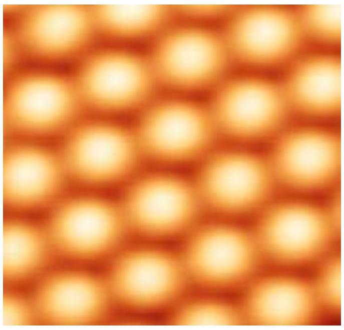

Silicon atoms observed at the surface of a silicon carbide crystal using a Scanning Tunnelling Microscope.
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UNIT 11

BARRIER POTENTIAL

Structure

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

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.

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 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 ~30 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 ~ 60 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.

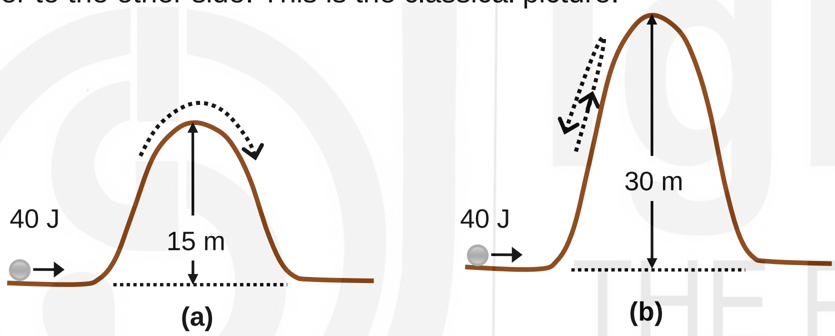

Fig. 11.1: A ball having a kinetic energy of 40 J trying to cross a hump of height a) 15.0 m , and b) 30.0 m.

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:

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

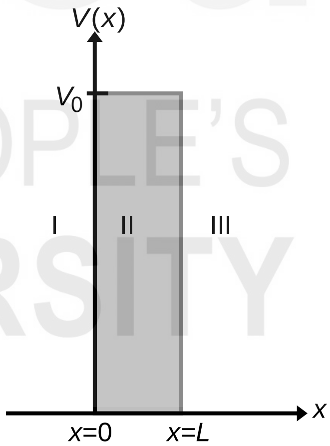

Fig. 11.2: A Potential Barrier.

$V(x)$ 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.

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):

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

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

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):

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

And

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

where

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

and:

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

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:

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

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

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

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

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

Then we rewrite Eq. (11.8) as:

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

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):

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

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 $0 \le x \le L$ and both terms in Eq. (11.11) would remain finite in this range.

Let us now summarize what you have studied so far.

Recap

ONE-DIMENSIONAL POTENTIAL BARRIER

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

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

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

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

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

The solutions of the Schrödinger equations are:

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

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

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

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:

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

Where:

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

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:

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

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

And

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

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

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:

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

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 $\psi_{III}(x)$.

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

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

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

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

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

and

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

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.

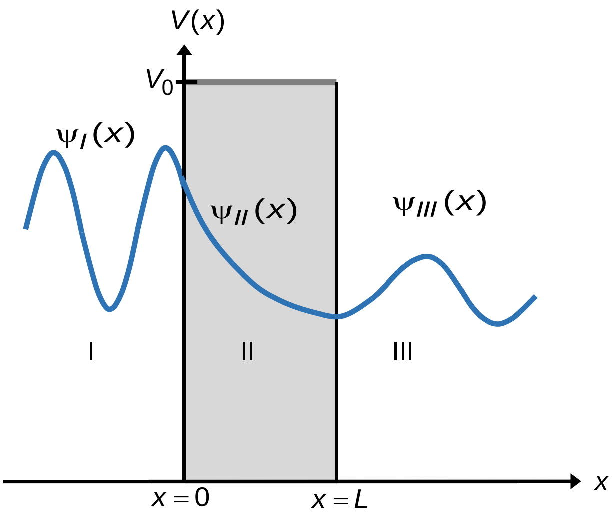

Fig. 11.3: The wave function for the one –dimensional potential barrier for a particle with an energy less than the barrier height.

