CHAPTER V

Simple potentials and quantum tunnelling

§ 1. Introduction

In this chapter we solve the one dimensional Schrödinger equation for three simple but important potentials $V(x)$ and these are usually called:

(i) The infinite square well or a particle in a box
(ii) The finite square well
(iii) The step potential or potential barrier

The last potential—the step potential or potential barrier—is a key example with which to illustrate the phenomenon of *quantum mechanical tunnelling*.

We finish the chapter with some remarks on tunnelling and scattering

§ 2. The infinite square well or a particle in a box

The potential V for an infinite square well is defined by

$$V(x) = \begin{cases} \infty & \text{if } -\infty < x \leq 0 \\ 0 & \text{if } \quad 0 < x < a \\ \infty & \text{if } \quad a \leq x < \infty \end{cases} \tag{5.1}$$

where a is some positive constant. V is displayed in figure 6

The Schrödinger equation says that the eigenfunctions ψ_n and their associated energies E_n are given by

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + V(x)\psi_n(x) = E_n\psi_n(x) \tag{5.2}$$

and to solve this equation it is natural to divide the x-axis up into the three ranges of x that appear in the definition 5.1 of the potential $V(x)$. Let us denote these regions by I, II and III so that we have

$$\begin{aligned} \text{I} &= \{x : -\infty < x \leq 0\} \\ \text{II} &= \{x : \quad 0 < x < a\} \\ \text{III} &= \{x : \quad a \leq x < \infty\} \end{aligned} \tag{5.3}$$

Consider first regions I and III throughout which $V = \infty$; since the product $V(x)\psi_n$ occurs in the Schrödinger equation then this product must always be *finite*, and the only way that

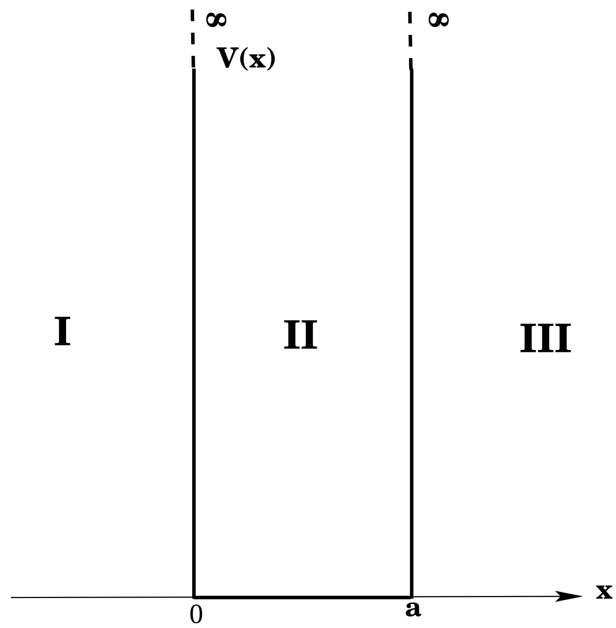

Fig. 6: The infinite square well

this can happen is if $\psi_n(x)$ *vanishes* in these two regions. Hence we deduce the important fact that

$$\psi_n(x) = 0 \quad \text{for} \begin{cases} x \in \text{I} \\ x \in \text{III} \end{cases} \tag{5.4}$$

or, more explicitly,

$$\psi_n(x) = 0 \quad \text{for} \begin{cases} -\infty < x \leq 0 \\ a \leq x < \infty \end{cases} \tag{5.5}$$

On the other hand, in region II, we have $V(x) = 0$, so that, in region II, the Schrödinger reduces to just

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} = E_n\psi(x), \quad \text{for} \quad 0 < x \leq a \tag{5.6}$$

Thus a complete summary of what holds for all three regions I, II and III is that

$$\begin{aligned} \psi_n(x) = 0 \quad &\text{for} \begin{cases} -\infty < x \leq 0 & \text{(I)} \\ a \leq x < \infty & \text{(III)} \end{cases} \\ -\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} = E_n\psi(x), \quad &\text{for } 0 < x < a \quad \text{(II)} \end{aligned} \tag{5.7}$$

This is now very easy to solve and we find that the solutions to the Schrödinger equation—which is just the SHM equation—are given by

$$\psi_n(x) = A\cos(\omega_n x) + B\sin(\omega_n x), \quad \text{with} \begin{cases} A, B \text{ constants} \\ \omega_n^2 = \dfrac{2mE_n}{\hbar^2} \end{cases} \tag{5.8}$$

But $\psi_n(x)$ must vanish in regions I and III and, more particularly, it must vanish[1] at the two points $x = 0$, a. Thus we have

$$\begin{aligned} \psi_n(0) = 0 &\Rightarrow A = 0 \\ \psi_n(a) = 0 &\Rightarrow A\cos(\omega_n a) + B\sin(\omega_n a) = 0 \end{aligned} \tag{5.9}$$

Thus 5.9 has just provided us with two simultaneous equations whose solutions are

$$\left\{ \begin{array}{c} A = 0 \\ \sin(\omega_n a) = 0 \end{array} \right. \Rightarrow \omega_n a = n\pi,\ n \in \mathbf{Z} \tag{5.10}$$

Notice that $n = 0$ will only give us the trivial solution $\psi_n(x) \equiv 0$ and so we exclude it; also changing n to $-n$ only changes the sign of $\psi_n(x)$ and so can be absorbed into B, hence we shall lose no generality by taking n to be *positive* which we now do.

