

Block

3

APPLICATIONS OF QUANTUM MECHANICS TO SIMPLE SYSTEMS

UNIT 9

Particle in a Box

7

UNIT 10

Step Potential

35

UNIT 11

Barrier Potential

51

UNIT 12

Finite Potential Well

79

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BLOCK 3 : APPLICATIONS OF QUANTUM MECHANICS TO SIMPLE SYSTEMS

In Block 2 of this course we have introduced you to the basic concepts of quantum mechanics. Quantum mechanics has forced us to reconsider our deepest convictions about the reality of nature. For example, the idea that wave-particle duality is an inherent property of all the elements that make up the physical universe does away with the distinction between matter and radiation (which is at the root of classical physics). Then you have seen how classical determinism and causality are called into question by quantum mechanics through the uncertainty principle and the probabilistic description. You learnt that our inability to measure certain pairs of variables with arbitrary accuracy is not a limitation of the experimental apparatus. Quantum mechanics tells us that uncertainty is not a matter of our inability to do better, rather it is inherent to the nature of the quantum world. That a particle may not have a well-defined position and momentum at the same time is a fundamentally new notion which many physicists including Einstein found hard to accept. It is indeed in the nature of things - either we define the particle's position and lose all information about its momentum, or we pinpoint its momentum and do not know where in space it is. This is surely a far cry from the deterministic depiction of classical mechanics. These fundamental ideas were built into a mathematical framework which you studied in Units 7 and 8.

The Schrödinger equation for the time evolution of matter waves led us to the probabilistic description of the quantum world. Quantum mechanics tells us that the probabilistic description is also the fundamental description; there is no deeper level. It gives us only the probability amplitude from which a probability can be computed. For example, we can compute the probability that an electron would have a certain velocity. But quantum mechanics does not give the velocity of a specific particle. Instead it claims that no such detailed information even exists.

The first idea of the energy quantum was introduced by Planck in 1900; it took about another thirty years to develop into a full-fledged theory. We can say that it is one of the most successful theories in the history of science. In the subsequent years since its birth, the fundamental ideas of quantum mechanics have been tested and verified with increasingly accurate experiments. It has continued to evolve into other important areas of research like quantum field theory, quantum electrodynamics and the quantum description of gravity. The methods of quantum mechanics become important when we talk of microscopic systems, far removed from our daily experiences. Yet it affects our lives in many different ways, because in today's world, a lot of the technology we take for granted owes its origins to quantum mechanics: shrinking transistor sizes to power laptops and mobiles, medical technology like MRI and PET and so on. This has become possible, in part, because of one important aspect of quantum mechanics: its ability to predict. You will discover its power in this block when you study its applications to some simple one-dimensional systems.

In **Unit 9** of this block, entitled **Particle in a Box**, you will solve the one-dimensional Schrödinger equation for the free particle and for a particle confined to a rigid one-dimensional box. You will study an important distinction between classical and quantum physics: that when a quantum particle is confined to a tiny region, its energies cannot be continuous. Rather the particle's energy can have only specified discrete values, which depend on the parameters of the system. This idea has important applications in semiconductor technology and in this context, you will study about the quantum dot.

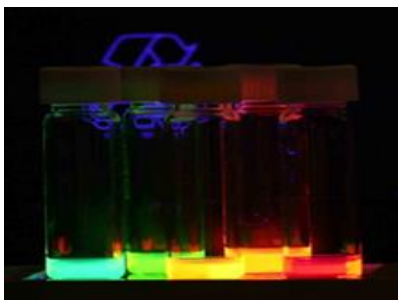
In **Unit 10** entitled **Step Potential** you will study the properties of a quantum particle moving in a one-dimensional step potential. You will learn that it is possible for quantum particles to be found in regions that are classically forbidden.

In **Unit 11** entitled **Barrier Potential**, we solve the Schrödinger equation for the one-dimensional potential barrier. You will find that it is possible for a particle to be transmitted across a potential barrier even when its kinetic energy is less than the barrier potential. This phenomenon of barrier penetration is called “**quantum tunnelling**” because it has no classical analogue. You will study applications of quantum tunnelling in alpha decay and scanning tunnelling microscopy.

Finally in **Unit 12** entitled **Finite Potential Well** you will study the motion of a particle in a finite potential well. This is important because an infinite well in which particles can be strictly confined is actually an idealization, rarely found in nature. Once again, you will see that a bound particle has discrete energy levels.

With this we end our study of the concepts of quantum mechanics and their applications. In higher courses at the Master’s level, you will solve the Schrödinger equation for more complex potentials. However, in this block you will learn the methods of solving the Schrödinger equation and how the properties of eigen functions and energy eigen values change with the parameters of the system.

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 are a lot of mathematical steps 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 wish to really understand it for 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!



Colloidal quantum dots of different sizes emit different colours of light when illuminated by ultraviolet radiation. [Walkman16, CC BY-SA 3.0

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UNIT 9

PARTICLE IN A BOX

Structure

- | | | | |
|-----|----------------------------------|-----|-----------------------|
| 9.1 | Introduction | 9.4 | Quantum Dot |
| | Expected Learning Outcomes | 9.5 | Summary |
| 9.2 | A Free Particle | 9.6 | Terminal Questions |
| 9.3 | Particle in a Box | 9.7 | Solutions and Answers |
| | Solving the Schrödinger Equation | | |
| | Eigen Functions and Eigen Values | | |
| | Time Dependent Wave Function | | |
| | Probability Density | | |

STUDY GUIDE

In this unit you will apply the Schrödinger equation to simple systems. You will be solving second order ordinary differential equations, obtaining normalized wave functions and calculating expectation values of dynamical variables. You should be familiar with ordinary differential and integral calculus which you have studied in school and the techniques of solving ODEs which you have studied in Unit 4 of BPHCT 131. Please be thorough with the concepts of Units 7 and 8 of Block 2 of this course before you start studying these units. You must work through all the examples, SAQs and TQs to get good practise in the methods taught here.

“A method is more important than a discovery, since the right method will lead to new and even more important discoveries.”

Lev Landau

9.1 INTRODUCTION

The Schrödinger equation cannot be derived, and like the other postulates of quantum mechanics, its validity lies in its agreement with experimental results. Schrödinger himself applied his equation to the hydrogen atom and in fact, it is in the field of atomic physics that this equation has been most successful. You should also know that one cannot obtain an exact solution for neutral atoms more complex than the hydrogen atom and one has to use approximation methods, which you study about in higher classes.

Note also that the Schrödinger equation is **not** a relativistic wave equation. So it is used only to study the nonrelativistic behaviour of atoms and molecules. Just like Newton's second law which gives way to the relativistic force law to study relativistic phenomena, there is also a relativistic wave equation which was developed by Dirac in 1928.

In Unit 7 of Block 2 you have studied the time independent Schrödinger equation. In this unit, you will how to solve Schrödinger equation in one dimension. 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 a number of more complicated physical problems can be reduced to the solution of equations similar to the one- dimensional Schrödinger equation.

In Sec. 9.2, you will first study a quantum mechanical free particle, that is one on which no force is being exerted. This is a particle that cannot be confined (bound) within a defined region of space by a potential, like a proton in a nucleus. You will see that a quantum mechanical free particle has a continuous spectrum of energy eigen values In Sec. 9.3 we solve the quantum mechanical problem of a particle moving within a limited space like in a rigid box. You will find that the energy eigen values of this system are different. Finally in Sec. 9.4 we discuss a quantum dot which is a practical realization of a particle in a box. A quantum dot is typically a nano sized semiconductor particle. The optical and electrical properties of the quantum dot change with size and material, and they have many applications in nano scale devices.

In the next unit you will solve the time independent Schrödinger equation for a one dimensional step potential function and study its applications.

Expected Learning Outcomes

After studying this unit, you should be able to:

- ❖ solve the time independent one-dimensional Schrödinger equation and obtain the eigen functions and energy eigen values for a free particle;
- ❖ solve the time independent one-dimensional Schrödinger equation and obtain the eigen functions and energy eigen values for a particle in a one dimensional box; and
- ❖ explain the properties of the quantum dot on the basis of the particle in a box model.

9.2. A FREE PARTICLE

Recall the time independent Schrödinger equation for the stationary state wave function $\psi(x)$ for a quantum particle of mass m from Unit 7 (Eq.7.47):

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x) \leftrightarrow \hat{H}\psi(x) = E\psi(x) \quad (9.1)$$

You know that this is the eigen value equation for the Hamiltonian operator $\hat{H}$. Any solution, $\psi(x)$, of this equation is the eigen function of $\hat{H}$. And the energy, E , is the eigen value of $\hat{H}$ corresponding to the eigen function $\psi(x)$.

Note that in Eq. (9.1), the partial derivative $\frac{\partial^2 \psi(x)}{\partial x^2}$ has been replaced by

$\frac{d^2 \psi(x)}{dx^2}$ because $\psi(x)$ is only a function of x . Now, you know that a free particle is one on which no force is being exerted. You have studied in BPHCT-131, that for a conservative system, force is related to the potential as follows:

$$F(x) = -\frac{dV(x)}{dx} \quad (9.2)$$

So, for a system on which no force is exerted, we will have:

$$F(x) = 0 \Rightarrow \frac{dV(x)}{dx} = 0 \Rightarrow V(x) = V_0 \quad (9.3)$$

where V_0 is a **constant** potential.

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. Putting $V(x) = 0$ in Eq. (9.1)

we can write the **time independent Schrödinger equation for a free particle** as follows:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} = E\psi(x) \quad (9.4)$$

In the classical picture, since the particle is not subjected to any force, its linear momentum p **does not change with time**. E , the total energy of the particle (which is equal to its kinetic energy) also does not change with time. E and p are related by the equation:

$$E = \frac{p^2}{2m} \quad (9.5)$$

From Eq. (5.3) you know that the linear momentum $\vec{p} = \hbar \vec{k}$. Since we are considering only one-dimensional motion, we can assume that both the momentum p and the wave vector k lie along the x -axis. So we write $p = p_x = \hbar k$. Then the expression for the energy of the particle is:

$$E = \frac{\hbar^2 k^2}{2m} \quad (9.6)$$

Let us now solve Eq. (9.1). Rearranging the terms we get:

$$\frac{d^2 \psi(x)}{dx^2} = -\frac{2mE}{\hbar^2} \psi(x) \quad (9.7)$$

Making the substitution $k^2 = \frac{2mE}{\hbar^2}$ we get the following second order ODE:

Block 3

Applications of Quantum Mechanics to Simple Systems

From Sec.4.3.3 of BPHCT-131 you can write the general solution of

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

As

$$\psi(x) = Ae^{m_1x} + Be^{m_2x}$$

Where m_1 and m_2 are the solutions of the indicial equation

$$m^2 + k^2 = 0$$

Here

$$m_1 = ik; m_2 = -ik$$

e^{m_1x} and e^{m_2x} are the two linearly independent solutions

$$\frac{d^2\psi(x)}{dx^2} = -k^2\psi(x) \quad (9.8)$$

For any given value of E and hence of k , there are two possible solutions to this equation, which are also linearly independent (read the margin remark):

$$\psi_1(x) = e^{ikx}; \psi_2(x) = e^{-ikx} \quad (9.9)$$

Thus for one value of E , we have two possible eigen functions, $\psi_1(x)$ and $\psi_2(x)$.

Recall from Sec. 8.3.4 that such eigen functions which have the same eigenvalue for a given eigenvalue equation are called degenerate eigen functions (otherwise they are non-degenerate). Thus, $\psi_1(x)$ and $\psi_2(x)$ are **degenerate eigen functions**. The general solution of Eq. (9.4) is the linear combination:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad (9.10)$$

You can check for yourself by solving SAQ 1, that $\psi(x)$ is also an eigen function of Eq.(9.4) with the same eigenvalue $E = \frac{\hbar^2 k^2}{2m}$.

The functions $\sin kx$ and $\cos kx$, as well as linear combinations of these functions are also solutions of the time independent Schrödinger equation for the free particle. You will see this for yourself when you work out SAQ 2

SAQ 1 - Free Particle in One Dimension

Show that $\psi(x) = Ae^{ikx} + Be^{-ikx}$ is an eigen function of the time independent Schrödinger equation for the quantum mechanical free particle with an eigenvalue $E = \frac{\hbar^2 k^2}{2m}$.

For the solution $\psi(x)$ to be physically acceptable, k cannot have an imaginary part. Can you say why?

To understand, let us take k to be complex: $k = \alpha + i\beta$. In that case,

$$\psi_1(x) = e^{i(\alpha+i\beta)x} = e^{i\alpha x} e^{-\beta x} \quad (9.11)$$

Now, if β is positive, you can see that the term $e^{-\beta x}$ would increase exponentially as $x \rightarrow -\infty$. If β is negative, the term $e^{-\beta x}$ would increase exponentially as $x \rightarrow \infty$. So this would **not** be an acceptable wave function, as you have studied in Sec. 7.5. You can also check for yourself that $\psi_2(x)$ would also would increase exponentially either as $x \rightarrow -\infty$ or as $x \rightarrow \infty$, if k had an imaginary part.

So, k should be a real number and therefore $k^2 \geq 0$. Therefore a quantum mechanical free particle can have **any non negative value of energy**:

$$E = \frac{\hbar^2 k^2}{2m} \geq 0 \quad (9.12)$$

Since any non-negative value of E is allowed, **the energy spectrum of a free particle is continuous**, extending from $E = 0$ to ∞ . This, of course, is not

surprising, since E is the kinetic energy of a free particle. It also corresponds to the classical result.

For a real value of k , $\psi_1(x)$ and $\psi_2(x)$ do not diverge at $x \rightarrow -\infty$ or as $x \rightarrow \infty$, but neither do they go to zero. For $\psi_1(x)$, you can see that :

$$\int_{-\infty}^{\infty} \psi_1^*(x) \psi_1(x) dx = \int_{-\infty}^{\infty} (e^{-ikx})(e^{ikx}) dx = \int_{-\infty}^{\infty} dx \quad (9.13)$$

which is clearly **NOT** finite. The same is true for $\psi_2(x)$. So, as you have studied in Sec. 7.3.3, the eigen functions $\psi_1(x)$ and $\psi_2(x)$ are **non-normalizable**.

We can also write down the time dependent wave function for the free particle. In Sec. 7.4 you have studied that for a stationary state $\psi(x)$, the time dependent wave function has the explicit form (Eq. 7.48):

$$\psi(x, t) = \psi(x) e^{-iEt/\hbar} \quad (9.14)$$

So the time dependent wave function for the free particle with an energy E is

$$\psi(x, t) = (Ae^{ikx} + Be^{-ikx}) e^{-iEt/\hbar} \quad (9.15)$$

If the quantum mechanical free particle is in a stationary state $\psi(x)$ which corresponds to the energy eigen value E (Eq. 9.1), while the wave function will evolve with time as given by Eq. (9.15), **the energy of the particle, E , will not change with time.**

Using $E = \hbar\omega$, we get:

$$\psi(x, t) = Ae^{i(kx - \omega t)} + Be^{-i(kx + \omega t)} \quad (9.16)$$

In order to interpret Eq. (9.16) physically, let us consider some special cases. If we set $B = 0$, the resulting wave function is the plane wave:

$$\psi(x, t) = Ae^{i(kx - \omega t)} \quad (9.17)$$

This function represents a travelling plane wave as shown in Fig. 9.1. This wave 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 $\frac{\hbar^2 k^2}{2m}$.

The probability density corresponding to the wave function of Eq. (9.17) is:

$$P(x, t) = \psi^*(x, t) \psi(x, t) = |A|^2 \quad (9.18)$$

which is independent of time t as well as position x . In other words, at any instant of time t , **the probability of finding the particle in an interval between x and $x + dx$ is the same ($|A|^2 dx$) for any value of x .** In other words, the position of the particle is completely unknown.

This result can also be deduced from the uncertainty principle. Since the momentum of the particle is precisely known, $\Delta p = \Delta p_x = 0$. Then, from the

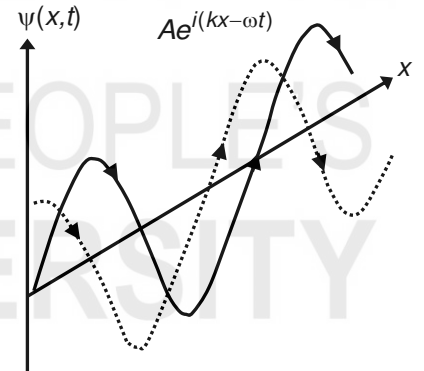


Fig. 9.1: A travelling wave

uncertainty principle, the uncertainty in the position of the particle $\Delta x = \infty$.

Further, since the energy of the particle is also known precisely, we also have $\Delta E = 0$. Hence, according to the energy-time uncertainty principle, we have an infinite time ($\Delta t = \infty$) to make a measurement of the energy of the particle.

You can carry out a similar analysis by setting $A = 0$ in Eq. (9.16). In this case the plane wave will be travelling in the **negative** x -direction.

It is possible to verify that $\psi_1(x)$ and $\psi_2(x)$ are also the eigen functions of the momentum operator. However the eigen values of the momentum operator are different for the two eigen functions. We work that out in the following example.

EXAMPLE 9.1: MOMENTUM EIGEN VALUES

Show that $\psi_1(x) = e^{ikx}$ and $\psi_2(x) = e^{-ikx}$ are eigen functions of the momentum operator and determine the corresponding eigen values.

SOLUTION ■ We have to show that the eigen value equation, Eq. (8.35), is valid for the wave functions $\psi_1(x) = e^{ikx}$ and $\psi_2(x) = e^{-ikx}$ with

$$\hat{D} = \hat{p}_x = -i\hbar \frac{d}{dx}.$$

Using $\psi_1(x) = e^{ikx}$ in Eq. (8.35) we get:

$$\hat{p}_x \psi_1(x) = -i\hbar \frac{d}{dx} \psi_1(x) = -i\hbar \frac{d}{dx} (e^{ikx}) = -i\hbar (ike^{ikx}) = \hbar k e^{ikx}$$

So $\hat{p}_x \psi_1(x) = (\hbar k) \psi_1(x)$. So $\psi_1(x)$ is an eigen function of the momentum operator $\hat{p}_x$ with the eigen value $\hbar k$.

Using $\psi_2(x) = e^{-ikx}$ in Eq. (8.35) we get:

$$\hat{p}_x \psi_2(x) = -i\hbar \frac{d}{dx} \psi_2(x) = -i\hbar \frac{d}{dx} (e^{-ikx}) = -i\hbar (-ike^{-ikx}) = -\hbar k e^{-ikx}$$

Since $\hat{p}_x \psi_2(x) = (-\hbar k) \psi_2(x)$, we can say that $\psi_2(x)$ is also an eigen function of the momentum operator $\hat{p}_x$ with the eigen value $-\hbar k$.

The energy $E[E(k)]$ and the momentum $p[p(k)]$ of a quantum mechanical free particle are both constants of motion and are defined in terms of k . k also characterises the eigen function $\psi(x)$ for the quantum mechanical free particle and hence we call k a **quantum number**.

Let us now summarize what you have studied so far.

FREE PARTICLE

Recap

The time independent Schrödinger equation for a quantum mechanical free particle of mass m is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad (9.4)$$

The general solution of Eq. (9.4) is:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad ; \text{ with } k^2 = \frac{2mE}{\hbar^2} \quad (9.10)$$

The quantum number k is real and the free particle can have **any non-negative value of energy**:

$$E = \frac{\hbar^2 k^2}{2m} \geq 0 \quad (9.12)$$

The energy of the particle does not change with time.

The time dependent wave function for the free particle with an energy $E = \hbar\omega$ is:

$$\psi(x, t) = Ae^{i(kx - \omega t)} + Be^{-i(kx + \omega t)} \quad (9.16)$$

You may now like to answer an SAQ.

SAQ 2 - Solutions of the free particle Schrödinger equation

Show that (i) $\psi(x) = \sin kx$ and (ii) $\psi(x) = \cos kx$ are solutions of the Schrödinger equation for the free particle (Eq. 9.7).

In the classical picture, a free particle has “unbounded motion” because it is not subjected to a force. In the corresponding quantum mechanical picture, the free particle can have any energy as defined by Eq. (9.6) and the energy eigen values E vary continuously with the value of k . So the energy spectrum is continuous and ranging between zero to infinity. Each energy state has a two-fold degeneracy corresponding to particles moving either along the positive x direction or along the negative x direction, except for the state corresponding to $k = 0$.

However, in the classical picture when the value of the momentum (p) is known exactly, you can locate the position of the particle at any instant of time, if the initial position is known. You have seen that this is not possible for a quantum mechanical free particle because of the uncertainty principle.

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

9.3. PARTICLE IN A BOX

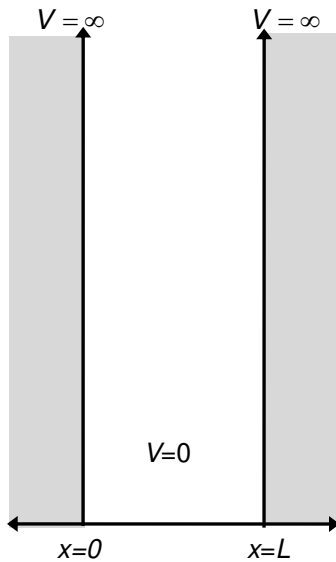


Fig. 9.2: Potential function for a one-dimensional box

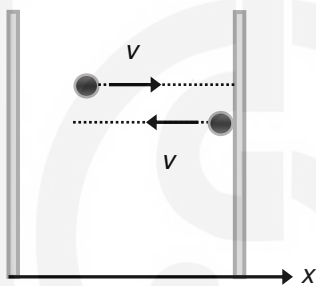


Fig. 9.3: A ball going back and forth between rigid walls.

Let us consider that a free particle is confined in a one-dimensional length segment lying between $x = 0$ and $x = L$. You can imagine that there are rigid barriers at $x = 0$ and $x = L$ that the particle cannot penetrate to move beyond these points: so the particle cannot move to the left of $x = 0$ or the right of $x = L$. This is also called a **rigid box**. We describe this system by saying that the potential $V(x)$ is **infinite** for all values of $x < 0$ and $x > L$. Between $0 \leq x \leq L$, the particle is free, and the potential is zero in this region. The potential function is shown in Fig 9.2 and is described as:

$$V(x) = \begin{cases} 0 & \text{for } 0 \leq x \leq L \\ \infty & \text{for } x < 0 \text{ and } x > L \end{cases} \quad (9.19)$$

The “particle in a box” problem is also called the “infinite potential well” or the “infinite square well potential” problem. A simple classical analogue of this system could be a ball bouncing elastically between two rigid walls (Fig. 9.3). Inside the box, the particle is “free” because the potential, and hence, the force on the particle is zero. As the particle bounces back and forth, its speed and kinetic energy remain constant. In the classical picture, the particle could have any speed inside the box, and any kinetic energy. Let us now solve the Schrödinger equation for this potential and determine the eigen functions and eigen values of the Hamiltonian operator for this system.

9.3.1 Solving the Schrödinger Equation

For the (free) particle inside the box, $V = 0$. The Schrödinger equation for the stationary state wave function $\psi(x)$ is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x) \text{ for } 0 \leq x \leq L \quad (9.20)$$

Since the walls of the box cannot be penetrated, the particle cannot be found beyond the walls (that is in the regions $x < 0$ and $x > L$). So, the quantum mechanical probability of finding the particle in the region beyond the box, should be zero. Therefore $\psi(x) = 0$ for $x < 0$ and $x > L$. Further, the wave functions for a physical system are always single-valued and continuous. To satisfy this condition, $\psi(x)$ should also be zero at the boundaries of the box, i.e. at $x = 0$ and $x = L$. So, we can write the **boundary conditions** for the wave function $\psi(x)$ as:

$$\psi(x=0) = \psi(x=L) = 0 \quad (9.21)$$

With these boundary conditions, we now solve Eq. (9.20). We put

$k^2 = \frac{2mE}{\hbar^2}$ in Eq. (9.20) and get the following second order ODE:

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \quad (9.22)$$

You have solved this equation in Sec. 9.2 (Eq. 9.8). From SAQ 2 you know that $\psi(x) = \sin kx$ and $\psi(x) = \cos kx$ are both solutions of this equation. So we can write the general solution for Eq. (9.22) as:

$$\psi(x) = A \sin kx + B \cos kx \quad (9.23)$$

To represent the particle in the box, this wave function must satisfy the boundary conditions given in Eq. (9.21). So, we now impose these conditions on the wave function $\psi(x)$ of Eq. (9.23).

$$\psi(x=0) = 0 \Rightarrow A \sin k(0) + B \cos k(0) = 0 \text{ or } B = 0 \quad (9.24)$$

With $B=0$, the expression for the wave function of Eq. (9.23) becomes

$$\psi(x) = A \sin kx \quad (9.25)$$

Applying the boundary condition on the wave function at $x=L$, we get:

$$\psi(x=L) = 0 \Rightarrow A \sin k(L) = 0 \quad (9.26)$$

Clearly, $A \neq 0$, because if it were, the wave function $\psi(x)$ would be zero at all values of x and the probability density ($P(x,t) = |\psi(x)|^2$) for finding the particle at any position x would also be zero. This is an unphysical solution and cannot be considered. In Eq. (9.26), since $A \neq 0$, we must have (read the margin remark):

$$\sin k(L) = 0 \Rightarrow kL = n\pi, \quad n = 0, 1, 2, 3, \dots \quad (9.27)$$

For $n=0$, k would be equal to zero and hence, $\psi(x)$ would be zero at all values of x , once again an unphysical solution. So we discard the value of $n=0$ in Eq. (9.27) and write the possible values of k , which satisfy the boundary conditions as:

$$k = \frac{n\pi}{L}, \text{ with } n = 1, 2, 3, \dots \quad (9.28)$$

Notice from Eq. (9.28) that the **all values of k are not permitted**. k can have only the following discrete or “**quantized**” values:

$$k = \frac{\pi}{L}, \frac{2\pi}{L}, \frac{3\pi}{L}, \dots$$

Therefore, we write k with a subscript n to denote the value of n :

$$k_n = \frac{n\pi}{L}, \text{ with } n = 1, 2, 3, \dots \quad (9.29)$$

We can now write down the possible stationary state solutions for this system (which are the eigen functions) and determine the corresponding energy eigen values.

9.3.2 Eigen functions and Eigen values

On substituting the value of k_n in Eq. (9.25) we can write the stationary state wave function as:

$$\psi_n(x) = A \sin k_n x = A \sin\left(\frac{n\pi x}{L}\right), \quad 0 < x < L \text{ and } n = 1, 2, 3, \dots \quad (9.30)$$

In general, for $\sin x = 0 \Rightarrow x = n\pi$ where $n = 0, \pm 1, \pm 2, \pm 3, \dots$. However the wave function for a negative value of n is not linearly independent of the wave function for the positive value of n . For example for $n=1$:

$$\psi_1(x) = A \sin\left(\frac{\pi x}{L}\right)$$

And for $n=-1$

$$\psi_{-1}(x) = A \sin\left(-\frac{\pi x}{L}\right)$$

So,

$$\psi_{-1}(x) = -\psi_1(x)$$

So we can consider only one of these solutions, either $n=1$ or $n=-1$. And so on for all values of n .

The subscript n once again indicates the value of $k = k_n = \frac{n\pi}{L}$ in the wave

function. As you can see, for each value of n we get a different wave function. Each of these functions $\psi_1(x), \psi_2(x), \dots$ is an eigen function of the Hamiltonian operator for the particle in a box. What are the corresponding eigen energies E_n ?

We determine the energy eigen value E_n from the Schrödinger equation for the eigen function $\psi_n(x)$:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_n(x)}{dx^2} = E_n \psi_n(x) \quad (9.31)$$

Since $\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right)$, we get

$$\frac{d\psi_n(x)}{dx} = A \left(\frac{n\pi}{L}\right) \cos\left(\frac{n\pi x}{L}\right)$$

and

$$\frac{d^2 \psi_n(x)}{dx^2} = -A \left(\frac{n\pi}{L}\right)^2 \sin\left(\frac{n\pi x}{L}\right) = -\left(\frac{n\pi}{L}\right)^2 \psi_n(x)$$

On substituting the second order derivative in Eq. (9.31), we get:

$$-\frac{\hbar^2}{2m} \left[-\left(\frac{n\pi}{L}\right)^2 \psi_n(x) \right] = E_n \psi_n(x) \Rightarrow E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad (9.32)$$

So the **energy eigen values** for the quantum mechanical particle in the box are:

$$E_n = \frac{\hbar^2 k_n^2}{2mL^2} = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad \text{with } n=1,2,3,\dots \quad (9.33)$$

As you can see, the particle can have only certain discrete values of energy. The energy spectrum is no longer continuous.

From Eq. (9.33) we can write for $n=1$:

$$E_1 = \frac{\hbar^2 k_1^2}{2mL^2} = \frac{\pi^2 \hbar^2}{2mL^2} \quad (9.34)$$

And therefore

$$E_n = n^2 E_1 \quad (9.35)$$

It is important to note the following properties of the energy eigen values of a particle in a box:

1. Now that when the particle has been confined to a box, you no longer have a continuous energy spectrum. Its energy can take only the discrete values given by Eq. (9.33) and shown in Fig. 9.4. This is in

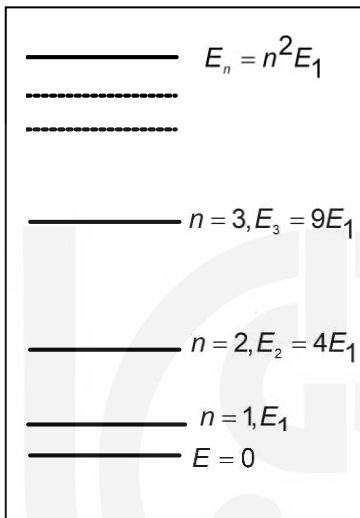


Fig. 9.4: The energy levels for a particle in a one-dimensional box. The ground state energy is E_1 .