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

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

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 probability density for Region I as:

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

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:

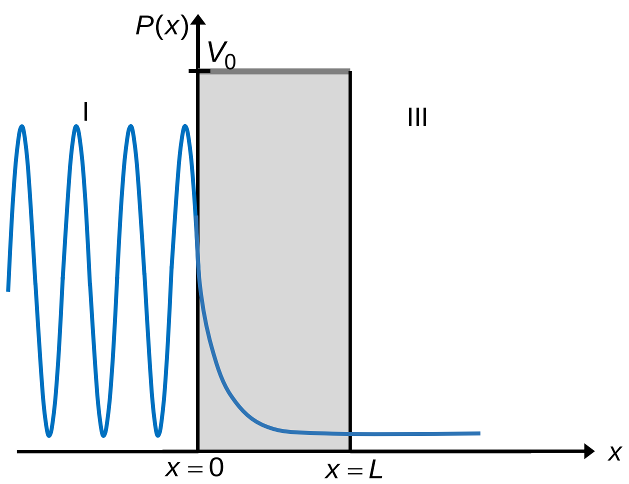

Fig. 11.4: The probability density as a function of position, for a quantum mechanical particle with an energy less than the barrier height.

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 xof the wave that is reflected back from the barrier as shown in Fig. 11.5.

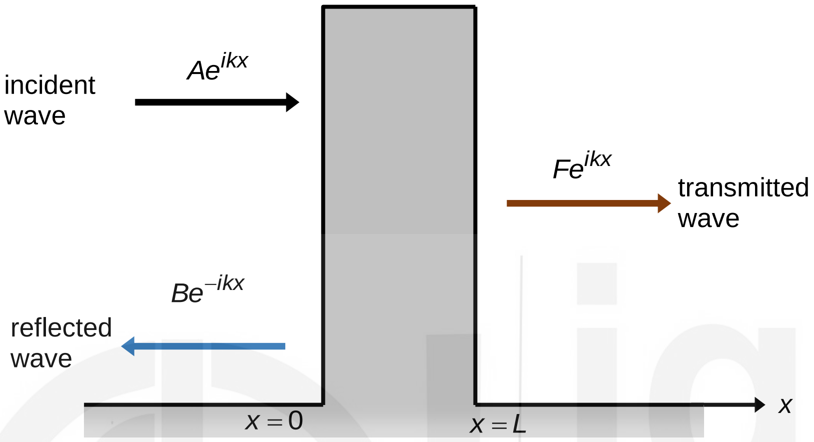

Fig. 11.5: Incident, reflected and transmitted waves at the one-dimensional potential barrier.

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:

$$R = \frac{|B|^2}{|A|^2} \tag{11.21}$$

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:

$$T = \frac{|F|^2}{|A|^2} \tag{11.22}$$

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:

$$R + T = 1 \tag{11.23}$$

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:

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

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

where

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

and

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

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:

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

or,

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

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**:

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

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:

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

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 $V_0 - E = 5.0\,\text{eV} = 8.0 \times 10^{-19}\,\text{J}$:

$$\lambda_T = \frac{\hbar}{\sqrt{2m(V_0 - E)}} = \frac{1.054 \times 10^{-34}\,\text{Js}}{\sqrt{2 \times (9.109 \times 10^{-31}\,\text{kg}) \times (8.0 \times 10^{-19}\,\text{J})}}$$

$$= .09 \times 10^{-9}\,\text{m} = .09\,\text{nm}$$

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

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

With $\lambda_T = .09\,\text{nm}$, the transmission coefficient for $L = 0.3\,\text{nm}$ 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 is: $\dfrac{T_2}{T_1} = \dfrac{f(E/V_0)e^{-4.4}}{f(E/V_0)e^{-6.7}} = e^{2.3} \approx 10$

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 nm and $k' = \dfrac{1}{\lambda_T}$. So,

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

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

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

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

Recap

RELECTION 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:

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

Recap

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

Where

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

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

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

The sum of the reflection and transmission coefficients is 1.

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

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

Where the **tunnelling length** λ_T is:

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

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:

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

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

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

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

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:

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

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

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 that while there is a finite probability of tunnelling , $R > T$.

