, \psi(x) = A(-x, -p_x)\, \psi(-x) = A(-x, -p_x)\, P\, \psi(x) = A(x, p_x) P\, \psi(x)$

Hence $(PA(x, p_x) - A(x, p_x)P)\, \psi(x) = 0$

Since $\psi(x)$ is arbitrary we have

$[P, A] = 0,$

6. Since ψ_1 and ψ_2 are degenerate, we have

$(\psi_1, [H, x^2]\, \psi_2) = 0$

Now $[H, x^2] = [p_x^2/2m + V(x), x^2]$

$= (1/2m)\, [p_x^2, x^2]$

$= (1/2m)\, 2(p_x x + xp_x]$

$= (1/m)\, (p_x x + xp_x]$ (Using the result of terminal question 2)

$\therefore\ (\psi_1, (p_x x + xp_x)\, \psi_2) = 0.$

7. $[L_z, L_x] = L_zL_x - L_xL_z$

Now from the definition of L_x and L_z (see SAQ 1(b)) we have

$$L_x = yp_z - zp_y \text{ and } L_z = xp_y - yp_x$$

Hence $[L_z, L_x] = [xp_y - yp_x, yp_z - zp_y]$

Using Eq. (7.11b) we get

$$[L_z, L_x] = [xp_y, yp_z] - [xp_y, zp_y] - [yp_x, yp_z] + [yp_x, zp_y]$$

Using Eqs. (7.11c and d)

$$[L_z, L_x] = y\,[xp_y, p_z] + [xp_y, y]p_z - 0 - 0 + y\,[p_x, zp_y] + [y, zp_y]p_x$$

$$= 0 - i\hbar\, xp_z + i\hbar\, zp_x$$

$$= i\hbar\,(zp_x - xp_z) = i\hbar\, L_y$$

Let $L_z\phi = m\,\phi$

But $L_zL_x - L_xL_z = i\hbar\, L_y$

$\therefore \quad (\phi, L_z L_x\phi) - (\phi, L_xL_z\phi) = i\hbar\,\langle L_y\rangle$

$m\,\langle L_x\rangle - m\,\langle L_x\rangle = i\hbar\,\langle L_y\rangle$

$\therefore \quad \langle L_y\rangle = 0.$

Similarly, $\langle L_x\rangle = 0.$

8. Since $\psi(x) = \sum_i c_i\,\phi_i(x)$

we have (D) $= \sum_i \sum_j c_i^*\, c_j\, d_j\,(\phi_i, \phi_j)$

$$= \sum_i \sum_j c_i^* c_j\, d_j\, \delta_{ij}$$

$$= \sum_i |c_i|^2\, d_i.$$

since only those terms of the j series will survive for which $j = i$.

FURTHER READING

1. Concepts of Modern Physics, A. Beiser, McGraw-Hill International Book Company, 1990.
2. Introduction to Quantum Mechanics, B.H. Bransden, C.J. Joachain, ELBS, 1990.
3. Quantum Mechanics, J.L. Powell, B. Crasemann, Addison Wesley Inc, 1961.
4. A Textbook of Quantum Mechanics, P.M. Mathews, K. Venkatesan, Tata McGraw Hill Publishing Company Limited, 1987.

A PERSPECTIVE ON QUANTUM MECHANICS

In this block we have introduced you to those basic ideas and concepts which form the bulwark of the new quantum mechanics. In the process, it may have seemed to you that the entire edifice of classical physics has been turned upside down: the classical ideas of causal determinism, continuity, unambiguous and precise language descriptions lie squarely challenged. What has replaced it is an entirely new way of thinking and understanding our world. And because the behaviour of objects in the quantum world is so unlike ordinary experience, you may have found it very difficult to get used to it, in the first instance. Do not worry. It appears peculiar and mysterious to everyone who encounters it for the first time — whether a novice or an experienced physicist.