In general, if we have a bounded system, or in the terms of classical mechanics, if the motion is confined to a finite region of space, solving the corresponding Schrödinger equation will give us a discrete energy spectrum.

contrast to the classical picture in which all finite values of the energy ($E \geq 0$) are allowed.

2. The quantization of energy follows from the boundary conditions imposed on the wave function due to the confinement of the particle.
3. The minimum energy of the particle in the box is **not zero** but has a finite value: $E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$. So in the quantum mechanical system, **the particle can never be at rest**. This is in keeping with the uncertainty principle and the concept of zero point energy that you have studied in Unit 6. E_1 is the zero point energy for this system.

Notice that the wave function defined by Eq. (9.30) is not normalized. Let us now determine the normalization constant A in the following example.

EXAMPLE 9.2 : NORMALIZING THE WAVE FUNCTION

Determine the normalization constant A for the following eigen function of a particle confined in a box of length L :

$$\psi_n(x) = A \sin k_n x = A \sin\left(\frac{n\pi x}{L}\right), \quad 0 < x < L$$

SOLUTION ■ We use the normalization condition given by Eq. (7.50) with

$\psi_n^*(x) = A^* \sin\left(\frac{n\pi x}{L}\right)$. We can write the normalization condition as:

$$\int_0^L A^* \sin\left(\frac{n\pi x}{L}\right) A \sin\left(\frac{n\pi x}{L}\right) dx = 1 \Rightarrow |A|^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = 1$$

On evaluating the integral we get (see the margin remark):

$$|A|^2 \left(\frac{L}{2}\right) = 1 \Rightarrow A = \sqrt{\frac{2}{L}}$$

$$\begin{aligned} & \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx \\ & \Rightarrow \frac{1}{2} \int_0^L \left[1 - \cos \frac{2n\pi x}{L}\right] dx \\ & = \frac{1}{2} \left[x - \frac{L}{2n\pi} \sin \frac{2n\pi x}{L} \right]_0^L \\ & = \frac{L}{2} \end{aligned}$$

Substituting the value of A from Example 9.2 into Eq. (9.30), we can write the eigen function $\psi_n(x)$ for a particle confined in a line segment of length L as:

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \text{ with } n = 1, 2, 3, \dots \quad (9.36)$$

The corresponding energy eigen values are given by Eq. (9.33). Let us write down the eigen functions and energy eigen values for the first three states of the system ($n = 1, 2$ and 3 respectively):

$$\psi_1(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right); E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \quad (9.37a)$$

$$\psi_2(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right); E_2 = \frac{2\pi^2 \hbar^2}{mL^2} = 4E_1 \quad (9.37b)$$

$$\psi_3(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{3\pi x}{L}\right); E_3 = \frac{9\pi^2 \hbar^2}{2mL^2} = 9E_1 \quad (9.37c)$$

These eigen functions are shown in Fig. 9.5.

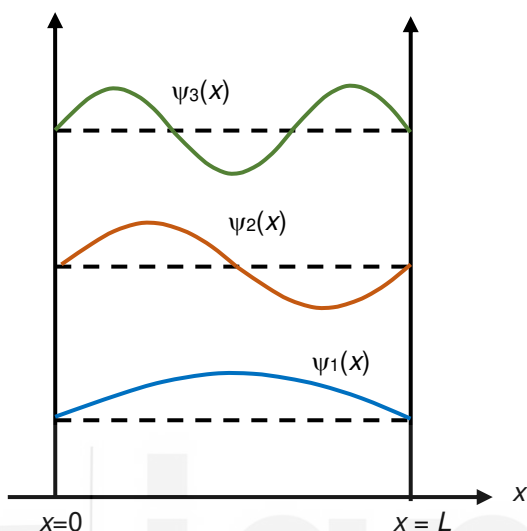


Fig: 9.5 : The first three eigen functions for a particle in a box.

You can see that each of the eigen functions has a node (a point where the wave function goes to zero) at $x=0$ and $x=L$. The number of nodes in the eigen function increases with the value of n . The eigen functions corresponding to different eigen values are orthogonal, as you can check for yourself in the next SAQ.

SAQ 3- Orthogonal eigen functions

Show that the eigen functions for the particle in a box are orthogonal.

So how do we reconcile the quantum mechanical picture with our experiences in the macroscopic world? By working through the following Example you will get an idea of value of the zero point energy of a typical macroscopic object.

EXAMPLE 9.3 : MACROSCOPIC OBJECT AS PARTICLE IN A BOX

A toy car of mass 0.2 kg is moving back and forth on a track 1.0 m long. Treating the car as a particle in a box, what would be the minimum energy of this car? Suppose it moves with a constant speed of 0.1 ms^{-1} , what is the value of n , corresponding to this speed.

SOLUTION ■ Assuming the toy car to be a particle of mass $m = 0.2 \text{ kg}$ confined to a region of length $L = 1.0 \text{ m}$, can say that its energy is (Eq. 9.33):

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2(0.2 \text{ kg}) \times (1.0 \text{ m})^2} = 2.5 n^2 \pi^2 \hbar^2 \text{ J} \quad (\text{i})$$

The minimum energy is the zero point energy:

$$E_1 = 2.5 \pi^2 \hbar^2 = 2.5 \times (\pi)^2 \times (1.054 \times 10^{-34})^2 \text{ J} = 2.7 \times 10^{-67} \text{ J}$$

The kinetic energy of the car is

$$K = \frac{1}{2} m v^2 = \frac{1}{2} \times (0.2 \text{ kg}) \times (0.1 \text{ ms}^{-1})^2 = 1.0 \times 10^{-3} \text{ J} \quad (\text{ii})$$

We calculate the value of n for which the energy of the bound state would be equal to the kinetic energy of the car. So using :

$$K = E_n \Rightarrow 1.0 \times 10^{-3} \text{ J} = n^2 E_1 \text{ and substituting for } E_1 \text{ we get:}$$

$$n^2 = \frac{1.0 \times 10^{-3} \text{ J}}{2.7 \times 10^{-67} \text{ J}} \Rightarrow n \approx 6 \times 10^{31}$$

So the minimum energy of the car is too small to be measured, and we can take it to be zero. Also the energy of the classical particle is characterized by an extremely large quantum number. As you have studied in Sec. (4.6.3), the Correspondence principle tells us that **we need not use the quantum formalism for such large quantum numbers**. We can use Newtonian mechanics. If n is small, on the other hand, we cannot use classical mechanics.

The **integer n** that is used to index the eigen functions $\psi_n(x)$ and the energy eigen values E_n is called the “**energy quantum number**” or the “**principle quantum number**”. As you can see in Fig. 9.4, corresponding to any allowed value of n you have a discrete eigen energy (level) . The state $\psi_1(x)$ is the **ground state eigenfunction** and E_1 , the **ground state energy**. The state $\psi_2(x)$ is the **first excited state** and E_2 , the energy of the first excited state. The state $\psi_3(x)$ is the second excited state and E_3 , the energy of the second excited state. You can think that these energy states are like the energy levels in an atom. Suppose a particle “occupies” the energy state (or energy level) E_1 . On being given an energy ($E_2 - E_1$), it can move into the first excited state E_2 . On the other hand, if the particle occupies the first excited state E_2 , it can emit an energy ($E_2 - E_1$) and move to the ground state E_1 .

Note from Eq. (9.33) that the eigen energy values depend upon the size of the box, L and the mass of the particle m . The energy difference between the corresponding energy levels also depends on L and m . The energy difference between the n^{th} and $(n+1)^{\text{th}}$ energy levels is:

Unlike for the free particle, for the particle in a box, the eigen functions of the Hamiltonian operator are not the simultaneous eigen functions of the momentum operator, which is why we call n the energy quantum number. You will see this for yourself in Terminal Question 8.

$$\Delta E = E_{n+1} - E_n = \frac{\pi^2 \hbar^2}{2mL^2} [(n+1)^2 - n^2] = (2n+1) \frac{\pi^2 \hbar^2}{2mL^2} \quad (9.38)$$

What does eq. (9.38) tell us? Smaller the region in which a particle is confined (L), the larger is the difference in energy (ΔE) between the consecutive energy levels. Conversely, as L increases, the energy separation decreases. 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, as you have seen in Example 9.3.

In fact in the limit when mL^2 becomes much larger than $\hbar^2$ ($mL^2 \gg \hbar^2$), which is typically true for everyday macroscopic objects, the spacing between the energy levels keeps getting smaller. So the energy of a classical particle in a box will vary continuously and quantum effects will not be visible.

Let us now try to model the electron in an atom like a particle in a box.

EXAMPLE 9.4: ELECTRON IN AN ATOMIC BOX

Calculate the energy levels of an electron confined to an atomic box of size $1.0 \text{ \AA}$.

SOLUTION ■ The energy levels for the electron are calculated using Eq. (9.33) with $L = 1.0 \text{ \AA} = 1.0 \times 10^{-10} \text{ m}$. Now,

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2m_e L^2} = \frac{n^2 \hbar^2}{8m_e L^2}, \quad n = 1, 2, 3, \dots$$

For $n=1$:

$$\begin{aligned} E_1 &= \frac{(1)^2 \hbar^2}{8m_e L^2} = \frac{\hbar^2}{8m_e L^2} = \frac{(6.626 \times 10^{-34} \text{ Js})^2}{8(9.109 \times 10^{-31} \text{ kg}) \times (1.0 \times 10^{-10} \text{ m})^2} \\ &= 0.602 \times 10^{-17} \text{ J} \approx 38 \text{ eV} \end{aligned}$$

So the remaining energy levels are:

$$E_n = n^2 E_1 = 38n^2 \text{ eV}$$

9.3.3 Time Dependent Wave Function

The complete time dependent wave function $\psi_n(x, t)$ corresponding to $\psi_n(x)$ is

$$\psi_n(x, t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-iE_n t/\hbar} \quad (9.39)$$

Using Euler's Formula, we can write:

$$\sin(k_n x) = \frac{1}{2i} (e^{ik_n x} + e^{-ik_n x}) \quad (9.40)$$

where $k_n = \frac{n\pi}{L}$, and $E_n = \hbar\omega_n$. Then we get:

$$\psi_n(x, t) = \frac{1}{2i} \sqrt{\frac{2}{L}} (e^{i(k_n x - \omega_n t)} + e^{-i(k_n x + \omega_n t)}) \quad (9.41)$$

This is the superposition of two travelling waves having the same frequency and amplitude. The first term in Eq. (9.40) represents the wave travelling along the positive x -direction. The second term is for the wave travelling in the negative x -direction, which is the second term. This is similar to the standing wave solutions of a vibrating string fixed at both ends.

We next determine the probability density corresponding to these eigen functions.

9.3.4 Probability Density

The probability density for a stationary state is time independent and we can write for the n^{th} eigen state:

$$P_n(x, t) = P_n(x) = |\psi_n(x)|^2 = \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right) \quad (9.42)$$

From Eq. (9.42), you can see that $P_n(x)$ depends on the position of the particle in the box. In Fig. 9.6 below, we have plotted the values of $P_n(x)$ corresponding to first three eigen functions of the system (for $n=1, 2, 3$).

The probability of finding the particle is maximum around the maxima (humps) of the probability distribution and is zero at the nodes. So the probability of finding the particle in any finite region of the box also changes with the eigen function.

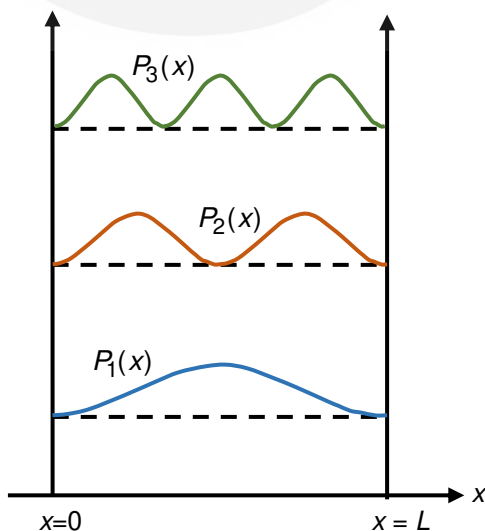


Fig: 9.6: The probability density $(|\psi_n(x)|^2)$ as a function of position for the first three eigen functions of a particle in a box.

To understand, let us work through the following example.

EXAMPLE 9.5: CALCULATING THE PROBABILITY

Calculate the probability of finding the particle between

- (i) $x = L/4$ and $x = 3L/4$, and
- (ii) $x = 0$ and $x = L/4$

when the particle is in the ground state.

SOLUTION ■ We use Eq. (7.15) to calculate the probability of finding the particle between two points x_1 and x_2 .

- (i) With $\psi(x) = \psi^*(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$ for the ground state, $x_1 = L/4$ and $x_2 = 3L/4$ in Eq.(7.15) we calculate the probability as:

$$\begin{aligned} P &= \int_{L/4}^{3L/4} \left(\sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \right)^2 dx = \left(\frac{1}{L} \right) \int_{L/4}^{3L/4} \left(1 - \cos \frac{2\pi x}{L} \right) dx \\ &= \frac{1}{L} \left[x - \frac{L}{2\pi} \sin \frac{2\pi x}{L} \right]_{L/4}^{3L/4} \\ &= \frac{1}{L} \left[\left(\frac{3L}{4} - \frac{L}{4} \right) - \frac{L}{2\pi} \sin \frac{2\pi}{L} \left(\frac{3L}{4} \right) + \frac{L}{2\pi} \sin \frac{2\pi}{L} \left(\frac{L}{4} \right) \right] \\ &= \frac{1}{L} \left[\frac{L}{2} - \frac{L}{2\pi} \sin \frac{3\pi}{2} + \frac{L}{2\pi} \sin \frac{\pi}{2} \right] = \frac{L}{L} \left[\frac{1}{2} + \frac{2}{2\pi} \right] = \left[\frac{1}{2} + \frac{1}{\pi} \right] \end{aligned}$$

- (ii) For $\psi(x) = \psi^*(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$, $x_1 = 0$ and $x_2 = L/4$ the probability is:

$$\begin{aligned} P &= \int_0^{L/4} \left(\sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \right)^2 dx = \frac{1}{L} \left[x - \frac{L}{2\pi} \sin \frac{2\pi x}{L} \right]_0^{L/4} \\ &= \frac{1}{L} \left[\frac{L}{4} - \frac{L}{2\pi} \sin \frac{2\pi}{L} \left(\frac{L}{4} \right) \right] = \frac{1}{L} \left[\frac{L}{4} - \frac{L}{2\pi} \right] = \left[\frac{1}{4} - \frac{1}{2\pi} \right] \end{aligned}$$

You may now like to work out an SAQ on calculating the probability.

SAQ 4 Calculating Probability

Calculate the probability of finding the particle between $x = L/4$ and $x = 3L/4$, when the particle is in the first excited state.

Let us compare this with the classical picture. Classically, the particle bounces back and forth between the walls. Since the kinetic energy of the particle is constant, it moves at a constant speed between collisions with the walls. Therefore, it spends the same amount of time in all intervals which have an equal length. So the normalized probability per unit distance, of the particle being found anywhere in the box is just $1/L$ which is independent of the position of the particle. This is clearly not the case for the quantum mechanical particle. However, when n is very large the wave function begins to have so many nodes and humps that in the limit as $n \rightarrow \infty$ each position of the particle is equally probable. Then the quantum mechanical probability distribution begins to look like the classical distribution.

For a large value of n , you would observe only the average value of the probability density which is

$$\langle P_n(x,t) \rangle = \frac{2}{L} \left\langle \sin^2 \left(\frac{n\pi x}{L} \right) \right\rangle = \frac{2}{L} \left(\frac{1}{2} \right) = \frac{1}{L} \quad (9.43)$$

(This is because the average of the square of the sine function over one or more cycles is always half.)

Let us now summarize what you have studied about the particle in a box.

PARTICLE IN A ONE-DIMENSIONAL BOX

Recap

- A particle is confined within a length segment lying between $x = 0$ and $x = L$ by the following potential function(infinite potential well):

$$V(x) = \begin{cases} 0 & \text{for } 0 \leq x \leq L \\ \infty & \text{for } x < 0 \text{ and } x > L \end{cases} \quad (9.19)$$

- The time independent Schrödinger equation for the particle is:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} = E \psi(x) \text{ for } 0 \leq x \leq L \quad (9.20)$$

- The boundary conditions to be satisfied by the wave function are:

$$\psi(x=0) = \psi(x=L) = 0 \quad (9.21)$$

- The normalized eigen functions of the Hamiltonian are

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad 0 < x < L \text{ for } n = 1, 2, 3, \dots \quad (9.30)$$

- The corresponding energy eigen values are:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \text{ with } n = 1, 2, 3, \dots \quad (9.33)$$

- n is called the energy quantum number.

*Recap***PARTICLE IN A ONE-DIMENSIONAL BOX (Contd.)**

- The energy of a particle bound inside an infinite potential well can have only discrete values.
- The minimum energy of the particle is not zero, it is $E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$.
- The complete time dependent wave function $\psi_n(x, t)$ corresponding to $\psi_n(x)$ is

$$\psi_n(x, t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-iE_n t/\hbar} \quad (9.36)$$

- The eigen functions of the system are orthogonal.

Our understanding of the way charge carriers behave in materials is also an application of quantum mechanics. Solving the Schrödinger equation using the exact potentials experienced by the charge carriers is very complicated. However, it is often possible to understand the observed phenomena using simple models of the potential which are easier to solve.

Some of you may have read(or you can read now) popular science articles about “nano” sized materials like quantum wells, quantum wires and quantum dots and how they have exciting applications, mainly because they exhibit **quantum effects**. In the next section we study about quantum dots. We can understand the special properties of a quantum dot by modelling a charge carrier inside the quantum dot as a particle in a box.

9.4 Quantum Dot

Quantum dots (sometimes called artificial atoms) are typically semiconductor (or metal) particles with sizes ranging from 1 to 100 nm. Their properties are very different from the bulk properties of the materials of which they are made and depend on the **size** of the particle.

You have all studied about conductors, insulators and semiconductors in your school physics courses. As you have studied in Bohr’s atomic model, in an isolated atom, the electrons occupy discrete energy levels. Whereas in bulk materials made up of several atoms, we have continuous energy bands which are collections of available energy states and energy gaps between these bands.

The quantum dot is a very tiny object. Therefore, the charge carriers inside the dot are confined within a very small region, very much like a particle in a rigid box. The simplest approximation for a quantum dot is an infinite potential

well where all the charge carriers are confined. So like a particle in a box (or an electron in an atom) , the charge carriers in the quantum occupy discrete energy levels.

While in a bulk semiconductor material you would have energy bands, in a quantum dot made out of the same material, the energy bands are replaced by discrete energy levels, as shown in Fig 9.7.

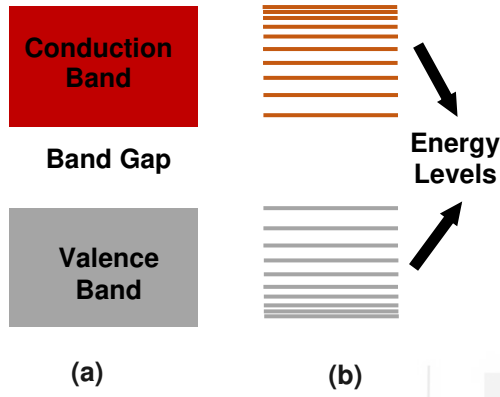


Fig. 9.7: Energy levels of (a) a bulk semiconductor and (b) a quantum dot of the same semiconductor.

Absorption and emission of light by these quantum dots (as in any atom or molecule) takes place by the transition of charge carriers between these energy levels.

Suppose an electron occupying the energy state j in a quantum dot of size D make a transition to state i . Let us assume that the quantum dot is a one-dimensional rigid box of size D (read the margin remark). Using Eq. (9.33) for the energy of the electron, we can write the expression for the energy emitted in this transition as:

$$\Delta E_{ji} = E_j - E_i = \frac{j^2 \hbar^2 \pi^2}{2m_e^* D^2} - \frac{i^2 \hbar^2 \pi^2}{2m_e^* D^2} = (j^2 - i^2) \frac{\hbar^2 \pi^2}{2m_e^* D^2} \quad (9.44)$$

Ideally you should think of an electron in a quantum dot as an electron confined in a three dimensional box. To understand the physical properties, here we assume it to be a one-dimensional box.

This energy difference depends on the size of the dot D . If D increases, other parameters remaining the same, the value of ΔE_{ji} decreases. This is depicted in Fig. 9.8 below.

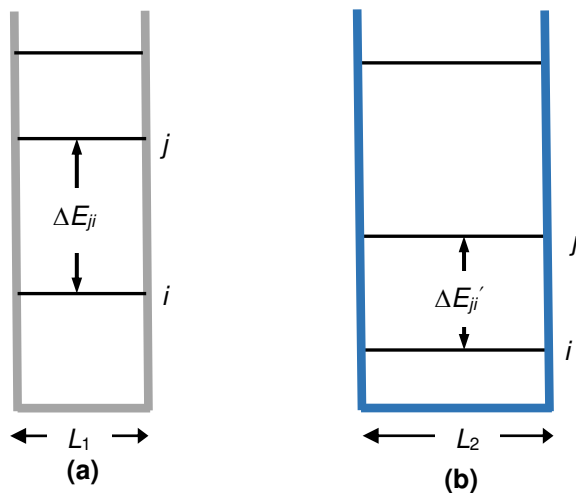


Fig. 9.8: Energy level variation with size. For a box of size (a) L_1 and (b) L_2 with $L_1 < L_2$, the difference between the energy levels $\Delta E_{ji} > \Delta E_{ji}'$.

Notice that for the electron in the semiconductor quantum dot we are writing the mass of the electron as m_e^* and not m_e . This is because in a semiconductor, the electron has an effective mass m_e^* (which is much less than the free electron mass m_e) which decides to a large extent how the electron behaves inside a semiconductor! It is because of this that the de Broglie wavelength in a semiconductor is typically of the order of nanometers, and not angstroms as for a conduction electron in a metal.

This energy difference is emitted from the dot as a photon of light. What is the wavelength of this photon? If the frequency of the emitted photon is ν and λ its wavelength ($\nu = c/\lambda$), then:

$$\Delta E_{ji} = h\nu = \frac{hc}{\lambda} = (j^2 - i^2) \frac{\hbar^2 \pi^2}{2m_e^* D^2} \quad (9.45)$$

So the wavelength of the emitted photon is directly proportional to the size of the dot D . As the size of the dot increases, the wavelength of the emitted photon also increases. As D increases, even though the material of the dot may remain the same, the wavelength of the emitted lights changes from the blue towards the red end of the visible spectrum! So by tuning the size of the quantum dot in the process of preparation, you can obtain a specific wavelength of the emitted light.

A real quantum dot is definitely more complicated than what we have described here. However as you can see it is possible to understand certain salient features of light emission from QDs using the particle in a box model. A more realistic estimate of the numbers is obtained by considering the confinement of an “electron-hole” pair also called an “exciton” inside a spherical quantum dot.

Several other applications of the quantum dot are also related to the fact that its energy levels can be tuned by its size. Quantum dots are used in single-electron transistors, solar cells, LEDs, lasers, single-photon sources, cell biology research, microscopy, and medical imaging.

Recap

QUANTUM DOT

- Quantum dots (sometimes called artificial atoms) are typically semiconductor (or metal) particles with sizes ranging from 1 to 100 nm with properties that are vastly different from the bulk material of which they are made and depend on the **size** of the particle.
- The simplest approximation for a quantum dot is an infinite potential well where all the charge carriers are confined to a region and occupy discrete energy levels, like electrons in a atom.
- A change in the size of the dot changes the spacing between the energy levels. This changes the energy released in the transition of the electron between the energy levels. So the wavelength of the light emitted by the quantum dot changes with the size of the dot.

Now we will summarize the concepts you have studied in this Unit.

9.5 SUMMARY

Concept	Description
Free Particle	■ The time independent Schrödinger equation for a quantum mechanical free particle of mass m is: $-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x)$ The general solution of Eq. (9.4) is: $\psi(x) = Ae^{ikx} + Be^{-ikx} \quad ; \text{ with } k^2 = \frac{2mE}{\hbar^2}$ The quantum number k is real and the free particle can have any non-negative value of energy: $E = \frac{\hbar^2 k^2}{2m} \geq 0$ The energy of the particle does not change with time. The time dependent wave function for the free particle with an energy $E = \hbar\omega$ is: $\psi(x,t) = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)}$
Particle in a one-dimensional box	■ A particle is confined within a length segment lying between $x = 0$ and $x = L$ by the following potential function(infinite potential well): $V(x) = \begin{cases} 0 & \text{for } 0 \leq x \leq L \\ \infty & \text{for } x < 0 \text{ and } x > L \end{cases}$ The time independent Schrödinger equation for the particle is: $-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x) \text{ for } 0 \leq x \leq L$ The boundary conditions to be satisfied by the wave function are: $\psi(x=0) = \psi(x=L) = 0$ The normalized eigen functions of the Hamiltonian are $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right), \quad 0 < x < L \text{ for } n = 1, 2, 3, \dots$ The corresponding energy eigen values are: $E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad \text{with } n = 1, 2, 3, \dots$ n is called the energy quantum number. The energy of a particle bound inside an infinite potential well can have only discrete values.

The minimum energy of the particle is not zero, it is $E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$.

The complete time dependent wave function $\psi_n(x, t)$ corresponding to $\psi_n(x)$ is

$$\psi_n(x, t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-iE_n t/\hbar}$$

The eigen functions of the system are orthogonal.

Quantum dot

- Quantum dots (sometimes called artificial atoms) are typically semiconductor (or metal) particles with sizes ranging from 1 to 100 nm with properties that are vastly different from the bulk material of which they are made and depend on the **size** of the particle.

The simplest approximation for a quantum dot is an infinite potential well where all the charge carriers are confined to a region and occupy discrete energy levels, like electrons in an atom.

A change in the size of the dot changes the spacing between the energy levels. This changes the energy released in the transition of the electron between the energy levels. So the wavelength of the light emitted by the quantum dot changes with the size of the dot.

9. 6 TERMINAL QUESTIONS

- A free quantum mechanical particle has a wave function given by $\psi(x, t) = Ae^{i(k_0 x - \omega_0 t)}$, $k_0 = 4.0 \times 10^{11} \text{ m}^{-1}$ and $\omega_0 = 5.0 \times 10^{15} \text{ s}^{-1}$. Determine its momentum and energy.
- Determine the eigen value of the operator $\hat{H} = i\hbar \frac{\partial}{\partial t}$ for the free particle wave function $\psi(x, t) = Ae^{i(kx - \omega t)}$.
- Let us model the proton in an atomic nucleus as a particle in a box. Suppose the proton is confined to a box of size $2.0 \times 10^{-14} \text{ m}$ (size of a nucleus). Calculate the frequency of the emitted photon if the proton makes a transition from the first excited state to the ground state.
- Suppose an electron confined to a box emits photons. The longest wavelength that is registered is 400.0 nm. What is the width of the box?
- The wave function of a particle of mass m inside an infinite square well of width $2a$ ($-a \leq x \leq a$) is given by:

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

Obtain the values of A and B and the eigen energy corresponding to the above eigen function.

6. A particle in a one-dimension box has an energy of 10 eV in its first excited state. Calculate its ground state energy and the energy in the second excited state.
7. Calculate the expectation value of $\langle p^2 \rangle$ for the wave function $\psi(x, t) = Ae^{i(kx - \omega t)}$.
8. Show that the eigen functions $\psi_n(x)$ are not the eigen functions of the momentum operator.
9. For the stationary state $\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$ show that

i) $\langle \hat{p}_x \rangle = 0$

ii) $\langle \hat{p}_x^2 \rangle = \frac{n^2 \pi^2 \hbar^2}{L^2}$

9.7 SOLUTIONS AND ANSWERS

Self-Assessment Questions

1. We use Eq. (9.4) with $\psi = Ae^{ikx} + Be^{-ikx}$. We first evaluate $\frac{d^2\psi}{dx^2}$:

$$\frac{d\psi}{dx} = \frac{d}{dx}(Ae^{ikx} + Be^{-ikx}) = ik(Ae^{ikx} - Be^{-ikx})$$

$$\frac{d^2\psi}{dx^2} = \frac{d}{dx}[ik(Ae^{ikx} - Be^{-ikx})] = (ik)^2(Ae^{ikx} + Be^{-ikx}) = -k^2\psi(x)$$

Substituting $\frac{d^2\psi}{dx^2} = -k^2\psi(x)$ in Eq.(9.4) we get,

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

2. (i) To show that $\psi(x) = \sin kx$ is solution of Eq. (9.4), we have to show:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2}(\sin kx) = E \sin kx \quad \text{with} \quad E = \frac{\hbar^2 k^2}{2m} \quad (i)$$

We have

$$\frac{d^2}{dx^2}(\sin kx) = \frac{d}{dx}\left(\frac{d}{dx}\sin kx\right) = k \frac{d}{dx}(\cos kx) = -k^2 \sin kx \quad (ii)$$

Substituting for $\frac{d^2}{dx^2}(\sin kx)$ from Eq. (ii) into the LHS of Eq. (i) we see that:

$$-\frac{\hbar^2}{2m}(-k^2 \sin kx) = \left(\frac{\hbar^2 k^2}{2m}\right) \sin kx \Rightarrow E = \frac{\hbar^2 k^2}{2m}$$

So Eq. (i) is true for $\psi(x) = \sin kx$.

ii) To show $\psi(x) = \cos kx$ is a solution of Eq. (9.4), we have to

$$\text{show: } -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} (\cos kx) = E \cos kx \text{ where } E = \frac{\hbar^2 k^2}{2m} \quad (\text{iii})$$

Since $\frac{d^2}{dx^2} (\cos kx) = -k^2 \cos kx$, we get:

$$-\frac{\hbar^2}{2m} \cdot (-k^2 \cos kx) = \left(\frac{\hbar^2 k^2}{2m}\right) \cos kx \Rightarrow E = \frac{\hbar^2 k^2}{2m}$$

So Eq. (iii) is true for $\psi(x) = \cos kx$.