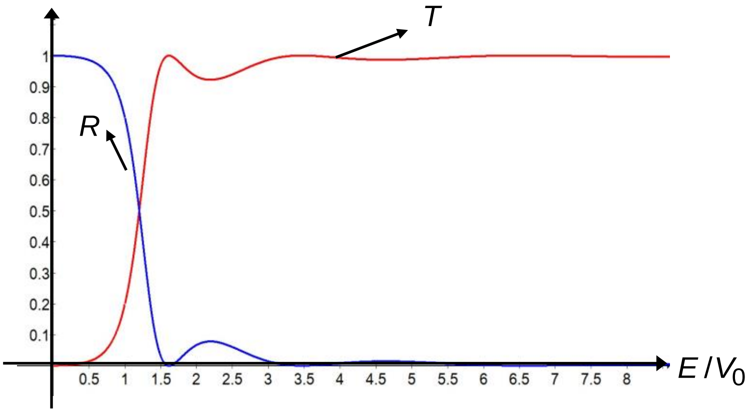

Fig. 11.6: The typical variation of the reflection coefficient *R* and transmission coefficient *T* with E/V_0, for $\frac{2mV_0L^2}{\hbar^2}=16$.

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:

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

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.

RELECTION AND TRANSMISSION COEFFICIENT ($E > V_0$)

Recap

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

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

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

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

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

The transmission and reflection coefficients are:

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

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

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

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 μs 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 that 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 (~10^{-15} m) and hence it is not significant outside the nucleus. Typically the radius of the nucleus is about 1 fm (~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:

$$V(r) = \frac{(Ze)(2e)}{4\pi\varepsilon_0 r} = \frac{Ze^2}{2\pi\varepsilon_0 r} \qquad (11.31)$$

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

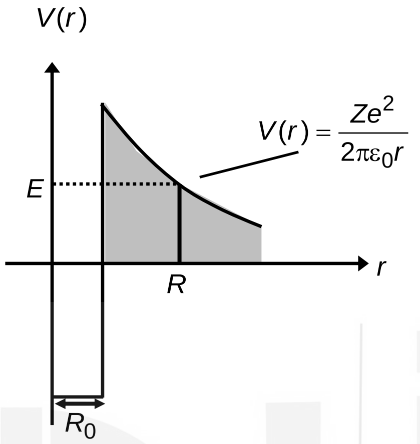

Fig. 11.7: Potential barrier for alpha-particle decay.

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 $r = R$,

$$E == \frac{Ze^2}{2\pi\varepsilon_0 R} \qquad (11.32)$$

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:

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

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

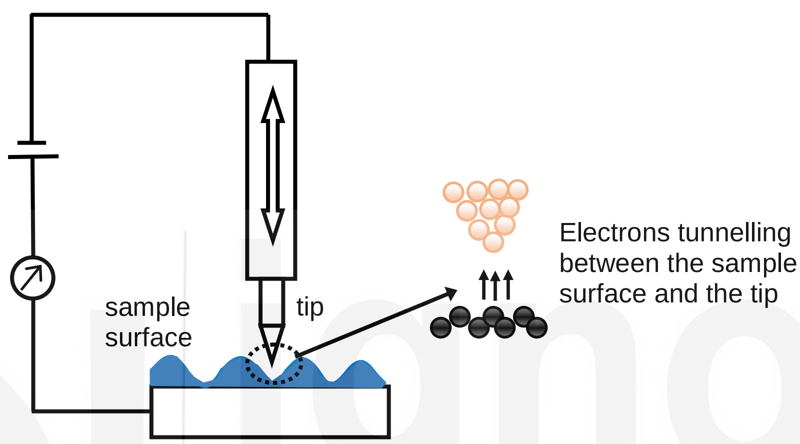

Fig. 11.7: Schematic Diagram of a Scanning Tunnelling Microscope

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 0.001nm, which is even less than the typical diameter of an atom.

Recap

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.

