

Having provided you once again with a **bird's** eye view of the fundamental concepts of quantum mechanics discussed in Block 2, we draw your attention to another feather in its cap — its ability to predict. You will discover its power in this block when you study its applications to various systems, such as the potential well and potential barrier, and the **harmonic** oscillator (Unit 8). The phenomenon of barrier penetration (also known as tunneling) by quantum particles, finds wide use today in tunnel diodes and scanning tunneling electron microscopes which enable us to 'see' the quantum world with much more clarity than hitherto possible (of course, without violating the uncertainty principle). When the formalism of quantum mechanics was developed, it was applied extensively to study the structure of hydrogen atom — its predicted energy levels were in beautiful agreement with the experimental results. And the optical spectrum resulting from the transition of an electron from a higher energy state to a lower one was explained very well. Therefore, in Unit 9 we discuss the application of quantum mechanics to spherically symmetric systems, and especially to hydrogen atom. The evolution of quantum mechanics has been guided from the beginning by discoveries in atomic spectroscopy. Explaining the internal structure of atoms and the resulting spectra (in the optical as well as X-ray regions) has been a major success of quantum mechanics and we take these up in Units 10 and 11, respectively.

As far as studying the material is concerned, follow the advice given in Block 2 — learn to think and calculate quantum mechanically! You may find the going tough initially as there is a lot of mathematical abstraction in this material. Our advice to you is to solve each and every step on your own. Do not try to rush through the material if you want to really understand it. In our estimate, you would need to spend 8 h on Unit 8, 7 h on Unit 9, 5 h on Unit 10 and just 3 h on Unit 11, for studying the material and assimilating the ideas. And at the end of it all, we hope that you experience a genuine sense of achievement and exhilaration at having understood one of the greatest and most beautiful intellectual creations of twentieth century science. Our best wishes are with you!

Acknowledgement

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UNIT 8 SOME SIMPLE SYSTEMS

Structure

- 8.1 Introduction
 - Objectives
- 8.2 A Free Particle
- 8.3 Particle in a Box
- 8.4 One-dimensional Rectangular Potential Barrier
- 8.5 One-dimensional Potential Well
- 8.6 One-dimensional Harmonic Oscillator
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- 8.9 Solutions and Answers

8.1 INTRODUCTION

In Unit 6 of Block 2 you have studied the time independent Schrodinger equation. In this unit we shall apply it to some simple one-dimensional systems so that you get some experience of solving the time-independent Schrodinger equation. You will learn how to solve it to obtain its eigenfunctions satisfying the conditions given in Sec. 6.4 of Unit 6 and determine the corresponding eigenvalues for these systems. Although the real world is three-dimensional, these one-dimensional systems are of great interest. This is not only because several physical situations are effectively one-dimensional but also because we can use them effectively to model the real world. A number of more complicated physical problems can be reduced to the solution of equations similar to the one-dimensional Schrodinger equation.

So in this unit we shall first study a free particle and then confine it to move within a limited space like a box. You will notice that the eigenvalues and eigenfunctions of the two systems are different. Then we shall solve the Schrödinger equation for a particle moving in a one-dimensional rectangular potential barrier and a one-dimensional potential well. These examples of simple potentials model natural processes like alpha decay of radioactive nuclei, and the energy spectrum of atoms, molecules and nuclei. Thus our models are expected to give us some insight into the physics of these systems. They will also bring out the difference between classical and quantum description of motion of objects. We shall end this unit by studying the quantum mechanical behaviour of a simple harmonic oscillator. As its application, we shall consider the vibrations of a diatomic molecule in terms of the oscillations of a simple harmonic oscillator. In the next unit, you will learn how to solve the Schrödinger equation, for the hydrogen atom.

Objectives

After studying this unit you should be able to

- solve the time independent one-dimensional Schrödinger equation and obtain the eigenfunctions and eigenvalues for simple one-dimensional systems like
 - free particle and particle in a box,
 - particle in a one-dimensional potential barrier and one-dimensional potential well,
 - simple harmonic oscillator,
- apply, the one-dimensional potential models to simple applications in quantum physics.

8.2 A FREE PARTICLE

Let us consider the simplest case of a potential which is constant:

$$V(x) = V_0$$

The force acting on the particle, $F(x) = -\frac{dV}{dx}$; then vanishes, so that the particle is free. Without loss of generality, we can take the constant V_0 to be zero. So now we have a particle of mass m moving freely in space. Since the particle is not subjected to any force, its total energy E , which is equal to its kinetic energy, and also its linear momentum p do not change with time. E and p are related by the equation

$$\frac{p^2}{2m} = E \quad (8.1)$$

Recall Eq. (6.28) from Unit 6. Putting $V(x) = 0$ in it, we can write the time independent Schrodinger equation for a free particle as follows:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad (8.2)$$

where the direction of the vector p is taken to be along x axis. Since $p = \hbar k$, where k is the wave number, we can combine Eqs. (8.1) and (8.2) to obtain

$$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x) \quad (8.3a)$$

$$\text{where} \quad E = \frac{\hbar^2 k^2}{2m} \quad (8.3b)$$

The two linearly independent solutions of Eq. (8.3a) are given by

$$\psi_{\pm k}(x) = e^{\pm ikx} \quad (8.4a)$$

Thus for one value of E we have two eigenfunctions e^{+ikx} and e^{-ikx} . We denote these eigenfunctions by $\psi_k(x)$ and $\psi_{-k}(x)$. Recall that such **eigenfunctions which have the same eigenvalue for a given eigenvalue-eigenfunction equation are called degenerate**. (Otherwise they are non-degenerate). Thus $\psi_k(x)$ and $\psi_{-k}(x)$ are degenerate eigenfunctions. The general solution of Eq. (8.3a) is the linear combination

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad (8.4b)$$

where A and B are arbitrary constants. It is clear that for the solution $\psi(x)$ to be physically acceptable, k cannot have an imaginary part. If it did, then $\psi(x)$ would increase exponentially at one of the limits $x = -\infty$ or $x = +\infty$, or possibly at both limits. You may know that the wavefronts of the waves represented by Eqs. (8.4) are planes, perpendicular to the direction of the propagation of the wave. Hence we call $e^{\pm ikx}$ as **plane waves**. They do not go to zero as $x \rightarrow \pm\infty$. Hence they are **unnormalizable** wave functions (recall Sec. 6.3.2 of Unit 6).

In order to interpret Eq. (8.4b) physically, let us consider some special cases. If we set $B = 0$, the resulting wavefunction is the plane wave

$$\psi(x, t) = Ae^{i(kx - \omega t)}$$

where we have included the **time** dependence (recall Eq. 6.27). This is associated with a free particle of **mass** m moving along the positive x -axis with a definite momentum of magnitude $\hbar k$ and an energy $\hbar^2 k^2/2m$. The probability density corresponding to it is $\psi^*\psi = |A|^2$. It is independent of time as well as position. Thus, the position of the **particle** is completely unknown. This is in accordance with the uncertainty principle. You can obtain a similar analysis by **setting** $A = 0$ in Eq. (8.4b). In this case the plane wave will be travelling in the negative x -direction.

You can also verify easily that $\psi_{\pm k}(x)$ are also eigenfunctions of the operator p with the eigenvalues $\pm\hbar k$. Thus as far as the linear momentum operator p is concerned, the

two eigenfunctions $\psi_{\pm k}(x)$ are non-degenerate, i.e., they have different eigenvalues. Why don't you do it as an exercise?

SAQ 1

Spend
2 min

Show that $p_{op} e^{\pm ikx} = \pm \hbar k e^{\pm ikx}$.

For the above system both the constants of motion E and p are given in terms of k . Thus k characterises the eigenfunction $\psi_k(x)$ and hence we call k a quantum number. Since $E = \hbar^2 k^2 / 2m$, we must have $E > 0$, i.e., the energy cannot remain lower than the potential (here $V = 0$) over the entire interval $(-\infty, +\infty)$. Since any non-negative value of E is allowed, the energy spectrum of a free particle is continuous, extending from $E = 0$ to $+\infty$. This, of course, is not surprising since E is the kinetic energy of a free particle. It also corresponds to the classical result.

Let us now see what happens when we confine the free particle to a box.

8.3 PARTICLE IN A BOX

Let us consider a one-dimensional system and confine a free particle in a length segment lying between $x = 0$ and $x = L$ (Fig. 8.1). Then the probability of finding the particle at $x = L - \epsilon$ and $x = L + \epsilon$, where ϵ is an infinitesimal quantity, should be zero. Further, since the wave functions are single-valued and continuous, they should also satisfy the condition that they are zero at the boundaries $x = 0$ and $x = L$, i.e.,

$$\lim_{\epsilon \rightarrow 0} \psi_k(-\epsilon) = \lim_{\epsilon \rightarrow 0} \psi_k(L + \epsilon) = 0 \tag{8.5a}$$

It follows from Eq. (8.5a) that

$$\psi_k(0) = \psi_k(L) = 0 \tag{8.5b}$$

Now we may also write the wave function as

$$\psi_k(x) = A \cos kx + B \sin kx$$

where $k = (2mE/\hbar^2)^{1/2}$. Since $\psi_k(0) = 0$, we have

$$A = 0$$

and since $\psi_k(L) = 0$, we get

$$B \sin kL = 0 \quad (\because B \neq 0)$$

whence $kL = n\pi, \quad n = 1, 2, 3, \dots$

Hence k is quantized; let us call it k_n :

$$k_n = \frac{n\pi}{L}, \quad n = 1, 2, 3, \dots \tag{8.6a}$$

Hence, energy E is also quantized; let us call it E_n :

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2mL^2}, \quad n = 1, 2, 3, \dots \tag{8.6b}$$

Notice that the quantization of energy follows from the condition of confinement or the boundary conditions imposed on the wave function. Thus, the moment we confine a free particle in a limited space, its energy can take only discrete values given by Eq. (8.6b); it is no longer continuous, it is quantized (Fig. 8.2). The eigenfunction of a state of quantized energy E_n of a particle in a box is, therefore, given by

$$\psi_k(x) = \psi_n(x) = N \sin \dots \tag{8.6c}$$

Notice that we still have to compute the normalisation constant N . You may like to do this exercise yourself. Here's an SAQ for you



Fig. 8.1: Particle confined in a line segment.

