Module P11.1 Reflection and transmission at steps and barriers

Exit module

1 Opening items

1.1 Module introduction

In 1954, the Nobel Prize for physics was awarded to Cockcroft and Walton for their initiation of nuclear physics twenty years previously. They made use of *quantum tunnelling* to induce nuclear reactions in circumstances which classical physics deemed impossible. In 1973, the Nobel Prize was awarded to three scientists for their work in developing useful devices called *tunnel diodes* which depend for their operation on the same effect. These devices have opened up whole new areas of physics and technology. In 1986, another Nobel Prize was awarded to Binnig and Rohrer for their invention of the scanning tunnelling electron microscope. All these prizes have been awarded for the exploitation of one quantum effect, carried out with great ingenuity and insight.

The behaviour of particles such as electrons, photons and nucleons is determined by their quantum mechanical characteristics, and we rely on the Born probability hypothesis to relate particle position to the amplitude squared of the associated wavefunction. Such particles may therefore be expected to exhibit wave-like characteristics. When light waves encounter a boundary where the refractive index changes, there may be both a reflected and a transmitted wave. If the boundary is between a transparent and an opaque material, the wave will still penetrate into the opaque material for a distance roughly equal to the wavelength. It follows that light can be transmitted through a layer of a metal provided its thickness is less than the *penetration depth* of the wave.

A good example of this is the layer of silver a few atoms thick on a glass slide forming a semi-reflecting mirror. In the context of quantum mechanics we might expect particles to show similar behaviour.

In the quantum mechanical case, one can think of the particle potential energy as roughly analogous to a refractive index. If the potential energy changes suddenly with position, then there is usually both a transmitted and a reflected quantum wave at the boundary, and the particles will be transmitted or reflected with calculable probability. If the increase in potential energy is greater than the particle kinetic energy, then the quantum wave will penetrate into the classically forbidden region though its amplitude will rapidly decrease. In consequence, if the region of high potential energy is narrow enough, the wave will emerge with reduced amplitude on the other side and there is a probability that the associated particle will tunnel through. A narrow region of high potential energy is called a *potential barrier*. Quantum mechanics therefore predicts two effects totally alien to the classical mechanics based on Newton's laws: (i) particles may be reflected by any sudden change in potential energy, and (ii) particles can tunnel through narrow potential barriers. Experiment confirms both of these remarkable predictions.

Study comment Having read the introduction you may feel that you are already familiar with the material covered by this module and that you do not need to study it. If so, try the *Fast track questions* given in Subsection 1.2. If not, proceed directly to *Ready to study?* in Subsection 1.3.

1.2 Fast track questions

Study comment Can you answer the following *Fast track questions*?. If you answer the questions successfully you need only glance through the module before looking at the *Module summary* (Subsection 5.1) and the *Achievements* listed in Subsection 5.2. If you are sure that you can meet each of these achievements, try the *Exit test* in Subsection 5.3. If you have difficulty with only one or two of the questions you should follow the guidance given in the answers and read the relevant parts of the module. However, *if you have difficulty with more than two of the Exit questions you are strongly advised to study the whole module*.

Question F1

A stationary state spatial wavefunction $\psi(x) = A\exp(ikx)$ represents a stream of particles. What is the number density of particles per unit length, the momentum of each particle, and the flux?

Question F2

A beam of electrons with kinetic energy 5 eV is incident on a region where the electron potential energy suddenly increases from 0 to 2.5 eV. Calculate the transmission and reflection coefficients at this 'step'. Sketch the electron density as a function of position. Account for the sequence of maxima and minima before the step. Assume the potential is constant before and after the step.

Question F3

Estimate the fraction of 2.5 eV electrons that pass through a potential barrier height 5 eV and width 0.5 nm.

Study comment

Having seen the *Fast track questions* you may feel that it would be wiser to follow the normal route through the module and to proceed directly to *Ready to study?* in Subsection 1.3.

Alternatively, you may still be sufficiently comfortable with the material covered by the module to proceed directly to the *Closing items*.