11.4 SUMMARY

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

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

The solutions of the Schrödinger equations are:

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

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

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

where

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

Reflection and transmission coefficients for E<V₀

- 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>V₀

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

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

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

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

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

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 $n = 1,2,3...$

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 is 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 (3.1eV).

6. Calculate the probability that an electron will tunnel through a 0.4nm gap from a metal to the STM probe if the work function is 3.0eV. 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 $m = 0.22 m_e$. So:

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

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

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 $m = m_e$:

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

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

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

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

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

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 = $8\,\text{e}V$, L = 0.80nm, $\frac{E}{V_0} = \frac{8.0\,\text{eV}}{10.0\,\text{eV}} = \frac{4}{5}$ and $\lambda_T = 0.14\,\text{nm}$, we get from Eq. (11.28):

$$T_2 = 16.\left(\frac{4}{5}\right)\left(1 - \frac{4}{5}\right) e^{-\frac{2\times 0.80\,\text{nm}}{0.14\,\text{nm}}} = \left(\frac{64}{25}\right) e^{-11.4} = (2.56)e^{-11.4} \qquad \text{(iii)}$$

We now calculate the ratios of the transmission coefficients T_1 and T_2 with respect to T_0:

$$\frac{T_1}{T_0} = \frac{(3.84)e^{-10}}{(3.84)e^{-20}} = e^{10}$$

and
$$\frac{T_2}{T_0} = \frac{(2.56)e^{-11.4}}{(3.84)e^{-20}} = (0.67)e^{8.6}$$

Since $e^{10} > 0.67e^{8.6}$ 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($m_P = 1836 m_e$) is

$$\lambda_{TP} = \frac{\hbar}{\sqrt{2m_P(V_0 - E)}}$$
$$= \frac{\hbar}{\sqrt{2(1836 m_e)(V_0 - E)}} = \frac{\hbar}{\sqrt{2m_e(V_0 - E)}\sqrt{1836}} = \frac{\lambda_{Te}}{43} \qquad \text{(i)}$$

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:

$$T_P = 16\left(\frac{E}{V_0}\right)\left(1-\frac{E}{V_0}\right)e^{-\frac{2L}{\lambda_{TP}}}$$

$$\therefore \frac{T_e}{T_P} = \frac{e^{-\frac{2L}{\lambda_{Te}}}}{e^{-\frac{2L}{\lambda_{Tp}}}} == \frac{e^{-\frac{2L}{\lambda_{Te}}}}{e^{-\frac{2L}{(\lambda_{Te}/43)}}} e^{42\left(\frac{2L}{\lambda_{Te}}\right)} \Rightarrow T_e >> T_P$$

4. We calculate the tunnelling length by using Eq.(11.27) with $V_0 - E = 2\,\text{eV} = 3.2\times10^{-19}$ J

$$\text{So } \lambda_T = \frac{(1.054\times10^{-34}\,\text{Js})}{\sqrt{2\times(9.109\times10^{-31}\,\text{kg})\times(3.2\times10^{-19}\,\text{J})}} = 0.14\,\text{nm} \qquad \text{(i)}$$

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:

$$T == \frac{1}{50} = 16\times\left(\frac{4}{5}\right)\left(1-\frac{4}{5}\right)e^{-\frac{2L}{0.14\,\text{nm}}}$$

$$\Rightarrow e^{-\frac{2L}{0.14\,\text{nm}}} = \frac{25}{64\times50} \quad \text{or} \quad e^{\frac{2L}{0.14\,\text{nm}}} = 128$$

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 $V_0 - E = (15.0-8.0)\text{eV} = 11.2\times10^{-19}$ J

$$\therefore \lambda_T = \frac{1.054\times10^{-34}\,\text{Js}}{\sqrt{2\times(9.109\times10^{-31}\,\text{kg})\times(11.2\times10^{-19}\,\text{J})}} = 0.074\times10^{-9}\,\text{m} = 0.074\,\text{nm} \qquad \text{(i)}$$