3. For any two eigen functions $\psi_n(x)$ and $\psi_m(x)$ to be orthogonal we must show that

$$\int_0^L \psi_n(x) \psi_m(x) dx = 0 \quad \text{when } m \neq n$$

$$\begin{aligned} 2 \sin A \sin B \\ = \cos(A-B) - \cos(A+B) \end{aligned}$$

Substituting for $\psi_n(x)$ and $\psi_m(x)$ in this integral we get:

$$\begin{aligned} \int_0^L \left[\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \right] \left[\sqrt{\frac{2}{L}} \sin\left(\frac{m\pi x}{L}\right) \right] dx &= \frac{2}{L} \int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx \\ &= \frac{1}{L} \int_0^L \left[\cos\left(\frac{(n-m)\pi x}{L}\right) - \cos\left(\frac{(n+m)\pi x}{L}\right) \right] dx \quad (\text{see the margin remark}) \\ &= \frac{1}{L} \left[\frac{L}{(n-m)\pi} \sin\left(\frac{(n-m)\pi x}{L}\right) - \frac{L}{(n+m)\pi} \sin\left(\frac{(n+m)\pi x}{L}\right) \right]_0^L \\ &= 0 \quad (\text{because } m \text{ and } n \text{ are integers } \sin(n-m)\pi = \sin(n+m)\pi = 0) \end{aligned}$$

4. To calculate the probability for the first excited state we use Eq. (7.15) with

$\psi(x) = \psi^*(x) = \sqrt{\frac{2}{L}} \sin \frac{2\pi x}{L}$, $x_1 = L/4$ and $x_2 = 3L/4$. So the probability is:

$$\begin{aligned} \therefore P &= \int_{L/4}^{3L/4} \left(\sqrt{\frac{2}{L}} \sin \frac{2\pi x}{L} \right)^2 dx = \frac{1}{L} \int_{L/4}^{3L/4} \left[1 - \cos \frac{4\pi x}{L} \right] dx \\ &= \frac{1}{L} \left[\left(\frac{3L}{4} - \frac{L}{4} \right) - \frac{L}{4\pi} \sin \frac{4\pi}{L} \left(\frac{3L}{4} \right) + \frac{L}{4\pi} \sin \frac{4\pi}{L} \left(\frac{L}{4} \right) \right] \\ &= \frac{1}{L} \left[\frac{L}{2} - \frac{L}{4\pi} \sin 3\pi + \frac{L}{4\pi} \sin \pi \right] = \frac{1}{2} \end{aligned}$$

Terminal Questions

1. Using Eq. (5.3) we can write

$$p = \hbar k = (1.054 \times 10^{-34} \text{ Js}) \times (4.0 \times 10^{11} \text{ m}^{-1}) = 4.2 \times 10^{-23} \text{ kg ms}^{-1}$$

$$E = \hbar \omega = (1.054 \times 10^{-34} \text{ Js}) \times (5.0 \times 10^{-5} \text{ s}^{-1}) = 5.3 \times 10^{-19} \text{ J}$$

2. The eigenvalue of $\hat{H} = i\hbar \frac{\partial}{\partial t}$ is determined using Eq. (8.35). With $\hat{D} = \hat{H}$ we can write:

$$\hat{H}\psi = E\psi \quad (\text{i})$$

Calculating the derivative, we get:

$$i\hbar \frac{\partial}{\partial t} [Ae^{i(kx - \omega t)}] = (i\hbar)(-i\omega)Ae^{i(kx - \omega t)} = \hbar \omega \psi \quad (\text{ii})$$

Substituting for $\hat{H}\psi$ in Eq. (i) we get

$$\hbar \omega \psi = E\psi \quad (\text{iii})$$

So the eigenvalue of $\hat{H}$ is $\hbar \omega$.

3. The ground state of the proton in the nucleus is calculated with $n = 1$, mass of the proton is $m_p = 1.673 \times 10^{-27} \text{ kg}$ and $L = 2.0 \times 10^{-14} \text{ m}$:

$$E_1 = \frac{h^2}{8m_p L^2} = \frac{(6.626 \times 10^{-34} \text{ Js})^2}{8 \times (1.673 \times 10^{-27} \text{ kg}) \times (2.0 \times 10^{-14} \text{ m})^2} \\ = 0.82 \times 10^{-13} \text{ J} = 0.51 \text{ MeV}$$

The first excited state: $E_2 = n^2 E_1 = (4) \times 0.51 \text{ MeV} = 2.1 \text{ MeV}$

When there is a transition from $E_2 \rightarrow E_1$, the emitted photon has an energy: $E_{ph} = E_2 - E_1 = (2.1 - 0.51) \text{ MeV} = 1.6 \text{ MeV}$

The frequency of the photon is,

$$\nu = \frac{E_{ph}}{h} = \frac{(1.6 \times 1.6 \times 10^{-13} \text{ J})}{(6.626 \times 10^{-34} \text{ Js})} = 0.39 \times 10^{21} \text{ Hz}$$

4. The longest wavelength will correspond to the minimum energy difference, because $\Delta E = h\nu = \frac{hc}{\lambda}$. The energy difference, ΔE , defined in Eq. (9.38) will be minimum for the lowest value of n which is $n=1$. Substituting $n=1$ in Eq. (9.38) we can write:

$$\Delta E_{\min} = \frac{3\pi^2 \hbar^2}{2m_e L^2} = \frac{3h^2}{8m_e L^2} \quad (\text{i})$$

Using $\Delta E = \frac{hc}{\lambda}$ in Eq. (i) we get

$$\frac{hc}{\lambda} = \frac{3h^2}{8m_e L^2} \quad \text{or} \quad L^2 = \left(\frac{3h\lambda}{8m_e c} \right) \quad (\text{ii})$$

So the size of the box, L , with $\lambda = 400 \text{ nm} = 4.0 \times 10^{-7} \text{ m}$ is:

$$L = \left[\frac{3 \times (6.626 \times 10^{-34} \text{ Js}) \times (4.0 \times 10^{-7} \text{ m})}{8 \times (9.109 \times 10^{-31} \text{ kg}) \times (3.0 \times 10^8 \text{ m s}^{-1})} \right]^{1/2}$$

$$= 0.60 \times 10^{-9} \text{ m} = 0.60 \text{ nm}.$$

5. We have the following boundary conditions to be satisfied at the boundaries of the potential well: $\psi(x=a) = \psi(x=-a) = 0$. Using $\psi(x=a) = 0$ we get:

$$\psi(a) = A \cos\left(\frac{3\pi a}{2a}\right) + B \sin\left(\frac{3\pi a}{2a}\right) = 0 \Rightarrow A \cos\left(\frac{3\pi}{2}\right) + B \sin\left(\frac{3\pi}{2}\right) \Rightarrow B = 0$$

So the wave function is:

$$\psi(x) = A \cos\left(\frac{3\pi x}{2a}\right)$$

Using the normalization condition of Eq. (7.50) we can get:

$$\int_{-a}^a A^* \cos\left(\frac{3\pi x}{2a}\right) A \cos\left(\frac{3\pi x}{2a}\right) dx = 1 \Rightarrow |A|^2 \int_{-a}^a \cos^2\left(\frac{3\pi x}{2a}\right) dx = 1$$

On evaluating the integral we get (see the margin remark):

$$|A|^2(a) = 1 \Rightarrow A = \sqrt{\frac{1}{a}}$$

Since $V(x)$ is zero inside the well, the Schrödinger equation is:

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

With $\psi(x) = A \cos\left(\frac{3\pi x}{2a}\right)$ we get:

$$\begin{aligned} -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \left[A \cos\left(\frac{3\pi x}{2a}\right) \right] &= -\frac{\hbar^2}{2m} \frac{d}{dx} \left[-A \left(\frac{3\pi}{2a}\right) \sin\left(\frac{3\pi x}{2a}\right) \right] \\ &= -\frac{\hbar^2}{2m} \left[-A \left(\frac{3\pi}{2a}\right)^2 \cos\left(\frac{3\pi x}{2a}\right) \right] = \frac{\hbar^2}{2m} \left(\frac{3\pi}{2a}\right)^2 \left[A \cos\left(\frac{3\pi x}{2a}\right) \right] \\ &= \frac{9\pi^2 \hbar^2}{8ma^2} \psi(x) \end{aligned}$$

On comparing with Eq. (i) we get the energy eigen value as:

$$E = \frac{9\pi^2 \hbar^2}{8ma^2}$$

$$\begin{aligned} &\int_{-a}^a \cos^2\left(\frac{3\pi x}{2a}\right) dx \\ &\Rightarrow \frac{1}{2} \int_{-a}^a \left[1 + \cos\left(\frac{3\pi x}{a}\right) \right] dx \\ &= \frac{1}{2} \left[x + \frac{a}{3\pi} \sin\left(\frac{3\pi x}{a}\right) \right]_{-a}^a \\ &= a \end{aligned}$$

6. From Eq. (9.35) we know that $E_n = n^2 E_1$. $n = 2$ corresponds to the first excited state and E_1 is the ground state. So,

$$E_2 = 10 \text{ eV} = (2^2) E_1 \Rightarrow E_1 = 2.5 \text{ eV}$$

∴ The second excited state is E_3 , with $n = 3$ in Eq. (9.35). So:

$$E_3 = (3)^2 E_1 = 9 \times 2.5 \text{ eV} = 22.5 \text{ eV}$$

7. Using Eq.(8.26), we can write for an unnormalized wave function $\psi(x)$:

$$\langle \hat{p}_x^2 \rangle = \frac{\int_{-\infty}^{\infty} \psi^* (\hat{p}_x^2 \psi) dx}{\int_{-\infty}^{\infty} \psi^* \psi dx} \quad (i)$$

$$\hat{p}_x = -i\hbar \frac{d}{dx} \Rightarrow \hat{p}_x^2 \psi = -\hbar^2 \frac{d^2 \psi}{dx^2} \quad (ii)$$

$$\text{And : } \frac{d^2 \psi}{dx^2} = \frac{d}{dx} \left[\frac{d}{dx} A e^{i(kx+\omega t)} \right] = \frac{d}{dx} [ik A e^{i(kx+\omega t)}] = -k^2 A e^{i(kx+\omega t)}$$

$$\begin{aligned} \therefore \langle p_x^2 \rangle &= \frac{\int_{-\infty}^{\infty} (A e^{i(kx+\omega t)})^* [-\hbar^2 (-k^2) (A e^{i(kx+\omega t)})] dx}{\int_{-\infty}^{\infty} (A e^{i(kx+\omega t)})^* (A e^{i(kx+\omega t)}) dx} \\ &= \hbar^2 k^2 \frac{\int_{-\infty}^{\infty} A^* e^{-i(kx+\omega t)} A e^{i(kx+\omega t)} dx}{\int_{-\infty}^{\infty} A^* e^{-i(kx+\omega t)} A e^{i(kx+\omega t)} dx} = \hbar^2 k^2 \end{aligned}$$

8. For $\psi_n(x)$ to be an eigen function of $\hat{p}_x$, we have to show (Eq. 8.35) :

$$\hat{p}_x \psi_n(x) = \phi \psi_n(x) \quad (i)$$

Using $\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$ in Eq. (i), we get :

$$\begin{aligned} \hat{p}_x \psi_n(x) &= -i\hbar \frac{d}{dx} \psi_n(x) = -i\hbar \frac{d}{dx} \left(\sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \right) \\ &= -i\hbar \sqrt{\frac{2}{L}} \left(\frac{n\pi}{L} \cos \frac{n\pi x}{L} \right) = -i\hbar n\pi \sqrt{\frac{2}{L^3}} \cos \frac{n\pi x}{L} \quad (ii) \end{aligned}$$

Since we cannot write $\hat{p}_x \psi_n(x)$ as $\phi \psi_n(x)$, $\psi_n(x)$ is not an eigen function of the momentum operator.

9. Since $\psi_n(x)$ is the normalized wave function we use Eq. (8.26) and

$$\psi_n^*(x) = \psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \text{ to calculate the expectation values.}$$

$$(i) \langle p_x \rangle = \int_0^L \left(\sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \right) \hat{p}_x \left(\sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \right) dx$$

As calculated in Eq. (ii) of Terminal Question 7,

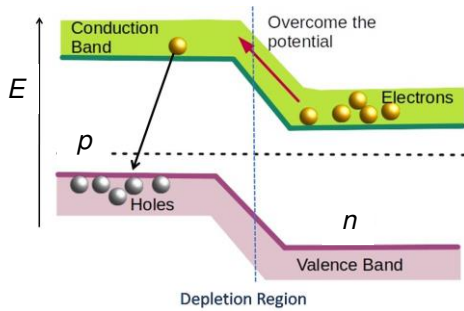
$$\begin{aligned} \hat{p}_x \psi_n(x) &= -i\hbar n\pi \sqrt{\frac{2}{L^3}} \cos \frac{n\pi x}{L} \\ \therefore \langle p_x \rangle &= -\frac{2i\hbar n\pi}{L^2} \int_0^L \sin \frac{n\pi x}{L} \cos \frac{n\pi x}{L} dx = -\frac{i\hbar n\pi}{L^2} \int_0^L \sin \frac{2n\pi x}{L} dx \\ &= \frac{i\hbar n\pi}{L^2} \left(\frac{L}{2n\pi} \right) \left[\cos \frac{2n\pi x}{L} \right]_0^L = \frac{i\hbar}{2L} [\cos 2n\pi - \cos 0] = 0 \\ \therefore \langle p_x \rangle &= 0 \end{aligned}$$

$$\begin{aligned} &\int_0^L \sin^2 \left(\frac{n\pi x}{L} \right) dx \\ &\Rightarrow \frac{1}{2} \int_0^L \left[1 - \cos \frac{2n\pi x}{L} \right] dx \\ &= \frac{1}{2} \left[x + \frac{L}{2n\pi} \sin \frac{n\pi x}{L} \right]_0^L \\ &= \frac{L}{2} \end{aligned}$$

$$\begin{aligned} (ii) \langle p_x^2 \rangle &= \int_0^L \psi_n^*(x) \hat{p}_x^2 \psi_n(x) dx \\ \hat{p}_x^2 \psi_n(x) &= \hat{p}_x [\hat{p}_x \psi_n(x)] = \hat{p}_x \left[-i\hbar \sqrt{\frac{2}{L}} \cdot \frac{n\pi}{L} \cos \frac{n\pi x}{L} \right] \\ &\quad \text{(using the results of Terminal Question 7)} \\ &= -\frac{i\hbar n\pi}{L} \sqrt{\frac{2}{L}} \left[-i\hbar \frac{d}{dx} \cos \frac{n\pi x}{L} \right] = -(i\hbar)^2 \left(\frac{n\pi}{L} \right)^2 \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} \\ \text{So } \langle p_x^2 \rangle &= \hbar^2 \left(\frac{n\pi}{L} \right)^2 \left(\frac{2}{L} \right) \int_0^L \sin^2 \left(\frac{n\pi x}{L} \right) dx \text{ (see the margin remark)} \\ &= \frac{2\hbar^2 n^2 \pi^2}{L^3} \left(\frac{L}{2} \right) = \frac{\hbar^2 n^2 \pi^2}{L^2} \end{aligned}$$

UNIT 10

STEP POTENTIAL



For a p - n junction in forward bias, the electrons in the n -type region in the conduction band diffuse across the potential barrier and find themselves at a higher energy than the holes in the p -type material. Combination of holes and electrons may occur which creates a continuous flow of current through the junction.

Structure

- | | | | |
|------|---|------|--|
| 10.1 | Introduction | 10.4 | Energy (E) of the Particle is greater than V_0 |
| | Expected Learning Outcomes | | Reflection and Transmission Coefficients |
| 10.2 | Step Potential and Schrödinger Equation | 10.5 | Summary |
| 10.3 | Energy (E) of the particle is less than V_0 | 10.6 | Terminal Questions |
| | Reflection and Transmission Coefficients | 10.7 | Solutions and Answers |

STUDY GUIDE

In the previous unit you have learnt how to solve the time independent Schrödinger equation for a particle in a box and obtained the energy eigenvalues for the problem. You have seen that the energy levels of the particle in the box are discrete. This is contrary to the results of classical physics where the energy of a system is continuous. In this unit, you will study the time independent Schrödinger equation for a step potential and learn how to solve it. The method of solving it is similar to what you have studied in Unit 9. Therefore, we advise you to revise Unit 9 before studying this unit. The mathematics in this unit is similar and we have used a great deal of algebra with which you are familiar since school. Work out all steps yourself and practice the SAQs and Terminal Questions to get a good grip of this unit.

“What quantum physics teaches us is that everything we thought was physical is not physical.”

Bruce H. Lipton

10.1 INTRODUCTION

In the previous units, you have studied the time independent Schrödinger equation of a free particle and a particle in a box. You have learnt how to solve it to obtain the eigenfunctions and energy eigenvalues for these systems. You have also learnt that a free particle has a continuous energy spectrum but a particle in a box has discrete energy levels.

In this unit, you will learn how to solve the time independent Schrödinger equation for a step potential. You will obtain the eigenfunctions and energy levels for such a potential. You are familiar with steps all around you. So, you can think of a step as a flat surface, which changes abruptly after a certain distance so that another flat surface is obtained at a higher level.

Similarly, the step potential changes abruptly, much like a single physical step. So, a step potential has an abrupt increase or decrease in its value. In Sec. 10.2, we first define the step potential and write down the time independent Schrödinger equation for a particle subjected to a step potential.

Then we take up two interesting cases: When the energy of the particle is less than the height of the step potential (Sec. 10.2.1), and when it is greater (Sec. 10.3). In both cases, we will get interesting results when we solve the time independent Schrödinger equation for the step potential.

The step potential can be used to model a variety of physical systems and some well known applications are seen in semiconductor devices, the physics of normal-metal superconductor interfaces, and alpha decay in the nucleus.

Solving the step potential problem in this unit will also serve as a good exercise for you to help you understand the next unit, where you will study about the barrier potential.

Expected Learning Outcomes

After studying this unit, you should be able to:

- ❖ define a step potential;
- ❖ solve time independent Schrödinger equation for step potential under given conditions;
- ❖ determine the reflection and transmission coefficients; and
- ❖ solve simple problems based on step potential.

10.2 STEP POTENTIAL AND SCHRÖDINGER EQUATION

A step potential is shown in Fig. 10.1. You can see that we can define it mathematically as:

$$V(x) = \begin{cases} 0, & \text{for } x < 0 \\ V_0 > 0, & \text{for } x > 0 \end{cases} \quad (10.1)$$

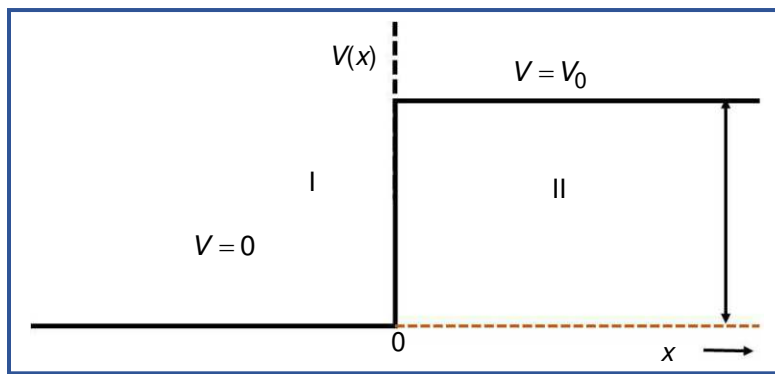


Fig. 10.1: A step potential. Note that the potential is zero in Region I and it has a non-zero value (V_0) in Region II.

In Fig. 10.1, note that the step potential $V(x)$ is zero in the region $x < 0$ and non-zero (equal to V_0) in the region $x > 0$. Note also from Fig. 10.1 that the step potential is discontinuous at $x = 0$.

You may like to ask: What does such a potential mean physically? To understand this, and to get a physical picture of the potential, let us see what happens to a particle subjected to the step potential.

Let us consider a particle of mass m having kinetic energy, E , and moving from left to right along the x -axis as shown in Fig. 10.2.

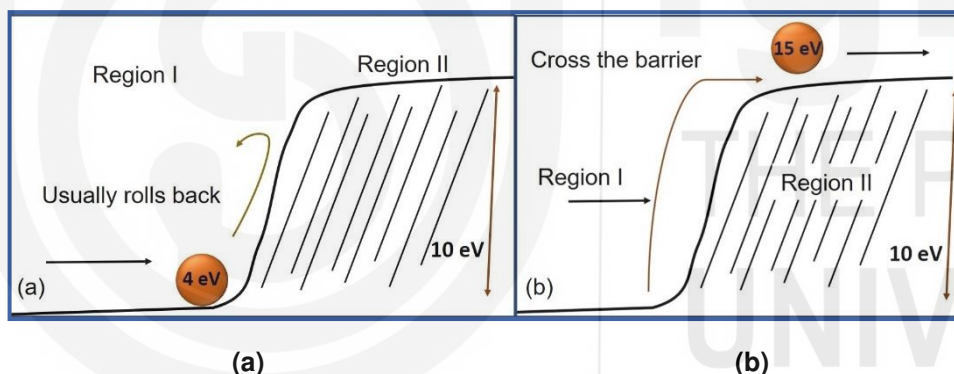


Fig. 10.2: Classical picture of a particle with energy (a) lower than the step potential V_0 and (b) higher than the step potential V_0 .

Let us first ask: What would happen if the particle was a classical particle? From classical mechanics, you know that if the energy (E) of the particle were less than the step potential V_0 , that is, if $E < V_0$, then the particle would not be able to enter Region II from Region I (see Fig. 10.2a). A classical particle for which $E < V_0$, would be reflected at the step. However, if the energy of the classical particle was greater than V_0 , it would be able to cross the step potential and move into Region II (see Fig. 10.2b).

Let us now ask: What would happen to a quantum particle subjected to this potential? Refer to Fig. 10.3. Note that the particle is incident from Region I of the step potential (V_0). Note that in the Region I, the energy (E) of the particle is purely kinetic energy, while in Region II, the energy is partly kinetic and partly potential. Now recall from Unit 9, how quantum mechanics differs fundamentally from classical physics. According to quantum mechanics, the wave function of the particle has finite value in Region II, which means that

there is a finite probability of finding the particle in Region II even when the particle has less energy than the potential!! This is the result we get when we solve the Schrödinger equation.

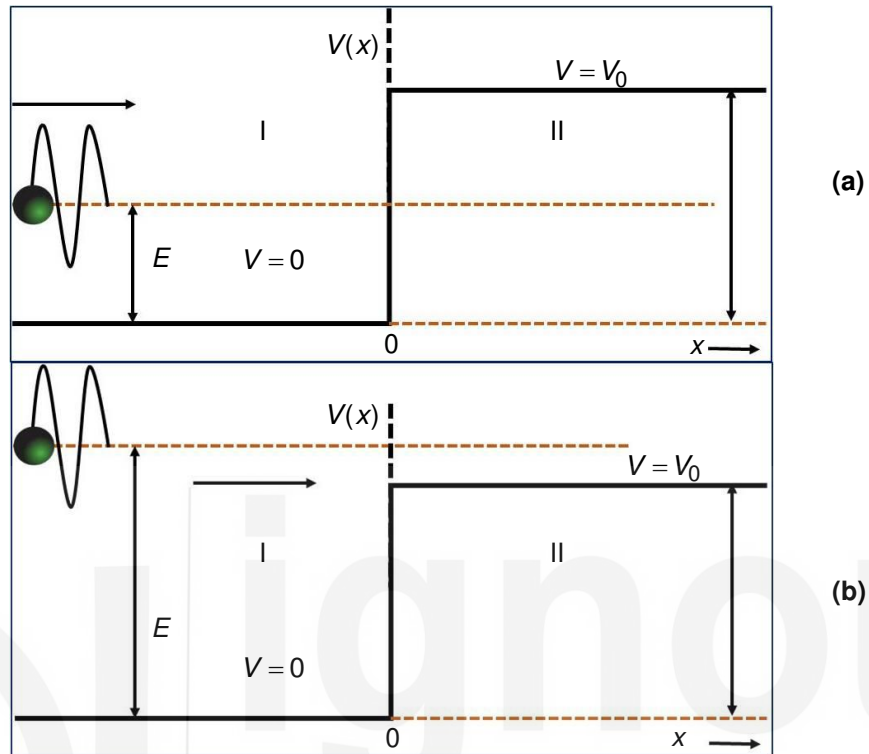


Fig. 10.3: A particle with energy E is incident from Region I and subjected to a step potential V_0 at $x = 0$. We consider two cases, a) when $E < V_0$; b) when $E > V_0$.

We now write the time independent Schrödinger equation for a particle in a step potential defined by Eq. (10.1). Note that there are two regions, Region I ($x < 0$) in which the potential is zero and Region II ($x > 0$) in which it is V_0 . So, we write the Schrödinger equation for a particle of mass m in the two regions (see Fig. 10.3) as:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_1}{dx^2} = E\psi_1 \quad x < 0 \quad (10.2a)$$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_2}{dx^2} + V_0\psi_2 = E\psi_2 \quad x > 0 \quad (10.2b)$$

We solve the Schrödinger equation for the two regions [Eqs. (10.2a and b)] using the method you have learnt in Unit 9. We also have to apply the boundary conditions to get acceptable wave functions. Note that we have denoted the solutions of the Schrödinger equation in Regions I and II as ψ_1 and ψ_2 in Eqs. (10.2a and b). The boundary conditions for this problem are: At $x = 0$

$$\psi_1(x=0) = \psi_2(x=0) \quad (10.3a)$$

and
$$\left(\frac{d\psi_1}{dx} \right) \Big|_{x=0} = \left(\frac{d\psi_2}{dx} \right) \Big|_{x=0} \quad (10.3b)$$

Now, there are two interesting possibilities regarding the energy of the particle with respect to the step potential. The first case is when the energy of the particles is less than the step potential V_0 and the second, when it is greater.

Therefore, in Secs. 10.3 and 10.4, we will solve Eqs. (10.2a and b) for the following two cases:

Case 1: The energy E of the particle is less than V_0 (Fig. 10.3a)

Case 2: The energy E of the particle is greater than V_0 (Fig. 10.3b)

10.3 ENERGY (E) OF THE PARTICLE IS LESS THAN V_0

Let us solve Eqs. (10.2a and b) for Regions I and II.

Region I: $-\infty \leq x < 0$ for which $V = 0$

Let $\psi_1(x)$ be the solution of the Schrödinger equation for the particle in Region I. Since the potential is zero in this region, the particle is free and the corresponding time independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_1}{dx^2} = E\psi_1 \quad (10.4a)$$

$$\Rightarrow \frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2} \psi_1 = 0 \quad (10.4b)$$

$$\Rightarrow \frac{d^2\psi_1}{dx^2} + k_1^2 \psi_1 = 0 \quad (10.4c)$$

$$\text{where } k_1 = \sqrt{\frac{2mE}{\hbar^2}} \quad (10.4d)$$

You know from Unit 9, [Eq. (9.10)], that the solution of Eq. (10.4c) is:

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad (10.5)$$

You know that, the term Ae^{ik_1x} in Eq. (10.5) represents a wave of amplitude A travelling in the positive x -direction while the term Be^{-ik_1x} represents a wave with amplitude B travelling in the negative x -direction. The second term in Eq. (10.5) is a **wave reflected at the step potential** (see Fig. 10.4).

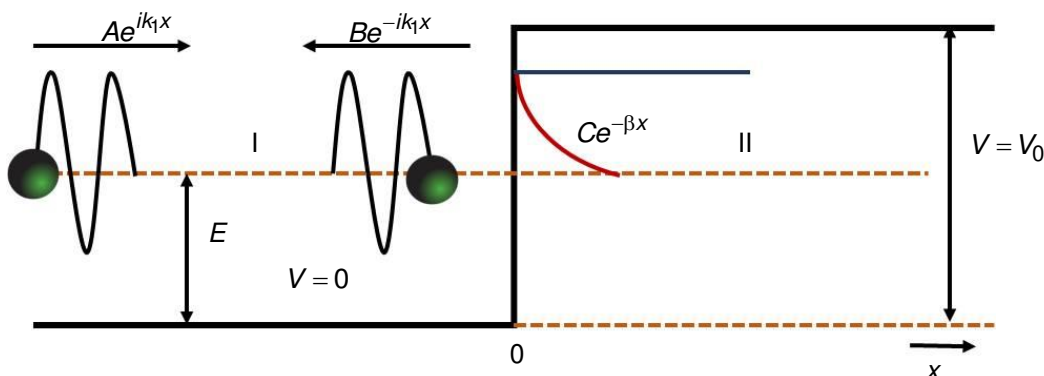


Fig. 10.4: The solutions [Eqs. (10.5 and 10.7)] of the Schrödinger equation for a free particle in Regions I and II of the step potential.

So, the solution of Eq. (10.2a) is a linear combination of wave functions representing an incident wave and a reflected wave.

Let us now solve Eq. (10.2b).

Region II: $-0 \leq x \leq +\infty$ for which $V = V_0$

Let $\psi_2(x)$ be the solution of the Schrödinger equation for the particle in Region II. The time independent Schrödinger equation for Region II is given as:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_2}{dx^2} + V_0\psi_2 = E\psi_2 \quad (10.6a)$$

$$\Rightarrow \frac{d^2\psi_2}{dx^2} - \frac{2m}{\hbar^2} (V_0 - E)\psi_2 = 0 \quad (10.6b)$$

We put $\beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$ (10.6c)

so that we can write Eq. (10.6b) as:

$$\frac{d^2\psi_2}{dx^2} - \beta^2\psi_2 = 0 \quad (10.6d)$$

The solution of Eq. (10.6d) is:

$$\psi_2(x) = Ce^{-\beta x} \quad (10.7)$$

In Eq. (10.7), the term $Ce^{-\beta x}$ represents an exponentially decreasing wave function for positive values of x (Fig. 10.4). This means that the wave function is finite in Region II of the step potential. Therefore, the probability of finding the particle in Region II is finite. You know from Unit 4 of BPHCT 131 that the general solution of Eq. (10.6d) is of the form $\psi_2(x) = Ce^{-\beta x} + De^{\beta x}$.