Finally since the relation 5.8 between the energies E_n and ω_n is that $\omega_n^2 = 2mE_n/\hbar^2$ then we find that the energies E_n are indeed quantised and given by

The energies for a particle in an infinite square well

$$E_n = \frac{n^2\hbar^2\pi^2}{2ma^2},\ n = 1, 2, \ldots \tag{5.11}$$

Notice that the lowest energy E_1 is *positive* rather than zero as it typical for quantum mechanical systems.

The terminology 'particle in a box' explained

Finally we point out that since any wave function $\psi(x)$ for this problem vanishes outside the region $0 < x < a$ then a particle moving under this potential is *confined* to this region—it has zero probability to be for its position to be measured anywhere else This situation is sometimes referred to as a particle in a (one dimensional) box. There are also two dimensional and three dimensional versions of the particle in a box where the particle is confined to a two dimensional rectangle, or a three dimensional box, by a potential which is infinite at the boundaries of the box.

We move on to our next problem.

§ 3. The finite square well

A finite square well has a potential V given by

$$V(x) = \begin{cases} V_0 & \text{if } -\infty < x \le 0 \\ 0 & \text{if } \quad 0 < x < a \\ V_0 & \text{if } \quad a \le x < \infty \end{cases} \tag{5.12}$$

The underlying physical problem is that of a particle beam

where a and V_0 are positive constants. A graph of $V(x)$ is shown in figure 7.

One can think of this problem physically as being that of a particle beam travelling along the x-axis towards a target represented by the potential in the region $0 < x < a$.

In region II the Schrödinger equation is the same as it is for the infinite well, namely

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} = E_n\psi(x), \quad \text{for } \ 0 < x < a \tag{5.13}$$

[1] Note that $\psi_n(x)$ it would also be discontinuous—and so not even differentiable—at the points $x = 0$, a if it didn't vanish there.

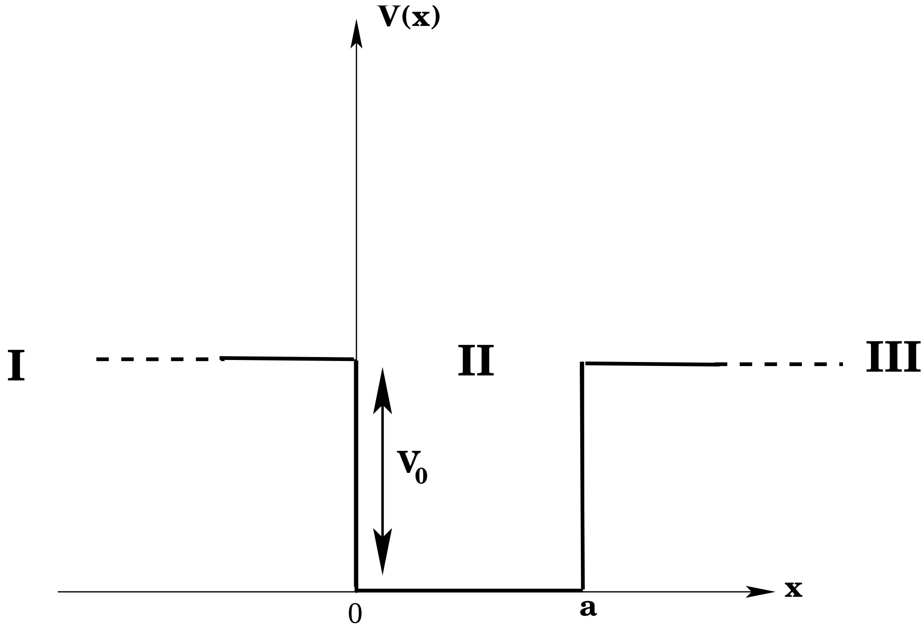

Fig. 7: The finite square well

while in regions I and III we have

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2}+V_0\psi_n(x)=E_n\psi(x),\quad \text{for}\ \begin{cases}-\infty<x\leq 0\\ \quad a\leq x<\infty\end{cases} \tag{5.14}$$

We deal with regions I and III first. The equation we have to solve is

$$\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2}-(V_0-E_n)\psi_n(x)=0 \tag{5.15}$$

i.e.

$$\frac{d^2\psi_n(x)}{dx^2}-\kappa^2\psi_n(x)=0,\quad \text{where}\ \kappa=\sqrt{\frac{2m(V_0-E_n)}{\hbar^2}} \tag{5.16}$$

Next we *assume* [2] that

$$E_n<V_0 \tag{5.17}$$

so that

$$\kappa^2>0\Rightarrow\kappa\ \text{is real} \tag{5.18}$$

[2] If this is not true—i.e. if $E_n\geq V_0$—the reader can easily adjust the argument here to construct the solutions. However all these states will be *scattering states* with $\langle\psi|\psi\rangle=\infty$ rather than quantised, or bound, states with $\langle\psi|\psi\rangle<\infty$. For the case where $E_n>V_0$, then κ will then be pure imaginary: $\kappa=i\theta$, with $\theta\in\mathbf{R}$, and the two solutions $\psi_n(x)$ are oscillatory functions of the form $e^{\pm i\theta}$. Finally when $E_n=V_0$ $\kappa=0$, and $\psi_n(x)$ just takes on the simple form $\psi_n(x)=A+Bx$.