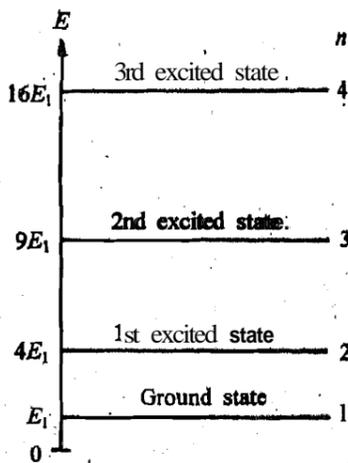


Fig. 8.2: The four lowest allowed energy levels for a particle in a one-dimensional box, where $E_1 = \hbar^2 / 8mL^2$.

Spend
5 min

SAQ 2

- (a) Show that $N = \left(\frac{2}{L}\right)^{1/2}$
 (b) Show that $\psi_n(x)$ and $\psi_m(x)$ are orthogonal when $m \neq n$.

Hence the eigenfunction for a free particle confined in a segment of length L is

$$\psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right) \quad (8.7a)$$

The complete solution for a stationary state of a particle in a box is then given as

$$\begin{aligned} \psi_n(x, t) &= \psi_n(x)e^{-iE_n t/\hbar} \\ &= \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n\pi x}{L}\right)e^{-iE_n t/\hbar} \end{aligned} \quad (8.7b)$$

and the probability for finding the particle at position x is independent of time:

$$P_n(x) = |\psi_n(x, t)|^2 = \left(\frac{2}{L}\right) \sin^2\left(\frac{n\pi x}{L}\right) \quad (8.7c)$$

However, it now depends on the position of the particle. Fig. 8.3 shows the probabilities per unit distance for a particle in a box for the three lowest energy states. The classical result is also shown for comparison.

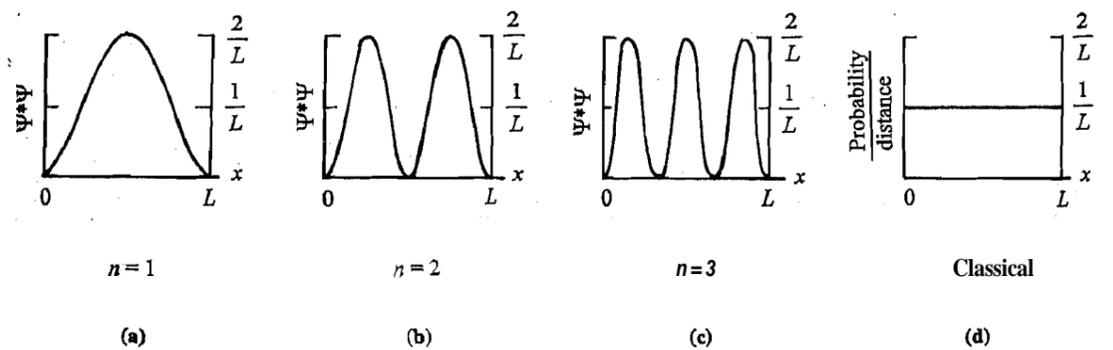


Fig. 8.3: The probability per unit distance for a particle in a box for the three lowest values of n , compared to the classical result.

The smallest value of n is $n = 0$, but $n = 0$ gives $\psi = 0$. This result means that the probability of an $n = 0$ state is zero. Now refer to Fig. 8.3. For $n = 1$, $\psi^*\psi = (2/L) \sin^2(\pi/L)x$; for $n = 2$, $\psi^*\psi = (2/L) \sin^2(2\pi/L)x$; and for $n = 3$, $\psi^*\psi = (2/L) \sin^2(3\pi/L)x$. Thus $\psi^*\psi$ oscillates between 0 and $2/L$ with an average value in the box of $1/L$.

Classically, the particle bounces back and forth between the walls. Since its kinetic energy is constant, it moves at a constant velocity between collisions with the walls. Therefore, it spends the same amount of time in all equal-distance intervals. This gives it the constant probability per unit distance of $1/L$ of being found anywhere in the box (Fig. 8.3d).

As you can see from Fig. 8.3a to c, $\psi^*\psi$ has n humps. This behaviour is easy to understand if you remember that k_n , the wave number for state n , equals $2\pi/\lambda_n$. Equating this wave number to $n\pi/L$ gives $L = n\lambda_n/2$. That is, n is the number of the particle's half wavelengths being fitted between the walls. In the limit of large quantum numbers, the number of humps with any finite Δx becomes so large that $\psi^*\psi \Delta x$ approaches the classical value, $(1/L)\Delta x$.

The linear momentum of the particle is given by

$$p_n = \pm k_n \hbar = \pm \frac{\hbar n \pi}{L}, \quad n = 1, 2, 3, \dots \quad (8.8)$$

You should note that the integer n in Eqs. (8.6a, b) and (8.8) now plays the same role as was played by k for a free particle. Hence n is called a **quantum number**. Since n takes only integer values, the momentum and the energy of the particle no longer vary in a continuous manner but take only discrete values.

Let us see what are the other implications of these results about a particle in a one-dimensional box. According to quantum mechanics, there is a minimum energy, the ground-state energy $E_1 = \pi^2 \hbar^2 / 2mL^2$ that the particle in a box must have. This result is in contrast to the classical result where all energy values including $E = 0$ are permitted. You can easily see that this is a consequence of the uncertainty principle. We are confining the particle within the length L . Thus there is an uncertainty in its position given by L . According to the uncertainty relation, Eq. (5.6a), there has to be a corresponding momentum uncertainty of \hbar/L . This means that the particle has to have a minimum energy; its energy can never be zero because that would contradict the uncertainty relation. This minimum energy is called the **zero point energy**.

Notice from Eq. (8.6b) that the energy separation between successive quantized levels increases with the decrease of L , the confining length. Conversely, as L increases, the energy separations decrease. When L is much larger than atomic dimensions, the energy separation is so small that we approach the classical correspondence limit. Note that for large L , the zero point energy also tends towards zero.

Thus far we have considered the qualitative situation. But what about the quantitative situation? Let us calculate the energy levels of an electron ($m = 9.1 \times 10^{-31}$ kg) confined to a box of atomic size ($L = 10^{-10}$ m). Substituting in the energy level formula, Eq. (8.6b), we get $E_n \approx 40n^2$ eV. The energy difference between the ground and the first excited state is then 120 eV. And a photon emitted from transition between these energy levels would have a frequency 3×10^{16} Hz, which is of the same order as that in many atomic transitions.

Now from Eq. (8.8) we have

$$p_{n+1} - p_n = \hbar \pi / L \quad (8.9)$$

Thus, the difference between p_{n+1} and p_n decreases with the increase of L . Now if we take a very large value of L , $(p_{n+1} - p_n)$ will approach zero, i.e., p will become continuous. Hence we may represent a free particle by a normalised wave function with a very large value of L . Such a procedure for the normalisation of a free particle is known as **box normalisation** and you can easily see that a one-dimensional box-normalised wave function is given by

$$\psi_k(x) = \left(\frac{1}{L}\right)^{1/2} e^{ikx} \quad (8.10)$$

We can generalise this analysis to a particle in a three-dimensional box. In fact, you should work this out yourself.

SAQ 3

Obtain eigenfunctions and eigenvalues of a particle confined in a three dimensional box having lengths L_x , L_y and L_z .

Spend
10 min

Let us now consider the problem of a particle in a one-dimensional rectangular potential barrier.

8.4 ONE-DIMENSIONAL RECTANGULAR POTENTIAL BARRIER

In Sec. 8.2, we considered the motion of a free particle, i.e., the potential in the entire

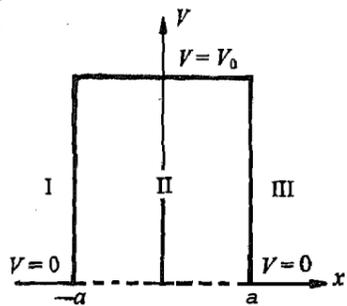


Fig. 8.4: one-dimensional potential barrier.

space was zero. Let us now modify that situation and consider a one-dimensional space in which the potential energy of a particle is V_0 between $x = -a$ and $x = a$ but zero otherwise:

$$\begin{aligned} V(x) &= 0 & x < -a \\ &= V_0 & -a < x < a \\ V(x) &= 0 & x > a \end{aligned} \quad (8.11)$$

Thus we divide the whole one-dimensional space in three regions. Region I extends from $-\infty$ to $-a$; region II from $-a$ to $+a$ and region III from $+a$ to $+\infty$ (see Fig. (8.4)). The central region is known as the potential barrier. Notice that as defined by Eq. (8.11), V is rectangular.