The tunnelling probability T_1 is calculated using Eq. (11.28) with L = 1.0 nm, $E/V_0 = \frac{8.0\,\text{eV}}{15.0\,\text{eV}}$ and $\lambda_T = \frac{1}{k'} = 0.074\,\text{nm}$

$$\therefore T_1 = 16\times\left(\frac{8}{15}\right)\left(1-\frac{8}{15}\right)e^{\frac{-2\times1.0\,\text{nm}}{0.074\,\text{nm}}} = (4.0)e^{-27} \qquad \text{(ii)}$$

When electron absorbs an photon of energy 3.1eV its kinetic energy becomes

$E = (8.0 + 3.1)\text{eV} = 11.1\text{eV}$. So $V_0 - E = 3.9\,\text{eV} = 6.24 \times 10^{-19}$ J

Now the tunnelling length is,

$$\lambda_T = \frac{1.054 \times 10^{-34}\text{ Js}}{\sqrt{2 \times (9.109 \times 10^{-31}\text{kg}) \times (6.24 \times 10^{-19}\text{ J})}} = 0.098\,\text{nm} \qquad \text{(iii)}$$

With $E / V_0 = \dfrac{11.1}{15.0}$ and λ_T given by Equation (iii) the tunnelling probability is:

$$T_2 = 16 \times \left(\frac{11.1}{15.0}\right)\left(1 - \frac{11.1}{15.0}\right) e^{\frac{-2 \times 1.0\,\text{nm}}{.098\,\text{nm}}} = (3.1)e^{-20.4}$$

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 $\approx 3\,\text{eV} = 4.8 \times 10^{-19}$ 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 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*:

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

$$e^{k'L}C + e^{-k'L}D = e^{ikL}F \qquad (11.15b)$$

$$ikA - ikB = k'C - k'D \qquad (11.17a)$$

$$k'e^{k'L}C - k'e^{-k'L}D = ike^{ikL}F \qquad (11.17b)$$

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:

$$k'A + k'B = k'C + k'D \qquad (i)$$

Adding Eqs.(11.17a) and (i) we get:

$$(k' + ik)A + (k' - ik)B = 2k'C \qquad (ii)$$

Subtracting Eq. (11.17a) from Eq. (i) we get

$$(k' - ik)A + (k' + ik)B = 2k'D \qquad (iii)$$

Multiplying Eq. (11.15b) by ik we get:

$$ike^{k'L}C + ike^{-k'L}D = ike^{ikL}F \qquad (iv)$$

Subtracting Eq. (iv) from Eq. (11.17b) we get

$$(k' - ik)e^{k'L}C - (k' + ik)e^{-k'L}D = 0 \qquad (v)$$

Which we can write as:

$$(k' - ik)e^{k'L}C = (k' + ik)e^{-k'L}D$$

or $$C = \frac{(k' + ik)e^{-k'L}}{(k' - ik)e^{k'L}}D \qquad (vi)$$

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:

$$\frac{(k' - ik)e^{k'L}}{(k' + ik)e^{-k'L}}\left[(k' + ik)A + (k' - ik)B\right] = 2k'D \qquad (vii)$$

You can see that the RHS of Eqs. (iii) and (vii) are equal. Equating the LHS of these two equations we get:

$$\frac{(k'-ik)e^{k'L}}{(k'+ik)e^{-k'L}}\left[(k'+ik)A+(k'-ik)B\right]=(k'-ik)A+(k'+ik)B \qquad \text{(viii)}$$

On simplifying, we can write Eq. (viii) as:

$$(k'-ik)e^{k'L}\left[(k'+ik)A+(k'-ik)B\right]=(k'+ik)e^{-k'L}\left[(k'-ik)A+(k'+ik)B\right]$$

Which is:

$$(k'-ik)(k'+ik)e^{k'L}A+(k'-ik)^2e^{k'L}B=(k'+ik)(k'-ik)e^{-k'L}A+(k'+ik)^2e^{-k'L}B$$

Using $(k'-ik)(k'+ik)=k'^2+k^2$ we can write:

$$(k'^2+k^2)e^{k'L}A+(k'-ik)^2e^{k'L}B=(k'^2+k^2)e^{-k'L}A+(k'+ik)^2e^{-k'L}B \qquad \text{(ix)}$$