We lose no generality by taking

$$\kappa > 0 \tag{5.19}$$

so we do so. This means that the solution to the Schrödinger equation in regions I and III can be written as

$$\psi_n(x) = \begin{cases} A_{\rm I}\, e^{\kappa x} + B_{\rm I}\, e^{-\kappa x}, & x < 0 \\ A_{\rm III}\, e^{\kappa x} + B_{\rm III}\, e^{-\kappa x}, & x > a \end{cases} \quad (\kappa > 0) \tag{5.20}$$

where $A_{\rm I}$, $A_{\rm III}$, $B_{\rm I}$ and $B_{\rm III}$ are constants. Now since

$$\lim_{x\to\mp\infty} \psi_n(x) \longrightarrow \infty \quad \text{is forbidden} \tag{5.21}$$

because it breaks normalisability and makes

$$\langle\psi_n|\psi_n\rangle = \int \overline{\psi_n(x)}\, \psi_n(x)\, dx\, dy\, dz = \infty \tag{5.22}$$

then we must set

$$B_{\rm I} = 0 \quad \text{in region I} \quad \text{and} \quad A_{\rm III} = 0 \quad \text{in region III} \tag{5.23}$$

In sum we have deduced that

$$\psi_n(x) = \begin{cases} A_{\rm I}\, e^{\kappa x}, & \text{for} \quad x < 0 \quad \text{(region I)} \\ B_{\rm III}\, e^{-\kappa x}, & \text{for} \quad x > a \quad \text{(region III)} \end{cases} \tag{5.24}$$

Coming now to region II we know that $\psi_n(x)$ satisfies equation 5.13 above which we write as

$$\frac{d^2\psi_n(x)}{dx^2} + \omega_n^2 \psi_n(x) = 0, \quad \text{with } \omega_n^2 = \frac{2mE_n}{\hbar^2} \tag{5.25}$$

and so, as in the infinite well problem, we have the solution

$$\psi_n(x) = C\cos(\omega_n x) + D\sin(\omega_n x), \quad \text{for } 0 < x < a \quad \text{(region II)} \tag{5.26}$$

with C and D constants.

Finally we must match up the solution in region II to those in regions I and III. This is done by imposing [3] the condition that

The matching condition for a finite potential well

$$\psi_n(x) \text{ and } \frac{d\psi_n(x)}{dx} \text{ are continuous where the regions join: i.e.. at } \begin{cases} x = 0 \\ x = a \end{cases} \tag{5.27}$$

On imposing these matching conditions we obtain the equations

$$\left.\begin{aligned} A_{\rm I} &= C & (i) \\ B_{\rm III} e^{-\kappa a} &= C\cos(\omega_n a) + D\sin(\omega_n a) & (ii) \end{aligned}\right\} \text{continuity of } \psi_n(x) \text{ at } x = 0,\, a \tag{5.28}$$

[3] That this condition is reasonable follows immediately from the fact that every Schrödinger equation contains the second derivative term $d^2\psi/dx^2$ whose very existence requires continuity of ψ and $d\psi/dx$.

$$\left.\begin{aligned} \kappa A_{\mathrm{I}} &= D\omega_n && (i)\\ -\kappa B_{\mathrm{III}}\, e^{-\kappa a} &= \omega_n\left(-C\sin(\omega_n a) + D\cos(\omega_n a)\right) && (ii)\end{aligned}\right\} \text{continuity of } \frac{d\psi_n(x)}{dx} \text{ at } x = 0,\, a \tag{5.29}$$

It is very straightforward to solve 5.28 and 5.29: first one uses 5.28 (i) in 5.29 (i) thereby deducing that

$$D = \frac{C\kappa}{\omega_n} \tag{5.30}$$

Then one substitutes this expression for D in 5.28 (ii) and 5.29 (ii) yielding the pair of equations

$$\begin{aligned} B_{\mathrm{III}}\, e^{-\kappa a} &= C\cos(\omega_n a) + \frac{C\kappa}{\omega_n}\sin(\omega_n a)\\ -\kappa B_{\mathrm{III}}\, e^{-\kappa a} &= \omega_n\left(-C\sin(\omega_n a) + \frac{C\kappa}{\omega_n}\cos(\omega_n a)\right)\end{aligned} \tag{5.31}$$

Now we multiply the first equation of 5.31 by κ and add it to the second. The result of this is the equation

$$0 = 2\kappa C\cos(\omega_n a) + C(\frac{\kappa^2}{\omega} - \omega_n)\sin(\omega_n a) \tag{5.32}$$

which we can instantly rewrite to read

$$\begin{aligned} \tan(\omega_n a) &= -\frac{2\kappa C}{C(\frac{\kappa^2}{\omega_n} - \omega_n)}\\ &= \frac{2\,\kappa\,\omega_n}{\omega_n^2 - \kappa^2}\end{aligned} \tag{5.33}$$