Let us consider the motion of a particle of mass m and total constant energy E in the above mentioned one-dimensional space. From purely physical considerations you can see that the particle is free in region I and there will be an incident plane wave as well as a plane wave reflected by the potential barrier. Hence, we may write the wave function for region I as

$$\psi_I(x) = A e^{ikx} + B e^{-ikx} \quad \text{for } x < -a \quad (8.12)$$

where

$$k = \sqrt{2mE}/\hbar \quad (8.13)$$

In region III the particle is again free ($V = 0$) but there we have only a transmitted wave. Hence

$$\psi_{III}(x) = F e^{ikx} \quad \text{for } x > a \quad (8.14)$$

However, in region II the Schrödinger equation is

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_{II}(x)}{dx^2} + V_0 \psi_{II}(x) = E\psi_{II}(x) \quad (8.15)$$

Let us rewrite this equation in the form

$$\frac{d^2\psi_{II}(x)}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \psi_{II}(x) = 0 \quad (8.16)$$

Introducing a real parameter γ , we may write Eq. (8.16) as

$$\frac{d^2\psi_{II}(x)}{dx^2} - \gamma^2 \psi_{II}(x) = 0 \quad (8.17a)$$

where

$$\gamma^2 = \frac{2m}{\hbar^2} (V_0 - E) \quad (8.17b)$$

The solution of Eq. (8.17a) is given as

$$\psi_{II}(x) = C e^{-\gamma x} + D e^{\gamma x}, \quad -a < x < a \quad (8.18)$$

Now, there are two possibilities: (i) E is less than V_0 and (ii) E is greater than V_0 . Let us consider the case when $E < V_0$. Then γ is real and the solution of Eq. (8.17a) becomes

$$\psi_{II}(x) = C e^{-\gamma x} + D e^{\gamma x} \quad \text{for } -a < x < a \quad (8.19)$$

With the help of Eqs. (6.19) and incident part ($A e^{ikx}$) of Eq. (8.12) we find that the incident flux from the left of the potential barrier is

$$S_i = \frac{\hbar k}{m} |A|^2 \quad (8.20)$$

Similarly, using the reflected part of the wave function ψ_I and the transmitted wave function ψ_{III} , we find that the reflected flux S_r and the transmitted flux S_t are given by

$$S_r = S_i |B/A|^2 \quad (8.21)$$

$$S_t = S_i |F/A|^2 \quad (8.22)$$

You should quickly verify Eqs. (8.20) to (8.22) before studying further. Thus we obtain

$$\text{Probability of reflection } P_r = S_r/S_i = |B/A|^2 \quad (8.23)$$

and

$$\text{Probability of transmission } P_t = S_t/S_i = |F/A|^2 \quad (8.24)$$

Now to determine P_r and P_t (i.e., the coefficients A, B and F) we match the appropriate wave functions ψ and their derivatives ψ' at the boundaries $x = -a$ and $x = a$. The boundary conditions are:

$$\psi_I(x = -a) = \psi_{II}(x = -a); \quad \psi'_I(x = -a) = \psi'_{II}(x = -a) \quad (8.25a)$$

and

$$\psi_{II}(x = a) = \psi_{III}(x = a); \quad \psi'_{II}(x = a) = \psi'_{III}(x = a) \quad (8.25b)$$

Substituting ψ_I , ψ_{II} and ψ_{III} from Eqs. (8.12), (8.19) and (8.14) and carrying out the necessary algebra we can obtain P_r and P_t as given below:

$$P_t = \left[1 + \frac{V_0 \sinh^2(2\gamma a)}{4E(V_0 - E)} \right]^{-1} \quad (8.26)$$

$$P_r = \left[1 + \frac{4E(V_0 - E)}{V_0 \sinh^2(2\gamma a)} \right]^{-1} \quad (8.27)$$

You may like to prove Eqs. (8.26) and (8.27) before studying further; So here is an exercise for you.

SAQ 4

Prove Eqs. (8.26) and (8.27).

You can easily verify that $P_t + P_r = 1$. One of the remarkable features of this analysis is that **there is a non-zero probability of transmission even though $E < V_0$, i.e., the energy of the object is less than the height of potential barrier.** This is in contrast to the classical situation. It is a purely quantum effect signifying the wave property of quantum objects. Hence, quantum objects are said to be able to **tunnel** through a classically impenetrable barrier. Thus, we conclude that the penetration through a potential barrier, usually referred to as **tunneling**, is a quantum mechanical phenomenon and should be taken into consideration for those objects for which wave-particle duality is significant. You may like to know that the phenomenon of tunneling has many applications. It explains the emission of α -particles in radioactive decay, and the passage of electrons through a forbidden region as in field emission. In electronics, it has been utilised in the construction of tunnel diodes. Let us take one of these applications, namely, alpha decay.

Example 1: Application to Alpha Decay

We are giving this application for the sake of interest only. You will not be tested on the mathematics given here.

Let us consider the case of alpha radioactivity of nuclei. This was the original application of the barrier transmission phenomenon worked out by **Gamow**, Gurney and Condon.

In this case of a physical barrier, the shape is not so square (Fig. 8.5). Now when $\gamma a \gg 0$, the probability of transmission becomes

$$P_t = |T|^2 = \frac{16 k^2 \gamma^2}{(k^2 + \gamma^2)^2} \exp(-4\gamma a) \approx \exp(-4\gamma a)$$

Spend 20 min

You should not **take** the word 'tunneling' **literally**. There is, of course, a finite probability for the **particle** to be inside the **classically forbidden barrier** region where its kinetic energy is negative. But the point is that nobody can "see" a **particle actually** go through a classically forbidden region. **Particle detectors can** detect only objects of kinetic energy **greater than zero**. **If you insert a detector** inside the **barrier** to 'see' the particle, you are not only **making** a hole in the **potential** but **also** in your objective, **because** the object will no longer belong to a **classically forbidden** region where you wanted to find it! Another way to **say** this is that **our effort** to observe the **object** with **any measuring instrument** will **impart** to it an **uncontrollable** amount of energy. This is how the **uncertainty** principle works in such measurement **situations!**

Similarly, we **cannot say** what kind of time the **particle takes** to tunnel through a barrier. It **may** do it now or later; quantum **mechanics** gives us only **average behaviour** — the **average** time it takes to travel to the other side. It seems best to think of quantum tunneling as "as if" tunneling — tunneling in potential. Alternatively, we **can** say that quantum objects go across a barrier for which they do not have enough energy by doing a quantum **"jump"** — **Bohr** style; they never go through, the intervening space, **and** they do not do it causally **taking** a finite amount of time. Now they **are** here, on this side of the barrier; and then they **are there**, on the **other** side.

We can write this as

$$P_t = e^{-2} [2m(V_0 - E)/\hbar^2]^{1/2} \cdot 2a$$

For a broad range of barriers, we can now make a generalised estimate of the order of magnitude. Generalising the expression of P_t for $V(x)$, we can write

$$P_t = \exp \left[-2 \int_a^b dx \left(\frac{2m}{\hbar^2} (V(x) - E) \right)^{1/2} \right]$$

Now we can approximate the situation for alpha emission from a nucleus by the potential barrier shown in Fig. 8.5b. Inside the nucleus, the alpha particle is a free particle, $E > 0$. (For, if the alpha particle were bound, how would the nucleus decay?). It has to tunnel through the coulomb barrier

$$V(r) = \frac{ZZ' e^2}{r}$$

where Z and Z' are the atomic numbers of the daughter nucleus and the alpha particle, respectively, into which the parent nucleus is splitting. Here r is the radial distance. Now, in the expression for P_t we can change the variable x to r , since x is just a dummy variable. Putting P_t equal to $\exp(-G)$, we obtain

$$G = 2 (2m/\hbar^2)^{1/2} \int_R^b \left[\frac{ZZ' e^2}{r} - E \right]^{1/2} dr$$

where R is the radius of the daughter nucleus (Fig. 8.5b) and the upper limit of the integral, b , is taken to be the classical "turning point" where the integrand vanishes, since

$$E = \frac{ZZ' e^2}{b}$$

Thus

$$G = 2 (2m/\hbar^2)^{1/2} (ZZ' e^2)^{1/2} \int_R^b \left(\frac{1}{r} - \frac{1}{b} \right)^{1/2} dr$$

The value of the integral is

$$\int_R^b dr \left(\frac{1}{r} - \frac{1}{b} \right)^{1/2} = \sqrt{b} \left[\cos^{-1} \left(\frac{R}{b} \right)^{1/2} - \left(\frac{R}{b} - \frac{R^2}{b^2} \right)^{1/2} \right]$$

For low energies and high barriers, $b \gg R$, and we get

$$G \approx 2 \left(\frac{2m ZZ' e^2 b}{\hbar^2} \right)^{1/2} \pi$$

But $b = ZZ' e^2/E = 2ZZ' e^2/mv^2$, where v is the velocity of the alpha particle inside the nucleus. Hence

$$G = \frac{2\pi ZZ' e^2}{\hbar v}$$

To calculate the alpha particle escape probability per second, we have to multiply the transmission coefficient $\exp(-G)$ by the rate of the alpha particles hitting the barrier, which is v/R . For a 1 MeV alpha particle, using $R = 1.2 \times 10^{-13} A^{1/3}$ cm with $A = 216$, we estimate $v/R = 10^{21} \text{ s}^{-1}$. Consequently, escape probability per second $= \tau^{-1} = 10^{21} e^{-G}$ where τ denotes the decay time. Noting that $Z' = 2$ and that the mass of alpha particle in energy units is $m \approx 4 \times 103 \text{ MeV}$, we get

$$G = \frac{2\pi ZZ' e^2}{\hbar (2E/m)^{1/2}} \approx \frac{4Z}{(E(\text{in MeV}))^{1/2}}$$

Therefore, we obtain

$$\log_{10} \frac{1}{\tau} = C_1 - C_2 \frac{Z}{(E \text{ MeV})^{1/2}}$$

where C_1 and C_2 are two constants, never mind our estimates for them. This formula, first derived by Gamow, Gurney and Condon, fits the data on alpha decay quite

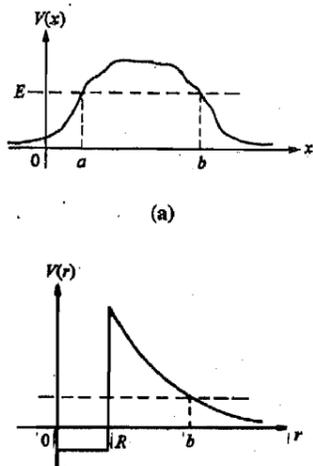


Fig. 8.5: (a) A realistic potential barrier has a more jagged look than a square barrier; (b) model potential barrier for alpha decay of nuclei.

remarkably. It is also remarkable that we can derive the formula from a one-dimensional calculation.