Can you say: Why have we not included the term $De^{\beta x}$ in Eq. (10.7)? Recall what you have learnt in Units 7 and 9 about physically acceptable wave functions.

You know that it is because the term $De^{\beta x}$ represents an exponentially increasing wave function in the Region II. It is not physically meaningful since an acceptable wave function must remain finite as $x \rightarrow \infty$. Thus, we must have $D = 0$.

Let us now put the solutions of the time independent Schrödinger equation for the step potential defined by Eqs. (10.4c and Eq. 10.6d), at one place. The solutions are:

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad \text{for Region I: } x < 0 \quad (10.5)$$

$$\psi_2(x) = Ce^{-\beta x} \quad \text{for Region II: } x > 0 \quad (10.7)$$

The next step, as you know, is to apply the boundary conditions at $x = 0$ to determine the constants A , B and C . Applying the first boundary condition [Eq. (10.3a)], we get:

$$A + B = C \quad (10.8a)$$

Remember that A and B are the amplitudes of the incident wave and the reflected wave in Region I and C represents the amplitude of a wave that decreases exponentially in Region II. Applying the second boundary condition [Eq. (10.3b)], we get:

$$\begin{aligned} \left(\frac{d\psi_1}{dx} \right) &= \left(\frac{d\psi_2}{dx} \right) \\ \Rightarrow Aik_1 - Bik_1 &= -C\beta \\ \Rightarrow A - B &= \frac{i\beta}{k_1} C \end{aligned} \quad (10.8b)$$

Let us now solve Eqs. (10.8a and b) to determine the constants A , B and C . Adding Eqs. (10.8a and b), we get:

$$\begin{aligned} 2A &= \left(1 + \frac{i\beta}{k_1} \right) C \\ \therefore C &= \left(\frac{2k_1}{k_1 + i\beta} \right) A \end{aligned} \quad (10.9a)$$

Subtracting Eq. (10.8b) from Eq. (10.8a), we get:

$$2B = \left(1 - \frac{i\beta}{k_1} \right) C \Rightarrow C = \left(\frac{2k_1}{k_1 - i\beta} \right) B \quad (10.9b)$$

Equating the LHS of Eqs. (10.9a and 10.9b) we can write:

$$B = \left(\frac{k_1 - i\beta}{k_1 + i\beta} \right) A \quad (10.9c)$$

Thus, we have obtained the constants B and C in terms of A . Let us now interpret these results.

10.3.1 Reflection and Transmission Coefficients

Let us first ask: What is the incident probability density, i.e., the probability of finding the particle in Region I? This is known as the **incident probability density**.

From Unit 7, you know that the probability density in any region is defined as:

$$P(x) = \psi^*(x) \psi(x) \quad (10.10)$$

Note that from Eq. (10.5) that the wave function for the incident wave is

$\psi_1(x) = Ae^{ik_1x}$. Therefore, the incident probability density is given as:

$$P_1(x) = \psi_1^*(x)\psi_1(x) = (A^*e^{-ik_1x})(Ae^{ik_1x}) = |A|^2$$

We would now like you to calculate the reflected and transmitted probability densities corresponding to the reflected and transmitted wave functions using Eqs. (10.5 and 10.7). Try SAQ 1.

SAQ 1 - Reflected and transmitted probability densities

Determine the reflected and the transmitted probability densities for a step potential.

Recall Eq. (7.31a) of Sec. 7.3.2 of Unit 7 from which the probability current density is given by:

$$J = \frac{\hbar}{2mi} \left[\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right] \Rightarrow J = -\frac{i\hbar}{2m} \left[\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right] \quad (10.11)$$

Substituting $\psi_1(x)$ and $\psi_2(x)$ in the Regions I and II, respectively, we obtain the reflected and transmitted probability current densities, respectively. Let J_r be the probability current density of the reflected wave. Let us take up an example to calculate it.

EXAMPLE 10.1: PROBABILITY CURRENT DENSITY J_r

What is the probability current density (J_r) of the reflected wave?

SOLUTION ■ We use Eq. (10.11) to determine J_r .

$$\text{Since } J = -\frac{i\hbar}{2m} \left[\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right]$$

$$J_r = -\frac{i\hbar}{2m} \left[(Be^{-ik_1x})^* \frac{d(Be^{-ik_1x})}{dx} - (Be^{-ik_1x}) \frac{d(Be^{-ik_1x})^*}{dx} \right]$$

$$\Rightarrow J_r = -\frac{i\hbar}{2m} [B^*B(-ik_1) - B^*B(ik_1)] = -\frac{\hbar k_1}{m} B^*B$$

$$\text{Hence, } J_r = -\frac{\hbar k_1}{m} B^*B = -\frac{\hbar k_1}{m} |B|^2$$

You can now calculate the incident probability current density corresponding to the incident wave function using Eqs. (10.5 and 10.11). Try SAQ 2.

SAQ 2 - Incident probability current density

Determine the probability current density (J_i) of the incident wave.

The reflection coefficient (R) is the probability that an incident particle is reflected from the step potential at $x=0$. It is defined as the ratio of the magnitudes of the probability current densities of the reflected wave and the incident wave:

$$R = \frac{|J_r|}{|J_i|} \quad (10.12)$$

The transmission coefficient (T) is the probability that the incident particle is transmitted and is defined as the ratio of the magnitudes of the probability current densities of the transmitted wave and the incident wave:

$$T = \frac{|J_t|}{|J_i|} \quad (10.13)$$

Using Eq. (10.12), we can determine the reflection coefficient for a step potential for $E < V_0$:

$$R = \frac{|B|^2}{|A|^2} \quad (10.14)$$

From Eq. (10.9c), we can see that $|B|^2 = \left(\frac{k_1 - i\beta}{k_1 + i\beta} \right) \left(\frac{k_1 + i\beta}{k_1 - i\beta} \right) |A|^2$ which means

that $|B|^2 = |A|^2$. Substituting this result in Eq. (10.14), we get $R = 1$.

Since the incident wave is either reflected or transmitted without any absorption, the sum of the reflection coefficient (R) and the transmission coefficient (T) should be unity:

$$R + T = 1$$

Therefore, for $R = 1$, we can see that the transmission coefficient is zero:

$$T = 0$$

This result agrees with the predictions of classical physics that when a particle possesses lower energy than the potential step, the particle cannot cross it! However, from Eq. (10.7) you have learnt that there is a finite probability of finding the particle in Region II since the wave function (ψ_2) in the region is non-zero.

You have already encountered a similar problem when you were dealing with bound state (particle in a box) where the wave function is non-zero in the classically forbidden region. So, how do we reconcile the two seemingly contradictory results?

In order to understand the result, it is important to remember how we have defined the step potential. You are aware that the step potential is an idealized potential and beyond $x > 0$, the potential (V_0) may extend to infinite distance. Hence, whatever is incident towards the barrier will eventually be reflected and it is for this very reason that we got $R = 1$. However, since the wave function is non-zero in Region II [Eq. (10.7)], we can conclude that the particle turns back eventually but before turning, it penetrates into classically forbidden region.

Thus, from the above result we can conclude that:

1. The reflection of incident wave at the step potential is total when $E < V_0$;
2. In the Region II, the wave function is non-zero. Therefore, there is a finite probability ($\psi_2^*(x)\psi_2(x) = C^*Ce^{-2\beta x}$) of finding the particle in Region II;
3. The wave function penetrates into classically forbidden region, $x > 0$. However, eventually it is completely reflected.

Let us explain the point 3 further.

Penetration in the Classically Forbidden Region

One of the most interesting outcomes of solving the Schrödinger equation for the step potential is that the wave function in the Region II ($x > 0$) is non-zero. This means that there is a finite probability of finding the particle in Region II even if $E < V_0$.

Note that according to classical mechanics, particles with energy $E < V_0$ cannot penetrate the step potential since it would lead to negative kinetic energy.

According to classical physics, when the initial energy of the particle is less than the height of the potential, the particle is reflected back with its original speed. The quantum particle's behaviour is in sharp contrast to the classical result. There is a finite probability of finding the particle in Region II given by Eq. (10.7). Let us now take up the case when the energy of the incident particle is greater than the height of the step potential.

10.4 ENERGY (E) OF THE PARTICLE IS GREATER THAN V_0

The case when the energy of the particle is greater than the potential step ($E > V_0$) is shown in Fig. 10. 3b. Again, we solve Eqs. (10.2a and b) in Regions I and II.

Region I: $-\infty \leq x < 0$ for which $V = 0$, the particle is free and the solutions remain the same as in Sec. 10.2 and are given by Eqs. (10.4c and 10.5), respectively.

Region II: For $0 < x < \infty$, the time independent Schrödinger equation is given as:

$$\begin{aligned}\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_2 &= 0 \\ \frac{d^2\psi_2}{dx^2} + k_2^2\psi_2 &= 0\end{aligned}\tag{10.15}$$

$$\text{where } k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$$

The solution of Eq. (10.15) is:

$$\psi_2(x) = F e^{ik_2 x} \quad (10.16)$$

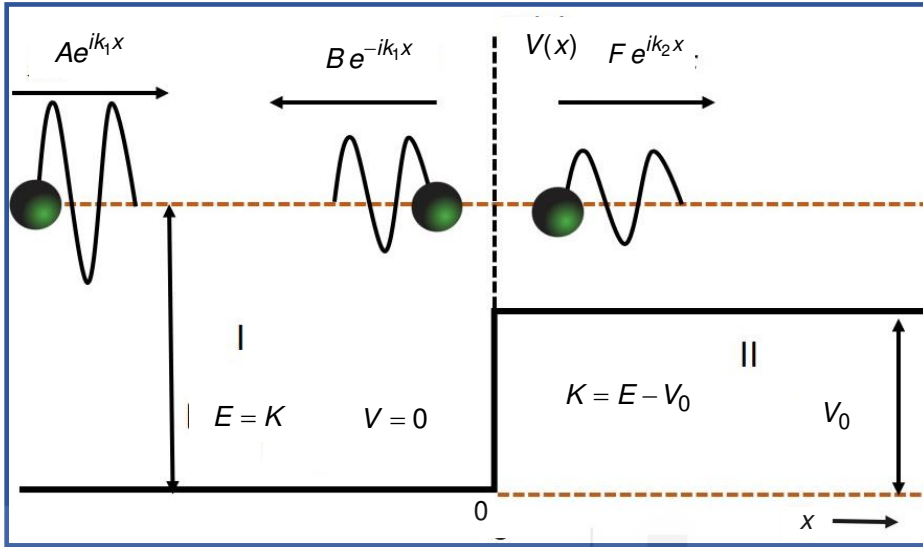


Fig. 10.5: The solutions of Schrödinger equation given by Eqs. (10.5 and 10.16).

The solution of Eq. (10.15) exhibits an oscillatory nature of the wave function (Fig. 10.5). The general solution of Eq. (10.15) is $\psi_2(x) = F e^{ik_2 x} + G e^{-ik_2 x}$. The term $F e^{ik_2 x}$ represents a wave travelling along the positive x -axis in the Region II, while a term like $G e^{-ik_2 x}$ would mean a wave travelling along the negative x -axis in Region II. However, since the particle is incident only from the left we can assume that $G = 0$.

Let us now apply the first boundary condition: At $x=0$, [Eq. (10.3a)], we have $\psi_1(x) = \psi_2(x)$. Hence, from Eqs. (10.5 and 10.16), we get:

$$A + B = F \quad (10.17a)$$

Here, F represents the amplitude of the wave in Region II. Similarly, applying the second boundary condition [Eq. (10.3b)], we get:

$$\left(\frac{d\psi_1}{dx} \right) = \left(\frac{d\psi_2}{dx} \right)$$

$$\Rightarrow Aik_1 - Bik_1 = iFk_2$$

$$\Rightarrow A - B = \frac{k_2}{k_1} F \quad (10.17b)$$

Adding Eqs. (10.17a and 10.17b), we get:

$$2A = \left(\frac{k_1 + k_2}{k_1} \right) F \quad \Rightarrow \quad F = \left(\frac{2k_1}{k_1 + k_2} \right) A \quad (10.18)$$

Subtracting Eq. (10.17b) from Eq. (10.17a), we get:

$$2B = \left(\frac{k_1 - k_2}{k_1} \right) F \quad \Rightarrow \quad B = \left(\frac{k_1 - k_2}{k_1 + k_2} \right) A \quad (10.19)$$

Once again, let us understand the results we have obtained for Case II.

10.4.1 Reflection and Transmission Coefficients

Let us now determine the reflection and the transmission coefficients for the case when the energy of the particle is greater than the potential: $E > V_0$. From Eq. (10.12), the reflection coefficient (R) is given by:

$$R = \frac{|J_r|}{|J_i|} = \frac{|B|^2}{|A|^2} = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 \quad (10.20)$$

Similarly, we determine the transmission coefficient (T) using Eq. (10.13) (read the margin remark):

$$T = \frac{|J_t|}{|J_i|} = \frac{\frac{\hbar k_2}{m} |F|^2}{\frac{\hbar k_1}{m} |A|^2} \quad (10.21a)$$

Substituting Eq. (10.18) in Eq. (10.21a), we get:

$$T = \frac{k_2}{k_1} \left(\frac{2k_1}{k_1 + k_2} \right)^2 = \frac{4k_1 k_2}{(k_1 + k_2)^2} \quad (10.21b)$$

You may like to attempt an SAQ on reflection and transmission coefficients.

SAQ 3 - Reflection and transmission coefficients

Show that $R + T = 1$ for $E > V_0$.

Let us now write the wave function for Region I in terms of the incident amplitude (A).

Substituting Eq. (10.19) in Eq. (10.5), we get the wave function for Region I when $E > V_0$ as:

$$\psi_1(x) = A \left[e^{ik_1 x} + \frac{k_1 - k_2}{k_1 + k_2} e^{-ik_1 x} \right] \text{ for } x < 0 \quad (10.22)$$

Attempt SAQ 4 to write the wave function for Region II.

SAQ 4 - Wave function for Region II

Write the wave function for Region II in terms of the incident amplitude when $E > V_0$.

Let us consider an example to apply the results obtained so far.

The wave function in region II is:

$$\psi = \psi_2(x) = F e^{ik_2 x}$$

$$\psi^* = \psi_2^*(x) = F^* e^{-ik_2 x}$$

And

$$\frac{d\psi}{dx} = \frac{d}{dx} (F e^{ik_2 x}) = ik_2 e^{ik_2 x} F$$

$$\frac{d\psi^*}{dx} = \frac{d}{dx} (F^* e^{-ik_2 x}) = -ik_2 e^{-ik_2 x} F^*$$

Substituting in Eq. (10.11) we get the probability current density of the transmitted wave as:

$$J_t = -\frac{i\hbar}{2m} \left[ik_2 F F^* + ik_2 F F^* \right] = \frac{\hbar k_2}{m} F^* F = \frac{\hbar k_2}{m} |F|^2$$

EXAMPLE 10.2 : REFLECTION AND TRANSMISSION COEFFICIENTS

A particle encounters a step potential of height V_0 . What is the reflection and transmission coefficient if $E = 2V_0$?

SOLUTION ■ We use Eqs. (10.20 and 10.21b).

$$\text{Since } R = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 = \left(\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}} \right)^2$$

$$\Rightarrow R = \left(\frac{\sqrt{2V_0} - \sqrt{2V_0 - V_0}}{\sqrt{2V_0} + \sqrt{2V_0 - V_0}} \right)^2$$

$$\Rightarrow R \approx 0.029$$

This means that about 3% of the wave is reflected even when the energy of the particle is greater than the height of the potential.

Similarly, from Eq. (10.21b), the transmission coefficient is given as:

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

$$\Rightarrow T = \frac{4\sqrt{E}\sqrt{E - V_0}}{(\sqrt{E} + \sqrt{E - V_0})^2}$$

$$\Rightarrow T = \frac{4\sqrt{2V_0}\sqrt{V_0}}{(\sqrt{2V_0} + \sqrt{2V_0 - V_0})^2}$$

$$T \approx 0.971$$

Thus, you can see that $R + T = 1$.

Let us now summarise the contents of the unit.

10.5 SUMMARY

Concept	Description
Step potential	■ A one-dimensional step potential is an idealized potential function which is zero for negative values of the independent variable and constant for positive values of the independent variable. The step potential is defined mathematically as:

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 > 0 & \text{for } x > 0 \end{cases}$$

It is discontinuous at the point $x = 0$ and constant on each side of the discontinuity.

Schrödinger equation for the step potential

- The **time independent Schrödinger equation** for the **step potential** is:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_1}{dx^2} = E \psi_1 \quad x < 0$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_2}{dx^2} + V_0 \psi_2 = E \psi_2 \quad x > 0$$

with the boundary conditions that at $x = 0$,

$$\psi_1(x) = \psi_2(x) \quad \text{and} \quad \left(\frac{d\psi_1}{dx} \right) = \left(\frac{d\psi_2}{dx} \right)$$

The Schrödinger equation is solved for two cases: 1) When the energy, E , of the particle is less than V_0 ; 2) when the energy, E , of the particle is greater than V_0 .

Solutions of the Schrödinger equation for the step potential for $E < V_0$

- When $E < V_0$, the solutions of the Schrödinger equation are:

$$\psi_1(x) = A e^{ik_1 x} + B e^{-ik_1 x} \quad \text{for } -\infty \leq x < 0$$

$$\psi_2(x) = C e^{-\beta x} \quad \text{for } 0 < x < \infty$$

$$\text{where } k_1 = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{and} \quad \beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$$\text{and } B = \left(\frac{k_1 - i\beta}{k_1 + i\beta} \right) A, \quad C = \left(\frac{2k_1}{k_1 + i\beta} \right) A$$

The **reflection coefficient (R)** is the ratio of J_r and J_i , where J_r and J_i are the probability current densities of the reflected and incident waves, respectively. The **transmission coefficient (T)** is the ratio of J_t and J_i , where J_t and J_i are the probability current densities of the transmitted and incident waves, respectively. The reflection and transmission coefficients are 1 and 0, in this case. Thus, $R + T = 1$. The particles with energy lower than the step potential have finite probability of penetrating through the classically forbidden region.

Solutions of the Schrödinger equation for the step potential for $E > V_0$

- When $E > V_0$, the solutions of the Schrödinger equation are:

$$\psi_1(x) = A e^{ik_1 x} + B e^{-ik_1 x} \quad \text{for } -\infty \leq x < 0$$

$$\text{and } \psi_2(x) = F e^{ik_2 x} \quad \text{for } 0 < x < \infty$$

$$\text{where } k_2 = \sqrt{\frac{2m(E - V_0)}{\hbar^2}},$$

$$\text{and } B = \left(\frac{k_1 - k_2}{k_1 + k_2} \right) A, \quad F = \left(\frac{2k_1}{k_1 + k_2} \right) A$$

In this case, the reflection and transmission coefficients are:

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 \quad \text{and} \quad T = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

such that $R + T = 1$. A particle with energy higher than the height of the step potential can get reflected back at the point of discontinuity.

10.6 TERMINAL QUESTIONS

1. A 1.1 mA beam of electrons enters a sharply defined boundary with a velocity $2.5 \times 10^6 \text{ ms}^{-1}$, and then its velocity reduces to $1.0 \times 10^6 \text{ ms}^{-1}$, due to the difference in potential. Determine the transmitted and reflected currents.
2. Determine the expression for the reflection coefficient when $E \approx V_0$.
3. A beam of particles with energy 7eV is sent towards a step potential of height 5eV. What fraction of the beam is reflected back?
4. A particle with energy 5 eV is incident on a potential with energy 7 eV. Calculate the distance in which the probability of finding the particle goes to 0.05 as it goes into the classically forbidden region.
5. A beam of free electrons are moving from left to right and suddenly encounters a step potential of height 8 eV. What should be the approximate energy (E) of the electrons such that 20% get reflected?

10.7 SOLUTIONS AND ANSWERS

Self-Assessment Questions

1. The reflected (P_r) and the transmitted (P_t) probability density is given as:

$$P_r(x) = |Be^{ik_1x}|^2 = |B|^2 \quad \text{and} \quad P_t(x) = |Ce^{\beta x}|^2 = |C|^2 e^{-2\beta x}$$

2. The probability current density of the incident wave can be obtain from Eq. (10.11):

$$J = -\frac{i\hbar}{2m} \left[\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right]$$

The incident wave function is $\psi(x) = Ae^{ik_1x}$, then the conjugate wave function is $\psi(x) = A^* e^{-ik_1x}$.

$$J_i = -\frac{i\hbar}{2m} \left[(Ae^{ik_1x})^* \frac{d(Ae^{ik_1x})}{dx} - (Ae^{ik_1x}) \frac{d(Ae^{ik_1x})^*}{dx} \right]$$

$$J_i = -\frac{i\hbar}{2m} [A^* A(ik_1) - A^* A(-ik_1)] = \frac{\hbar k_1}{m} A^* A = \frac{\hbar k_1}{m} |A|^2$$

3. From Eqs. (10.20 and 10.21b) we have:

$$R = \frac{|J_r|}{|J_i|} = \frac{|B|^2}{|A|^2} = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 \quad \text{and} \quad T = \frac{k_2}{k_1} \left(\frac{2k_1}{k_1 + k_2} \right)^2 = \frac{4k_1k_2}{(k_1 + k_2)^2}$$

$$\text{or } R + T = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 + \frac{4k_1k_2}{(k_1 + k_2)^2} = \frac{(k_1 - k_2)^2 + 4k_1k_2}{(k_1 + k_2)^2}$$

$$\therefore R + T = \frac{(k_1 + k_2)^2}{(k_1 + k_2)^2} = 1$$

4. Substituting Eq. (10.18) in Eq. (10.16), the wave function for Region II for $E > V_0$:

$$\psi_2(x) = A \left(\frac{2k_1}{k_1 + k_2} \right) e^{ik_2x} \quad \text{for } x > 0$$

Terminal Questions

1. From Eq. (10.21b)

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2} = \frac{4k_1/k_2}{(k_1/k_2 + 1)^2}$$

For the given condition, $\frac{k_1}{k_2} = \frac{v_1}{v_2} = 2.5$. Hence, $T = \frac{10}{12.25}$

The transmitted current is $T \times 1.1 \text{ mA} = 0.816 \times 1.1 \text{ mA} = 0.898 \text{ mA}$
and the reflected current is 0.102 mA.

2. From Eq. (10.20), $R = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 = \left(\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}} \right)^2$

Thus, $R \rightarrow 1$ as $E \approx V_0$.

3. From Eq. (10.20), $R = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 = \left(\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}} \right)^2$

or $R = \left(\frac{\sqrt{7} - \sqrt{2}}{7 + \sqrt{2}} \right)^2 = 0.092$. Thus, 9.2% is reflected back.

4. Here, $E < V_0$. From Eq. (10.7), $\psi_2(x) = C e^{-\beta x}$

where $\beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$. So, $\beta = \sqrt{\frac{(7 - 5) \text{ eV}}{38 \times 10^3 \text{ eV nm}^{-2}}} = 7.25 \text{ nm}^{-1}$

If the probability of finding the particle at $x = 0$ is P , then the probability of finding the particle at $x = d$ is $0.05P$. Thus,

$$P = |C|^2 \quad \text{or} \quad |C|^2 e^{-2\beta d} = 0.05P$$

Dividing the two relations, we get

$$e^{2\beta d} = 20 \quad \text{or} \quad 2\beta d = \ln 20 \quad \text{and} \quad d \approx 0.21 \text{ nm}$$

5. $R = \left(\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}} \right)^2 = 0.2 \Rightarrow \left(\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}} \right) = 0.447$

For (see the margin remark) $V_0 = 8 \text{ eV}$, $E = 9.35 \text{ eV} \approx 9 \text{ eV}$

Using

$$\frac{\sqrt{E} - \sqrt{E - V_0}}{\sqrt{E} + \sqrt{E - V_0}} = \frac{1 - \sqrt{\frac{E - V_0}{E}}}{1 + \sqrt{\frac{E - V_0}{E}}}$$

And

$$x = \sqrt{\frac{E - V_0}{E}}$$

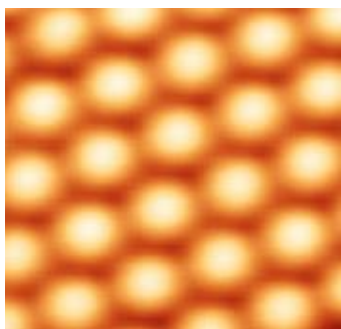
We can write :

$$\frac{1 - x}{1 + x} = 0.447 \Rightarrow x = 0.38$$

$$\therefore \sqrt{\frac{E - V_0}{E}} = 0.38$$

$$\Rightarrow \frac{E - V_0}{E} = 0.146$$

$$\Rightarrow E = 9.35$$



Silicon atoms observed at the surface of a silicon carbide crystal using a Scanning Tunnelling Microscope.

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UNIT 11

BARRIER POTENTIAL

Structure

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| <p>11.1 Introduction</p> <p>Expected Learning Outcomes</p> <p>11.2 One-Dimensional Barrier Potential</p> <p>Solving the Schrödinger equation</p> <p>Reflection and Transmission Coefficient for $E < V_0$.</p> <p>Reflection and Transmission Coefficient for $E > V_0$</p> | <p>11.3 Applications of Quantum Tunnelling</p> <p>Alpha Decay</p> <p>Scanning Tunnelling Microscope</p> <p>11.4 Summary</p> <p>11.5 Terminal Questions</p> <p>11.6 Solutions and Answers</p> |
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STUDY GUIDE

In this unit you will solve the one-dimensional Schrödinger equation for another physical system, which is the potential barrier. You will use the same techniques that you have learnt in the last two units: differential and integral calculus and second order ODEs. You should also be comfortable with complex numbers. You must work out all the steps of each derivation and work through all the SAQs and TQS. We have added an Appendix on the derivation of the reflection and transmission coefficients which you may like to go through.

“The simplicities of natural laws arise through the complexities of the language we use for their expression.”

Eugene Wigner

11.1 INTRODUCTION

The idea of quantum tunnelling was used by George Gamow in 1928 to explain α -decay and by Cockcroft and Watson in 1932, in their experiment to split an atom at energies forbidden by classical physics. Over the years several Nobel Prizes have been awarded for research based on the idea of quantum tunnelling: to Cockcroft and Watson in 1954, to Esaki in 1973 for discovering tunnelling in semiconductors, also in the same year to Giaever and Josephson for tunnelling in superconductors and to Binnig and Rohrer in 1986 for the scanning tunnelling microscope. Since tunnelling across potential barriers is a purely quantum mechanical phenomenon, it is also seen as an important success of quantum theory.

In Unit 9 you have solved the time independent Schrödinger equation for a free particle and for a particle confined to a certain region of space. You have seen that for a free particle you can have a continuous spectrum of energies, whereas when the particle is localized to a small region, you have a discrete energy spectrum. In general, whenever you solve the time independent Schrödinger equation for a potential $V(x)$, you will have either (i) “**bound**” states with discrete energy values, or (ii) “**unbound**” states with continuous energy values. In Unit 10 you solved the Schrödinger equation for a quantum mechanical particle incident on a step potential.

In this unit we solve the time independent Schrödinger equation for a particle incident on a potential barrier. Just like a potential well tends to attract and localize a particle, a barrier, as the name suggests, has a tendency to deflect particles. When a classical particle is incident on a barrier, it will cross the barrier if its energy is greater than the barrier potential. It will be reflected at the barrier if its energy is less than the barrier potential. What about a quantum particle? Will it be reflected or transmitted through the barrier? No matter what the energy of a quantum particle is, because the matter wave associated with it is finite everywhere – there is no region of space that is forbidden to a quantum particle. In Unit 10 also you have seen that there is a finite probability of finding a quantum particle in a classically forbidden region. The phenomenon in which a quantum particle is transmitted through a potential barrier and penetrates into regions which are classically forbidden to it is called “**quantum tunnelling**”. Quantum tunnelling was first noticed in 1927 by Friedrich Hund and since then it has been used to explain many physical phenomena and has several important applications (read the margin remark).

In Sec. 11.2 we solve the Schrödinger equation for the barrier potential and calculate the reflection and transmission probabilities at the barrier. In Sec. 11.3 we study some important applications of the concept of quantum tunnelling in explaining α -decay and in scanning tunnelling microscopy.

In the next unit we solve the Schrödinger equation for the one-dimensional finite potential well.

Expected Learning Outcomes

After studying this unit, you should be able to:

- ❖ solve the time independent one-dimensional Schrödinger equation for a quantum particle incident on a potential barrier;
- ❖ carry out calculations using the reflection and transmission coefficients;
- ❖ identify the factors on which the tunnelling probability depends;
- ❖ explain how tunnelling enables alpha decay; and
- ❖ describe the working of a scanning tunnelling microscope.

11.2 ONE-DIMENSIONAL BARRIER POTENTIAL

Let us first look at the classical version of a potential barrier. Recall Sec. 10.5 of BPHCT 131, where you have studied the **principle of conservation of energy**. Consider a ball of mass 200 g (a cricket ball, for example) rolling along a (frictionless surface) with a constant speed of 20 ms^{-1} . So its kinetic energy is 40 J. Now suppose it comes to a hump in the surface which has a height of 15 m as shown in Fig.11.1a below. If the ball were to reach the top of the hump, its potential energy at the top of the hump would be $\sim 30 \text{ J}$. So you expect that the ball will easily reach the top of the hump and roll over it to come down the other side. This is an application of this principle of conservation of energy (recall Terminal Question 6 of Unit 10 of BPHCT 131). What if the height of the hump is 30 m (Fig. 11.1b)? Then the potential of the ball at the top of the hump would be $\sim 60 \text{ J}$. In this case, the ball would not be able to cross over to the other side of the hump. It would roll back at some point as is shown in the figure. Therefore, if the potential energy is greater than the kinetic energy, the ball **is not able to cross the hump**. You can imagine that the hump is the potential barrier which prevents the ball from rolling over to the other side. This is the classical picture.