But κ and ω_n are not independent: indeed, from their definitions in 5.16 and 5.25, we have that

$$\begin{aligned} \kappa^2 &= \frac{2m(V_0 - E_n)}{\hbar^2}, \quad \omega_n^2 = \frac{2mE_n}{\hbar^2}\\ \Rightarrow \kappa^2 &= \frac{2mV_0}{\hbar^2} - \omega_n^2\\ \Rightarrow \kappa &= \sqrt{\frac{2mV_0}{\hbar^2} - \omega_n^2}\end{aligned} \tag{5.34}$$

and so if we use this value for κ in 5.33 above we find that

$$\tan(\omega_n a) = \frac{2\omega_n\sqrt{\frac{2mV_0}{\hbar^2} - \omega_n^2}}{2\omega_n^2 - 2mV_0/\hbar^2} \tag{5.35}$$

that is

$$\tan(\omega_n a) = \frac{\omega_n\sqrt{\frac{2mV_0}{\hbar^2} - \omega_n^2}}{\omega_n^2 - mV_0/\hbar^2}, \quad \text{where } \omega_n^2 = \frac{2mE_n}{\hbar^2} \tag{5.36}$$

Here is the quantisation condition for the finite square well energies E_n

So 5.36 gives the energies E_n of the finite square well which we see are quantised. These energies E_n have to be found numerically or graphically as there is no simple formula for ω_n coming from 5.36. Let use $g(\omega_n)$ to denote the RHS of 5.36 so that

$$g(\omega_n) = \frac{\omega_n\sqrt{\frac{2mV_0}{\hbar^2} - \omega_n^2}}{\omega_n^2 - mV_0/\hbar^2} \tag{5.37}$$

then we show how a value of ω_n arises graphically in figure 8. The point is that the *intersection points* of the two functions are solutions to 5.36 and hence values of $\omega_n a$ giving a quantised energy E_n; note that there are four of these in figure 8.

There will always be a finite number of such quantised E_n since E_n is required to satisfy $E_n < V_0$, also there will always be at least one positive E_n as long as V_0 is non zero. Recall, too, that states with $E_n > V_0$ are not normalisable states but scattering states.

Notice that a finite square well has only a finite number of bound states

The intersection of $\tan(\omega_n a)$ **and** $g(\omega_n)$

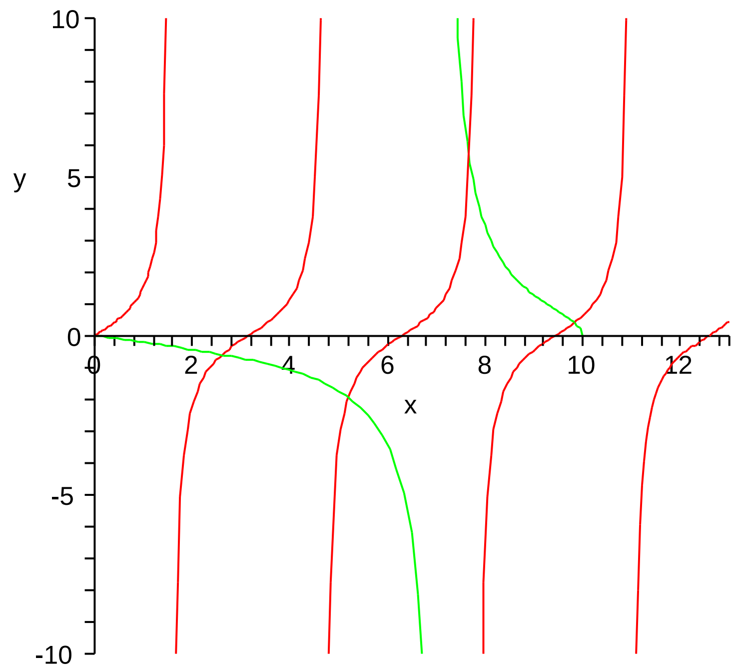

Fig. 8: Energy values for a finite square well ($a = 1$, $x = \omega_n$, $2mV_0/\hbar^2 = 100$)

We close this section with some pictures of the energy level structure for various potentials.