Dividing Eq. (ix) by A we get

$$(k'^2+k^2)e^{k'L}+(k'-ik)^2e^{k'L}\frac{B}{A}=(k'^2+k^2)e^{-k'L}+(k'+ik)^2e^{-k'L}\frac{B}{A} \qquad \text{(x)}$$

Therefore we have

$$\frac{B}{A}=\frac{(k'^2+k^2)\left(e^{-k'L}-e^{k'L}\right)}{(k'-ik)^2e^{k'L}-(k'+ik)^2e^{-k'L}} \qquad \text{(xi)}$$

which is:

$$\frac{B}{A}=\frac{(k'^2+k^2)\left(e^{-k'L}-e^{k'L}\right)}{(k'^2-k^2)\left(e^{k'L}-e^{-k'L}\right)-(2ik'k)\left(e^{k'L}+e^{-k'L}\right)} \qquad \text{(xii)}$$

Or

$$\frac{B}{A}=\frac{(k'^2+k^2)\sinh(k'L)}{(k^2-k'^2)\sinh(k'L)+2ik'k\cosh(k'L)} \qquad \text{(xii)}$$

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):

$$R=\frac{(k'^2+k^2)^2\sinh^2(k'L)}{(k^2-k'^2)^2\sinh^2(k'L)+4k'^2k^2\cosh^2(k'L)} \qquad \text{(xiii)}$$

Using the identity $\sinh^2(k'L)-\cosh^2(k'L)=1$, we can simplify the denominator of the RHS of Eq. (xiii) as

$$(k^2-k'^2)^2\sinh^2(k'L)+4k'^2k^2\cosh^2(k'L)$$
$$=(k^2-k'^2)^2\sinh^2(k'L)+4k'^2k^2\sinh^2(k'L)+4k'^2k^2\cosh^2(k'L)-4k'^2k^2\sinh^2(k'L)$$
$$=(k^2-k'^2)^2\sinh^2(k'L)+4k'^2k^2$$

Notice that B/A given in Eq. (xii) is complex and it has the general form:

$$\frac{B}{A}=\frac{u}{v+iw}=\frac{u}{v+iw}\left(\frac{v-iw}{v-iw}\right)=\frac{uv-iuw}{v^2+w^2}$$

$$\left|\frac{B}{A}\right|^2=\frac{(uv)^2+(uw)^2}{\left(v^2+w^2\right)^2}=\frac{u^2\left(v^2+w^2\right)}{\left(v^2+w^2\right)^2}=\frac{u^2}{\left(v^2+w^2\right)}$$

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

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

From Eqs.(11.6 and 11.9) we also know that $k = \sqrt{\frac{2mE}{\hbar^2}}$ and

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

So, $k^2 = \frac{2mE}{\hbar^2}$; and $k'^2 = \frac{2m(V_0 - E)}{\hbar^2}$

and

$$k'^2 + k^2 = \frac{2m(V_0 - E)}{\hbar^2} + \frac{2mE}{\hbar^2} = \frac{2mV_0}{\hbar^2}; \; k'^2k^2 = \frac{2m(V_0 - E)}{\hbar^2} \times \frac{2mE}{\hbar^2} \quad \text{(xv)}$$

Substituting from Eq. (xv) into Eq. (xiv) we get the result of Eq. (11.24b):

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

To calculate *T* we use Eq. (11.23). Hence *T*=1-*R*. Using the value of *R* from Eq. (xiv) we get:

$$T = 1 - R = 1 - \frac{(k'^2 + k^2)^2 \sinh^2(k'L)}{(k^2 + k'^2)^2 \sinh^2(k'L) + 4k'^2k^2} = \frac{4k'^2k^2}{(k^2 + k'^2)^2 \sinh^2(k'L) + 4k'^2k^2}$$
$$= \left[1 + \frac{(k^2 + k'^2)^2 \sinh^2(k'L)}{4k'^2k^2}\right]^{-1} \quad \text{(xvi)}$$

Substituting from Eq. (xv) into Eq.(xvi) we get the following result of Eq.(11.24a):

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