All of us know how large objects act — all of our direct experience and intuition applies to such objects. But as you have studied in this block, things on a small scale just do not act that way. Quantum objects are wave-particles represented by wave functions. Though the time-evolution of wave functions is governed by an equation of motion, its solutions give us only a probability of finding the wave-parlicles in a certain region at a given time. Measurement of the physical observables like position, momenta, energy, etc. (which can be determined precisely for classical objects) is governed by the uncertainty principle in the quantum mechanical world. Then there is the idea of quantum jumps (or discontinuities) in quantum mechanics. To put it in a nutshell, as per the Copenhagen interpretation of quantum mechanics cleveloped through the ideas of Born, Heisenberg and Bohr, we calculate quantum objects probabilistically, we determine their attributes somewhat uncertainly and we understand them complementarily. Quantum mechanics, thus, presents a new and exciting world-view that challenges old concepts such as deterministic trajectories of motion and causal continuity. It springs unexpected surprises on us, and keeps our minds in a constant flurry of animated activity.

For those of you philosophically inclined, we present here an excerpt from Feynman's Lectures on Physics which gives us a perspective on quantum mechanics. It is a masterly reflection upon one of the most fundamental concepts of quantum mechanics — the uncertainty principle which has unendingly troubled the best of minds. Through Feynman's eyes, we, the students of physics, get to look deeply and philosophically into the nature of quantum mechanics and the nature of science. This, in our opinion, constitutes a befitting final6 to an introductory foray into the world of quantum mechanics.

"Philosophical Implications

Let us consider briefly some philosophical implications of quantum mechanics. As always, there are two aspects of the problem; one is the philosophical implication for physics, and the other is the extrapolation of philosophical matters to other fields. When philosophical ideas associated with science are dragged into another field, they are usually completely distorted. Therefore we shall confine our remarks as much as possible to physics itself.

First of all, the most interesting aspect is the idea of the uncertainty principle; making an observation affects a phenomenon. It has always been known that making observations affects a phenomenon, but the point is that the effect cannot be disregarded or minimized or decreased arbitrarily by rearranging the apparatus. When we look for a certain phenomenon we cannot help but disturb it in a certain minimum way, and ***the disturbance is necessary for the consistency of the viewpoint.*** The observer was sometimes important in prequantum physics, but only in a rather trivial sense. The problem has been raised: if a tree falls in a forest and there is nobody there to hear it, does it make a noise? ***A real*** tree falling in a ***real*** iorest makes a sound, of course, even if nobody is there. Even if no one is present to hear it, there are other traces left. The sound will shake some leaves, and if wc were careful enough we might find somewhere that some thorn had rubbed against a leaf and made a tiny scratch that could not be explained unless we assumed the leaf were vibrating. So in a certain sense we would have to admit that there is sound made. We might ask; was there a ***sensation*** of sound? No, sensations have to do, presumably, with consciousness. And whether ants are conscious and whether there were ants in the forest, or whether the tree was conscious, we do not know. Let us leave the problem in that form.

Another thing that people have emphasized since quantum mechanics was developed is the idea that we should not speak about those things which we cannot measure. (Actually relativity theory also said this.) Unless a thing can be defined by measurement, it has no place in a theory. And since an accurate value of the momentum of a localized particle cannot be defined by measurement it therefore has no place in the theory. The idea that this is what was the matter with classical theory is a ***false position.*** It is a careless analysis of the situation. Just because we cannot measure position and momentum precisely does not ***a priori*** mean that we ***cannot*** talk about them. It only means that we ***need*** not talk about them. The situation in the sciences is this: A concept or an idea which cannot be measured or cannot be referred directly to experiment may or may not be useful. It need not exist in a theory. In other words, suppose we compare the classical theory of the world with the quantum theory of the world, 'and suppose that it is true experimentally that we can measure position and momentum only imprecisely. The question is whether the ***ideas*** of the exact position of a particle and the exact momentum of a particle are valid or not. The classioal theory admits the ideas: the quantum theory does not. This does not in itself mean that classical physics is wrong. When the new quantum mechanics was discovered, the classical people—which included everybody except Heisenberg, Schrodinger, and Born—said: "Look, your theory is not any good because you cannot answer certain questions like: what is the exact position of a particle?, which hole does it go through?, and some others." Heinsenberg's answer was: "I do not need to ask such questions because you cannot ask such a question experimentally." It is that we do not have to. Consider two theories (a) and (b): (a) contains an idea that cannot be checked directly but which is used in the analysis, and the other, (b) does not contain the idea. If they disagree in their predictions, one could not claim that (b) is false because it cannot explain this idea that is in (a) because that idea is one of the things that cannot be checked directly. It is always good to know which ideas cannot be checked directly, but it is not necessary to remove them all. It is not true that we can pursue science completely by using only those concepts which are directly subject to experiment.