1.3 Ready to study?

Study comment In order to study this module, you will need to be familiar with the following physics terms: *de Broglie wave*, *eigenfunction* (of momentum), *time-independent Schrödinger equation*, *wavefunction*, *Born probability interpretation* of the wavefunction, the (*stationary state*) *probability density* function $P(x) = |\,\psi(x)\,|^2$. You should be familiar with the solutions of the Schrödinger equation for a particle moving in one dimension, in a region where the potential energy is constant. In particular, you should know the different forms of the solutions: (a) when the total energy of the particle is greater than the potential energy, and (b) when the total energy is less than the potential energy. Some knowledge of classical Newtonian mechanics is assumed, especially the treatment of particle motion in terms of the total energy, kinetic energy and potential energy. The module assumes some familiarity with the treatment of *transverse waves* on a string and the reflection of *travelling waves* at a boundary. If you are uncertain of any of these terms, you can review them now by referring to the *Glossary* which will indicate where in *FLAP* they are developed. We have to use *complex numbers*, so you must be familiar with them in *Cartesian form* $z = a + ib$, *polar form* $z = A(\cos\theta + i\sin\theta)$ and *exponential form* $z = A\exp(i\theta)$. You must be confident using a spatial wavefunction written as a complex number: for example $\psi(x) = A\exp(ikx)$, and with the manipulation of complex numbers. We will frequently use *differential calculus*, including *differentiation* of elementary functions such as sine, cosine and exponential. The following *Ready to study questions* will allow you to establish whether you need to review some of the topics before embarking on this module.

Question R1

Write down the spatial part of the wavefunction of a particle travelling in the positive x-direction with definite momentum p. If the total energy of the particle is E and the potential energy has the constant value V, what is the relation between p, E, and V? What is the relation between the angular wavenumber k, the de Broglie wavelength, and the momentum magnitude p?

Question R2

Write down the time-independent Schrödinger equation for a particle moving in one dimension (x) in a region of space where the total energy is less than the constant potential energy V. Show by substitution that the spatial wavefunction $\psi(x) = A\exp(-\alpha x) + B\exp(\alpha x)$, where A and B are constants, is a solution of this equation and find α in terms of E and V.

Question R3

Define the (stationary state) probability density function $P(x)$, for a particle moving in one dimension, and describe its physical interpretation. A particle has the spatial wavefunction $\psi(x) = A\exp(-\alpha x)$, in the region $x \geq 0$, with A and α real, and $\psi(x) = 0$ elsewhere. Write down an expression for the probability density $P(x)$. Find a real positive value of A if the total probability of finding the particle somewhere between $x = 0$ and $x \to \infty$ is one (i.e. normalize the wavefunction).

Question R4

(a) Write $z = a + i\,b$ in the form $z = A\exp(i\phi)$ by relating A and ϕ to a and b.

(b) Show that the complex number $z = \dfrac{a - ib}{a + ib}$ may be written as $z = \exp(-2i\phi)$.

(c) Show that the complex number $z = \dfrac{2a}{a + ib}$ may be written $z = 2\cos\phi\,\exp(-i\phi\,)$.

2 Reflection and transmission at a potential step when $E > V$

2.1 Classical description of the problem

The physical situation we are modelling is quite simple. A particle is moving with constant velocity in the positive x-direction and encounters at some point a strong force directed in the negative x-direction. The force is constant in time and acts over a short distance d. It is usually best to represent the situation in classical (Newtonian) mechanics with a potential energy function $U(x)$. The derivative of the potential energy function with respect to x gives the force component in the negative x-direction:

$$F_x(x) = -\frac{dU(x)}{dx}$$

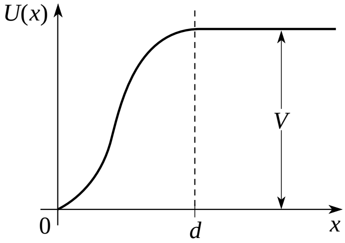

Figure 1 The potential energy function $U(x)$ for a particle acted on by a repulsive force between $x = 0$ and $x = d$.

The potential energy function looks like that drawn in Figure 1. Notice that for convenience we have taken $U(x) = 0$ for $x < 0$ and $U(x) = V$ for $x \geq d$. It is the *change* in the potential energy that is physically significant, and the force acts in the region between 0 and d. For obvious reasons, the situation is referred to as a **potential step**, and we wish to know what happens to a particle encountering it.

Classical mechanics gives a definite answer, and all we need to know is the initial speed of the particle, its mass m and the potential energy function. Classically, the total energy E of the particle, kinetic plus potential, must be constant everywhere. So, if we let the speed of the particle be u as it approaches the step, and if we let υ be its speed beyond the step, then

$$E = \tfrac{1}{2}mu^2 + 0 = \tfrac{1}{2}m\upsilon^2 + V$$

Hence $$\upsilon = \sqrt{\frac{2(E-V)}{m}}$$ ☞

This equation has a real solution only if $E \geq V$. The particle then passes across the step and continues with reduced speed. If the potential energy has a value greater than E beyond the step, then the solution for υ is purely *imaginary* and does not represent a physical situation. In fact, the particle is reflected from the step and is not seen in the region $x \geq d$.