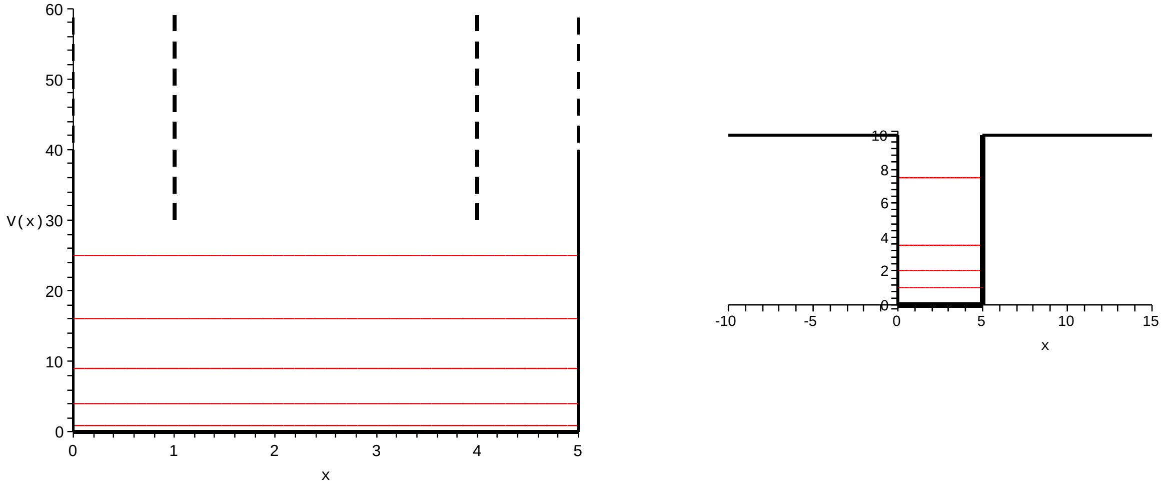

Fig. 9: Energy levels for an infinite and a finite potential well

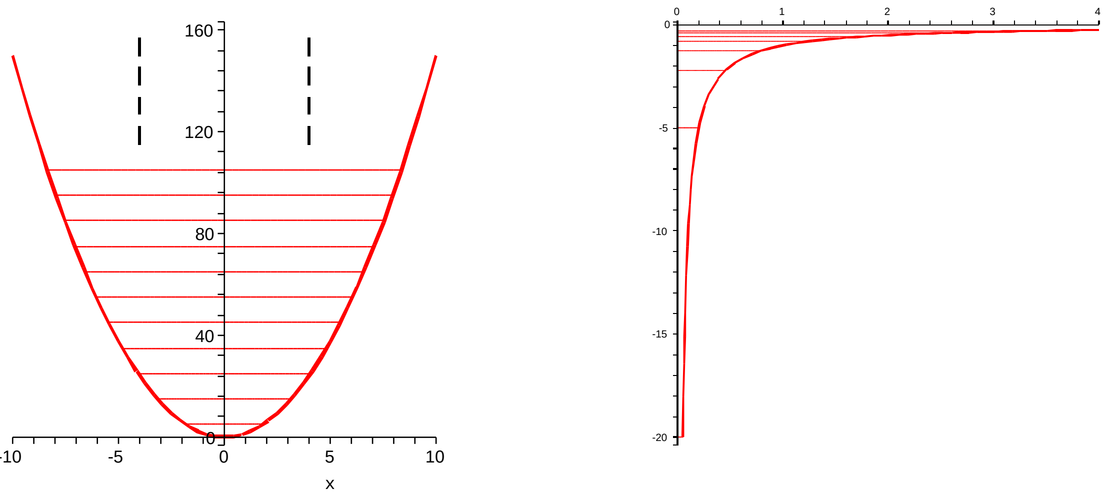

Fig. 10: Energy levels for the harmonic oscillator and the hydrogen atom

§ 4. A potential step or potential barrier

A step potential or potential barrier $V(x)$ is defined by

$$V(x) = \begin{cases} 0 & \text{if } -\infty < x \leq 0 \\ V_0 & \text{if } \quad 0 < x < a \\ 0 & \text{if } \quad a \leq x < \infty \end{cases} \tag{5.38}$$

and is displayed in figure 11.

We see that there are similarities to the finite potential well problem of the preceding section and also we still have precisely the same regions I, II and III of the x-axis that we defined for the finite potential well. This means that we will be able to draw on the calculation done there to deduce what happens in the present problem.

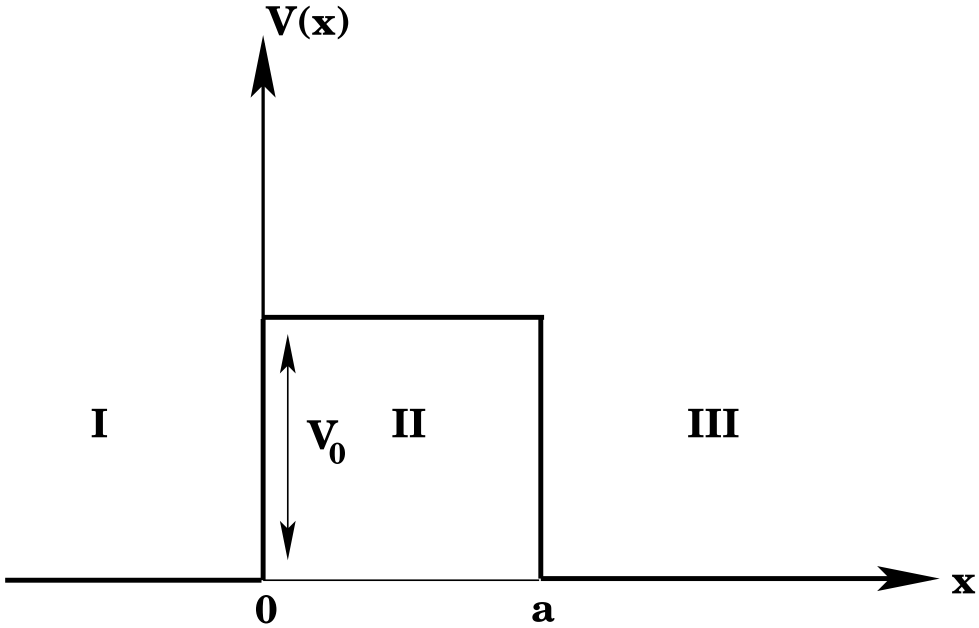

Fig. 11: The step potential or potential barrier

Tunnelling introduced

The most interesting case—and this is the one that gives rise to what is called *tunnelling*—is when

$$E < V_0 \tag{5.39}$$

which we now assume.