Let us now consider the situation for $E > V_0$. Classically the particle with $E > V_0$ will be transmitted with cent per cent probability. The quantum mechanical prediction may be easily obtained by appropriately modifying the above formulae for this case. The only modification is in γ which is now imaginary. Hence taking $\gamma = iq$ with $q^2 = (2m/\hbar^2)(E - V_0)$, we get

$$P_t = |T|^2 = \left[1 + \frac{V_0^2 \sin^2(2qa)}{4E(-V_0 + E)} \right]^{-1} \quad (8.28)$$

and

$$P_r = |R|^2 = \left[1 + \frac{4E(-V_0 + E)}{V_0^2 \sin^2(2qa)} \right]^{-1} \quad (8.29)$$

Thus, we see that quantum mechanically $P_r \neq 0$ and hence, even if $E > V_0$, a part of the incident flux is reflected. In Fig. 8.6 we have shown the variation of the transmission probability with the barrier height. We see in the figure that P_t is low for low E and for high E it approaches unity.

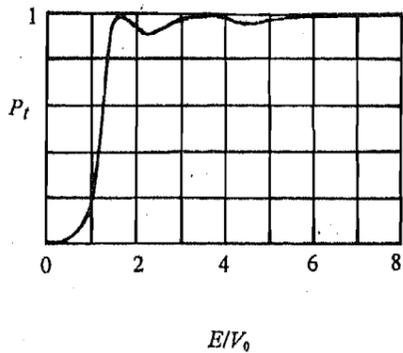


Fig. 8.6: Transmission probability of a particle of energy E through a rectangular potential barrier of height V_0 .

An interesting feature of the above curve is that for a certain value of (E/V_0) , the transmission probability P_t is unity and hence $P_r = 0$ (see Fig. 8.6). This happens whenever $2qa = n\pi$ with $n = 0, 1, 2, \dots$. The two boundaries at $x = \pm a$ where the reflection is taking place are producing reflected waves of equal amplitudes and opposite phases. Hence, there is no reflection at all.

Let us now study the case of a particle in a one-dimensional potential well.

8.5 ONE-DIMENSIONAL POTENTIAL WELL

Let us obtain the eigenvalues and eigenfunctions of a potential well, shown in Fig. 8.7. The well is such that a particle has V_0 potential energy for $x < -a$ as well as for $x > a$ but for $-a < x < a$ the potential energy is zero:

$$V = V_0 \quad x < -a$$

$$V = 0 \quad -a < x < a$$

$$V = V_0 \quad x > a$$

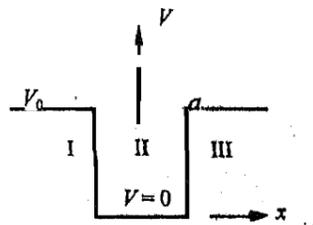


Fig. 8.7: Rectangular potential well,

The total energy E of a particle of mass m is again a constant of motion. Hence the Schrödinger equations of the particle in regions I and III are given by

$$H\psi = E\psi \quad (8.30a)$$

where

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \quad (8.30b)$$

Substituting for $V(x)$, we obtain for region I

$$\psi''(x) + \frac{2m}{\hbar^2} (E - V_0) \psi(x) = 0 \quad \text{for } |x| > a \quad (8.31a)$$

and in region II it is

$$\psi''(x) + \frac{2mE}{\hbar^2} \psi(x) = 0 \quad \text{for } |x| < a \quad (8.31b)$$

We define

$$\gamma^2 = \frac{2m}{\hbar^2} (V_0 - E) \quad \text{and} \quad q^2 = \frac{2mE}{\hbar^2} \quad (8.32)$$

and consider the case when $V_0 > E$, i.e., γ is real. In region II the wave function is given by

$$\psi_{II}(x) = B \cos(qx) + C \sin(qx) \quad (8.33)$$

Similarly, general solutions in regions I and III are given by

$$\psi_I(x) = A \exp(\gamma x) \quad (8.34a)$$

$$\text{and} \quad \psi_{III}(x) = D \exp(-\gamma x) \quad (8.34b)$$

Let us further examine the wave function $\psi_{II}(x)$. Notice that the Hamiltonian (Eq. 8.30b) of *this* system does not change when x is replaced by $-x$. This leads to an interesting result that H commutes with the parity operator P . We can prove this as follows:

$$P[H\psi(x)] = H(-x) \psi(-x) = H\psi(-x) = H(x) [P\psi(x)]$$

Hence

$$PH - HP = 0, \text{ since } \psi(x) \neq 0$$

$$\text{or} \quad [P, H] = 0$$

Now recall this result from Unit 7, Sec. 7.3: If an operator A commutes with the parity operator, then the non-degenerate eigenfunctions of A have definite parity, i.e., they are either of odd parity or of even parity. Let us again demonstrate this for H . Let

$$H(x, p_x) \psi(x) = \lambda \psi(x)$$

Then operating with P from the left we get

$$PH(x, p_x) \psi(x) = \lambda P \psi(x)$$

$$\text{or} \quad H(P\psi) = \lambda(P\psi) \quad (\because PH = HP)$$

Thus both ψ and $P\psi$ are eigenfunctions of H for the same eigenvalue λ . Since $\psi(x)$ is a non-degenerate wave function, the two functions can differ at the most by a constant. Hence

$$P\psi(x) = p\psi(x)$$

where p is a constant.

Thus, $\psi(x)$ is an eigenfunction of P with p as the eigenvalue. Operating P once again on the left we get

$$P^2\psi(x) = P p\psi(x) = p^2\psi(x)$$

and

$$P^2\psi(x) = P\psi(-x) = \psi(x)$$

implying $p^2 = 1$ and $p = \pm 1$. The wave functions for which $p = +1$ are called **wave functions of even parity** and those for which $p = -1$ are called **wave functions of odd parity**. Since p can take only one of these values at one time, $\psi(x)$ has to be of either even or odd parity.

$\psi_{II}(x)$, as given by Eq. (8.33) is of mixed parity. Hence the above discussion shows that it is unacceptable. Therefore, either C or B should be zero. If we take $C = 0$ in Eq. (8.33) we get even parity solutions while $B = 0$ yields odd parity solutions. You can verify that equating the wave functions at boundaries of the well yields $D = \pm A$ for the even and odd parity solutions, respectively. Thus the **even parity solutions of the well** are given by

$$\psi_I(x) = A \exp(\gamma x) \quad \text{for } x < -a \quad (8.35a)$$

$$\psi_{II}(x) = B \cos(qx) \quad \text{for } -a < x < a \quad (8.35b)$$

and

$$\psi_{III}(x) = A \exp(-\gamma x) \quad \text{for } x > a \quad (8.35c)$$

On the other hand, the **odd parity solutions** are given by

$$\psi_I(x) = D \exp(\gamma x) \quad \text{for } x < -a \quad (8.36a)$$

$$\psi_{III}(x) = C \sin(qx) \quad \text{for } -a < x < a \quad (8.36b)$$

and

$$\psi_{III}(x) = -D \exp(-\gamma x) \quad \text{for } x > a \quad (8.36c)$$

Since ψ and $\partial\psi/\partial x$ have to be continuous, the logarithmic derivative $\partial/\partial x (\ln \psi)$, i.e., $1/\psi(\partial\psi/\partial x)$ too has to be continuous at the boundaries. Imposing the continuity condition of the logarithmic derivatives at $x = \pm a$ on the even parity solution we obtain the condition that

$$\eta = \xi (\tan \xi) \quad (8.37)$$

where

$$\eta = \gamma a \quad \text{and} \quad \xi = qa \quad (8.38)$$

You may like to prove Eq. (8.37) before studying further.

SAQ 5

Prove Eq. (8.37).

*Spend
5 min*

Eqs. (8.38) and (8.32) yield

$$\eta^2 + \xi^2 = 2m V_0 a^2 / \hbar^2 = R^2 \quad (8.39)$$

The energy eigenvalues can now be obtained by solving Eqs. (8.37) and (8.39) for η and ξ , from which γ and q may be determined. A graphical method of solving these equations is illustrated in Fig. 8.8a.

The possible values of η and ξ and hence of γ and q are obtained from the intersections of the circle $\eta^2 + \xi^2 = R^2$ (where $R^2 = 2mV_0a^2/\hbar^2$) with the curve $\eta = \xi (\tan \xi)$. Since γ and q are real, the circle and the curve are to be considered in the first quadrant only. It is clear from the figure that the allowed values of ξ and hence E are discrete and the number of allowed values of E increases as R increases. It is easy to see that for $R = 1$, there is only one solution. The same is true for $R = 2$ but at $R = 3.5$ the number of even parity solutions are two.

$$\eta = -\xi \cot \xi \quad (8.40)$$

For the above case $R = 1$ yields no solution; however $R = 2$ and 3 support one bound state (Fig. 8.8b).