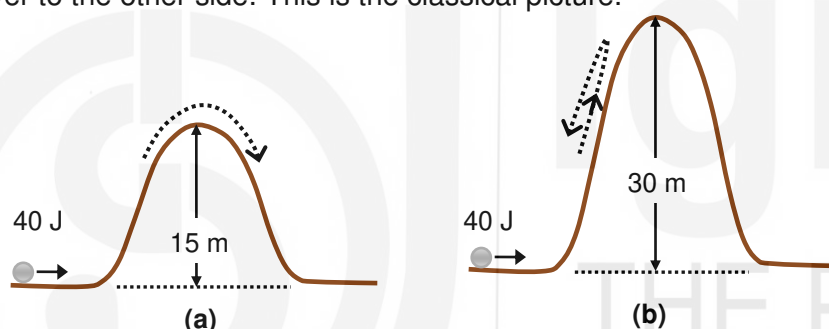


Fig. 11.1: A ball having a kinetic energy of 40 J trying to cross a hump of height a) 15.0 m , and b) 30.0 m.

Let us now look at the quantum mechanical analogue of this. In quantum mechanics the hump can be represented by a potential barrier. We define the potential energy function for a one-dimensional potential barrier as follows:

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } 0 \leq x \leq L \\ 0 & \text{for } x > L \end{cases} \quad (11.1)$$

$V(x)$ is shown in Fig. 11.2.

We divide the entire one-dimensional space into three regions as shown in the figure. Region I extends from $-\infty$ to 0 ; region II from 0 to L and Region III from L to ∞ . The central region is known as the potential barrier. You can see that the shape of the barrier is rectangular. In text books you may come across the term “**rectangular potential barrier**” for this or “**square potential barrier**” when the potential barrier has a square shape. They refer to the same problem.

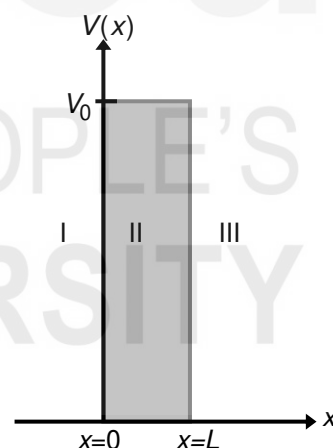


Fig. 11.2: A Potential Barrier.

A classical particle incident on the barrier from the left cannot cross the barrier if the energy (E) of the particle is less than the barrier potential V_0 i.e. if

$E < V_0$. If $E > V_0$, the particle continues its motion over the barrier with a kinetic energy $E - V_0$ and crosses it. So Region II and Region III are inaccessible to a particle which has an energy $E < V_0$.

We now solve the time independent Schrödinger equation for a quantum mechanical particle incident on the barrier with (i) an energy $E < V_0$ and (ii) $E > V_0$.

11.2.1 Solving the Schrödinger Equation

Let us consider the motion of a particle of mass m and total constant energy E in the above mentioned one-dimensional space. Let us first write down the time independent Schrödinger equations for the particle in regions I and III. Since the potential energy in these two regions is zero, we have (putting $V(x)=0$ in Eq. 7.47):

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad (\text{for Regions I and III}) \quad (11.2)$$

Recall that you have already solved this equation in Sec. 9.2. We therefore write down the solutions (as in Eq. 9.10) for Regions I and III, which are $\psi_I(x)$ and $\psi_{III}(x)$, respectively (see also the margin remark):

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad (\text{for Region I}) \quad (11.3)$$

And

$$\psi_{III}(x) = Fe^{ikx} + Ge^{-ikx} \quad (\text{for Region III}) \quad (11.4)$$

where

$$E = \frac{\hbar^2 k^2}{2m} \quad (11.5)$$

and:

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad (11.6)$$

You have studied in Unit 9 that the function e^{ikx} represents a particle moving along the positive x - direction. And the function e^{-ikx} represents a free particle moving along the negative x - direction.

In the expression for $\psi_I(x)$, Ae^{ikx} represents the plane wave that is incident on the barrier at $x = 0$, which has an amplitude A and is travelling to the right. Be^{-ikx} represents the plane wave reflected at the barrier, which has an amplitude B and is moving towards the left from $x = 0$. So in Eq. (11.4) both A and B are non-zero. In Region III, since there is only the wave that is transmitted through the barrier and moving towards the right, and no wave travelling to the left, we can set $G = 0$. So, the wave function for Region III is:

Notice that we use either:

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

or

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

as the general solution of the Schrödinger equation for $V(x)=0$. Both solutions are equivalent. The choice of the form of the solution is made for convenience.

$$\psi_{III}(x) = Fe^{ikx} \quad (\text{for Region III}) \quad (11.7)$$

We next write the time independent Schrödinger equation for the particle in Region II ($0 \leq x \leq L$), where the function is denoted by $\psi_{II}(x)$:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_{II}(x)}{dx^2} + V_0\psi_{II}(x) = E\psi_{II}(x) \quad (\text{for Region II}) \quad (11.8)$$

Let us now define a parameter k' similar to k in Eq. (11.6):

$$k' = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad (11.9)$$

Then we rewrite Eq. (11.8) as:

$$\frac{d^2\psi_{II}(x)}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi_{II}(x) = 0 \quad \text{or} \quad \frac{d^2\psi_{II}(x)}{dx^2} - (k')^2\psi_{II}(x) = 0 \quad (11.10)$$

From your knowledge of homogeneous second order ODEs (Unit 4 of BPHCT 131) you know that the solution of Eq. (11.10) is (see the margin remark):

$$\psi_{II}(x) = Ce^{k'x} + De^{-k'x} \quad (\text{for Region II}) \quad (11.11)$$

Let us now summarize what you have studied so far.

Note that unlike in Eq. (10.7), in Eq. (11.11) we retain both the terms $Ce^{k'x}$ and $De^{-k'x}$ in the solution for region II. That is because, in this case this solution is valid only over the range $0 \leq x \leq L$ and both terms in Eq. (11.11) would remain finite in this range.

ONE-DIMENSIONAL POTENTIAL BARRIER

Recap

The potential energy function for a one-dimensional potential barrier of width L is:

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } 0 \leq x \leq L \\ 0 & \text{for } x > L \end{cases} \quad (11.1)$$

The time independent Schrödinger equation for a particle of mass m is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad (\text{for } x < 0 \text{ and } x > L) \quad (11.2)$$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi_{II}(x)}{dx^2} + V_0\psi_{II}(x) = E\psi_{II}(x) \quad (\text{for } 0 \leq x \leq L) \quad (11.8)$$

The solutions of the Schrödinger equations are:

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad (\text{for } x < 0) \quad (11.3)$$

$$\psi_{II}(x) = Ce^{k'x} + De^{-k'x} \quad (\text{for } 0 \leq x \leq L) \quad (11.11)$$

$$\psi_{III}(x) = Fe^{ikx} \quad (\text{for } x > L) \quad (11.7)$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{and} \quad k' = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Now we consider the following two cases:

- I. The energy of the particle: $E < V_0$.

In this case $(V_0 - E)$ is positive and the solution is given by Eq. (11.11) with a real value of the parameter k' .

- II. The energy of the particle: $E > V_0$.

In this case $(V_0 - E)$ is negative and the parameter k' is complex. If we write $k' = i\alpha$, where α is real, then the solution is:

$$\psi_{II}(x) = Ce^{i\alpha x} + De^{-i\alpha x} \quad (11.12)$$

Where:

$$\alpha = \sqrt{\frac{2m(E - V_0)}{\hbar^2}} \quad (11.13)$$

Let us now study the two cases separately.

CASE I: $E < V_0$

To determine the constants A , B , C , D and F we use the properties of an acceptable wave function for a physical system.

Let us first write down the boundary conditions. You know that for $\psi(x)$ to be an acceptable wave function in a physical system, $\psi(x)$ and $\frac{d\psi(x)}{dx}$ must be continuous for all x . So, the wave functions in the three regions and their derivatives must be equal at the boundaries of the potential barrier and satisfy the following conditions:

$$\psi_I(x=0) = \psi_{II}(x=0) \quad (11.14a)$$

$$\psi_{II}(x=L) = \psi_{III}(x=L) \quad (11.14b)$$

And

$$\left. \frac{d\psi_I(x)}{dx} \right|_{(x=0)} = \left. \frac{d\psi_{II}(x)}{dx} \right|_{(x=0)} \quad (11.14c)$$

$$\left. \frac{d\psi_{II}(x)}{dx} \right|_{(x=L)} = \left. \frac{d\psi_{III}(x)}{dx} \right|_{(x=L)} \quad (11.14d)$$

We first apply the boundary condition given by Eq. (11.14a). From Eq. (11.3) we can write $\psi_I(x=0) = A + B$. From Eq. (11.11) for $\psi_{II}(x)$ we get $\psi_{II}(x=0) = C + D$. Therefore, from Eq. (11.14a) we have:

$$A + B = C + D \quad (11.15a)$$

To apply Eq.(11.14b), we set $x = L$ in Eqs. (11.11 and 11.7) for $\psi_{II}(x)$ and

$\psi_{III}(x)$, respectively, and get:

$$Ce^{k'L} + De^{-k'L} = Fe^{ikL} \quad (11.15b)$$

To apply Eqs. (11.14c and d), we first write down the derivatives of $\psi_I(x)$, $\psi_{II}(x)$ and $\psi_{III}(x)$.

$$\frac{d\psi_I}{dx} = \frac{d}{dx}(Ae^{ikx} + Be^{-ikx}) = ik(Ae^{ikx} - Be^{-ikx}) \quad (11.16a)$$

$$\frac{d\psi_{II}}{dx} = \frac{d}{dx}(Ce^{k'x} + De^{-k'x}) = k'(Ce^{k'x} - De^{-k'x}) \quad (11.16b)$$

$$\frac{d\psi_{III}}{dx} = \frac{d}{dx}(Fe^{ikx}) = ik(Fe^{ikx}) \quad (11.16c)$$

From Eqs. (11.14c and d) we can write:

$$ik(A - B) = k'(C - D) \quad (11.17a)$$

and

$$k'(Ce^{k'L} - De^{-k'L}) = ikFe^{ikL} \quad (11.17b)$$

Now we have four equations (11.15a and b, and 11.17a and b), but there are five unknowns: A , B , C , D and F . However, as you will see in the next section, we are interested in calculating the probability of reflection and transmission, for which we need the ratios B/A and F/A . If we divide the equations (11.15a and b, and 11.17a and b) by A , we will be left with just four unknowns as you can see below:

$$\frac{C}{A} + \frac{D}{A} = 1 + \frac{B}{A} \quad (11.18a)$$

$$\frac{C}{A}e^{k'L} + \frac{D}{A}e^{-k'L} = \frac{F}{A}e^{ikL} \quad (11.18b)$$

$$k'\left(\frac{C}{A} - \frac{D}{A}\right) = ik\left(1 - \frac{B}{A}\right) \quad (11.18c)$$

$$k'\left(\frac{C}{A}e^{k'L} - \frac{D}{A}e^{-k'L}\right) = ik\frac{F}{A}e^{ikL} \quad (11.18d)$$

The four unknowns now are B/A , C/A , D/A and F/A . We can determine these constants by solving Eqs. (11.18a – 11.18d).

However, even without calculating the constants, we can see that the wave function has an oscillatory behaviour in Regions I and III, but in Region II the wave function is exponential. The typical wave function in all the three regions for $E < V_0$, is shown in the Fig. 11.3.

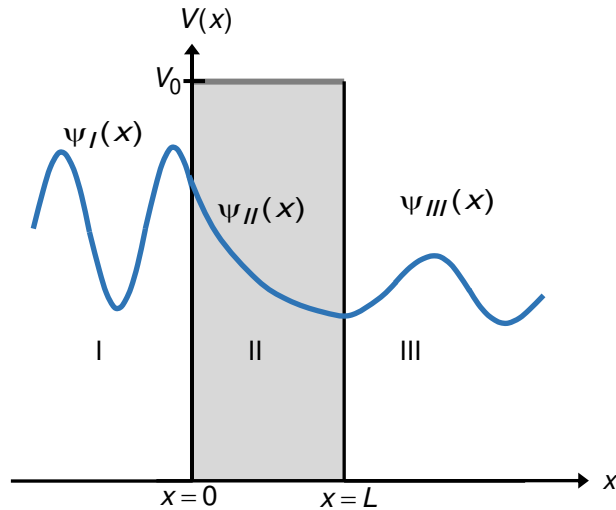


Fig. 11.3: The wave function for the one –dimensional potential barrier for a particle with an energy less than the barrier height.

In region III, the wave function is purely a travelling wave. We can calculate the probability density of the wave in this region as:

$$P_{III}(x) = \psi_{III}^*(x)\psi_{III}(x) = |F|^2 \text{ (which is a constant)} \quad (11.19)$$

In region I, the wave function is primarily a standing wave because we have a wave travelling to the right as well as a wave travelling to the left. Note that the amplitude of the reflected wave is necessarily less than that of the incident wave. We can write the probability density for Region I as:

$$P_I(x) = \psi_I^*(x)\psi_I(x) = |A|^2 + |B|^2 + AB^*e^{2ikx} + A^*Be^{-2ikx} \quad (11.20)$$

So, the probability density in Region I has an oscillatory component (last two terms of Eq. 11.20) as well as a constant component (first two terms of Eq. 11.20). So the minimum probability density in Region I is always slightly greater than zero as it is in Region III.

Within the barrier, although we have both the exponential terms, the decreasing exponential term ($De^{-k'x}$) is dominant. Hence, the probability density decreases exponentially as $P_{II}(x) = |D|^2 e^{-2k'x}$. The probability density for all three regions is shown in Fig.11.4 below:

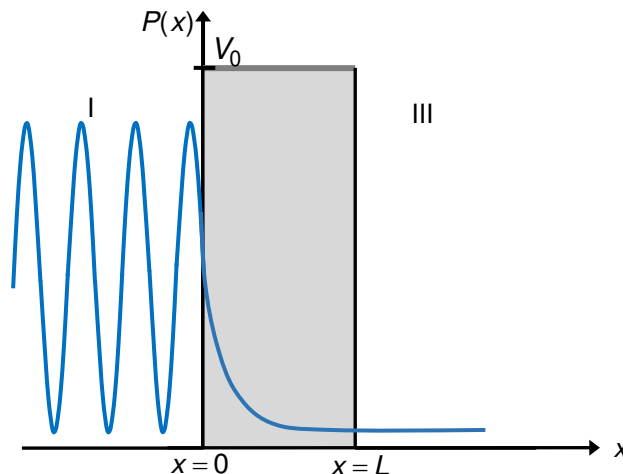


Fig. 11.4: The probability density as a function of position, for a quantum mechanical particle with an energy less than the barrier height.

We next calculate the reflection and transmission coefficients which are a measure of the probability of the particle being reflected or transmitted at the barrier.

11.2.2 Reflection and Transmission Coefficient for $E < V_0$

For the wave function $\psi_I(x)$, $\psi_0(x) = Ae^{ikx}$ is the part of the wave that is incident on the barrier from the left, whereas $\psi_R(x) = Be^{-ikx}$ represents the part of the wave that is reflected back from the barrier as shown in Fig. 11.5.

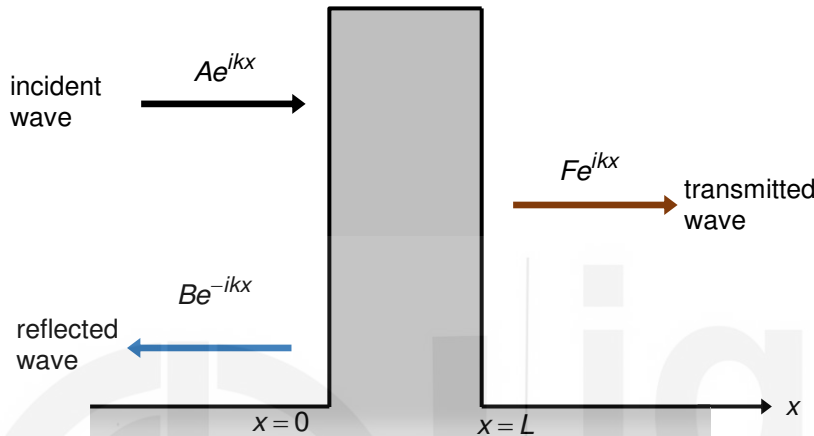


Fig. 11.5: Incident, reflected and transmitted waves at the one-dimensional potential barrier.

As you have studied in Unit 10, the reflection coefficient is given by the ratio of the magnitude of the probability current density associated with the reflected wave to the magnitude of probability current density associated with the incident wave (Eq.10.12). So we write the reflection coefficient R as:

$$R = \frac{|B|^2}{|A|^2} \quad (11.21)$$

You have studied that the intensity of a wave is proportional to its amplitude. The reflection coefficient is, therefore, the fraction of the intensity of the incident wave that is carried by the reflected wave. It also gives us the probability that a particle having an energy E incident on a potential barrier V_0 (such that $E < V_0$) is reflected back by the barrier.

We next define the transmission coefficient which tell us the probability of a particle being transmitted through the barrier. The transmission coefficient, T , is the ratio of the magnitudes of the probability current densities associated with the transmitted wave and the incident wave (Eq. 10.13), which is:

$$T = \frac{|F|^2}{|A|^2} \quad (11.22)$$

This is the ratio of the intensity of the transmitted wave to the intensity of the incident wave.

Since the incident wave is either reflected or transmitted, we must also have the sum of the reflection and transmission coefficient to be one:

$$R + T = 1 \quad (11.23)$$

To calculate R and T for the system we have to calculate B/A and F/A using Eqs. (11.18 a to d). The algebra is lengthy but straightforward and is worked out for you in the Appendix to this unit (you will not be tested on this derivation). We write down the results for T and R :

$$T = \left[1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(k'L) \right]^{-1} \quad (11.24a)$$

$$R = \left[1 + \frac{4E(V_0 - E)}{V_0^2 \sinh^2(k'L)} \right]^{-1} \quad (11.24b)$$

where

$$\sinh(k'L) = \frac{e^{k'L} - e^{-k'L}}{2} \quad (11.24c)$$

and

$$k'L = \sqrt{\frac{2mL^2(V_0 - E)}{\hbar^2}} = \sqrt{\frac{2mV_0L^2}{\hbar^2} \left(1 - \frac{E}{V_0} \right)} \quad (11.24d)$$

The transmission coefficient tells us about the extent of the penetration of the barrier by the particle. It is also called the **tunnelling probability**.

Notice that Eq. (11.24a) tells us something that is totally at odds with classical behaviour. For a classical particle, for $E < V_0$, the particle is always reflected at the barrier. So $R = 1$ and $T = 0$. But, for a quantum mechanical particle there is always a **small but finite probability** for the particle to penetrate the barrier and appear on the other side. This phenomenon is called “**barrier penetration**”. You can see that the transmission coefficient becomes vanishingly small in the limit of large values of $k'L$, because the factor $e^{-2k'L}$ in Eq. (11.24a) would be very small.

For large values of $k'L$, $\sinh(k'L) \approx e^{k'L}/2$ and we can write the expression for the transmission coefficient as:

$$T \approx \left[\frac{V_0^2}{4E(V_0 - E)} \left(\frac{e^{2k'L}}{4} \right) \right]^{-1} \quad (11.25)$$

or,

$$T \approx \frac{16E}{V_0} \left(1 - \frac{E}{V_0} \right) e^{-2k'L} \quad \text{for } k'L \gg 1 \quad (11.26)$$

Eq. (11.26) holds **for wide barriers and large values of V_0** .

The transmission coefficient T decreases exponentially as $e^{-2k'L}$ and $T \ll 1$.
The factor $k'L$ in the exponent (refer to Eq. 11.24d) is very large because Planck's constant is a very small number.

We define a **tunnelling length**:

$$\lambda_T = \frac{1}{k'} = \frac{\hbar}{\sqrt{2m(V_0 - E)}} \quad (11.27)$$

λ_T is a measure of the opacity of the barrier. It is also known as the **barrier penetration depth**. At a distance λ_T into the barrier, the wave function has fallen to $1/e$ of its value at the barrier edge; thus, the probability of finding the particle is appreciable only within about λ_T of the barrier edge. Notice that T decreases exponentially with L , the barrier width (beyond the tunnelling length) and the energy difference $(V_0 - E)$.

In terms of the tunnelling length, Eq. (11.26) can be written as:

$$T \approx \frac{16E}{V_0} \left(1 - \frac{E}{V_0}\right) e^{-\frac{2L}{\lambda_T}} \quad \text{for} \quad \frac{L}{\lambda_T} \gg 1 \quad (11.28)$$

Let us estimate how the transmission coefficient changes with the barrier width L for a fixed value of the tunnelling length λ_T .

EXAMPLE 11.1: TUNNELLING LENGTH AND TRANSMISSION COEFFICIENT

Consider an electron bound inside a typical metal. Typically the effective value of $(V_0 - E)$ that prevents the electron from escaping the metal is ~ 5.0 eV. Calculate the tunnelling length and the ratio of the transmission coefficients for $L=0.3$ nm and 0.2 nm.

SOLUTION ■ We calculate the tunnelling length using Eq. (11.27) with $V_0 - E = 5.0$ eV $= 8.0 \times 10^{-19}$ J:

$$\begin{aligned} \lambda_T &= \frac{\hbar}{\sqrt{2m(V_0 - E)}} = \frac{1.054 \times 10^{-34} \text{ Js}}{\sqrt{2 \times (9.109 \times 10^{-31} \text{ kg}) \times (8.0 \times 10^{-19} \text{ J})}} \\ &= .09 \times 10^{-9} \text{ m} = .09 \text{ nm} \end{aligned}$$

Notice that the transmission coefficient of Eq. (11.28) can be written as

$$T = f(E/V_0) e^{-2k'L} = f(E/V_0) e^{-\frac{2L}{\lambda_T}} \quad (i)$$

With $\lambda_T = .09$ nm, the transmission coefficient for $L = 0.3$ nm is

$$T_1 = f(E/V_0) e^{-\frac{2 \times 0.3 \text{ nm}}{0.09 \text{ nm}}} \approx f(E/V_0) e^{-6.7}$$

For $L = 0.2\text{nm}$ the transmission coefficient is:

$$T_2 = f(E/V_0)e^{-\frac{2 \times 0.2\text{nm}}{0.09\text{nm}}} \approx f(E/V_0)e^{-4.4}$$

So the ratio of the transmission coefficients

$$\text{is: } \frac{T_2}{T_1} = \frac{f(E/V_0)e^{-4.4}}{f(E/V_0)e^{-6.7}} = e^{2.3} \approx 10$$

So the transmission through a barrier of width 0.2 nm is almost **ten times more** probable than a barrier of width 0.3 nm .

Let us work out another example on calculating the transmission coefficient.

EXAMPLE 11.2 : TRANSMISSION COEFFICIENT

Calculate the transmission coefficient for an electron of energy 1.5 eV incident on a potential barrier of 2.0 eV , if the width of the barrier is 0.50 nm .

SOLUTION ■ We calculate first calculate λ_T using Eq. (11.27) with $E = 1.5\text{ eV}$, $V_0 = 2.0\text{ eV}$ and then calculate the value of T from Eq. (11.26), with using $L = 0.50\text{ nm}$ and $k' = \frac{1}{\lambda_T}$. So,

$$V_0 - E = 0.50\text{ eV} = 0.80 \times 10^{-19}\text{ J}.$$

$$\lambda_T = \frac{(1.054 \times 10^{-34}\text{ Js})}{\sqrt{2 \times (9.109 \times 10^{-31}\text{ kg}) \times (0.80 \times 10^{-19}\text{ J})}} = 0.28 \times 10^{-9}\text{ m} = 0.28\text{ nm}$$

$$\therefore T = 16 \frac{E}{V_0} \left(1 - \frac{E}{V_0}\right) e^{-\frac{2L}{\lambda_T}} = 16 \times \left(\frac{1.5\text{ eV}}{2.0\text{ eV}}\right) \left(1 - \frac{1.5\text{ eV}}{2.0\text{ eV}}\right) e^{-\frac{2 \times 0.50\text{ nm}}{0.28\text{ nm}}} = 3e^{-3.6}$$

Let us now summarize what we have studied about the reflection and transmission coefficient

Recap

REFLECTION AND TRANSMISSION COEFFICIENT ($E < V_0$)

The transmission coefficient T is the probability of a particle being transmitted through the barrier and is given by:

$$T = \left[1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(k'L)\right]^{-1} \quad (11.24a)$$

REFLECTION AND TRANSMISSION COEFFICIENT ($E < V_0$)(Contd.)

Recap

Where

$$k'L = \sqrt{\frac{2mL^2(V_0 - E)}{\hbar^2}} = \sqrt{\frac{2mV_0L^2}{\hbar^2} \left(1 - \frac{E}{V_0}\right)} \quad (11.24d)$$

The reflection coefficient R is the probability of the particle being reflected at the barrier edge and is given by:

$$R = \left[1 + \frac{4E(V_0 - E)}{V_0^2 \sinh^2(k'L)} \right]^{-1} \quad (11.24b)$$

The sum of the reflection and transmission coefficients is 1.

For wide barriers and large values of V_0 the transmission coefficient is:

$$T \approx \left[\frac{V_0^2}{4E(V_0 - E)} \left(\frac{e^{2k'L}}{4} \right) \right]^{-1} = \frac{16E}{V_0} \left(1 - \frac{E}{V_0} \right) e^{-\frac{2L}{\lambda_T}} \quad (11.25)$$

Where the **tunnelling length** λ_T is:

$$\lambda_T = \frac{1}{k'} = \frac{\hbar}{\sqrt{2m(V_0 - E)}} \quad (11.27)$$

The probability of finding the particle is appreciable only within about λ_T of the barrier edge.

You may like to work through the following SAQ.

SAQ 1 - Transmission Coefficient

Calculate the transmission coefficient for an electron in a semiconductor (having an energy of 1.5 eV incident on a potential barrier 2.0 eV if the width of the barrier is 0.10 nm. The effective mass of the electron is $0.22 m_e$).

You should not take the word 'tunnelling' 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. Suppose you are able to tunnel through a barrier to insert a detector inside it to 'see' the particle. Then, you are not only making a hole in the potential but also in your objective. Why so? 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 give it an uncontrollable amount of energy. This is how the uncertainty principle works in such measurement situations!

Quantum tunnelling should be taken into consideration only in those systems where wave particle duality is significant. In the Sec 11.3 we will take up certain important applications of quantum tunnelling.

We now study the reflection and transmission coefficient for Case II in which the energy of the particle $E > V_0$

11.2.3 Reflection and Transmission Coefficient for $E > V_0$

Let us write down the wave function for the three regions for $E > V_0$ (Eqs. 11.4, 11.12 and 11.5) once again:

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad (\text{for Region I}) \quad (11.3)$$

$$\psi_{II}(x) = Ce^{i\alpha x} + De^{-i\alpha x} \quad (\text{for Region II}) \quad (11.12)$$

$$\psi_{III}(x) = Fe^{ikx} \quad (\text{for Region III}) \quad (11.5)$$

where $\alpha = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$ and $k = \sqrt{\frac{2mE}{\hbar^2}}$.

You can see that the wave function is oscillatory in all three regions. Applying the boundary conditions Eqs. (11.14a to d) at $x=0$ and $x=L$ for the wave function and its derivatives as stated in Sec. 11.2.2, we can derive the expressions for the transmission and reflection coefficients as:

$$T = \left[1 + \frac{V_0^2}{4E(E - V_0)} \sin^2(\alpha L) \right]^{-1} \quad (11.29a)$$

$$R = \left[1 + \frac{4E(E - V_0)}{V_0^2 \sin^2(\alpha L)} \right]^{-1} \quad (11.29b)$$

From the expressions you can see that both R and T have an oscillatory component. Notice here that even when $E > V_0$, there is a finite probability for the particle to be reflected at the barrier.

Once again this behaviour is **NOT** what is predicted by classical mechanics. A classical particle which has an energy $E > V_0$ would be transmitted and not reflected ($T=1$ and $R=0$).

The typical variation of the transmission coefficient with the ratio of the particle energy E to the value of the potential at the barrier which is V_0 , is plotted in Fig. 11.6. For $E/V_0 < 1$, T is defined by Eq. (11.24a) and for $E/V_0 > 1$, T is given by Eq. (11.29a). For $E/V_0 < 1$, you can see that while there is a finite probability of tunnelling, $R > T$.

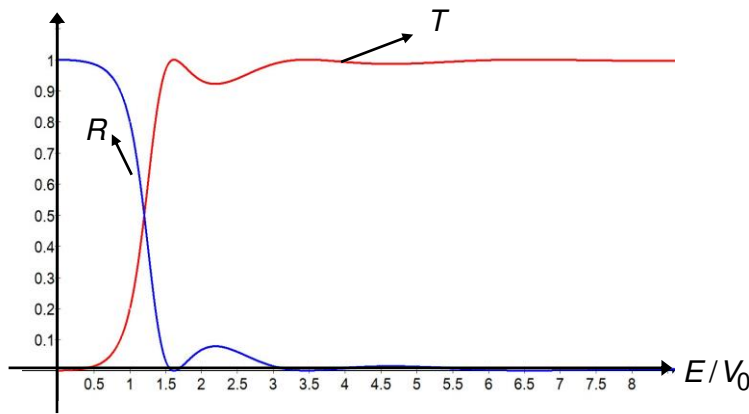


Fig. 11.6: The typical variation of the reflection coefficient R and transmission coefficient T with E/V_0 , for $\frac{2mV_0L^2}{\hbar^2} = 16$.