First consider a classical free particle with energy $E < V_0$ moving along the negative x-axis so as to encounter the barrier at $x = 0$; such a particle will never penetrate into the barrier since it requires energy $E > V_0$ to do so [4] . However quantum mechanically this is *false*: such a particle can not only penetrate the barrier but also move through it to the other side where $x > a$. The particle is said to *tunnel* through the barrier.

[4] Think of a ball with kinetic energy E moving towards the bottom of a hill of height h. If the ball has mass m, and manages to get to the top of the hill, it will have potential energy V_0, where $V_0 = mgh$. But if $E < V_0$ it will never get to the top: it will only get part of the way up.

Notice, too, that in the quantum mechanical problem the analogy is with a hill of infinite slope since the potential jumps discontinuously from the value 0 to the value V_0 at $x = 0$. This discontinuous jump is not necessary and is an idealisation, which would not happen in nature where the jump would be gradual: the only reason we have it here is because the mathematics is more simple if the potential is made up of vertical and horizontal straight line pieces.

It is quite easy to see why this is so: we shall calculate that a particle incident on the barrier from the *left* has a wave function $\psi(x)$ which is *non zero on the right* of the barrier and so has a non zero probability of being measured there—in fact the wave function ψ is non zero in all three regions I, II and III.

The key point: the particle's wave function is non zero to the right of the barrier (as well as everywhere else).

Now for the calculation of the wave function ψ. In region I the potential $V(x)$ is zero and so the Schrödinger equation is just

$$\frac{d^2\psi(x)}{dx^2} + \omega^2\psi(x) = 0, \quad \text{with } \omega^2 = \frac{2mE}{\hbar^2} \quad \text{for } -\infty < x < 0 \tag{5.40}$$

and so we have oscillatory solutions which we can take to be combinations of $\cos(\omega x)$ and $\sin(\omega x)$ or $e^{i\omega x}$ and $e^{-i\omega x}$ the latter being more convenient for the present problem. Hence we can write[5]

$$\begin{aligned} &\psi(x) = C\cos(\omega x) + D\sin(\omega x) \\ \text{or} \quad &\psi(x) = Ae^{i\omega x} + Be^{-i\omega x} \text{ (more convenient here)} \end{aligned} \quad \text{for } -\infty < x < 0 \tag{5.41}$$

The reason for the exponentials $e^{i\omega x}$ and $e^{-i\omega x}$ being more convenient is that $e^{i\omega x}$ represents a wave travelling from left to right and $e^{-i\omega x}$ a wave travelling from right to left[6] The expression $Ae^{i\omega x}$ represents a (plane) wave incident on the barrier from the left and $Be^{-i\omega x}$ represents a wave which is *reflected* by the barrier.

Take note that the reflected wave must be included despite the fact that the particle can penetrate the barrier; one has to remember that, though there is a non vanishing probability for transmission through the barrier, not all particles will pass through the barrier some will be *reflected* and the probability for reflection is also non vanishing.

Some particles are reflected as well as transmitted

In any case, in region I, we have

$$\psi(x) = Ae^{i\omega x} + Be^{-i\omega x}, \quad \text{for } -\infty < x < 0 \tag{5.42}$$

with A and B constant.

Passing now to region II—inside the barrier—we have, as in 5.16,

$$\frac{d^2\psi(x)}{dx^2} - \kappa^2\psi(x) = 0, \quad \text{where } \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}, \quad 0 < x < a \tag{5.43}$$

But

$$E < V_0 \Rightarrow \kappa \text{ is real} \tag{5.44}$$

and so we have

$$\psi(x) = Ce^{\kappa x} + De^{-\kappa x}, \quad 0 < x < a \tag{5.45}$$

[5] Notice that we write E instead of E_n and ω instead of ω_n. This is because the energy can vary continuously here: the potential does not trap the particle since it is not a well but a step, there is no energy quantisation.

[6] To see this recall (cf. 3.33) that the time dependence of ψ can be supplied by multiplying $\psi(x)$ by the factor $e^{-iEt/\hbar}$ giving here the two possibilities $\psi(x,t) = e^{\mp i\omega x}e^{-iEt/\hbar} = e^{\mp i\omega x - iEt/\hbar}$, an expression which we see represents the pair of waves mentioned above.

with C and D constant.

Finally in region III, $a < x < \infty$ we have, as in region I,

$$\frac{d^2\psi(x)}{dx^2} + \omega^2\psi(x) = 0, \quad \text{with } \omega^2 = \frac{2mE}{\hbar^2}, \quad a < x < \infty \tag{5.46}$$

from which we shall select only the right travelling solution since we know that there are no particles incident from infinity on the right. Hence we write

$$\psi(x) = Ee^{i\omega x}, \quad a < x < \infty \tag{5.47}$$

with E constant.