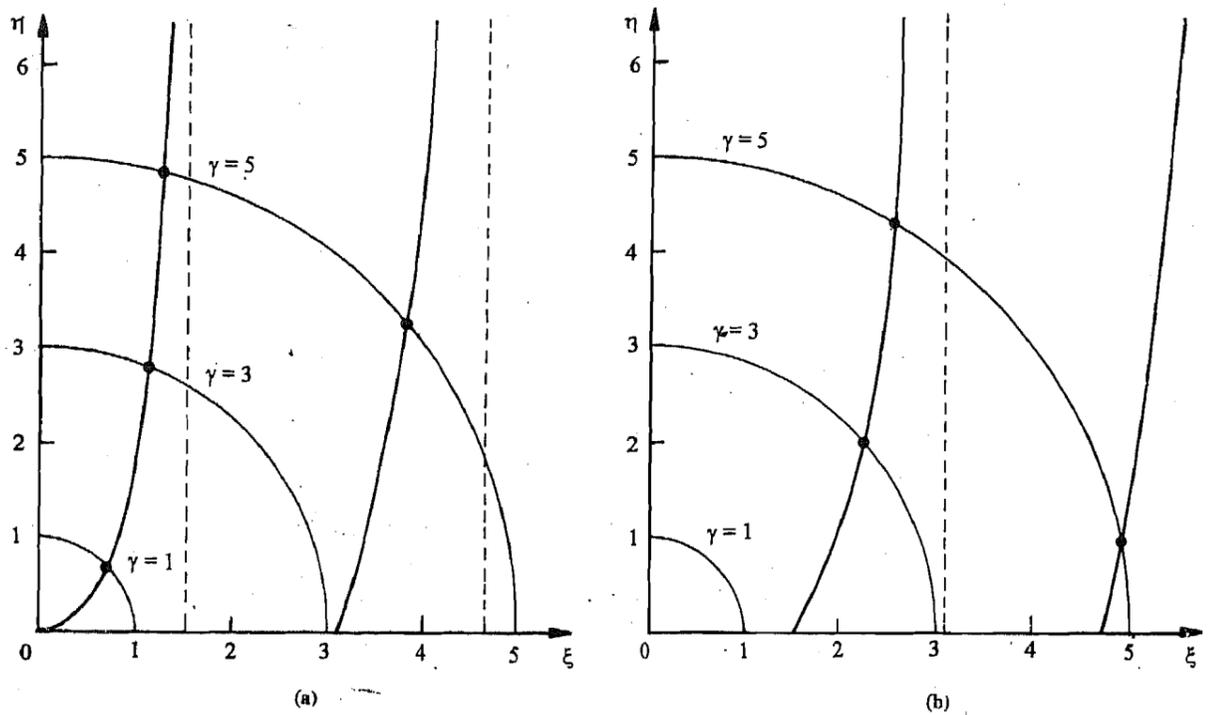


Fig. 8.8: (a) Variation of η with ξ in the two equations $\eta^2 + \xi^2 = R^2$ and $\eta = \xi \tan \xi$. The intersections give the solutions; (b) Variation of η with ξ in the two equations $\eta^2 + \xi^2 = R^2$ and $\eta = -\xi \cot \xi$. The intersections give the solutions.

We summarize that for $E < V_0$, the energy levels of a particle in a potential well depend upon the well parameters V_0 and a . For R lying between 0 and $\pi/2$, i.e., for V_0 (a^2) lying between 0 and $(\hbar^2/2m)(\pi/2)^2$ there is just one energy level of even class; for R between $(\pi/2)$ and $2(\pi/2)$ there is one even and one odd class solution. As R increases the total number of energy levels increases. Thus for $E < V_0$ the particle is bound to the well and the energy spectrum is discrete. On the other hand for $E > V_0$ we can show that the particle is in the continuum state and energy E varies continuously from V_0 to ∞ .

Finally, let us consider a potential well having infinite depth. In this case the probability of finding the particle outside the well will be zero and the wave function will be non-zero only for $|x| < a$. The even and odd parity solutions will again be given by Eqs. (8.35b) and (8.36b), respectively. Equating $\psi_{II}(x)$ at $x = \pm a$ to zero yields

$$qa = (n+1)\pi/2 \quad (8.41)$$

where n is a positive integer including zero. Putting Eq. (8.41) into (8.32) we obtain

$$E_n = \frac{\hbar^2 \pi^2 (n+1)^2}{8m a^2} \quad \text{with } n = 0, 1, 2, \dots \quad (8.42)$$

It is interesting to note that even for $n = 0$ the energy is finite. This energy $E_0 (= \hbar^2/8ma^2)$ is known as **zero point** energy and is a consequence of the **Heisenberg** uncertainty principle. Since the width of the well is $2a$, the maximum uncertainty in the position of the particle is $2a$. Hence the uncertainty in the momentum of the particle is $\hbar/2a$. This may be taken as the **minimum** momentum of the particle. Thus the minimum energy of the particle will be $\hbar^2/8ma^2$. This energy is of the same order as E_0 . Hence the zero point energy is consistent with the uncertainty principle.

You should note that in the present problem we have only one constant of motion, namely, total energy. Hence, the energy levels are specified by only one quantum number n . Again although $E < V_0$, the probability of finding the particle outside the well is non-zero. This result is non-classical. However, you should remember that this probability decreases exponentially with the increase of $|x|$.

Let us now consider the case of the one dimensional harmonic oscillator.

8.6 ONE DIMENSIONAL HARMONIC OSCILLATOR

The problem of a one-dimensional harmonic oscillator is of direct physical interest. Actually, a large number of systems are governed exactly or approximately by the harmonic oscillator equation. Recall the classical definition of a harmonic oscillator: It obeys Hooke's law according to which the force F on the particle is directly proportional to the displacement and is always directed towards the mean position, i.e., $F = -kx$; k , the constant of proportionality, is known as force constant (Fig. 8.9). It is related to the classical frequency ν of the oscillator and is given by $k = 4\pi^2 \nu^2 m$ where m is the mass of the particle. The potential energy of the particle at x is given by $\frac{1}{2} kx^2$ or $\frac{1}{2} m \omega^2 x^2$, where $\omega = 2\pi\nu$ is the angular frequency. Hence the time independent Schrödinger equation is

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2 \right] \psi(x) = E \psi(x) \quad (8.43)$$

where E is the total energy of the oscillator and is independent of time. It is evident from the above equation that the Hamiltonian of the system is invariant under space inversion, i.e., it commutes with the parity operator. Hence the eigenfunctions are of definite parity.

Now we define

$$\xi = ax, \text{ with } a^2 = m\omega/\hbar \quad (8.44)$$

and

$$E = \frac{\lambda \hbar \omega}{2}$$

With the help of the above definitions, Eq. (8.43) reduces to

$$\frac{d^2 \psi(\xi)}{d\xi^2} + (\lambda - \xi^2) \psi(\xi) = 0 \quad (8.45)$$

You should quickly check out Eq. (8.45).

SAQ 6

Verify Eq. (8.45).

Spend
5 min

To obtain acceptable solutions of Eq. (8.45) we are required to go through a fairly lengthy algebra which is unnecessary at this stage. Here we simply state the results. For the solution to be acceptable λ must satisfy the relation

$$\lambda = 2n + 1, \quad n = 0, 1, 2, \dots \quad (8.46)$$

Hence from Eq. (8.46) it follows that

$$E_n = \left(n + \frac{1}{2}\right) \hbar \omega, \quad n = 0, 1, 2, \dots \quad (8.47)$$

The integer n is known as energy quantum number. Since our simple harmonic oscillator is a one-dimensional system we have only one quantum number. Notice from Fig. 8.10 that

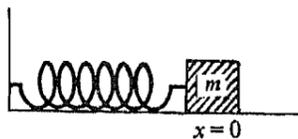


Fig. 8.9: Mass on a spring as a one-dimensional harmonic oscillator.

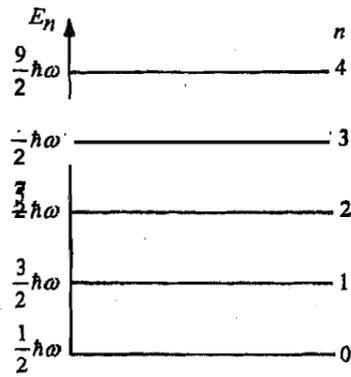


Fig. 8.10 : Energy level diagram of a simple harmonic oscillator.

● The energy levels of a quantum mechanical oscillator are equally spaced. This is a characteristic of some parts of the molecular and nuclear experimental spectra. The harmonic oscillator provides a good model description of these spectra, so much so that the spectra are referred to as vibrational spectra. There are also excitations in solids called phonons that fall in the same category.

● For each eigenvalue, there will be only one eigenfunction. Thus there is no degeneracy. This property seems to be a common characteristic of bound states for one-dimensional potentials that remain finite for all finite values of x .

We have zero point energy given by

$$E_0 = \frac{\hbar\omega}{2} \quad \text{for } n=0 \quad (8.48)$$

This zero point energy is again a consequence of the Heisenberg uncertainty principle. This can be seen as follows. Since

$$E = \frac{p^2}{2m} + \frac{1}{2} kx^2$$

E can be zero only when p and x both are equal to zero simultaneously. Under such a circumstance p and x will become definite (equal to zero) simultaneously. This will violate uncertainty principle. Therefore, the lowest eigenenergy has to be non-zero.

The normalised eigenfunctions of a simple harmonic oscillator are given by

$$\Psi_n(x) = \left(\frac{a}{\sqrt{\pi} 2^n n!}\right)^{1/2} H_n(ax) \exp(-a^2 x^2/2), \quad n = 0, 1, 2, \dots \quad (8.49)$$

where $H_n(ax)$ are Hermite polynomials. A few of the lower order $H_n(\xi)$ are given by

$$\begin{aligned} H_0(\xi) &= 1; \\ H_1(\xi) &= 2\xi; \\ H_2(\xi) &= 4\xi^2 - 2; \\ H_3(\xi) &= 8\xi^3 - 12\xi; \\ H_4(\xi) &= 16\xi^4 - 48\xi^2 + 12; \\ H_5(\xi) &= 32\xi^5 - 160\xi^3 + 120\xi. \end{aligned} \quad (8.50)$$

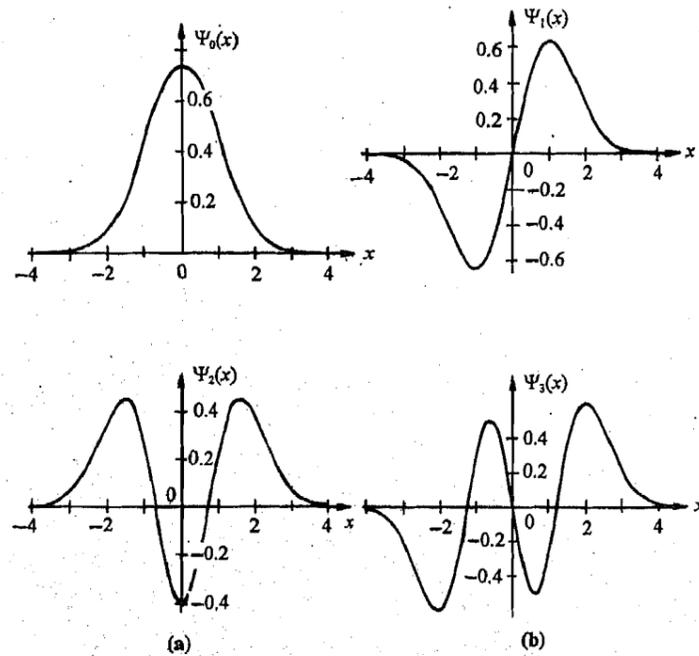


Fig. 8.11 : (a) Even parity solutions and (b) odd parity solutions for the one-dimensional harmonic oscillator.