In the classical sense, reflected means that the repulsive force is so strong that the particle comes to rest and then moves back in the direction from which it came.

Question T1

Suppose the potential energy function in Figure 1 is $U(x) = 0$ for $x < 0$ and $U(x) = 6\,\mathrm{J}$ for $x \geq d$. A particle of mass 6 kg approaches from the left with speed $2\,\mathrm{m\,s^{-1}}$. Find its speed after the step. ❑

If the force on the particle is in the positive x-direction, then the potential energy decreases and we have a *step down* rather than a step up! It is easy to show that the particle will always gain speed at this step and classical physics predicts that it will never be reflected.

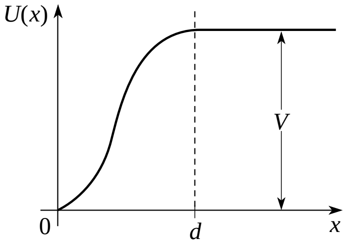

Figure 1 The potential energy function $U(x)$ for a particle acted on by a repulsive force between $x = 0$ and $x = d$.

Often we have to model this kind of situation when the distance d is *small* compared with any other dimension in the problem. Figure 2 represents a potential step with the distance d negligibly small; the potential suddenly increases at the origin from zero to a constant value V. Remember that this diagram can only be an *approximation* to the truth, since such a sudden increase in potential represents an infinite force acting over zero distance. However, it is a useful device, and it is also convenient to represent the total energy E on the diagram. Classical mechanics then makes the following definite predictions for a particle approaching from the left ($x < 0$) with zero potential energy initially:

Particle transmitted across the step if $E > V$ and $V > 0$
Particle reflected at the step if $E < V$ and $V > 0$
Particle always transmitted across step if $V \le 0$

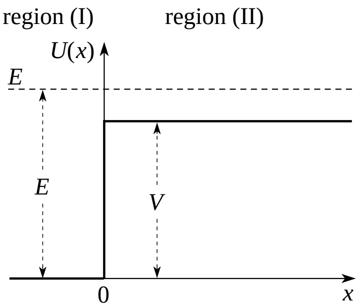

Figure 2 A schematic representation of a potential step. The distance over which the force acts is assumed to be negligible. The total energy of the particle is E.

2.2 The time-independent Schrödinger equation and its solutions

In order to find out what quantum mechanics can tell us about a physical situation, we have to make a simple model and then solve the *Schrödinger equation* to find the appropriate *wavefunctions*. As in classical mechanics, we model the potential function as a step and make the approximation that d is small, but small compared with what? ☞

The relevant dimension is now the de Broglie wavelength of the incident particle $\lambda = h/p$, where h is Planck's constant and p is the magnitude of the *particle momentum* initially. The potential energy diagram is the same as Figure 2, and it is convenient to call the space $x < 0$ region (I) and the space $x \geq 0$ region (II). The time-independent Schrödinger equation in one dimension is:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\,\psi(x) = E\,\psi(x) \tag{1}$$

where E is the total energy of the particle, $U(x)$ the potential energy function and $\psi(x)$ the spatial part of the wavefunction.

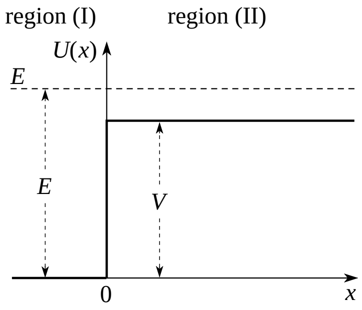

Figure 2 A schematic representation of a potential step. The distance over which the force acts is assumed to be negligible. The total energy of the particle is E.