Notice that the value of T is close to 1 for $E > V_0$ and actually equal to 1 at some points. These are the points at which $T=1$ in Eq. (11.29a) and so we must have:

$$\sin^2(\alpha L) = 0 \Rightarrow \alpha L = n\pi \text{ for } n=1,2,3\dots \quad (11.30)$$

These points of perfect transmission, or $T=1$ are called “transmission resonances and the energies at which they occur can be calculated from Eq. (11.30). At these energies, a quantum particle will cross the potential barrier without any reflection.

REFLECTION AND TRANSMISSION COEFFICIENT ($E > V_0$)

Recap

The wave function for the three regions for $E > V_0$ are:

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad (\text{for } x < 0) \quad (11.3)$$

$$\psi_{II}(x) = Ce^{i\alpha x} + De^{-i\alpha x} \quad (\text{for } 0 \leq x \leq L) \quad (11.12)$$

$$\psi_{III}(x) = Fe^{ikx} \quad (\text{for } x > L) \quad (11.5)$$

where $\alpha = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$ and $k = \sqrt{\frac{2mE}{\hbar^2}}$.

The transmission and reflection coefficients are:

$$T = \left[1 + \frac{V_0^2}{4E(E - V_0)} \sin^2(\alpha L) \right]^{-1} \quad (11.29a)$$

$$R = \left[1 + \frac{4E(E - V_0)}{V_0^2 \sin^2(\alpha L)} \right]^{-1} \quad (11.29b)$$

The points of perfect transmission at which $T=1$ and $R=0$, are called “transmission resonances” and are given by the condition:

$$\alpha L = n\pi, n=1,2,3\dots$$

Let us now look at some interesting applications of quantum tunnelling which also point towards the success of quantum mechanics.

11.3 APPLICATIONS OF QUANTUM TUNNELLING

We discuss two important applications which are alpha decay and scanning tunnelling microscopy.

11.3.1 Alpha Decay

Alpha decay is the process in which the isotopes of certain radioactive elements like uranium, radium and bismuth, decay by emitting alpha (α) particles. Alpha particles are helium nuclei with two neutrons and two protons. After emitting the alpha particle, the original nucleus (parent nucleus) is transformed into a different atomic nucleus (the daughter nucleus), with the mass number reduced by four and the atomic number reduced by two. The following two aspects of the alpha decay process were not explained for a long time:

- All alpha particles emitted from the same source have almost the same kinetic energy. If they are emitted from different sources, the kinetic energies all lie within a narrow range of 4.0 to 9.0 MeV.
- The half-life of the radioactive element from which the alpha particle is emitted, however varies over a very large range: for example the half-life for polonium-214 is 160 μ s and the half life of uranium-238 is around 4.5 billion years. Incidentally the kinetic energies of the emitted alpha particles are ~ 7.7 MeV for polonium and 4.3 MeV for uranium.

This large variation in the half-lives of the parent element in the alpha decay process was explained by George Gamow using the concept of quantum tunnelling. He assumed that before the alpha decay takes place, an alpha particle exists inside the parent nucleus and is bound by the attractive potential of the strong nuclear force. You may consider the nucleus to be a kind of rigid spherical box inside which the alpha particle is confined. The alpha particle is free to move between the walls of the box. It does have a finite kinetic energy but this kinetic energy is much less than what required to escape from the nucleus, leaving behind the daughter nucleus. So classically, the alpha particle should remain forever remain bound inside the parent nucleus.

We consider a somewhat simplified picture as shown in Fig. 11.7, in which the potential function is plotted as a function of the distance from the centre of the nucleus. In this the nuclear potential which binds the alpha particle is represented by a square well. The nuclear force itself is extremely short-ranged ($\sim 10^{-15}$ m) and hence it is not significant outside the nucleus. Typically the radius of the nucleus is about 1 fm ($\sim 10^{-14}$ m). Suppose the alpha particle now tunnels out of the nucleus, leaving behind the daughter nucleus. Once the alpha particle escapes the nucleus by tunnelling through the nuclear potential barrier, the only force acting on it is the Coulomb repulsive force due to the (daughter) nucleus. Therefore outside the radius of the nucleus ($r > R_0$)

), the potential is modified by the Coulomb repulsion $V(r)$ between the alpha particle(which has a charge $2e$) and the daughter nucleus(which has a charge Ze). r is the distance between alpha particle and the nucleus. $V(r)$ is given by:

$$V(r) = \frac{(Ze)(2e)}{4\pi\epsilon_0 r} = \frac{Ze^2}{2\pi\epsilon_0 r} \quad (11.31)$$

The shaded region shows the forbidden region for the alpha – particle.

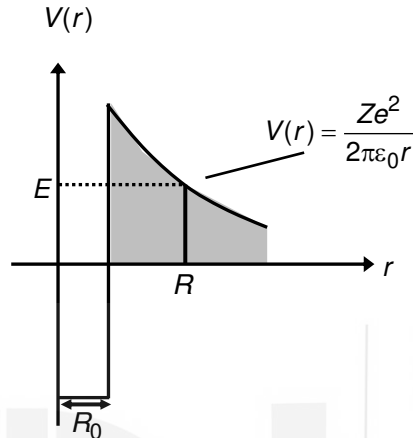


Fig. 11.7: Potential barrier for alpha-particle decay.

The kinetic energy of the alpha particle is E . At the point R , at which the alpha particle escapes the nucleus, the kinetic energy of the alpha particle is at least equal to the electrostatic energy between it and the daughter nucleus. So, at $r = R$,

$$E = \frac{Ze^2}{2\pi\epsilon_0 R} \quad (11.32)$$

It is possible to calculate the **tunnelling probability for the alpha particle**, which is just the transmission coefficient T which you have studied in Sec. 11.2.2. Instead of the potential barrier of constant height which you have studied earlier in this unit, here the potential barrier is described by the function $V(r)$ defined in Eq. (11.31). The transmission coefficient (of Eq. 11.26) now looks like:

$$T \approx e^{-2K'L} = e^{-2 \int_{R_0}^R \sqrt{\frac{2m}{\hbar^2}(V(r)-E)} dr} \quad (11.33)$$

This tunnelling probability, T , is the probability of emission of an alpha particle from a nucleus. T is used to calculate the decay rate λ for the nucleus, which is the **alpha particle emission probability per unit time**. To calculate λ , we multiply T by the number of times the alpha particle approaches the barrier per second. This number is just $\frac{v}{2R_0}$, where v is the speed of the alpha particle inside the nucleus. v can be calculated from the kinetic energy E of the alpha particle, when it escapes from the nucleus. Typically $\frac{v}{2R_0} \approx 10^{21}$ collisions per second and the decay rate $\lambda = 10^{21}T$.

The decay rate is used to calculate the half-life of the parent nucleus using the relation $T_{1/2} = .693 / \lambda$. From Eq. (11.33), you can see that for a very small change in E , there will be a disproportionately large change in λ and hence in $T_{1/2}$. So the more energetic α -particles have a better chance to escape the nucleus, and, for such nuclei, the nuclear disintegration half-life will be shorter.

We now describe in brief another important device based on the tunnelling phenomena, which is extensively used in materials science research today.

11.3.2 Scanning Tunnelling Microscope

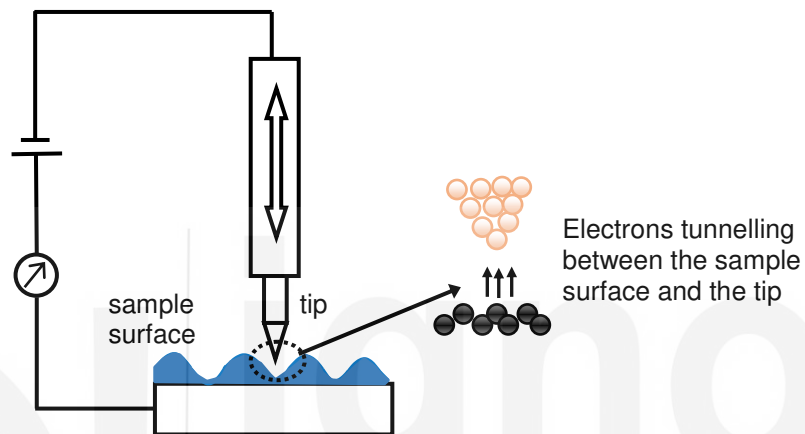


Fig. 11.7: Schematic Diagram of a Scanning Tunnelling Microscope

The Scanning Tunnelling Microscope (STM) is a type of microscope which is used for imaging surfaces at the atomic level. It is based on the phenomenon of field emission, in which electrons bound inside a metal are removed from its surface by a very strong electric field. This happens by the quantum tunnelling of electrons through the potential barrier.

The STM consists of

- a very sharp, conducting (typically tungsten, gold, or platinum—iridium) tip (**probe**), which scans the surface to be imaged;
- a piezoelectric device which can control the height of the tip above the surface to be scanned (typically 0.4 to 0.7 nm); and
- a mechanism to move the tip over the surface being studied.

There is of course a complex instrumentation that converts the inputs into a computer imagery of the surface. Here we shall discuss only the basic principle of the microscope.

When the tip is brought very close to the surface and a voltage difference exists between the tip and the surface, electrons tunnel through the gap between the tip and the surface and set up a tunnelling current. The tunnelling current (which is proportional to the tunnelling probability of the electron through the barrier) will depend on the distance between the tip and the surface (this is the width of the barrier). So as we scan the tip over the sample at a fixed height, the distance and hence the tunnelling current will depend on

the corrugations on the surface of the material. The variations in current are converted into an image of the topography of the surface of the material. The sensitivity of the microscope is such that the resolution is of the order of 0.001 nm, which is even less than the typical diameter of an atom.

APPLICATIONS OF QUANTUM TUNNELLING

Recap

Alpha Decay

The process of emission of alpha particles from a radioactive nucleus takes place by the quantum tunnelling. The alpha particle is initially trapped in a potential well by the nucleus. Classically, it cannot escape from the nucleus. However quantum mechanics allows for a finite probability of tunnelling of the alpha particle through the potential barrier created by the nuclear potential. The lifetime of the radioactive nucleus is calculated from tunnelling probability.

Scanning Tunnelling Microscope

The Scanning Tunnelling Microscope (STM) is a type of microscope which is used for imaging surfaces at the atomic level and works on the principle of quantum tunnelling. When the tip of the STM is very close to the surface, the voltage difference between the tip and the surface causes electrons to tunnel through the gap and set up a tunnelling current which depends on the distance between the tip and the surface. This is used to create an image of the surface.

11.4 SUMMARY

Concept	Description
One-dimensional Potential Barrier	■ The potential energy function for a one-dimensional potential barrier of width L is: $V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } 0 \leq x \leq L \\ 0 & \text{for } x > L \end{cases}$ The time independent Schrödinger equation for a particle of mass m is: $-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad (\text{for } x < 0 \text{ and } x > L)$

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

The solutions of the Schrödinger equations are:

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad (\text{for } x < 0)$$

$$\psi_{II}(x) = Ce^{k'x} + De^{-k'x} \quad (\text{for } 0 \leq x \leq L)$$

$$\psi_{III}(x) = Fe^{ikx} \quad (\text{for } x > L)$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad \text{and} \quad k' = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

Reflection and transmission coefficients for $E < V_0$

- The transmission coefficient T is the probability of a particle being transmitted through the barrier and is given by:

$$T = \left[1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(k'L) \right]^{-1}$$

Where

$$k'L = \sqrt{\frac{2mL^2(V_0 - E)}{\hbar^2}} = \sqrt{\frac{2mV_0L^2}{\hbar^2} \left(1 - \frac{E}{V_0} \right)}$$

The reflection coefficient R is the probability of the particle being reflected at the barrier edge and is given by:

$$R = \left[1 + \frac{4E(V_0 - E)}{V_0^2 \sinh^2(k'L)} \right]^{-1}$$

The sum of the reflection and transmission coefficients is 1.

For wide barriers and large values of V_0 the transmission coefficient is:

$$T \approx \left[\frac{V_0^2}{4E(V_0 - E)} \left(\frac{e^{2k'L}}{4} \right) \right]^{-1} = \frac{16E}{V_0} \left(1 - \frac{E}{V_0} \right) e^{-\frac{2L}{\lambda_T}}$$

where the **tunnelling length** λ_T is:

$$\lambda_T = \frac{1}{k'} = \frac{\hbar}{\sqrt{2m(V_0 - E)}}$$

The probability of finding the particle is appreciable only within about λ_T of the barrier edge.

Reflection and transmission coefficients for $E > V_0$

- The wave function for the three regions for $E > V_0$ are:

$$\psi_I(x) = Ae^{ikx} + Be^{-ikx} \quad (\text{for } x < 0)$$

$$\psi_{II}(x) = Ce^{i\alpha x} + De^{-i\alpha x} \quad (\text{for } 0 \leq x \leq L)$$

$$\psi_{III}(x) = Fe^{ikx} \quad (\text{for } x > L)$$

where $\alpha = \sqrt{\frac{2m(E - V_0)}{\hbar^2}}$ and $k = \sqrt{\frac{2mE}{\hbar^2}}$.

The reflection and transmission coefficients are:

$$T = \left[1 + \frac{V_0^2}{4E(E - V_0)} \sin^2(\alpha L) \right]^{-1}$$

$$R = \left[1 + \frac{4E(E - V_0)}{V_0^2 \sin^2(\alpha L)} \right]^{-1}$$

The points of perfect transmission at which $T=1$ and $R=0$ are called “transmission resonances and are given by the condition: $\alpha L = n\pi$ for $n = 1, 2, 3, \dots$

Applications of quantum tunnelling ■ Alpha Decay

The process of emission of alpha particles from a radioactive nucleus takes place by the quantum tunnelling. The alpha particle is initially trapped in a potential well by the nucleus. Classically, it cannot escape from the nucleus. However quantum mechanics allows for a finite probability of tunnelling of the alpha particle through the potential barrier created by the nuclear potential. The lifetime of the radioactive nucleus is calculated from tunnelling probability.

Scanning Tunnelling Microscope

The Scanning Tunnelling Microscope (STM) is a type of microscope which is used for imaging surfaces at the atomic level and works on the principle of quantum tunnelling. When the tip of the STM is very close to the surface, the voltage difference between the tip and the surface causes electrons to tunnel through the gap and set up a tunnelling current which depends on the distance between the tip and the surface. This is used to create an image of the surface.

11.5 TERMINAL QUESTIONS

1. An electron with a kinetic energy 4.0 eV is incident on a potential barrier of height 10.0 V and width 0.80 nm. Calculate the tunnelling length and tunnelling probability of the electron to tunnel through the barrier (use Eq. 11.28).
2. For the electron of TQ1, calculate in which case the tunnelling probability increases more:
 - (i) when the width of the barrier is reduced to 0.4 nm, other parameters remaining the same.

- (ii) when energy of the electron increases to 8 eV, other parameters remaining the same.
3. An electron and a proton with the same kinetic energy E are incident on a potential barrier of height V_0 and width L . Calculate the ratio of their tunnelling probabilities.
 4. An electron with a energy of 8.0 eV strikes a potential barrier of energy 10.0 eV. If the tunnelling probability is 2.0 percent, determine the width of the barrier (use Eq. 11.28).
 5. An electron has a kinetic energy of 8.0 eV. The electron is incident upon a rectangular barrier of height 15.0 eV which has a thickness of 1.0 nm. Calculate the increase in the tunnelling probability of the electron if it absorbs all the energy of a photon of blue light (3.1 eV).
 6. Calculate the probability that an electron will tunnel through a 0.4 nm gap from a metal to the STM probe if the work function is 3.0 eV. By what factor does the tunnelling probability change if we increase the gap to 0.50 nm.

11.6 SOLUTIONS AND ANSWERS

Self-Assessment Questions

1. Following the steps of Example 11.2, we first calculate the tunnelling length λ_T using Eq. (11.27) with $E = 1.5 \text{ eV}$, $V_0 = 2.0 \text{ eV}$ and $m = 0.22m_e$. So:

$$V_0 - E = 0.50 \text{ eV} = 0.80 \times 10^{-19} \text{ J}$$

$$\lambda_T = \frac{1.054 \times 10^{-34} \text{ Js}}{\sqrt{2 \times (0.22 \times 9.109 \times 10^{-31} \text{ kg}) \times (0.80 \times 10^{-19} \text{ J})}} = 0.58 \text{ nm} \quad (\text{i})$$

Using Eq. (11.28) with $\frac{E}{V_0} = \frac{1.5 \text{ eV}}{2.0 \text{ eV}} = \frac{3}{4}$, $L = 0.10 \text{ nm}$, and λ_T as

calculated in Eq. (i) we calculate the transmission coefficient T :

$$T = 16 \times \left(\frac{3}{4}\right) \times \left(1 - \frac{3}{4}\right) e^{-\frac{2 \times 0.10 \text{ nm}}{0.58 \text{ nm}}} = 3 e^{-0.34}$$

Terminal Questions

1. We first calculate the tunnelling length λ_T using Eq. (11.27) with $E = 4.0 \text{ eV}$, $V_0 = 10.0 \text{ eV}$ and $m = m_e$:

$$\therefore \lambda_T = \frac{1.054 \times 10^{-34} \text{ Js}}{\sqrt{2 \times (9.109 \times 10^{-31} \text{ kg}) \times (9.6 \times 10^{-19} \text{ J})}} = 0.08 \text{ nm} \quad (\text{i})$$

With $\frac{E}{V_0} = \frac{4.0 \text{ eV}}{10.0 \text{ eV}} = \frac{2}{5}$, $L = 0.80 \text{ nm}$ and $\lambda_T = 0.8 \text{ nm}$ in Eq. (11.28):

$$T = 16 \times \left(\frac{2}{5}\right) \times \left(1 - \frac{2}{5}\right) e^{\frac{-2 \times 0.80 \text{ nm}}{0.08 \text{ nm}}} = \left(\frac{96}{25}\right) e^{-20} = (3.84) e^{-20}$$

2. Let us denote the transmission coefficient calculated in TQ 1 by T_0

$$\text{So } T_0 = (3.84) e^{-20} \quad (\text{i})$$

i) With $L = 0.40 \text{ nm}$, $\lambda_T = 0.08 \text{ nm}$ and $\frac{E}{V_0} = \frac{2}{5}$ in Eq. (11.28) :

$$T_1 = 16 \left(\frac{2}{5}\right) \left(1 - \frac{2}{5}\right) e^{\frac{-2 \times 0.40 \text{ nm}}{0.08 \text{ nm}}} = (3.84) e^{-10} \quad (\text{ii})$$

ii) We first calculate λ_T with $E = 8.0 \text{ eV}$, $V_0 = 10 \text{ eV}$ and $m = m_e$

$$\lambda_T = \frac{(1.054 \times 10^{-34} \text{ Js})}{\sqrt{2 \times (9.109 \times 10^{-31} \text{ kg}) \times (3.2 \times 10^{-19} \text{ J})}} = 0.14 \text{ nm}$$

Then with $E = 8 \text{ eV}$, $L = 0.80 \text{ nm}$, $\frac{E}{V_0} = \frac{8.0 \text{ eV}}{10.0 \text{ eV}} = \frac{4}{5}$ and

$\lambda_T = 0.14 \text{ nm}$, we get from Eq. (11.28):

$$T_2 = 16 \left(\frac{4}{5}\right) \left(1 - \frac{4}{5}\right) e^{\frac{-2 \times 0.80 \text{ nm}}{0.14 \text{ nm}}} = \left(\frac{64}{25}\right) e^{-11.4} = (2.56) e^{-11.4} \quad (\text{iii})$$

We now calculate the ratios of the transmission coefficients T_1 and T_2 with respect to T_0 :

$$\frac{T_1}{T_0} = \frac{(3.84) e^{-10}}{(3.84) e^{-20}} = e^{10}$$

$$\text{and } \frac{T_2}{T_0} = \frac{(2.56) e^{-11.4}}{(3.84) e^{-20}} = (0.67) e^{8.6}$$

Since $e^{10} > 0.67 e^{8.6}$ we can say that the tunnelling probability increases more in case (i) when width of the barrier is decreased.

3. Let us say that the tunnelling length for the electron is

$$\lambda_{TE} = \frac{\hbar}{\sqrt{2m_e(V_0 - E)}}$$

And the tunnelling length for the proton ($m_P = 1836m_e$) is

$$\begin{aligned} \lambda_{TP} &= \frac{\hbar}{\sqrt{2m_P(V_0 - E)}} \\ &= \frac{\hbar}{\sqrt{2(1836m_e)(V_0 - E)}} = \frac{\hbar}{\sqrt{2m_e(V_0 - E)} \sqrt{1836}} = \frac{\lambda_{Te}}{43} \end{aligned} \quad (\text{i})$$

The transmission coefficient for the electron is

$$T_e = 16 \left(\frac{E}{V_0} \right) \left(1 - \frac{E}{V_0} \right) e^{-\frac{2L}{\lambda_{Te}}}$$

and for the proton it is:

$$T_p = 16 \left(\frac{E}{V_0} \right) \left(1 - \frac{E}{V_0} \right) e^{-\frac{2L}{\lambda_{Tp}}}$$

$$\therefore \frac{T_e}{T_p} = \frac{e^{-\frac{2L}{\lambda_{Te}}}}{e^{-\frac{2L}{\lambda_{Tp}}}} = \frac{e^{-\frac{2L}{\lambda_{Te}}}}{e^{-\frac{2L}{(\lambda_{Te}/43)}}} = e^{42 \left(\frac{2L}{\lambda_{Te}} \right)} \Rightarrow T_e \gg T_p$$

4. We calculate the tunnelling length by using Eq.(11.27) with $V_0 - E = 2 \text{ eV} = 3.2 \times 10^{-19} \text{ J}$

$$\text{So } \lambda_T = \frac{(1.054 \times 10^{-34} \text{ Js})}{\sqrt{2 \times (9.109 \times 10^{-31} \text{ kg}) \times (3.2 \times 10^{-19} \text{ J})}} = 0.14 \text{ nm} \quad (\text{i})$$

The tunnelling probability is calculated using Eq.(11.28) with $\frac{E}{V_0} = \frac{8 \text{ eV}}{10 \text{ eV}} = \frac{4}{5}$ and $\lambda_T = 0.14 \text{ nm}$. Given that $T = 2\% = \frac{1}{50}$ we can write:

$$\begin{aligned} T &= \frac{1}{50} = 16 \times \left(\frac{4}{5} \right) \left(1 - \frac{4}{5} \right) e^{-\frac{2L}{0.14 \text{ nm}}} \\ \Rightarrow e^{-\frac{2L}{0.14 \text{ nm}}} &= \frac{25}{64 \times 50} \text{ or } e^{\frac{2L}{0.14 \text{ nm}}} = 128 \end{aligned}$$

Taking the logarithm of both sides,

$$\frac{2L}{0.14 \text{ nm}} = \ln(128) \Rightarrow L = 0.07 \times (4.85) \text{ nm} = 0.34 \text{ nm}$$

5. We first calculate the tunnelling length using Eq. (11.27), with $V_0 - E = (15.0 - 8.0) \text{ eV} = 11.2 \times 10^{-19} \text{ J}$

$$\therefore \lambda_T = \frac{1.054 \times 10^{-34} \text{ Js}}{\sqrt{2 \times (9.109 \times 10^{-31} \text{ kg}) \times (11.2 \times 10^{-19} \text{ J})}} = 0.074 \times 10^{-9} \text{ m} = 0.074 \text{ nm} \quad (\text{i})$$

The tunnelling probability T_1 is calculated using Eq. (11.28) with $L = 1.0 \text{ nm}$, $E/V_0 = \frac{8.0 \text{ eV}}{15.0 \text{ eV}}$ and $\lambda_T = \frac{1}{k'} = 0.074 \text{ nm}$

$$\therefore T_1 = 16 \times \left(\frac{8}{15} \right) \left(1 - \frac{8}{15} \right) e^{-\frac{2 \times 1.0 \text{ nm}}{0.074 \text{ nm}}} = (4.0) e^{-27} \quad (\text{ii})$$

When electron absorbs an photon of energy 3.1eV its kinetic energy becomes

$$E = (8.0 + 3.1)\text{eV} = 11.1\text{eV}. \text{ So } V_0 - E = 3.9\text{eV} = 6.24 \times 10^{-19} \text{ J}$$

Now the tunnelling length is,

$$\lambda_T = \frac{1.054 \times 10^{-34} \text{ Js}}{\sqrt{2 \times (9.109 \times 10^{-31} \text{ kg}) \times (6.24 \times 10^{-19} \text{ J})}} = 0.098 \text{ nm} \quad (\text{iii})$$

With $E/V_0 = \frac{11.1}{15.0}$ and λ_T given by Equation (iii) the tunnelling probability is:

$$T_2 = 16 \times \left(\frac{11.1}{15.0} \right) \left(1 - \frac{11.1}{15.0} \right) e^{\frac{-2 \times 1.0 \text{ nm}}{0.098 \text{ nm}}} = (3.1) e^{-20.4}$$

So the increase in the tunnelling probability is:

$$\frac{T_2}{T_1} = \frac{(3.1) e^{-20.4}}{(4.0) e^{-27.0}} = \left(\frac{3.1}{4.0} \right) \times e^{6.6} \approx 570$$

So the tunnelling probability increases about 570 times.

6. Since the electron must overcome the work function, we can assume that the value of $V_0 - E$ is at least $\approx 3\text{eV} = 4.8 \times 10^{-19} \text{ J}$

So the typical tunnelling length can be calculated using Eq. (11.27)

$$\lambda_T = \frac{1.054 \times 10^{-34} \text{ Js}}{\sqrt{2 \times (9.109 \times 10^{-31} \text{ kg}) \times (4.8 \times 10^{-19} \text{ J})}} = 0.11 \text{ nm}$$

Given that E, V_0 are fixed we can write that the tunnelling probability is a function only of the gap between the tip of the STM probe and the surface

$$\text{i.e. } T = f(E/V_0) e^{-2L/\lambda_T}.$$

For $L = 0.40 \text{ nm}$, the transmission coefficient is

$$T_1 = f(E/V_0) e^{\frac{2 \times (0.40 \text{ nm})}{(0.11 \text{ nm})}} = f(E/V_0) e^{-7.3}$$

For $L = 0.50 \text{ nm}$ the transmission coefficient is

$$T_2 = f(E/V_0) e^{\frac{2 \times 0.50 \text{ nm}}{0.11 \text{ nm}}} = f(E/V_0) e^{-9.1}$$

$$\therefore \frac{T_2}{T_1} = \frac{f(E/V_0) e^{-9.1}}{f(t/V_0) e^{-7.3}} = e^{-1.8} \approx \frac{1}{6}$$

The tunnelling probability reduces by $1/6$ when the distance between the tip and the surface increases by 0.10 nm . The tunnelling current also changes proportionally. This is why the STM can detect variations even of the order of 0.10 nm on the surface of a material.

APPENDIX 11A: CALCULATING THE REFLECTION AND TRANSMISSION COEFFICIENTS

After applying the boundary conditions on the wave functions and their derivatives for $E < V_0$, we have derived the following equations for A , B , C , D and F :

$$A + B = C + D \quad (11.15a)$$

$$e^{k'L}C + e^{-k'L}D = e^{ikL}F \quad (11.15b)$$

$$ikA - ikB = k'C - k'D \quad (11.17a)$$

$$k'e^{k'L}C - k'e^{-k'L}D = ike^{ikL}F \quad (11.17b)$$

Let us first calculate the value of B/A from these equations. For this we eliminate the constants C and D from the Eqs. (11.15a, 11.15b, 11.17a and 11.17b). Multiplying Eq. (11.15a) by k' we get:

$$k'A + k'B = k'C + k'D \quad (i)$$

Adding Eqs. (11.17a) and (i) we get:

$$(k' + ik)A + (k' - ik)B = 2k'C \quad (ii)$$

Subtracting Eq. (11.17a) from Eq. (i) we get

$$(k' - ik)A + (k' + ik)B = 2k'D \quad (iii)$$

Multiplying Eq. (11.15b) by ik we get:

$$ike^{k'L}C + ike^{-k'L}D = ike^{ikL}F \quad (iv)$$

Subtracting Eq. (iv) from Eq. (11.17b) we get

$$(k' - ik)e^{k'L}C - (k' + ik)e^{-k'L}D = 0 \quad (v)$$

Which we can write as:

$$(k' - ik)e^{k'L}C = (k' + ik)e^{-k'L}D$$

$$\text{or } C = \frac{(k' + ik)e^{-k'L}}{(k' - ik)e^{k'L}} D \quad (vi)$$

Eq. (vi) gives us the relation between C and D . Substituting for C from Eq. (vi) into Eq. (ii) we get:

$$(k' + ik)A + (k' - ik)B = 2k' \frac{(k' + ik)e^{-k'L}}{(k' - ik)e^{k'L}} D$$

Which is:

$$\frac{(k' - ik)e^{k'L}}{(k' + ik)e^{-k'L}} [(k' + ik)A + (k' - ik)B] = 2k'D \quad (vii)$$

You can see that the RHS of Eqs. (iii) and (vii) are equal. Equating the LHS of these two equations we get:

$$\frac{(k' - ik)e^{k'L}}{(k' + ik)e^{-k'L}} [(k' + ik)A + (k' - ik)B] = (k' - ik)A + (k' + ik)B \quad (\text{viii})$$

On simplifying, we can write Eq. (viii) as:

$$(k' - ik)e^{k'L} [(k' + ik)A + (k' - ik)B] = (k' + ik)e^{-k'L} [(k' - ik)A + (k' + ik)B]$$

Which is:

$$(k' - ik)(k' + ik)e^{k'L}A + (k' - ik)^2 e^{k'L}B = (k' + ik)(k' - ik)e^{-k'L}A + (k' + ik)^2 e^{-k'L}B$$

Using $(k' - ik)(k' + ik) = k'^2 + k^2$ we can write:

$$(k'^2 + k^2)e^{k'L}A + (k' - ik)^2 e^{k'L}B = (k'^2 + k^2)e^{-k'L}A + (k' + ik)^2 e^{-k'L}B \quad (\text{ix})$$

Dividing Eq. (ix) by A we get

$$(k'^2 + k^2)e^{k'L} + (k' - ik)^2 e^{k'L} \frac{B}{A} = (k'^2 + k^2)e^{-k'L} + (k' + ik)^2 e^{-k'L} \frac{B}{A} \quad (\text{x})$$

Therefore we have

$$\frac{B}{A} = \frac{(k'^2 + k^2)(e^{-k'L} - e^{k'L})}{(k' - ik)^2 e^{k'L} - (k' + ik)^2 e^{-k'L}} \quad (\text{xi})$$

which is:

$$\frac{B}{A} = \frac{(k'^2 + k^2)(e^{-k'L} - e^{k'L})}{(k'^2 - k^2)(e^{k'L} - e^{-k'L}) - (2ik'k)(e^{k'L} + e^{-k'L})} \quad (\text{xii})$$

Or

$$\frac{B}{A} = \frac{(k'^2 + k^2) \sinh(k'L)}{(k^2 - k'^2) \sinh(k'L) + 2ik'k \cosh(k'L)} \quad (\text{xii})$$

The reflection coefficient is $R = \frac{|B|^2}{|A|^2}$ (Eq. 11.21). Using the value of B/A

obtained in Eq. (xii) we can write (see the margin remark):

$$R = \frac{(k'^2 + k^2)^2 \sinh^2(k'L)}{(k^2 - k'^2)^2 \sinh^2(k'L) + 4k'^2 k^2 \cosh^2(k'L)} \quad (\text{xiii})$$

Using the identity $\sinh^2(k'L) - \cosh^2(k'L) = 1$, we can simplify the denominator of the RHS of Eq. (xiii) as

$$\begin{aligned} & (k^2 - k'^2)^2 \sinh^2(k'L) + 4k'^2 k^2 \cosh^2(k'L) \\ &= (k^2 - k'^2)^2 \sinh^2(k'L) + 4k'^2 k^2 \sinh^2(k'L) + 4k'^2 k^2 \cosh^2(k'L) - 4k'^2 k^2 \sinh^2(k'L) \\ &= (k^2 - k'^2)^2 \sinh^2(k'L) + 4k'^2 k^2 \end{aligned}$$

Notice that B/A given in Eq. (xii) is complex and it has the general form:

$$\begin{aligned} \frac{B}{A} &= \frac{u}{v + iw} \\ &= \frac{u}{v + iw} \left(\frac{v - iw}{v - iw} \right) \\ &= \frac{uv - iuw}{v^2 + w^2} \end{aligned}$$

$$\begin{aligned} \left| \frac{B}{A} \right|^2 &= \frac{(uv)^2 + (uw)^2}{(v^2 + w^2)^2} \\ &= \frac{u^2(v^2 + w^2)}{(v^2 + w^2)^2} \\ &= \frac{u^2}{(v^2 + w^2)} \end{aligned}$$

With :

$$u = (k'^2 + k^2) \sinh(k'L)$$

$$v = (k^2 - k'^2) \sinh(k'L)$$

And

$$w = 2k'k \cosh(k'L)$$

We get the result of Eq. (xiii).