We can show that the eigenfunctions of the Hamiltonian are also eigenfunctions of the parity operator. It is evident from Eqs. (8.49) and (8.50) that the eigenfunctions corresponding to zero or even value of n are of even parity. On the other hand odd parity eigenfunctions have odd values of n . The variation of even parity functions for $n = 0, 2$ and 4 with ξ are shown in Fig. (8.11a). The odd parity functions for $n = 1, 3$ and 5 are shown in Fig. (8.11b).

Let us now compare the quantum oscillator with the classical oscillator. Let us first take up the question of time dependence. Classically, the simple harmonic oscillator oscillates in such a manner that the position of the particle represented by the oscillator changes from one moment to another. Quantum mechanics, on the other hand, tells us that for any state of energy E , although there is a distribution of probabilities for various positions, this distribution is constant as far as time is concerned; (these probabilities are 'frozen' in time). This is the usual meaning of energy eigenstates being stationary. Is it possible to reconcile these two very different pictures?

The answer lies in considering not one single eigenfunction but a superposition of eigenfunctions as in a wave packet. Consider, for example, the superposition $\psi(x, t)$ of the first two oscillator eigenfunctions:

$$\psi(x, t) = \frac{1}{\sqrt{2}} [\exp(-iE_0 t/\hbar) \psi_0(x) + \exp(-iE_1 t/\hbar) \psi_1(x)]$$

If we plot $|\psi(x, t)|^2$, we get Fig. 8.12, where the plot is made for four different values of time. Clearly, the probability oscillates with time with just the frequency of the harmonic oscillator as expected classically. It is therefore reasonable to expect that when we take a superposition of a large number of oscillator eigenfunctions we will get a classical behaviour

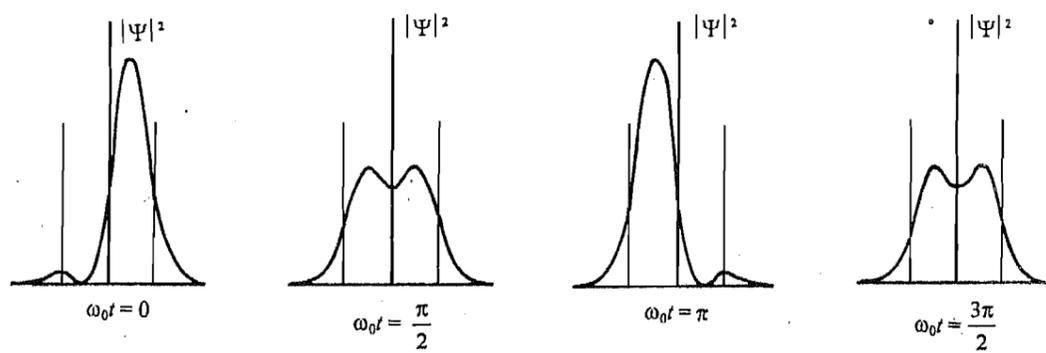


Fig. 8.12: The probability corresponding to the superposition of the first two oscillator eigenfunctions of equal amplitude (with their time dependence included) plotted at four different times. Classical oscillatory behaviour is clearly seen. The vertical lines indicate the classical limits of motion, assuming an energy $E = \langle H \rangle = \hbar\omega$.

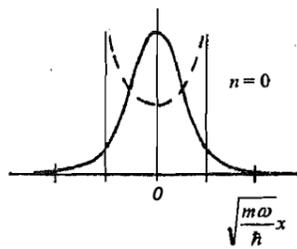
You should be very clear, however, that the quantum solution of the harmonic oscillator is radically different from that for the classical oscillator. In classical mechanics, the oscillator is forbidden to go beyond the potential, beyond the turning points where its kinetic energy turns negative. But clearly, the quantum wave functions extend beyond the potential, and thus there is a finite probability for the oscillator to be found in a classically forbidden region.

To be specific, let us compare the quantum and classical probabilities for the states corresponding to $n = 0$ and $n = 1$. The quantum probabilities are easily calculated by taking the square of the appropriate wave functions, ψ_0 and ψ_1 .

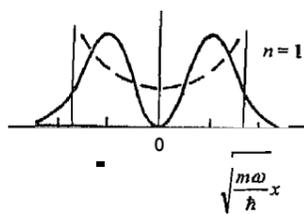
The expression for the probability of finding a classical harmonic oscillator of mass m and energy E governed by the equation $x = A \sin \omega t$ in a region Δx is given as

$$P(x) \Delta x = \frac{1}{2\pi A} \frac{1}{(1 - x^2/A^2)^{1/2}} \Delta x$$

where $A = (2E/m\omega^2)^{1/2}$. As expected, the classical probability is non-zero only for $-A < x < A$; the oscillator is confined within the turning points. For $x > A$, it is clear that the potential energy $\frac{1}{2} m\omega^2 x^2 > E$, and classically this is impossible.



(a)



(b)

Fig. 8.13 : Comparison of quantum (solid curve) and classical probability densities (dashed curve) for the harmonic oscillator for the two oscillator states having the same total energy, corresponding to $n = 0$ and $n = 1$.

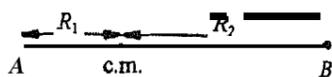


Fig. 8.14 : Vibration of two atoms A and B in a diatomic molecule.

Spend
20 min

The quantum and classical probabilities are compared in Figs. 8.13 (a) and (b) for $n = 0$ and $n = 1$, respectively. In both cases, the quantum probability does not vanish in the classically forbidden region. For $n = 1$, the classical probability is maximum at the turning points. But the quantum probability reaches the maximum much closer to the point of equilibrium. For large n , the average of the quantum mechanical probability distribution is found to be given by the classical probability curve.

Let us now consider an application of the simple harmonic oscillator to physical systems: the vibrations of the two atoms of a diatomic molecule.

Example 2: Diatomic Molecule

Let us assume that both the atoms in the molecule execute simple harmonic motion about their equilibrium positions. Hence, they satisfy the following equations

$$M_1 \frac{d^2 R_1}{dt^2} = -k(R - R_e) \quad (8.51)$$

and

$$M_2 \frac{d^2 R_2}{dt^2} = -k(R - R_e)$$

where R_1 and R_2 are the distance of the two atoms A and B from their centre of mass and $R = R_1 + R_2$ (Fig. 8.14). The masses of the two atoms are M_1 and M_2 , k is the force constant and at equilibrium, the distance between the two atoms is R_e . Considering the moment about A (see Fig. 8.14) we obtain

$$M_2 \dot{R} = (M_1 + M_2) \dot{R}_1 \quad (8.52)$$

Putting Eq. (8.52) in Eq. (8.51) we obtain

$$\frac{M_1 M_2}{M_1 + M_2} \frac{d^2 R}{dt^2} = -k(R - R_e) \quad (8.53)$$

or

$$\mu \frac{d^2 x}{dt^2} = -kx \quad (8.54)$$

with $x = R - R_e$.

Thus we have reduced a two body problem of masses M_1 and M_2 to a one-body problem of mass μ and the whole molecule behaves as a simple harmonic oscillator of mass μ (reduced mass of the molecule) having force constant k . Hence the eigenfunctions and eigenvalues of the molecules are given by Eq. (8.49) and Eq. (8.47), respectively. These equations have been very useful in understanding the vibrational spectrum (obtained in the near infrared region of the electromagnetic waves) of diatomic molecules. The analysis of the experimental spectrum has yielded force constants of a large number of heteronuclear molecules.

Would you like to apply the ideas discussed so far to some concrete situations? Try the following SAQ.

SAQ 7

- Consider a proton as a bound oscillator with a natural frequency of 3×10^{21} Hz. What is the energy of its ground and first excited states?
- Calculate $\langle x \rangle$ and $\langle p \rangle$ for the ground state harmonic oscillator eigenfunctions.

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

8.7 SUMMARY

In this unit you have solved time independent Schrödinger equation for a number of simple one-dimensional conservative systems. Some of the important results are summarised below:

- The eigenenergy E of a **free** particle moving in a one-dimensional space is given by $E = \frac{\hbar^2 k^2}{2m}$. It can take any value continuously from 0 to ∞ . Hence its energy spectrum is continuous. The eigenfunctions are incoming and outgoing plane waves given by $\psi_{\pm k}(x) = Ae^{\pm ikx}$ and are unnormalizable. However, if the particle is confined to a finite line segment then the eigenenergies vary in a discrete manner and the bound state eigenfunctions can be normalised. The plane waves can also be box-normalised.