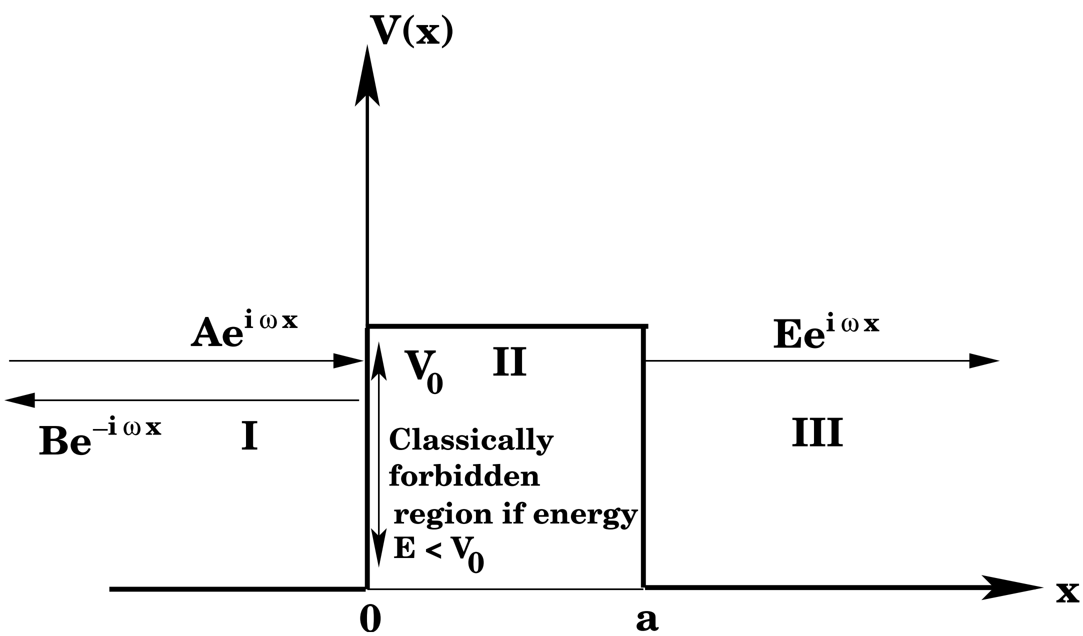

Fig. 12: The potential barrier and its incident, reflected and transmitted waves

The solution for $\psi(x)$ in all three regions just requires us to determine the unknown constants A, B, C, D, E. This simply means applying the boundary conditions of continuity for $\psi(x)$ and $d\psi(x)/dx$ at $x = 0, a$, just as had to be done for the finite well—cf. 5.27 above. The details vary slightly of course—in any case we find that we obtain

The boundary conditions for the barrier problem

$$\begin{aligned} &A + B = C + D \quad (i) && i\omega(A - B) = \kappa(C - D) \quad (iii) \\ &Ce^{\kappa a} + De^{-\kappa a} = Ee^{i\omega a} \quad (ii) && \kappa(Ce^{\kappa a} - De^{-\kappa a}) = i\omega Ee^{i\omega a} \quad (iv) \end{aligned} \tag{5.48}$$

We shall solve for these details in the next section where we calculate the tunnelling probability.

§ 5. The tunnelling probability

The numerical measure of the tunnelling is the fraction of the incident particles—whose wave function is $\psi_{incident}(x) = Ae^{i\omega x}$—which are transmitted through the barrier—where the wave function is $\psi_{transmitted}(x) = Ee^{i\omega x}$. This is simply the ratio of the probability density of the transmitted beam to that of the incident beam: in other words it is

The tunnelling probability

$$\frac{|\psi_{transmitted}(x)|^2}{|\psi_{incident}(x)|^2} = \frac{|Ee^{i\omega x}|^2}{|Ae^{i\omega x}|^2} = \frac{|E|^2}{|A|^2} \tag{5.49}$$

and this is called the *tunnelling probability* and we shall denote it by T writing

T denotes the tunnelling probability

$$T = \frac{|E|^2}{|A|^2} \tag{5.50}$$

We must now finish off by solving the equations of 5.48 to get an expression for the tunnelling probability. Eliminating B from 5.48 (i) and (iii), dividing 5.48 (iv) by κ, and then adding and subtracting the resulting equation to 5.48 (ii) yields the three equations

$$\begin{aligned} A &= \frac{1}{2}\left(1+\frac{\kappa}{i\omega}\right)C + \frac{1}{2}\left(1-\frac{\kappa}{i\omega}\right)D \\ Ce^{\kappa a} &= \frac{1}{2}\left(1+\frac{i\omega}{\kappa}\right)Ee^{i\omega a} \\ De^{-\kappa a} &= \frac{1}{2}\left(1-\frac{i\omega}{\kappa}\right)Ee^{i\omega a} \end{aligned} \tag{5.51}$$

Now if we substitute for C and D from the second and third equations of 5.51 into the first we immediately discover that

$$\begin{aligned} \frac{E}{A} &= \frac{4i\omega\kappa e^{-i\omega a}}{(\kappa^2-\omega^2+2i\omega\kappa)e^{-\kappa a} + (-\kappa^2+\omega^2+2i\omega\kappa)e^{\kappa a}} \\ &= \frac{4i\omega\kappa e^{-i\omega a}}{(\kappa+i\omega)^2 e^{-\kappa a} - (\kappa-i\omega)^2 e^{\kappa a}} \end{aligned} \tag{5.52}$$

Thus T is given by [7]

The full expression for T

$$T = \frac{|E|^2}{|A|^2} = \frac{16\omega^2\kappa^2}{|(\kappa+i\omega)^2 e^{-\kappa a} - (\kappa-i\omega)^2 e^{\kappa a}|^2} \tag{5.53}$$

and so we have our expression for the tunnelling probability T which we see is non-zero.