In quantum mechanics itself there is a wave function amplitude, there is a potential, and there are many constructs that we cannot measure directly. The basis of a science is its ability to ***predict.*** To predict means to tell what will happen in an experiment that has never been done. How can we do that? By assuming that we know what is there, independent of the experiment. We must extrapolate the experiments to a region where they have not been done. We must take out concepts and extend them to places where they have not yet been checked. If we do not do that, we have no prediction. So it was perfectly sensible for the classical physicists to go happily along and suppose that the position—which obviously means something for a baseball—meant something also for an electron. It was not stupidity. It was a sensible procedure. Today we say that the law of relativity is supposed to be true at all energies, but somebody may come along and say how stupid we were. We do not know where we are "stupid" until we "stick our neck out;" and so the whole idea is to put our neck out. And the only way to find out that we are wrong is to find out ***what*** our predictions are. It is absolutely necessary to make constructs.

We have already made a few remarks about the indeterminacy of quantum mechanics. That is, that we are unable now to predict what will happen in physics in a given physical circumstance which is arranged as carefully as possible. If we have an atom that is in an excited state and so is going to emit a photon, we cannot say ***when*** it will emit the photon. It has a certain amplitude to emit the photon at any time, and we can predict only a probability for emission; we cannot predict the future exactly. This has given rise to all kind of nonsense and questions on the meaning of freedom of will, and of the ideas that the world is uncertain.

Of course we must emphasise that classical physics is also indeterminate, in a sense. It is usually thought that this indeterminacy, that we cannot predict the future, is an 'important quantum-mechanical thing, and this is said to explain the behaviour of the mind, feelings of free will, etc. But if the world were classical—if the laws of mechanics were classical—it is not quite obvious that the mind would not feel more or less the same. It is true classically that if we knew the position and the velocity of

In science we go by experiments — even conceptual experiments. And if the limitation is not of the nctunl measuring devices used hut is set by the fundamental processes of measurement then we have to accept it.

Let us give you an idea about the debate on determinism (cnusnlity) versus free will: According to Newtonian dynamics, if the position, velocity and the forces acting on a body at any instant of time are known its 'state' nt all later times can be predicted accurately. Thnt is, if know the 'cause' we can predict the effect. This applies to any object, however large or small. Extending this to all objects in the universe it was thought thnt every event and its time evolution can be determined for all times to come. This determinism would apply even to human body and mind. This means that even the humnn mind has no free will, no freedom of choice; the future of every living creature, being a part of the mechanistic universe is completely determined.

Now things are entirely different In qunntum mechanics. We can only predict the probability of an event taking plnce nnd the attributes of a system are governed by the uncertainty principle. Thus, there seems to be a complete brenkdown of determinism (or the cause-effect relationship in the microscopic world). This is interpreted by some as restoration of 'freedom of will' to choose an alternative in the probabilistic world which is also uncertain.

every particle in the world, or in a box of gas. we could predict exactly what would happen. And therefore the classical world is deterministic. Suppose, however, that we have a finite accuracy and do not know ***exactly*** where just one atom is, say to one part in a billion. Then as it goes along it hits another atom, and because we did not know the position better than to one part in a billion, we find an even larger error in the position after the collision. And that is amplified, of course, in the next collision, so that if we start with only a tiny error it rapidly magnifies to a very great uncertainty. To give an example: if water falls over a dam, it splashes. If we stand nearby, every now and then a drop will land on our nose. This appears to be completely random, yet such a behavior would be predicted by purely classical laws. The exact position of all the drops depends upon the precise wigglings of the water before it goes over the dam. How? The tiniest irregularities are magnified in falling, so that we get complete randomness. Obviously, we cannot really predict the position of the drops unless we know the motion of the water ***absolutely exactly.***