For a one-dimensional rectangular potential barrier, the eigenenergies vary continuously from 0 to ∞ . However, unlike in classical mechanics the quantum mechanical probabilities of reflection and transmission of the particle by the barrier are, in general, finite. Thus even for $E < V_0$, the particle can **tunnel** through the barrier. Another interesting result is that for

$$E = \frac{1}{2m} \left(\frac{n\hbar\pi}{2a} \right)^2 + V_0$$

there is a hundred percent transmission with no reflection. Here symbols have the meanings discussed in the text.

- For a one-dimensional potential well the eigenenergy spectrum breaks into two parts. For $E > V_0$, the eigenenergy varies in a continuous manner. On the other hand for $E < V_0$ the eigenenergy varies in a discrete manner and bound states are obtained. The lowest eigenenergy is non-zero and is in accordance with the Heisenberg uncertainty relation. The number of permissible bound states increase with V_0 : the eigenfunctions being alternately of even and odd parities, the lowest being of even parity.
- for a particle executing **simple harmonic motion** along a line all the eigenstates are bound states and eigenenergies vary in a discrete manner. Consecutive eigenenergy states are separated from each other by the same amount $\hbar\omega$. The eigenfunctions are given in terms of Hermite polynomials and are of definite parity, alternately of even and odd parities. The finite value of the lowest eigenenergy is again a consequence of the uncertainty principle. The results obtained for a simple harmonic oscillator can be applied to study the vibrational spectrum of diatomic molecules.

8.8 TERMINAL QUESTIONS

Spend 45 min

1. The wave function of a particle of mass m inside an infinite square well of width $2a$ ($-a$ to $+a$) is given by

$$\psi(x) = A \cos \frac{3\pi x}{2a} + B \sin \frac{3\pi x}{2a}$$

Obtain the values of A and B and the eigenenergy corresponding to the above eigenfunction.

2. The potential energy of a particle of mass m is given by

$$V(x) = \begin{cases} \frac{1}{2} m\omega^2 x^2 & \text{for } x > 0 \\ \infty & \text{for } x < 0. \end{cases}$$

Show that its eigenenergies are given by

$$E_{2m+1} = 2 \left(m + \frac{3}{4} \right) \hbar\omega \text{ for } m = 0, 1, 2, \dots$$

3. Show that the average value of x for a simple harmonic oscillator in the n^{th} quantum state is zero.
4. Calculate the mean kinetic and potential energies of a simple harmonic oscillator which is in its ground state.

Self-Assessment Questions

$$1. \quad p_{op} e^{\pm ikx} = -i\hbar \frac{\partial}{\partial x} e^{\pm ikx} \left[\because p_{op} = -i\hbar \frac{\partial}{\partial x} \right]$$

$$= -i\hbar (\pm ik) e^{\pm ikx}$$

$$= \pm k\hbar e^{\pm ikx}$$

2. (a) The normalisation condition is

$$\int_{-\infty}^{\infty} \psi_n^*(x) \psi_n(x) dx = 1$$

or

$$N^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1 \quad \left[\because \psi_n(x) \text{ is finite only for } 0 < x < L \right]$$

or

$$N^2 \left(\frac{L}{2}\right) = 1 \quad \left[\because \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = \frac{L}{2} \right]$$

or

$$N = \left(\frac{2}{L}\right)^{1/2}$$

(b) To prove that $\psi_m(x)$ and $\psi_n(x)$ are orthogonal for $m \neq n$, we have to show that

$$I = \int_{-\infty}^{\infty} \psi_m^*(x) \psi_n(x) dx = 0 \text{ for } m \neq n$$

or

$$I = N^2 \int_{-\infty}^{\infty} \sin \frac{n\pi x}{L} \sin \frac{m\pi x}{L} dx = \int_0^L \sin \frac{n\pi x}{L} \sin \frac{m\pi x}{L} dx$$

$$= 0, \text{ for } m \neq n \quad \left[\because \int_0^L \sin \frac{n\pi x}{L} \sin \frac{m\pi x}{L} dx = 0 \text{ for } m \neq n \right]$$

3. A three-dimensional extension of Eq. (8.3a) is

$$\left[\frac{d^2}{dx^2} + \frac{d^2}{dy^2} + \frac{d^2}{dz^2} \right] \psi(x, y, z) = -(k_x^2 + k_y^2 + k_z^2) \psi(x, y, z)$$

Since x, y, z are independent variables, we may write

$$\psi(x, y, z) = \phi_{n_x}(x) \phi_{n_y}(y) \phi_{n_z}(z) \quad (1)$$

where

$$\phi_{n_x}(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{n_x \pi x}{L_x}\right) \text{ etc.} \quad (2)$$

and

$$E_{n_x, n_y, n_z} = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right) \quad (3)$$

Here n_x, n_y and n_z are positive integers ranging from zero to infinity, but all the three can't be zero simultaneously. It is evident from (3) that E_{n_x, n_y, n_z} takes only discrete values. Hence the energy spectrum of a particle enclosed in a box is discrete and the eigenfunctions given by (1) and (2) form an orthonormal set.

4. Applying the boundary conditions given by Eqs. (8.25a and b) to the wave functions ψ_I, ψ_{II} and ψ_{III} we obtain the following set of equations:

$$Ae^{-ika} + Be^{ika} = Ce^{\gamma a} + De^{-\gamma a} \quad (1)$$

$$Ae^{-ika} - Be^{ika} = \frac{i\gamma}{k} (Ce^{\gamma a} - De^{-\gamma a}) \quad (2)$$

$$Ce^{-\gamma a} + De^{\gamma a} = Fe^{ika} \quad (3)$$

$$Ce^{-\gamma a} - De^{\gamma a} = -\frac{i\gamma}{k} Fe^{ika} \quad (4)$$

To obtain P_r we have to eliminate C and D from Eqs. (1 and 2). Adding Eqs. 1 and 2 and subtracting Eq. 2 from Eq. 1, we get

$$2Ae^{-ika} = Ce^{\gamma a} \left(1 + \frac{i\gamma}{k}\right) + De^{-\gamma a} \left(1 - \frac{i\gamma}{k}\right) \quad (5)$$

$$2Beika = Ce^{\gamma a} \left(1 - \frac{i\gamma}{k}\right) + De^{-\gamma a} \left(1 + \frac{i\gamma}{k}\right) \quad (6)$$

Similarly, adding (3) and (4) and subtracting (4) from (3), we get

$$2Ce^{-\gamma a} = Feika \left(1 - \frac{ik}{\gamma}\right)$$

$$2De^{\gamma a} = Feika \left(1 + \frac{ik}{\gamma}\right)$$

whence

$$Ce^{\gamma a} = \frac{Feika+2\gamma a}{2} \left(1 - \frac{ik}{\gamma}\right)$$

and

$$De^{-\gamma a} = \frac{Feika-2\gamma a}{2} \left(1 + \frac{ik}{\gamma}\right)$$

Substituting these expressions in Eqs. (5) and (6) we get

$$2Ae^{-ika} = \frac{F}{2} eika \left[e^{2\gamma a} \left(1 - \frac{ik}{\gamma}\right) \left(1 + \frac{i\gamma}{k}\right) + e^{-2\gamma a} \left(1 + \frac{ik}{\gamma}\right) \left(1 - \frac{i\gamma}{k}\right) \right] \quad (7)$$

and

$$2Beika = \frac{F}{2} eika \left[e^{2\gamma a} \left(1 - \frac{ik}{\gamma}\right) \left(1 - \frac{i\gamma}{k}\right) + e^{-2\gamma a} \left(1 + \frac{ik}{\gamma}\right) \left(1 + \frac{i\gamma}{k}\right) \right] \quad (8)$$

Dividing Eq. (8) by (7) we have

$$\begin{aligned} \frac{B}{A} e^{2ika} &= \frac{e^{2\gamma a} (\gamma - ik) (k - i\gamma) + e^{-2\gamma a} (\gamma + ik) (k + i\gamma)}{e^{2\gamma a} (\gamma - ik) (k + i\gamma) + e^{-2\gamma a} (\gamma + ik) (k - i\gamma)} \\ &= \frac{-ie^{2\gamma a} (\gamma^2 + k^2) + ie^{-2\gamma a} (\gamma^2 + k^2)}{-ie^{2\gamma a} (k + i\gamma)^2 + ie^{-2\gamma a} (k - i\gamma)^2} \\ &= \frac{(\gamma^2 + k^2) (e^{2\gamma a} - e^{-2\gamma a})}{e^{2\gamma a} (k + i\gamma)^2 - e^{-2\gamma a} (k - i\gamma)^2} \\ &= \frac{2(\gamma^2 + k^2) \sinh 2\gamma a}{(k^2 - \gamma^2) (e^{2\gamma a} - e^{-2\gamma a}) + 2ik\gamma (e^{2\gamma a} + e^{-2\gamma a})} \\ &= \frac{2(\gamma^2 + k^2) \sinh 2\gamma a}{2(k^2 - \gamma^2) \sinh 2\gamma a + 4ik\gamma \cosh 2\gamma a} \end{aligned}$$

Now

$$\begin{aligned} P_r &= \left| \frac{B}{A} \right|^2 = \frac{(\gamma^2 + k^2)^2 \sinh^2 2\gamma a}{(k^2 - \gamma^2)^2 \sinh^2 2\gamma a + 4k^2\gamma^2 \cosh^2 2\gamma a} \\ &= \frac{(\gamma^2 + k^2)^2 \sinh^2 2\gamma a}{(k^4 + \gamma^4 - 2k^2\gamma^2) \sinh 2\gamma a + 4k^2\gamma^2 \cosh^2 2\gamma a} \\ &= \frac{(\gamma^2 + k^2)^2 \sinh^2 2\gamma a}{(k^4 + \gamma^4 + 2k^2\gamma^2) \sinh^2 2\gamma a + 4k^2\gamma^2} \end{aligned}$$

where we have added and subtracted $4k^2\gamma^2 \sinh^2 2\gamma a$ in the denominator and used the relation $\cosh^2 \theta - \sinh^2 \theta = 1$.