A useful fact to remember is that T becomes very small when the width of the barrier is large enough. [8]

[7] Another widely used name for T is the *transmission coefficient*.

[8] Note that if the width the barrier is very large and such that

$$\kappa a >> 0 \tag{5.54}$$

As well as tunnelling through the barrier particles can be *reflected*: the reflected wave is just $\psi_{reflected}(x)$ where

Particles can be reflected as well as transmitted

$$\psi_{reflected}(x) = Be^{-i\omega x} \tag{5.56}$$

and the *reflection probability*, which we denote by R, is then defined by [9]

R denotes the reflection probability

$$R = \frac{|\psi_{reflected}(x)|^2}{|\psi_{incident}(x)|^2} = \frac{|Be^{-i\omega x}|^2}{|Ae^{i\omega x}|^2} = \frac{|B|^2}{|A|^2} \tag{5.57}$$

Now particles must be either reflected or transmitted, and since probability is conserved, it must be that

$$R + T = 1 \tag{5.58}$$

One can easily verify this: a very similar calculation to that done above for T shows that the reflection probability is given by

The detailed expression for R

$$R = \frac{|(\kappa^2 + \omega^2)(e^{\kappa a} - e^{-\kappa a})|^2}{|(\kappa + i\omega)^2 e^{-\kappa a} - (\kappa - i\omega)^2 e^{\kappa a}|^2} \tag{5.59}$$

and a little algebra then readily allows us to verify that

R and T do add up to one as they should

$$R + T = 1 \tag{5.60}$$

as claimed.

An important fact to note about reflection is that *classically* reflection *only happens* if $E < V_0$ but quantum mechanically reflection can occur—that is $R \neq 0$—both when $E < V_0$ *and* when $E \geq V_0$.

Here is a comparison of the classical and quantum mechanical situations:

then we may drop the $e^{-\kappa a}$ in the denominator of 5.53 above, since it is then very small, and write

$$\begin{aligned} T = \frac{|E|^2}{|A|^2} \simeq \frac{16\omega^2\kappa^2}{|-(\kappa - i\omega)^2 e^{\kappa a}|^2} &= \frac{16\omega^2\kappa^2 e^{-2\kappa a}}{(\omega^2 + \kappa^2)^2} \\ &= \frac{16E(V_o - E)}{V_0^2} e^{-2(\sqrt{2m(V_0 - E)})(a/\hbar)} \end{aligned} \qquad \text{valid when } \kappa a >> 0 \tag{5.55}$$

an expression which can be useful (in the last line we have re-expressed ω and κ in terms of E and V_0).

Finally a point to remember *only* if the reader ever goes on to study the (special) relativistic version of quantum mechanics known as *quantum field theory*. If we examine T in the limit as Planck's constant $\hbar \to 0$ we find that $T \to 0$ very rapidly because it contains a factor of the form $e^{-c/\hbar}$, $c > 0$. This means that $T \to 0$ more rapidly than any power of $\hbar$ and so cannot be calculated by perturbation theory in $\hbar$. So tunnelling cannot be seen in quantum field theory by using perturbation theory rather it has to do with special non-perturbative effects known as *instantons*.

[9] R is also referred to as the *reflection coefficient*.

Energy E	**Classically**	**Quantum mechanically** ($R+T=1$)
$E<V_0$	$R=1,\ T=0$	$R\neq 0,\ T\neq 0$
$E=V_0$	$R=0,\ T=0$	$R\neq 0,\ T\neq 0$
$E>V_0$	$R=0,\ T=1$	$R\neq 0,\ T\neq 0$

The quantum and the classical barrier compared

Notice that, in the *classical case*, when $E=V_0$, one has $R=T=0$. This means that the particle just comes to a halt at the barrier; if one uses the hill analogy given in the footnote on p. 74 it means that the particle comes to rest at the top of the hill.

Tunnelling and the STEM

Tunnelling enables one to understand the process of alpha decay. It is also the physical mechanism used by the *scanning tunnelling electron microscope* or STEM where electrons can tunnel across the gap between a sample and an ultra fine tungsten needle whose tip is one atom across: individual atoms can then be seen easily.

Tunnelling and other areas of physics

Tunnelling is important in many other parts of physics, for example: nuclear physics, solid state physics and the physics of superconductors (the *Josephson junction*).[10]

We finish here.

[10] The Josephson junction consists of a thin insulator between two superconductors. Electrons can tunnel across the insulator and many interesting phenomena occur. The Josephson junction plays a crucial part in measuring magnetic fields very accurately using a device called a SQUID, where the acronym stands for *superconducting quantum interference device.*

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