Speaking more precisely, given an arbitrary accuracy, no matter how precise, one can find a time long enough that we cannot make predictions valid for that long a time. Now the point is that this length of time is not very large. It is not that the time is millions of years if the accuracy is one part in a billion. The time goes, in fact, only logarithmically with the error, and it turns out that in only a very, very tiny time we lose all our information. If the accuracy is taken to be one part in billions and billions and billions—no matter how many billions we wish, provided we do stop somewhere—then we can find a time less than the time it took to state the accuracy—after which we can no longer predict what is going to happen! It is therefore not fair to say that from the apparent freedom and indeterminancy of the human mind, we should have realized that classical "deterministic" physics could not even hope to understand it, and to welcome quantum mechanics as a release from a "completely mechanistic" universe. For already in classical mechanics there was indeterminability from a practical point of view."

Table of fundamental constants

Quantity	Symbol	Value
Planck's constant	h	6.62618×10^{-34} J s
	$\hbar = \frac{h}{2\pi}$	1.05459×10^{-34} J s
Velocity of light in vacuum	c	2.99792×10^{8} m s^{-1}
Elementary charge (absolute value of electron charge)	e	1.60219×10^{-19} C
Permeability of free space	μ_0	$4\pi \times 10^{-7}$ H m^{-1} = $1.256\,64 \times 10^{-6}$ H m^{-1}
Permittivity of free space	$\varepsilon_0 = \frac{1}{\mu_0 c^2}$	$8.854\,19 \times 10^{-12}$ F m^{-1}
Gravitational constant	G	6.672×10^{-11} N m^2 kg^{-2}
Fine structure constant	$\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c}$	$\frac{1}{137.036} = 7.297\,35 \times 10^{-3}$
Avogadro's number	N_A	$6.022\,05 \times 10^{23}$ mol^{-1}
Faraday's constant	$F = N_A e$	$9.648\,46 \times 10^{4}$ C mol^{-1}
Boltzmann's constant	k	$1.380\,66 \times 10^{-23}$ J K^{-1}
Gas constant	$R = N_A k$	$8.314\,41$ J mol^{-1} K^{-1}
Atomic mass unit	a.m.u. $= \frac{1}{12} M_{^{12}C}$	$1.660\,57 \times 10^{-27}$ kg
Electron mass	m or m_e	$9.109\,53 \times 10^{-31}$ kg = $5.485\,80 \times 10^{-4}$ a.m.u.
Proton mass	M_p	$1.672\,65 \times 10^{-27}$ kg = 1.007 276 a.m.u.
Neutron mass	M_n	$1.674\,92 \times 10^{-27}$ kg = 1.008 665 a.m.u.
Ratio of proton to electron mass	M_p/m_e	1836.15
Electron charge to mass ratio	$\lvert e \rvert / m_e$	$1.758\,80 \times 10^{11}$ C kg^{-1}
Classical radius of electron	$r_0 = \frac{e^2}{4\pi\varepsilon_0 mc^2}$	$2.817\,84 \times 10^{-15}$ m
Bohr radius for atomic hydrogen (with infinite nuclear mass)	$a_0 = \frac{4\pi\varepsilon_0 \hbar^2}{me^2}$	5.29177×10^{-11} m
Rydberg's constant for infinite nuclear mass	$R_\infty = \frac{me^2}{8\varepsilon_0^2 h^3 c} = \frac{\alpha}{4\pi a_0}$	1.09737×10^{7} m^{-1}
Rydberg's constant for atomic hydrogen	R_H	$1.096\,78 \times 10^{7}$ m^{-1}
Bohr magneton	$\mu_B = \frac{e\hbar}{2m}$	9.27408×10^{-24} J T^{-1}
Nuclear magneton	$\mu_N = \frac{e\hbar}{2M_p}$	5.05082×10^{-27} J T^{-1}