$$\text{or } P_r = \frac{(\gamma^2 + k^2)^2 \sinh^2 2\gamma a}{(\gamma^2 + k^2)^2 \sinh^2 2\gamma a + 4k^2\gamma^2}$$

$$\text{Now } \gamma^2 + k^2 = \frac{2m}{\hbar^2} (V_0 - E + E) = \frac{2m}{\hbar^2} V_0$$

$$\text{and } \gamma^2 k^2 = \left(\frac{2m}{\hbar^2}\right)^2 E (V_0 - E)$$

Therefore

$$\begin{aligned} P_r &= \frac{V_0^2 \sinh^2 2\gamma a}{V_0^2 \sinh^2 2\gamma a + 4E (V_0 - E)} \\ &= \left[\frac{V_0^2 \sinh^2 2\gamma a + 4E (V_0 - E)}{V_0^2 \sinh^2 2\gamma a} \right]^{-1} \\ &= \left[1 + \frac{4E (V_0 - E)}{V_0^2 \sinh^2 2\gamma a} \right]^{-1} \end{aligned}$$

To obtain an expression for P_t , we can use Eq. (7) whence

$$\frac{F}{A} = \frac{4e^{-2ika}}{e^{2\gamma a} \left(1 - \frac{ik}{\gamma}\right) \left(1 + \frac{i\gamma}{k}\right) + e^{-2\gamma a} \left(1 + \frac{ik}{\gamma}\right) \left(1 - \frac{i\gamma}{k}\right)}$$

$$\frac{F}{A} = \frac{4e^{-2ika}}{e^{2\gamma a} \left(2 - \frac{ik}{\gamma} + \frac{i\gamma}{k}\right) + e^{-2\gamma a} \left(2 + \frac{ik}{\gamma} - \frac{i\gamma}{k}\right)}$$

$$= \frac{4e^{-2ika}}{4 \cosh 2\gamma a + 2i \left(\frac{\gamma}{k} - \frac{k}{\gamma}\right) \sinh 2\gamma a}$$

Thus

$$P_t = \left| \frac{F}{A} \right|^2 = \frac{4}{4 \cosh^2 2\gamma a + \left(\frac{\gamma}{k} - \frac{k}{\gamma}\right)^2 \sinh^2 2\gamma a}$$

$$\text{Now } \left(\frac{\gamma}{k} - \frac{k}{\gamma}\right)^2 = \frac{(\gamma^2 - k^2)^2}{k^2\gamma^2} = \frac{\left(\frac{2m}{\hbar^2}\right)^2 (V_0 - E - E)^2}{\left(\frac{2m}{\hbar^2}\right)^2 (V_0 - E) E}$$

$$= \frac{(V_0 - 2E)^2}{E (V_0 - E)}$$

Therefore,

$$P_t = \frac{4E (V_0 - E)}{4 \cosh^2 2\gamma a (EV_0 - E^2) + (V_0^2 + 4E^2 - 4V_0E) \sinh^2 2\gamma a}$$

$$= \frac{4E (V_0 - E)}{4E V_0 - 4E^2 + V_0^2 \sinh^2 2\gamma a}$$

$$= \frac{4E (V_0 - E)}{4E (V_0 - E) + V_0^2 \sinh^2 2\gamma a}$$

$$= \left[\frac{4E(V_0 - E) + V_0^2 \sinh^2 2\gamma a}{4E(V_0 - E)} \right]^{-1}$$

$$= \left[1 + \frac{V_0^2 \sinh^2 2\gamma a}{4E(V_0 - E)} \right]^{-1}$$

5. The condition

$$\frac{1}{\psi_I} \frac{\partial \psi_I}{\partial x} \Big|_{x=-a} = \frac{1}{\psi_{II}} \frac{\partial \psi_{II}}{\partial x} \Big|_{x=-a}$$

yields

$$\frac{-\gamma A e^{-\gamma a}}{A e^{-\gamma a}} = \frac{-q B \sin qa}{B \cos qa}$$

or

$$-\gamma a = -qa \tan qa$$

or

$$\eta = \xi \tan \xi$$

where

$$\eta = \gamma a \text{ and } \xi = qa$$

6. Since $\xi = ax$

$$\frac{d\psi}{dx} = \frac{d\psi}{d\xi} \frac{d\xi}{dx} = a \frac{d\psi}{d\xi}$$

and

$$\frac{d^2\psi}{dx^2} = a^2 \frac{d^2\psi}{d\xi^2}$$

Thus Eq. (8.43) may be written as

$$-\frac{\hbar^2 a^2}{2m} \frac{d^2\psi}{d\xi^2} + \frac{1}{2} \frac{m\omega^2}{a^2} \xi^2 \psi = \frac{\lambda \hbar \omega}{2} \psi(\xi)$$

or

$$-\frac{\hbar^2 m \omega}{2m\hbar} \frac{d^2\psi}{d\xi^2} + \frac{1}{2} \frac{m\omega^2 \hbar}{m\omega} \xi^2 \psi = \frac{\lambda \hbar \omega}{2} \psi$$

or

$$-\frac{\hbar \omega}{2} \frac{d^2\psi}{d\xi^2} + \frac{\hbar \omega}{2} \xi^2 \psi = \frac{\lambda \hbar \omega}{2} \psi$$

or

$$\frac{d^2\psi}{d\xi^2} + (\lambda - \xi^2) \psi(\xi) = 0$$

$$7. (a) E_n = \left(n + \frac{1}{2}\right) \hbar \omega$$

$$\text{For the ground state } n = 0, E_0 = \frac{1}{2} \hbar \omega = \frac{1}{2} h\nu$$

$$= \frac{1}{2} \times 6.626 \times 10^{-34} \text{ Js} \times 3 \times 10^{21} \text{ Hz}$$

$$= 9.939 \times 10^{-13} \text{ J}$$

For the first excited state, $n = 1$

$$E_1 = \frac{3}{2} \hbar \omega = \frac{3}{2} h\nu$$

$$= 3E_0 = 2.982 \times 10^{-12} \text{ J}$$

(b) For the ground state harmonic oscillator wavefunction

$$\langle x \rangle = \int_{-\infty}^{\infty} dx \psi_0^*(x) x \psi_0(x)$$

where
$$\psi_0(x) = \left(\frac{a}{\sqrt{\pi}}\right)^{1/2} H_0(ax) \exp\left(-\frac{a^2 x^2}{2}\right)$$

$$= \left(\frac{a}{\sqrt{\pi}}\right)^{1/2} \exp\left(-\frac{a^2 x^2}{2}\right) \text{ since } H_0(\xi) = 1$$

Thus

$$\langle x \rangle = \left(\frac{a}{\sqrt{\pi}}\right) \int_{-\infty}^{\infty} x \exp(-a^2 x^2) dx$$

The integrand is an odd function. Hence the integral over the interval will be zero.

$$\therefore \langle x \rangle = 0$$

Similarly

$$\begin{aligned} \langle p_x \rangle &= -i\hbar \int_{-\infty}^{\infty} \psi_0^*(x) \frac{\partial}{\partial x} \psi_0(x) dx \\ &= -i\hbar \left(\frac{a}{\sqrt{\pi}}\right) \int_{-\infty}^{\infty} \exp\left(-\frac{a^2 x^2}{2}\right) (-a^2 x) \exp\left(-\frac{a^2 x^2}{2}\right) dx \\ &= i \frac{a^3}{\sqrt{\pi}} \hbar \int_{-\infty}^{\infty} x \exp(-a^2 x^2) dx \end{aligned}$$

Again the integrand is an odd function of x . Hence the integral over this interval will be zero.

$$\therefore \langle p_x \rangle = 0$$

Terminal Questions

1. Since the well is of infinite depth $\psi(+a) = 0$. Hence $B = 0$. A is obtained as follows:

$$A^2 \int_{-a}^{+a} \cos^2 \frac{3\pi x}{2a} dx = 1$$

or

$$A = \left(\frac{1}{a}\right)^{1/2}$$

Now inside the well $V(x) = 0$ and the Schrödinger equation yields

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} (A \cos \frac{3\pi x}{2a}) = +A \frac{\hbar^2}{2m} \left(\frac{3\pi}{2a}\right)^2 \cos\left(\frac{3\pi x}{2a}\right)$$

$$\therefore E = \frac{9\pi^2 \hbar^2}{8m a^2}$$

2. The problem is similar to that of a simple harmonic oscillator but

$$\psi(0) = 0.$$

Hence n must be odd (See Eq. 8.50).

Therefore,

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega, \text{ with } n = 1, 3, 5, \dots$$

Putting $n = 2m + 1$ we get

$$E_{2m+1} = 2\left(m + \frac{3}{4}\right) \hbar\omega \text{ with } m = 0, 1, 2, 3, \dots$$

3. $\langle x \rangle = \langle \psi_n, x\psi_n \rangle = \int_{-\infty}^{\infty} \psi_n^*(x) x \psi_n(x) dx$

Since $\psi_n(x)$ is of definite parity, it is either an odd or an even function of x . In either case, the product $\psi_n^*(x) \psi_n(x)$ will be even. Since x is odd, the integrand will be an odd function of x and hence the integral will be zero.

4. The average value of the potential energy V is given by

$$\langle V \rangle = \int_{-\infty}^{\infty} \psi_0^*(x) \frac{1}{2} kx^2 \psi_0(x) dx.$$

Evaluation of the integral with $\psi_0 = \left(\frac{a}{\sqrt{\pi}}\right)^{1/2} \exp\left(-\frac{a^2 x^2}{2}\right)$ yields

$$\langle V \rangle = \frac{1}{4} \hbar\omega$$

Since $E_0 = \frac{1}{2} \hbar\omega$

$$\therefore \langle \text{K.E.} \rangle = E_0 - \frac{1}{4} \hbar\omega = \frac{1}{4} \hbar\omega.$$