Therefore

$$R = \frac{(k'^2 + k^2)^2 \sinh^2(k'L)}{(k^2 + k'^2)^2 \sinh^2(k'L) + 4k'^2 k^2} = \left[\frac{(k^2 + k'^2)^2 \sinh^2(k'L) + 4k'^2 k^2}{(k'^2 + k^2)^2 \sinh^2(k'L)} \right]^{-1} \quad (\text{xiv})$$

From Eqs.(11.6 and 11.9) we also know that $k = \sqrt{\frac{2mE}{\hbar^2}}$ and

$$k' = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}.$$

$$\text{So, } k^2 = \frac{2mE}{\hbar^2}; \text{ and } k'^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

and

$$k'^2 + k^2 = \frac{2m(V_0 - E)}{\hbar^2} + \frac{2mE}{\hbar^2} = \frac{2mV_0}{\hbar^2}; k'^2 k^2 = \frac{2m(V_0 - E)}{\hbar^2} \times \frac{2mE}{\hbar^2} \quad (\text{xv})$$

Substituting from Eq. (xv) into Eq. (xiv) we get the result of Eq. (11.24b):

$$R = \left[1 + \frac{4k'^2 k^2}{(k'^2 + k^2)^2 \sinh^2(k'L)} \right]^{-1} = \left[1 + \frac{4E(V_0 - E)}{V_0^2 \sinh^2(k'L)} \right]^{-1}$$

To calculate T we use Eq. (11.23). Hence $T=1-R$. Using the value of R from Eq. (xiv) we get:

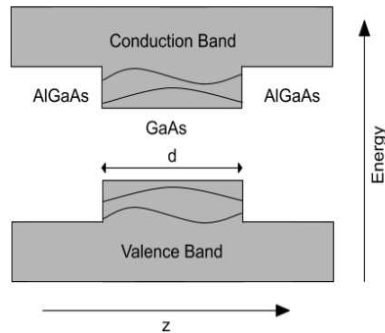
$$\begin{aligned} T = 1 - R &= 1 - \frac{(k'^2 + k^2)^2 \sinh^2(k'L)}{(k^2 + k'^2)^2 \sinh^2(k'L) + 4k'^2 k^2} = \frac{4k'^2 k^2}{(k^2 + k'^2)^2 \sinh^2(k'L) + 4k'^2 k^2} \\ &= \left[1 + \frac{(k^2 + k'^2)^2 \sinh^2(k'L)}{4k'^2 k^2} \right]^{-1} \end{aligned} \quad (\text{xvi})$$

Substituting from Eq. (xv) into Eq.(xvi) we get the following result of Eq.(11.24a):

$$T = \left[1 + \frac{V_0^2 \sinh^2(k'L)}{4E(V_0 - E)} \right]^{-1}$$

UNIT 12

FINITE POTENTIAL WELL



A quantum well system can be constructed by inserting a thin layer of one type of semiconductor material between two layers of another with a different band-gap. [PFMoses, CC BY-SA 4.0 <<https://creativecommons.org/licenses/by-sa/4.0/>>, via Wikimedia Commons]

Structure

- 12.1 Introduction
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 - Parity of the Eigen Functions
 - Energy Eigen Values
 - Symmetric Infinite Potential Well

- 12.3 Summary
- 12.4 Terminal Questions
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STUDY GUIDE

In this unit you will solve the one-dimensional Schrödinger equation for a finite potential well. You have already solved the Schrödinger equation for the infinite potential well in Unit 9. Here the mathematical solution of the differential equation with the relevant boundary conditions are slightly more difficult, so please study this carefully. You must also understand how the finite well is different from the infinite well. You will use the concepts of differential and integral calculus, second order ODEs and complex number. You must work out all the steps of each derivation and work through all the SAQs and TQS.

“Once again I repeat : the aim of physics at its most fundamental level is not just to describe the world but to explain why it is the way it is.”

Steven Weinberg

12.1 INTRODUCTION

In Unit 9 you have solved the time independent Schrödinger equation for a particle confined to a one-dimensional box. That was modelled by a one-dimensional infinite potential well, in which the probability of finding the box outside the well was exactly zero. A particle rigidly confined by an infinite potential well is an idealization which does not correspond to any real physical situation. Given sufficient energy, it is always possible for a particle to escape the confines of a well. Hence, it is important that we study the behaviour of a quantum particle in a finite potential well. The important difference between the two systems is that in this case, even if the kinetic energy of the particle in the well is less than the potential energy, there is a finite probability of finding the quantum particle outside the well.

In Sec. 12.2 we solve the Schrödinger equation for the quantum particle in the symmetric finite potential well. As you have studied, whenever a particle is bound to a certain region of space, the energy spectrum is discrete and not continuous. We learn how to calculate the energy eigen values and the corresponding eigen functions. You will see that the eigen functions have a definite parity which is a consequence of the symmetry of the potential function. We also study the symmetric infinite potential well.

With this unit we complete our study of quantum mechanics. In the next block you will study the fundamental concepts of nuclear physics.

Expected Learning Outcomes

After studying this unit, you should be able to:

- ❖ solve the time independent one-dimensional Schrödinger equation for the finite potential well;
- ❖ determine the eigen functions and eigenvalues for a particle in a one-dimensional finite potential well;
- ❖ determine the zero-point energy;
- ❖ determine the eigen functions and eigenvalues for a particle in a one-dimensional symmetric infinite potential well; and
- ❖ state the parity of the stationary state wave functions.

12.2 ONE-DIMENSIONAL FINITE POTENTIAL WELL

Let us first define the potential function $V(x)$ for the one-dimensional finite potential well:

$$V(x) = \begin{cases} V_0 & \text{for } x < -a \\ 0 & \text{for } -a \leq x \leq a \\ V_0 & \text{for } x > a \end{cases} \quad (12.1)$$

Note that the well defined by Eq. (12.1) has the following features:

- The potential energy V_0 is finite for $x < -a$ as well as for $x > a$.
- The potential energy is zero for $-a \leq x \leq a$.
- The potential function $V(x)$ is symmetric, i.e. $V(x) = V(-x)$

This potential is sometimes referred to as the square potential well in text books. $V(x)$ is shown in Fig. 12.1.

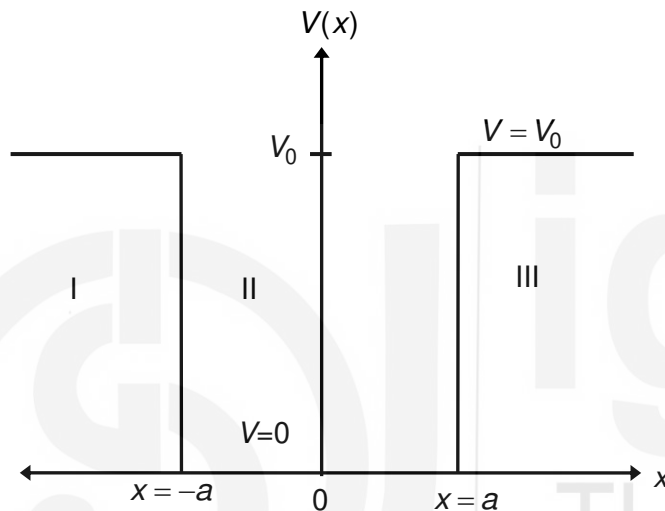


Fig. 12.1: A one-dimensional finite potential well. The potential energy is V_0 for $x < -a$ (Region I) and for $x > a$ (Region III). It is zero for $-a \leq x \leq a$ (Region II).

If the total energy (E) of a classical particle is greater than the barrier height V_0 , it can move freely in the entire region, including the region $x < -a$ and $x > a$. Its kinetic energy would be $E - V_0$ in the region $x < -a$ and $x > a$ and E in the region $-a \leq x \leq a$. However, if E is less than V_0 , the classical particle would remain bound forever in the region $-a \leq x \leq a$. It would move back and forth in the region with a constant speed (and a momentum of constant magnitude) and the total energy of the particle could have any value $E \geq 0$. Quantum mechanically, however, a bound particle can only have certain discrete values of the energy. Further, as you have also seen in Units 10 and 11, there is a finite probability for the quantum mechanical particle to penetrate the classically forbidden region i.e., $x < -a$ as well as $x > a$ even if its energy $E < V_0$.

The square shape of the potential is an over-simplification. However we study this simpler shape because it is relatively easier to solve and it does capture the physics for a microscopic particle bound in a region by certain forces. An example of such a system would be a conduction electron bound inside a metal block or a charge carrier trapped in a thin layer of

semiconductor sandwiched between two layers of a different semiconductor with larger band gap than its own.

We now solve the time independent Schrödinger equation for a quantum mechanical particle in this potential well.

12.2.1 Solving the Schrödinger Equation

Let us consider the motion of a quantum particle of mass m and total constant energy E in the one-dimensional potential well described by Eq. (12.1). We solve the Schrödinger equation in the three regions shown in Fig. 12.1. Region I extends from $-\infty$ to a ; Region II from $-a$ to a and Region III from a to ∞ . The central region is the potential well.

Let us first write down the time independent Schrödinger equation for the particle in region II. Since the potential energy in this region is zero, we have (with $V(x)=0$ in Eq. 7.47):

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad (\text{for Region II}) \quad (12.2)$$

Inside the well we have a free particle. You already know the solution of the Schrödinger equation for a free particle (Eq. 9.23). It is:

$$\psi_{II}(x) = A\sin kx + B\cos kx \quad (\text{for Region II: } -a \leq x \leq a) \quad (12.3)$$

The total energy is

$$E = \frac{\hbar^2 k^2}{2m} \quad (12.4)$$

and:

$$k = \sqrt{\frac{2mE}{\hbar^2}} \quad (12.5)$$

We next write the time independent Schrödinger equation for the particle in Regions I and III ($x < -a$ and $x > a$, respectively) which is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E\psi(x) \quad (12.6)$$

You have learnt how to solve such an equation in Unit 10 and 11. We define a parameter k' :

$$k' = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad (12.7)$$

We can rewrite Eq. (12.6) as:

$$\frac{d^2\psi(x)}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\psi(x) = 0 \quad \text{or} \quad \frac{d^2\psi(x)}{dx^2} - (k')^2\psi(x) = 0 \quad (12.8)$$

Let us write the solution for this equation for Regions I and III separately (recall Eq. 11.10) where the wave functions are $\psi_I(x)$ and $\psi_{III}(x)$, respectively:

$$\psi_I(x) = Ce^{k'x} + De^{-k'x} \quad (\text{for Region I : } x < -a) \quad (12.9)$$

And

$$\psi_{III}(x) = Fe^{-k'x} + Ge^{k'x} \quad (\text{for Region III : } x > a) \quad (12.10)$$

Let us consider that the total energy of the particle $E < V_0$. Therefore, $(V_0 - E)$ is positive and the parameter k' is real. We know that an acceptable wave function must be finite for all values of x . Since the term $De^{-k'x}$ in Eq. (12.8) diverges as $x \rightarrow -\infty$ and the term $Ge^{k'x}$ in Eq. (12.9) diverges as $x \rightarrow \infty$, for the wave function be finite in all regions we must have :

$$D = G = 0 \quad (12.11)$$

So, we can write:

$$\psi_I(x) = Ce^{k'x} \quad (\text{for Region I}) \quad (12.12)$$

and

$$\psi_{III}(x) = Fe^{-k'x} \quad (\text{for Region III}) \quad (12.13)$$

Let us summarize what we have studied so far.

PARTICLE IN A FINITE POTENTIAL WELL

Recap

The potential function for the one-dimension finite potential well is

$$V(x) = \begin{cases} V_0 & \text{for } x < -a & \text{Region I} \\ 0 & \text{for } -a \leq x \leq a & \text{Region II} \\ V_0 & \text{for } x > a & \text{Region III} \end{cases} \quad (12.1)$$

The time independent Schrödinger equation for the particle of mass m in the three regions is:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V_0\psi(x) = E\psi(x) \quad (\text{for Region I and III}) \quad (12.6)$$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad (\text{for Region II}) \quad (12.2)$$

The solutions of the Schrödinger equation in the three regions are:

$$\psi_I(x) = Ce^{k'x} \quad (\text{for Region I: } x < -a) \quad (12.12)$$

$$\psi_{II}(x) = A\sin kx + B\cos kx \quad (\text{for Region II: } -a < x < a) \quad (12.3)$$

$$\psi_{III}(x) = Fe^{-k'x} \quad (\text{for Region III: } x > a) \quad (12.13)$$

$$\text{with: } k' = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad \text{and } k = \sqrt{\frac{2mE}{\hbar^2}}$$

Next we evaluate the constants A , B , C and F using the boundary conditions on the wave function and its derivatives. Notice that the wave functions are different in the three regions of the potential. In order that the wave function and its derivatives are continuous in the entire region,

we must match the wave functions and their derivatives at the boundaries of the potential well.

Before we do that, let us examine a special property of a symmetric potential function. This will help us simplify the solution for Schrödinger equation in Region II.

EXAMPLE 12.1 : PARITY OPERATOR AND THE SYMMETRIC POTENTIAL FUNCTION

Show that, for a symmetric potential function ($V(x) = V(-x)$), the parity operator commutes with the Hamiltonian.

SOLUTION ■ The commutator of $\hat{P}$ and $\hat{H}$ can be written as follows:

$$[\hat{P}, \hat{H}] = \hat{P}\hat{H} - \hat{H}\hat{P} \quad (i)$$

To determine the value of this commutator, we operate it on the wave function $\psi(x)$:

$$(\hat{P}\hat{H} - \hat{H}\hat{P})\psi(x) = \hat{P}(\hat{H}\psi(x)) - \hat{H}(\hat{P}\psi(x)) \quad (ii)$$

Now

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

In Unit 8 you have studied that the parity operator is the space inversion operator ($x \rightarrow -x$) and $\hat{P}\psi(x) = \psi(-x)$. So the first term on the RHS of Eq. (ii) is:

$$\begin{aligned} \hat{P}(\hat{H}\psi(x)) &= -\frac{\hbar^2}{2m} \frac{d^2\psi(-x)}{dx^2} + V(-x)\psi(-x) \\ &= -\frac{\hbar^2}{2m} \frac{d^2\psi(-x)}{dx^2} + V(x)\psi(-x) \quad (\text{since } V(x) = V(-x)) \\ &= \left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \psi(-x) = \hat{H}\psi(-x) \quad (iv) \end{aligned}$$

For the second term on the RHS of Eq. (ii) we get

$$\hat{H}(\hat{P}\psi(x)) = \hat{H}\psi(-x) \quad (v)$$

So, using Eqs. (iv) and (v) in Eq. (ii) we get:

$$[\hat{P}, \hat{H}] = 0$$

Let us now apply this property to the potential function in Eq. (12.1).

12.2.2 Parity of the Eigen Functions

Recall that the finite well potential function defined by Eq. (12.1) is symmetric, that is $V(x) = V(-x)$. So, as you have learnt by

solving Example 12.1, the Hamiltonian $\hat{H}$ of the symmetric potential well commutes with the parity operator $\hat{P}$.

Now recall another result from Example 8.9 of Unit 8: If an operator $\hat{A}$ commutes with the parity operator $\hat{P}$, then the non-degenerate eigen functions of $\hat{A}$ have a definite parity, i.e., they are either of odd parity or of even parity. So the solutions of the Schrödinger equation for the symmetric finite potential well, which are the eigen functions of $\hat{H}$, will have a definite parity. That is: **the eigen functions will either be even or odd.**

Now this helps us to simplify the wave function for Region II given by $\psi_{II}(x) = A\sin kx + B\cos kx$.

Notice that this wave function does not have a definite parity because $\sin kx$ is an odd function [$\sin k(-x) = -\sin kx$] and $\cos kx$ is an even function [$\cos k(-x) = \cos kx$]. We have already established that the wave function must have a definite parity. Therefore, **either A or B should be zero.**

If we take $A = 0$ we get even parity solutions:

$$\psi_{II}(x) = B\cos kx \quad (\text{even parity : } \psi(-x) = \psi(x)) \quad (12.14)$$

With $B = 0$ we get the odd parity solutions:

$$\psi_{II}(x) = A\sin kx \quad (\text{odd parity : } \psi(-x) = -\psi(x)) \quad (12.15)$$

Both solutions are valid. Now let us apply the boundary conditions. The wave functions must match at the boundaries of the potential well and so the boundary conditions are:

$$\psi_I(x = -a) = \psi_{II}(x = -a) \quad (12.16a)$$

and

$$\psi_{II}(x = a) = \psi_{III}(x = a) \quad (12.16b)$$

Let us first work out the relation between the constants for the even parity solution: $\psi_{II}(x) = B\cos kx$. Substituting $x = -a$ in Eqs. (12.12 and 12.14), we get from Eq. (12.16a):

$$Ce^{-k'a} = B\cos k(-a) = B\cos ka \quad (12.17)$$

Substituting $x = a$ in Eqs. (12.13 and 12.14), we get from Eq. (12.16b):

$$Fe^{-k'a} = B\cos ka \quad (12.18)$$

The RHS of Eqs. (12.18 and 12.17) are the same, so we can write:

$$Ce^{-k'a} = Fe^{-k'a} \Rightarrow (C - F)e^{-k'a} = 0 \quad (12.19)$$

Since $e^{-k'a} \neq 0$, the following must be true for the even parity solution:

$$C = F \quad (12.20)$$

For the odd parity solution, $\psi_{II}(x) = A \sin kx$ using Eqs.(12.16a and b) respectively we get:

$$C = -F \quad (12.21)$$

You can verify Eq. (12.21) for yourself by solving SAQ 1.

SAQ 1 - Odd parity solution for the finite potential well

Show that for the odd parity solution $\psi_{II}(x) = A \sin kx$, $C = -F$.

Now we can write the complete set of solutions for the finite potential well.

The **even parity** solutions are (using $C = F$):

$$\psi_I(x) = Ce^{k'x} \quad (\text{for } x < -a) \quad (12.22a)$$

$$\psi_{II}(x) = B \cos kx \quad (\text{for } -a \leq x \leq a) \quad (12.22b)$$

$$\psi_{III}(x) = Ce^{-k'x} \quad (\text{for } x > a) \quad (12.22c)$$

The **odd parity** solutions are (using $C = -F$):

$$\psi_I(x) = Ce^{k'x} \quad (\text{for } x < -a) \quad (12.23a)$$

$$\psi_{II}(x) = B \sin kx \quad (\text{for } -a \leq x \leq a) \quad (12.23b)$$

$$\psi_{III}(x) = -Ce^{-k'x} \quad (\text{for } x > a) \quad (12.23c)$$

Recap

SOLUTIONS OF THE SCHRÖDINGER EQUATION

- The potential function for the one-dimension finite potential well is symmetric, hence the Hamiltonian commutes with the parity operator.
- The eigen functions of the Hamiltonian have a definite parity.
- The **even parity** solutions for $E < V_0$ are:

$$\psi_I(x) = Ce^{k'x} \quad (\text{for } x < -a) \quad (12.22a)$$

$$\psi_{II}(x) = B \cos kx \quad (\text{for } -a \leq x \leq a) \quad (12.22b)$$

$$\psi_{III}(x) = Ce^{-k'x} \quad (\text{for } x > a) \quad (12.22c)$$

- The **odd parity** solutions for $E < V_0$ are:

$$\psi_I(x) = Ce^{k'x} \quad (\text{for } x < -a) \quad (12.23a)$$

$$\psi_{II}(x) = B \sin kx \quad (\text{for } -a \leq x \leq a) \quad (12.23b)$$

$$\psi_{III}(x) = -Ce^{-k'x} \quad (\text{for } x > a) \quad (12.23c)$$

The purpose of solving the Schrödinger equation is to obtain the eigen functions of the Hamiltonian and the corresponding energy eigen values. We have written down the even and odd parity eigen functions for the bound state of the particle ($E < V_0$). However we have yet to determine

the constants B and C and the energy eigen values which are values of E corresponding to these bound state eigen functions. Let us now determine E .

12.2.3 Energy Eigen Values

We determine the constants B and C using the boundary conditions for the continuity of the derivatives of the wave function.

You know that for $\psi(x)$ to be an acceptable wave function, $\psi(x)$ and $\frac{d\psi(x)}{dx}$ should be continuous for all x . Therefore the derivative of the

logarithm of $\psi(x)$ which is $\frac{d}{dx}(\ln \psi(x)) = \frac{1}{\psi(x)} \frac{d\psi(x)}{dx}$, should also be

continuous. We now write the condition of continuity for the derivatives of $\ln \psi(x)$ at the boundary of Regions I and II:

$$\left. \frac{1}{\psi_I(x=-a)} \frac{d\psi_I(x)}{dx} \right|_{x=-a} = \left. \frac{1}{\psi_{II}(x=-a)} \frac{d\psi_{II}(x)}{dx} \right|_{x=-a} \quad (12.24)$$

Since

$$\frac{d\psi_I}{dx} = \frac{d}{dx}(Ce^{k'x}) = Ck'e^{k'x} \quad (12.25)$$

and for the even parity solution $\psi_{II}(x) = B\cos kx$:

$$\frac{d\psi_{II}}{dx} = \frac{d}{dx}(B\cos kx) = -B\sin kx \quad (12.26)$$

On imposing the condition given by Eq. (12.24) on the even parity solution, we get for $x = -a$:

$$\frac{1}{Ce^{-k'a}}(Ck'e^{-k'a}) = \frac{1}{B\cos ka}(Bk\sin ka) \Rightarrow k' = k \tan ka \quad (12.27)$$

Multiplying both sides of Eq. (12.26) by a we get:

$$ak' = ak \tan ka \Rightarrow \eta = \xi \tan \xi \quad (12.28)$$

We have introduced the variables η and ξ , which are defined as follows:

$$\eta = k'a = \sqrt{\frac{2m(V_0 - E)a^2}{\hbar^2}} \text{ and } \xi = ka = \sqrt{\frac{2mEa^2}{\hbar^2}} \quad (12.29)$$

Notice that η and ξ are dimensionless quantities, but both η and ξ are functions of the energy of the particle E .

From Eq. (12.28) we get:

$$\eta^2 + \xi^2 = (k'a)^2 + (ka)^2 = \frac{2m(V_0 - E)a^2}{\hbar^2} + \frac{2mEa^2}{\hbar^2} = \frac{2mV_0a^2}{\hbar^2} = R^2 \quad (12.30)$$

where R is a constant that depends on the depth of the well (V_0) and its width $2a$:

$$R = \sqrt{\frac{2mV_0a^2}{\hbar^2}} \quad (12.31)$$

The energy eigen values can now be obtained by solving Eqs. (12.28) and (12.30) for η and ξ for a fixed value of R . Combining these equation we can write:

$$\eta^2 + \xi^2 = R^2; \eta = \xi \tan \xi; \eta, \xi > 0 \quad \text{for even parity states} \quad (12.32a)$$

Before we solve these equations you can derive the conditions equivalent to Eq. (12.32a) for the odd parity states

SAQ 2 - Energy eigen values for the odd parity solution

Show that for the odd parity solutions given by Eqs. (12.23 a,b,c) the boundary conditions on the continuity of the derivatives of the wave function lead to the following conditions:

$$\eta^2 + \xi^2 = R^2; \eta = -\xi \cot \xi; \eta, \xi > 0 \quad \text{for odd parity states} \quad (12.32b)$$

Eqs. (12.32a and 12.32b) are what are known as **transcendental** equations, where the variable appears both as an argument to a transcendental function and elsewhere in the equation. These equations are not solvable in closed form. So we have to solve them numerically or graphically

Eq. (12.32 a and b) are solved graphically as shown in Fig. 12.2. For this, we plot ξ along the x-axis and η along the y-axis. Since both η and ξ are greater than zero, we plot only the first quadrant. The equation $\eta^2 + \xi^2 = R^2$ represents a circle with a radius R and is plotted in Fig. 12.2 for four different values of R . For each value of R (corresponding to the value of the product V_0a^2), we get a different circle.

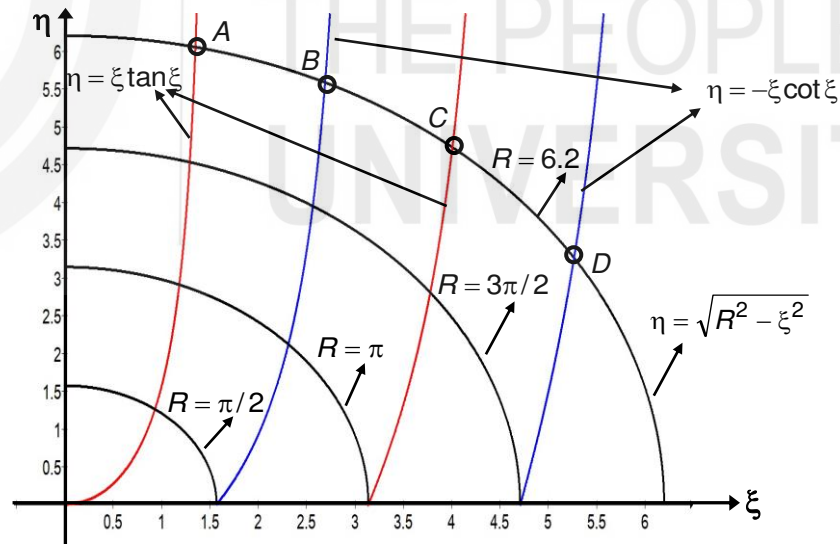


Fig. 12.2: Graphical Solution of Eqs. 12.32a and b. The red, blue and black curves represent the functions $\eta = \xi \tan \xi$, $\eta = -\xi \cot \xi$ and $\eta^2 + \xi^2 = R^2$ respectively.

The equation $\eta = \xi \tan \xi$ and $\eta = -\xi \cot \xi$ are plotted by the red and blue lines respectively in Fig. 12.2. The solutions of Eq. (12.32a) are the points at which the plot of the function $\eta^2 + \xi^2 = R^2$ and $\eta = \xi \tan \xi$ intersect. In Fig 12.2, for $R = 6.2$, these points of intersection are A and C. At any point of intersection we get a value of ξ , say $\xi = \xi_n$. This value of ξ_n can be used to calculate the energy eigen value

E_n using the relation $E_n = \frac{\hbar^2 \xi_n^2}{2m}$ (from Eq. 12.29). Remember that this is for a particular value of R .

The solutions of Eq. (12.32b) are the points at which the plot of the function $\eta^2 + \xi^2 = R^2$ and $\eta = -\xi \cot \xi$ intersect, which are the points B and D in Fig.12.2 for $R = 6.2$. Once again, at the point of intersection, we can calculate the energy eigen value using Eq. (12.29).

Note from Fig. 12.2 that the allowed values of ξ and hence E are discrete and the number of allowed values of E increases as R increases. The solutions of Eq. (12.32a) give us the energy eigen values for the even parity states and the solutions of Eq.(12.32b) give us the energy eigen values for the odd parity states.

Therefore for $E < V_0$, the energy levels of a particle in a finite potential well are discrete and depend upon the well parameters (V_0) and its width

a. From Fig. 2.2, note that:

- For a value of R lying between 0 and $\pi/2$, there is **just one** possible solution of the set of Eqs. (12.32a and b) and that corresponds to a state of even parity (obtained from the intersection of the curves $\eta^2 + \xi^2 = R^2$ and $\eta = \xi \tan \xi$). We can write:

$$R < \frac{\pi}{2} \Rightarrow R^2 < \frac{\pi^2}{4} \Rightarrow V_0 a^2 < \frac{\hbar^2 \pi^2}{8m}$$

So for $0 < V_0 a^2 < \frac{\hbar^2 \pi^2}{8m}$ you can have **just one bound state of even parity**. There are no odd parity states for a value of R between 0 and $\pi/2$.

- For a value of R in the range $\pi/2 \leq R < \pi$, you have one solution of even parity and one solution of odd parity, **hence two bound states**.
- For a value of R in the range $\pi/2 \leq R < 3\pi/2$, you have two solutions of even parity and one solution of odd parity, **hence three bound states**.
- The number of bound states depends on the value of R . **The greater the value of R (larger the value of V_0), the greater the number of bound states**. As the value R increases, more bound states of even and odd parities get added to the eigen functions.
- For the value of $R = 6.2$, you can see that there are four bound states. The first intersection is at A , corresponds to a value of $\xi = \xi_1$ and it gives us the ground state energy for $R = 6.2$. It is a state of even parity. The next intersection is at B , which corresponds to $\xi = \xi_2$ and gives us the energy of the first excited state, and so on.
- However small be the value of R , there will always be a solution corresponding to an intersection of the curves $\eta^2 + \xi^2 = R^2$ and $\eta = \xi \tan \xi$. This ensures there will always be **at least one bound state and that this state corresponds to an even parity state**.

- For any value of value of R , the lowest energy state is always an even parity state

Clearly, for $E < V_0$ the particle is bound to the well and the energy spectrum is discrete. What if the energy of the particle is greater than V_0 ?

In that case the particle is no longer confined to the well and the energy of the particle varies continuously from V_0 to ∞ .

In Fig. 12.3, you can see typical energy level diagram for a particle in a finite potential well. For $E < V_0$, you have discrete energy levels. For

$E > V_0$, you have a continuum of energies.

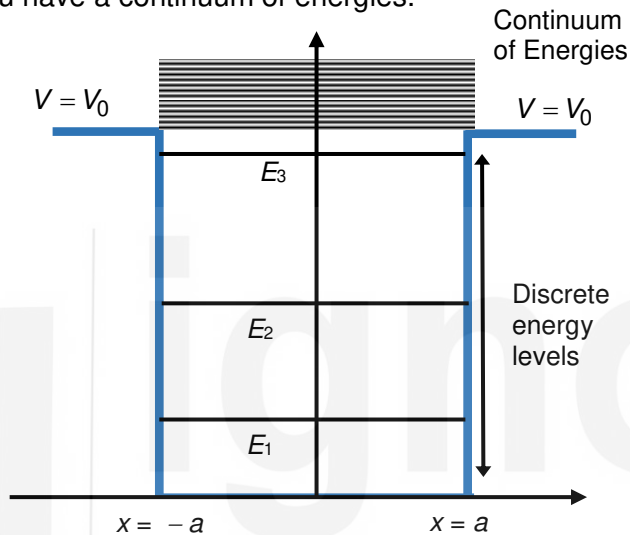


Fig. 12.3: Typical energy eigen values for a finite potential well.

Recap

ENERGY EIGEN VALUES

- The energy eigen values can be obtained by solving the transcendental equations:

$$\eta^2 + \xi^2 = R^2; \eta = \xi \tan \xi; \eta, \xi > 0 \text{ for even parity states} \quad (12.32a)$$

$$\eta^2 + \xi^2 = R^2; \eta = -\xi \cot \xi; \eta, \xi > 0 \text{ for odd parity states} \quad (12.32b)$$

for η and ξ for a fixed value of R , where

$$\eta = k'a = \sqrt{\frac{2m(V_0 - E)a^2}{\hbar^2}}; \xi = ka = \sqrt{\frac{2mEa^2}{\hbar^2}}; R = \sqrt{\frac{2mV_0a^2}{\hbar^2}}$$

- For $E < V_0$ the particle is bound to the well and the energy spectrum is discrete.
- The lowest energy state is always an even parity state and there is always at least one bound state.
- The number of bound states depends on the radius of the circle, R . **The greater the value of R (larger the value of V_0), the greater the number of bound states.**

Once the energy eigen values are known, the corresponding eigen functions can be determined by matching the wave function and its derivatives at one of the boundaries $x=a$ or $x=-a$. The calculation is

however complex. But we can deduce the nature of the eigen functions by looking at the corresponding symmetric infinite square well (i.e. $V_0 \rightarrow \infty$).

12.2.4 Symmetric Infinite Potential Well

The symmetric infinite potential well can be written as

$$V(x) = \begin{cases} \infty & \text{for } x < -a \\ 0 & \text{for } -a < x < a \\ \infty & \text{for } x > a \end{cases} \quad (12.33)$$

where we have replaced V_0 by ∞ in Eq. (12.1). Recall that we have solved the infinite potential well in Unit 9. However, the potential well we studied in Unit 9 was not symmetric about $x = 0$.

Since there is an infinite potential for $x < -a$ and $x > a$, we can say that the wave function will not extend beyond the boundaries of the well.

Therefore, for both the even and odd parity solutions:

$$\psi_I(x) = \psi_{III}(x) = 0$$

And for $-a < x < a$, we can write for the infinite symmetric potential well:

$$\text{Even Parity Solution : } \psi(x) = A \cos kx \quad (\text{for } -a < x < a) \quad (12.34a)$$

$$\text{Odd Parity Solution : } \psi(x) = B \sin kx \quad (\text{for } -a < x < a) \quad (12.34b)$$

The constants A and B are determined by the normalization condition for the wave function. We can also write the following boundary condition for the wave function going to zero at the boundaries of the potential well:

$$\psi(x = -a) = \psi(x = a) = 0 \quad (12.35)$$

Using this condition for Eq. (12.34a), we get:

$$\psi(x = -a) = A \cos ka = 0 \Rightarrow ka = (n) \frac{\pi}{2} \text{ with } n = 1, 3, 5, \dots \quad (12.36)$$

So the eigen function for the even parity state is:

Even Parity Eigen function :

$$\psi_{\text{even}}(x) = A \cos\left(\frac{n\pi x}{2a}\right) \text{ with } n = 1, 3, 5, \dots \quad (12.37a)$$

The corresponding eigen energy for the even parity states is found using

$$E = \frac{\hbar^2 k^2}{2m} \text{ and the value of } k \text{ as obtained in Eq. (12.36) :}$$

$$E_{n,\text{even}} = \frac{\hbar^2}{2m} \left[\frac{n\pi}{2a} \right]^2 \text{ with } n = 1, 3, 5, \dots \quad (12.37b)$$

You can obtain the corresponding odd parity eigen functions and the eigen energies by applying Eq. (12.35) to Eq. (12.34b). You may like to work this out for yourself.

***SAQ 3* - Odd parity eigen functions and eigen energies.**

Show that the odd parity eigen functions and eigen energies of the symmetric infinite potential well are:

$$\psi_{odd}(x) = B \sin\left(\frac{n\pi x}{2a}\right) \text{ with } n = 2, 4, 6, \dots \quad (12.38a)$$

and

$$E_{n,odd} = \frac{\hbar^2}{2m} \left[\frac{n\pi}{2a} \right]^2 \text{ with } n = 2, 4, 6, \dots \quad (12.38b)$$

You can see for yourself that the lowest possible energy is for $n = 1$ in Eq. (12.37b) which is:

$$E_1 = \frac{\hbar^2 \pi^2}{8ma^2} \quad (12.39a)$$

This corresponds to the even parity eigen function $\psi_1(x) = A \cos\left(\frac{\pi x}{2a}\right)$.

This is the ground state and this energy is the zero point energy. Notice that the minimum energy is not zero.

The next energy eigenvalue is found by substituting $n = 2$ in Eq. (12.38b):

$$E_2 = \frac{\hbar^2 \pi^2}{2ma^2} = 4 \left(\frac{\hbar^2 \pi^2}{8ma^2} \right) = 4E_1 \quad (12.39b)$$

This corresponds to the odd parity eigen function $\psi_2(x) = B \sin\left(\frac{\pi x}{a}\right)$.

The next energy eigen value corresponds to a even parity state, so we evaluate it from Eq. (12.37b) with $n = 3$ and get:

$$E_3 = \frac{9\hbar^2 \pi^2}{8ma^2} = 9E_1 \quad (12.39c)$$

And the corresponding even parity eigen function is $\psi_3(x) = A \cos\left(\frac{3\pi x}{2a}\right)$.

So as you can see, the eigen functions are alternately of even and odd parity.

Now that we know the form of the eigen functions for the infinite potential well, we can deduce what the eigen functions of a finite potential well would look like. Unlike in the infinite potential well, the wave function for a finite potential well would not go to zero at the boundaries of the potential well. Rather the wave function would decay exponentially on both sides of the potential well and the form of the wave function is given by $\psi_I(x)$ and $\psi_{III}(x)$ as described in Eqs. (12.22a and 12.22c) or Eqs. (12.23a and 12.23c) depending on the parity of the solution.

In Fig. 12. 4(a) and (b) we plot the first three eigen functions for the infinite and finite symmetric potential well respectively.

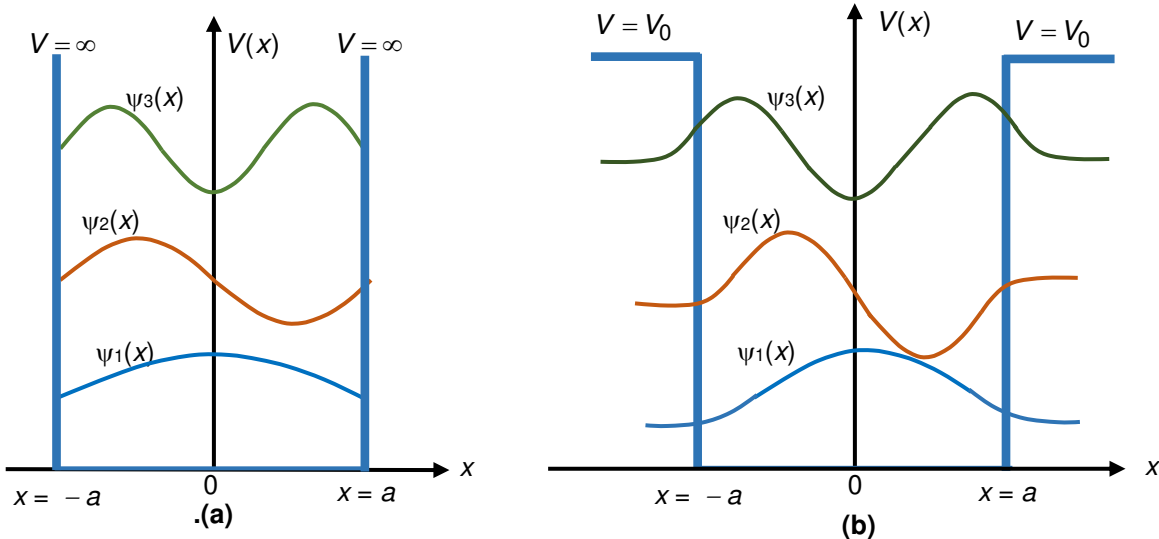


Fig. 12.4: The first three eigen functions for (a) a symmetric infinite potential well, and (b) a symmetric finite potential well

Note that the wave function extends into the classically forbidden region on either side of the boundary of the finite potential well.

We define what is known as the penetration depth, which is the distance to which the wave function penetrates the region beyond the boundaries of the potential as:

$$\delta = \frac{1}{k'} = \frac{\hbar}{\sqrt{2m(V_0 - E)}} \quad (12.40)$$

At a distance δ beyond the boundary of the well the amplitude of the wave function falls to $1/e$ of its value at the boundary. At this distance, the wave function in the exterior of the well is almost zero.

Also the eigen energies for a finite well are typically less than that for an infinite square well of the same width. This is because when the wave functions extend upto a distance of δ beyond the boundaries of the well, we can say that the effective size of the box increases. So the typical energies are lower.

PARTICLE IN A SYMMETRIC INFINITE POTENTIAL WELL

Recap

The potential function for the symmetric one-dimensional infinite potential well is

$$V(x) = \begin{cases} \infty & \text{for } x < -a & \text{Region I} \\ 0 & \text{for } -a \leq x \leq a & \text{Region II} \\ \infty & \text{for } x > a & \text{Region III} \end{cases} \quad (12.1)$$

The solutions of the Schrödinger equation for a particle of mass m in the symmetric infinite well have a definite parity:

Recap

PARTICLE IN A SYMMETRIC INFINITE POTENTIAL WELL

$$\psi_{\text{even}}(x) = A \cos\left(\frac{n\pi x}{2a}\right) \text{ with } n = 1, 3, 5, \dots \quad (12.37a)$$

$$\psi_{\text{odd}}(x) = B \sin\left(\frac{n\pi x}{2a}\right) \text{ with } n = 2, 4, 6, \dots \quad (12.38a)$$

The eigen energies are:

$$E_{n,\text{even}} = \frac{\hbar^2}{2m} \left[\frac{n\pi}{2a} \right]^2 \text{ with } n = 1, 3, 5, \dots \quad (12.37b)$$

$$E_{n,\text{odd}} = \frac{\hbar^2}{2m} \left[\frac{n\pi}{2a} \right]^2 \text{ with } n = 2, 4, 6, \dots \quad (12.38b)$$

The ground state energy is: $E_1 = \frac{\hbar^2 \pi^2}{8ma^2}$

12.3 SUMMARY

Concept

Description

**Particle in a finite
potential well**

- The potential function for the one-dimension finite potential well is

$$V(x) = \begin{cases} V_0 & \text{for } x < a & \text{Region I} \\ 0 & \text{for } -a \leq x \leq a & \text{Region II} \\ V_0 & \text{for } x > a & \text{Region III} \end{cases}$$

The time independent Schrödinger equation for the particle of mass m in the three regions is:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_{II}(x)}{dx^2} + V_0 \psi(x) = E \psi(x) \quad (\text{for Region I and III})$$

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} = E \psi(x) \quad (\text{for Region II})$$

The solutions of the Schrödinger equation in the three regions are:

$$\psi_I(x) = C e^{k'x} \quad (\text{for Region I})$$

$$\psi_{II}(x) = A \sin kx + B \cos kx \quad (\text{for Region II: } -a < x < a)$$

$$\psi_{III}(x) = F e^{-k'x} \quad (\text{for Region III})$$

With:

$$k' = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad \text{and} \quad k = \sqrt{\frac{2mE}{\hbar^2}}$$

Solutions of the Schrödinger equation

- The potential function for the one-dimension finite potential well is symmetric, hence the Hamiltonian commutes with the parity operator.

The eigen functions of the Hamiltonian have a definite parity.

The **even parity** solutions for $E < V_0$ are:

$$\psi_I(x) = Ce^{k'x} \quad (\text{for } x < -a)$$

$$\psi_{II}(x) = B\cos kx \quad (\text{for } -a \leq x \leq a)$$

$$\psi_{III}(x) = Ce^{-k'x} \quad (\text{for } x > a)$$

The **odd parity** solutions for $E < V_0$ are:

$$\psi_I(x) = Ce^{k'x} \quad (\text{for } x < -a)$$

$$\psi_{II}(x) = B\sin kx \quad (\text{for } -a \leq x \leq a)$$

$$\psi_{III}(x) = -Ce^{-k'x} \quad (\text{for } x > a)$$

Energy eigen values

- The energy eigen values can be obtained by solving the transcendental equations:

$$\eta^2 + \xi^2 = R^2; \eta = \xi \tan \xi; \eta, \xi > 0 \quad \text{for even parity states}$$

$$\eta^2 + \xi^2 = R^2; \eta = -\xi \cot \xi; \eta, \xi > 0 \quad \text{for odd parity states}$$

for η and ξ for a fixed value of R , where

$$\eta = k'a = \sqrt{\frac{2m(V_0 - E)a^2}{\hbar^2}}; \xi = ka = \sqrt{\frac{2mEa^2}{\hbar^2}}; R = \sqrt{\frac{2mV_0a^2}{\hbar^2}}$$

For $E < V_0$ the particle is bound to the well and the energy spectrum is discrete.

The lowest energy state is always an even parity state and there is always at least one bound state.

The number of bound states depends on the radius of the circle, R . **The greater the value of R (larger the value of V_0), the greater the number of bound states.**

Particle in a symmetric infinite potential well

- The potential function for the symmetric one-dimensional infinite potential well is

$$V(x) = \begin{cases} \infty & \text{for } x < -a & \text{Region I} \\ 0 & \text{for } -a \leq x \leq a & \text{Region II} \\ \infty & \text{for } x > a & \text{Region III} \end{cases}$$

The solutions of the Schrödinger equation for a particle of mass m in the symmetric infinite well have a definite parity:

$$\psi_{\text{even}}(x) = A\cos\left(\frac{n\pi x}{2a}\right) \quad \text{with } n = 1, 3, 5, \dots$$

$$\psi_{\text{odd}}(x) = B\sin\left(\frac{n\pi x}{2a}\right) \quad \text{with } n = 2, 4, 6, \dots$$

The eigen energies are:

$$E_{n,even} = \frac{\hbar^2}{2m} \left[\frac{n\pi}{2a} \right]^2 \text{ with } n = 1, 3, 5, \dots$$

$$E_{n,odd} = \frac{\hbar^2}{2m} \left[\frac{n\pi}{2a} \right]^2 \text{ with } n = 2, 4, 6, \dots$$

The ground state energy is: $E_1 = \frac{\hbar^2 \pi^2}{8ma^2}$

12. 4 TERMINAL QUESTIONS

1. Explain whether the eigen functions of the following Hamiltonian for a particle of mass m will have a definite parity:

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

2. Calculate the normalization constants for the wave functions of Eqs. 12.34 and b

$$(i) \quad \psi(x) = A \cos kx \quad (\text{for } -a < x < a)$$

$$(ii) \quad \psi(x) = B \sin kx \quad (\text{for } -a < x < a)$$

3. Calculate the penetration depth for an electron of energy 40 eV, trapped by an electrostatic potential of 100 eV.
4. The penetration depth for an electron is 2.0 nm. How much energy would be required to “free” the electron from the well?

12.5 SOLUTIONS AND ANSWERS

Self-Assessment Questions

1. We use the condition given in Eq. (12.16 a), with $\psi_{11}(x) = A \sin kx$ to get,

$$C e^{-k'a} = A \sin k(-a) = -A \sin ka \Rightarrow A \sin ka = -C e^{-k'a} \quad (i)$$

and applying the condition of Eq. (12.16a) we get

$$A \sin ka = F e^{-k'a} \quad (ii)$$

Equating the LHS of Eqs. (i) and (ii) we get:

$$-C e^{-k'a} = F e^{-k'a} \Rightarrow (C + F) e^{-k'a} = 0$$

$$\therefore e^{-k'a} \neq 0 \text{ we must have } C = -F$$

2. Taking $\psi_{II}(x) = A \sin kx$ we impose the condition

$$\frac{1}{\psi_I(x=-a)} \frac{d\psi_I}{dx}(x=-a) = \frac{1}{\psi_{II}(x=-a)} \frac{d\psi_{II}}{dX}(x=-a) \quad (i)$$

$$\text{From Eq. (12.25) we know: } \frac{d\psi_I}{dx} = C k' e^{k'x} \quad (ii)$$

$$\text{And } \frac{d\psi_{II}}{dx} = \frac{d}{dx}(A \sin kx) = Ak \cos kx \quad (iii)$$

So, using Eq. (i) and the results of Eqs. (ii) and (iii) we get:

$$\frac{1}{C e^{-k'a}} [C k' e^{-k'a}] = \frac{1}{-A \sin ka} Ak \cos ka \Rightarrow k' = -k \cot ka \quad (iv)$$

$$\text{or } k'a = -ka \cot ka \quad (v)$$

With $\eta = k'a$ and $\xi = ka$, we get

$$\eta = -\xi \cot \xi$$

$$\text{And from Eq. (12.30) } \eta^2 + \xi^2 = R^2$$

So, we can write the conditions for odd parity states as:

$$\eta^2 + \xi^2 = R^2; \eta = -\xi \cot \xi, \eta, \xi > 0$$

3. Using $\psi(x) = B \sin kx$ and applying Eq. (12.35) we get,

$$B \sin ka = 0 \Rightarrow \sin ka = 0 \text{ or } ka = n \left(\frac{\pi}{2} \right), n = 2, 4, 6, \dots$$

$$\therefore k = \frac{n\pi}{2a}, n = 2, 4, 6, \dots$$

$$\text{So } \psi_n(x) = B \sin \left(\frac{n\pi x}{2a} \right), n = 2, 4, 6, \dots$$

$$\text{And } E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left[\frac{n\pi}{2a} \right]^2, n = 2, 4, 6, \dots$$

Terminal Questions

1. Following the steps of Example 12.1 we can write,

$$[\hat{P}, \hat{H}] \psi = \hat{P}[\hat{H} \psi(x)] - \hat{H}[\hat{P} \psi(x)] \quad (i)$$

where

$$\hat{H} = -\hbar^2 \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2$$

$$\text{So } \hat{P}[\hat{H} \psi(x)] = \hat{P} \left[-\frac{\hbar^2}{2} \frac{d^2 \psi}{dx^2} + \frac{1}{2} m \omega^2 x^2 \psi(x) \right]$$

$$= -\hbar^2 \frac{d^2 \psi(-x)}{dx^2} + \frac{1}{2} m \omega^2 x^2 \psi(x) \quad (\text{ii})$$

and

$$\hat{H}[\hat{P}\psi(x)] = -\frac{\hbar^2}{2m} \frac{d^2 \psi(-x)}{dx^2} + \frac{1}{2} m \omega^2 x^2 \psi(-x) \quad (\text{iii})$$

From Eq. (ii) and (iii) we can write

$$\hat{P}(\hat{H}\psi) = \hat{H}(\hat{P}\psi)$$

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

$\therefore$ the parity operator commutes with the Hamiltonian, the eigen functions will have a definite parity

2. i) The normalization condition is

$$\int_{-a}^a \psi^*(x) \psi(x) dx = 1 \Rightarrow |A|^2 \int_{-a}^a \cos^2 kx dx = 1 \text{ where}$$

$$k = \frac{n\pi}{2a} \quad (n = 1, 3, 5, \dots)$$

$$\Rightarrow \frac{|A|^2}{2} \int_{-a}^a [1 + \cos 2kx] dx = 1 \Rightarrow \frac{|A|^2}{2} \left[x + \frac{1}{2k} \sin 2kx \right]_{-a}^a = 1$$

$$\Rightarrow \frac{|A|^2}{2} \left[2a + \frac{2}{2k} \sin 2ka \right] = 1$$

Given that

$$k = \frac{n\pi}{2a} \quad (n = 1, 3, 5, \dots) \Rightarrow \sin 2ka = \sin 2 \left(\frac{n\pi}{2a} \right) a = \sin(n\pi) = 0$$

$$\therefore \frac{|A|^2}{2} [2a] = 1 \text{ and } A = |A| = \sqrt{\frac{1}{a}}$$

(ii) The normalization condition is written as

$$|B|^2 \int_{-a}^a \sin^2 kx dx = 1 \text{ where } k = \frac{n\pi}{2a}, \quad n = 2, 4, 6, \dots$$

$$\Rightarrow \frac{|B|^2}{2} \int_{-a}^a [1 - \cos 2kx] dx = 1$$

$$\text{or } \frac{|B|^2}{2} \left[x - \frac{1}{2k} \sin 2kx \right]_{-a}^a = 1$$

$$\text{or } \frac{|B|^2}{2} \left[2a - \frac{1}{2k} \sin 2ka \right] = 1$$

$$\sin 2ka = \sin \frac{2n\pi}{2a} (a) = \sin n\pi = 0$$

$$\Rightarrow \frac{|B|^2}{2} [2a] = 1 \text{ or } |B| = B = \sqrt{\frac{1}{a}}$$

3. We calculate penetration depth δ using Eq.(12.40)

With $V_0 = 100 \text{ eV}$ and $E = 40 \text{ eV}$

$$\begin{aligned} \text{So } \delta &= \frac{1.054 \times 10^{-34} \text{ Js}}{\sqrt{2 \times (9.109 \times 10^{-31} \text{ kg}) \times (60 \times 1.6 \times 10^{-19} \text{ J})}} \\ &= .025 \times 10^{-9} \text{ m} = .025 \text{ nm} \end{aligned}$$

4. The energy required to free the electron is $(V_0 - E)$.

Using Eq. (12.40) for the penetration depth δ , we can write

$$V_0 - E = \frac{(\hbar)^2}{2m_e \delta^2} \quad (i)$$

with $\delta = 2.0 \text{ nm} = 2.0 \times 10^{-9} \text{ m}$

we get,

$$\begin{aligned} V_0 - E &= \frac{(1.054 \times 10^{-34} \text{ Js})^2}{2 \times (9.109 \times 10^{-31} \text{ kg}) \times (2.0 \times 10^{-9} \text{ m})^2} = 0.015 \times 10^{-19} \text{ J} \\ &= 0.01 \text{ eV} \end{aligned}$$

FURTHER READINGS

1. Quantum Physics of Atoms, Molecules, Solids, Nuclei and Particles, Robert Eisberg and Robert Resnick, Wiley Student Edition (2006).
2. Modern Physics, Raymond Serway, Clement Moses and Curt Moyer, 3rd Edition, Cengage Learning (2012).

TABLE OF PHYSICAL CONSTANTS

Symbol	Quantity	Value
c	Speed of light in vacuum	$2.998 \times 10^8 \text{ ms}^{-1}$
μ_0	Permeability of free space	$1.257 \times 10^{-6} \text{ NA}^{-2}$
ϵ_0	Permittivity of free space	$8.854 \times 10^{-12} \text{ C}^2 \text{ N}^{-1} \text{ m}^{-2}$
$1/4\pi\epsilon_0$		$8.988 \times 10^9 \text{ Nm}^2\text{C}^{-2}$
e	Charge of the proton	$1.602 \times 10^{-19} \text{ C}$
$-e$	Charge of the electron	$1.602 \times 10^{-19} \text{ C}$
h	Planck's constant	$6.626 \times 10^{-34} \text{ Js}$
$\hbar$	$h / 2\pi$	$1.054 \times 10^{-34} \text{ Js}$
m_e	Electron rest mass	$9.109 \times 10^{-31} \text{ kg}$
$-e/m_e$	Electron charge to mass ratio	$1.759 \times 10^{-19} \text{ Ckg}^{-1}$
m_p	Proton rest mass	$1.673 \times 10^{-27} \text{ kg}$
m_n	Neutron rest mass	$1.675 \times 10^{-27} \text{ kg}$
a_0	Bohr radius	$5.292 \times 10^{-11} \text{ m}$
N_A	Avogadro constant	$6.022 \times 10^{23} \text{ mol}^{-1}$
R	Universal gas constant	$8.315 \text{ J mol}^{-1}\text{K}^{-1}$
k_B	Boltzmann constant	$1.381 \times 10^{-23} \text{ JK}^{-1}$
G	Universal gravitational constant	$6.673 \times 10^{-11} \text{ Nm}^2\text{kg}^{-2}$

LIST OF BLOCKS AND UNITS: BPHET-141

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Special Theory of Relativity: Constancy of Speed of Light, Postulates of Special Theory of Relativity, Lorentz Transformation, Length Contraction, Time Dilation, Examples, Velocity Addition Theorem, Doppler Effect, Variation of Mass with Velocity, Energy-Mass Equivalence, Relativistic Energy and Momentum.

An Introduction to Quantum Mechanics: Birth of Quantum Physics, Blackbody Radiation, Planck's Quantum Hypothesis, Planck's constant and light as a collection of photons; Photo-electric effect and Compton scattering. Problems with Rutherford model – instability of atoms and observation of discrete atomic spectra; Bohr Model, Bohr's quantization rule and atomic stability; calculation of energy levels for hydrogen like atoms and their spectra.

de-Broglie hypothesis and matter waves; Davisson-Germer experiment, Wave-Particle Duality, Matter waves and wave amplitude, Wave Packet, Group Velocity.

The Uncertainty Principle and its Consequences, Thought Experiments: Position measurement – gamma ray microscope thought experiment; Two slit interference experiment with photons, atoms and particles; Complementarity; Estimating minimum energy of a confined particle using uncertainty principle; Energy-time uncertainty principle.

Postulates of Quantum Mechanics, Time Dependent and Time Independent Schrödinger Equation in One Dimension, Statistical Interpretation of Wave Function, Probability Current Density and Continuity Equation, Normalization of Wave Functions, Wave Function in Momentum Space; Observables and Operators, Linear Momentum and Energy Operators; Parity Operator and its Eigenvalues; Commutation Relations, Expectation Values.

Applications of Quantum Mechanics: One Dimensional Infinitely Rigid Box – energy eigen values and eigen functions, normalization, quantum dot as an example, Particle in a Box, Free Particle, Step Potential and Rectangular Potential Barrier, Quantum mechanical scattering and Tunneling; One Dimensional Potential Well and barrier.

Nuclear Physics: Radioactivity: Stability of nucleus; Law of Radioactive Decay, Mean life and half-life; Radioactive Equilibria, Natural Radioactive Series, Law of α decay, β decay – energy released, spectrum and Pauli's prediction of neutrino; γ -ray emission. General Properties of Nuclei: Size and structure of atomic nucleus and its relation with atomic weight; Impossibility of an electron being in the nucleus as a consequence of the uncertainty principle. Nature of nuclear force, NZ graph, semi-empirical mass formula and binding energy; Stability of Nuclei: Binding Energy Curve. Fission and fusion – mass defect, generation of energy; Fission – nature of fragments and emission of neutrons. Nuclear reactor: slow neutrons and their interactions with Uranium 235; Fusion and thermonuclear reactions.