Study comment The full wavefunction $\Psi(x,\ t)$ is time-dependent and satisfies the *time-dependent Schrödinger equation*. For a stationary state of definite energy E the wavefunction takes the form

$$\Psi(x,t) = \psi(x)\exp\left(-i\frac{E}{\hbar}t\right)$$

Since this module is entirely concerned with states of given energy E, we need only determine $\psi(x)$, which we may therefore conveniently refer to as the wavefunction. The full wavefunction $\Psi(x,\ t)$ follows immediately. Similarly, we may refer to Equation 1 as the Schrödinger equation. ❏

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\,\psi(x) = E\,\psi(x) \qquad \text{(Eqn 1)}$$

In region (I), $U(x) = 0$ and $\psi(x) = \psi_1(x)$ so the Schrödinger equation is

$$\frac{-\hbar^2}{2m}\frac{d^2\psi_1(x)}{dx^2} = E\,\psi_1(x)$$

The solution of this equation takes the form:

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \qquad (2)$$

with A and B arbitrary complex constants and $k_1 = \sqrt{2mE}/\hbar$.

In region (II), $U(x) = V$ and the Schrödinger equation is:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi_2(x)}{dx^2} = (E - V)\,\psi_2(x)$$

The solution then has the form:

$$\psi_2(x) = C\exp(ik_2x) + D\exp(-ik_2x) \qquad (3)$$

with C and D arbitrary complex constants and $k_2 = \sqrt{2m(E - V)}\big/\hbar$.
Notice that k_2 is a real number because $E > V$.

The first term on the right-hand side of Equation 2

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \qquad \text{(Eqn 2)}$$

represents a particle moving with momentum component $\hbar k_1$ in the x-direction, ☞ and the second term represents a reflected particle moving with momentum component $-\hbar k_1$. The first term in Equation 3 represents a particle transmitted across the step moving with momentum component $\hbar k_2$, and the second term represents a particle moving in the negative x-direction. Clearly, we must set coefficient $D = 0$, since this physical problem involves a particle approaching the barrier from the left, not from the right and here it cannot return from infinity.

In summary, the solutions to the Schrödinger equation in the two regions are:

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \quad \text{in region (I)} \qquad (4a)$$

$$\psi_2(x) = C\exp(ik_2x) \quad \text{in region (II)} \qquad (4b)$$

The important question of normalization of the wavefunctions must be postponed until we have discussed fully the constraints imposed on the constants A, B and C by the conditions at the boundary between the two regions.

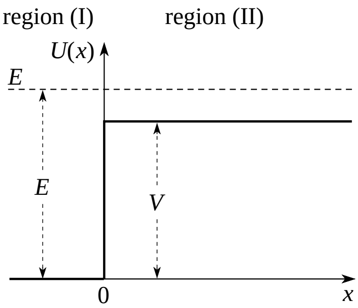

Figure 2 A schematic representation of a potential step. The distance over which the force acts is assumed to be negligible. The total energy of the particle is E.

2.3 Relations imposed by the boundary conditions

General solutions of differential equations always contain arbitrary constants, and we can determine these from the conditions assumed to apply at certain positions or times. For example, the general solution of the wave equation for transverse waves on a string stretched between two fixed points has two arbitrary constants. ☞ We can determine these constants from the initial configuration of the string including the requirement that its displacement is zero at the ends.

We can apply two **boundary conditions**, at $x = 0$, to the solutions of the Schrödinger equation in this application. We will state them and then make some justification.

boundary condition (1) $\quad \psi_1(x) = \psi_2(x) \quad$ at $x = 0$

boundary condition (2) $\quad \dfrac{d\psi_1(x)}{dx} = \dfrac{d\psi_2(x)}{dx} \quad$ at $x = 0$

The first condition ensures that the wavefunction has a single value at $x = 0$. The *Born probability hypothesis* says that the probability density is given by $|\,\psi(x)\,|^2$, so that the solution in region (I) must match the solution in region (II) at the boundary between the regions.

The second condition

boundary condition (2) $$\frac{d\psi_1(x)}{dx} = \frac{d\psi_2(x)}{dx} \qquad \text{at } x = 0$$

is clear when we examine the Schrödinger equation itself (Equation 1).

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\,\psi(x) = E\,\psi(x) \qquad \text{(Eqn 1)}$$

If both E and $U(x)$ are finite quantities everywhere, then the second derivative $d^2\psi_1(x)/dx^2$ must also be finite. This means that the first derivative of the wavefunction $d\psi_1(x)/dx$ cannot suddenly change at any point, including the boundary at $x = 0$. Therefore the slope of the wavefunction in region (I) at $x = 0$ is equal to the slope of the wavefunction in region (II) also evaluated at $x = 0$.

The possibilities are illustrated in Figure 3:

(a) shows a discontinuity in ψ at $x = 0$,

(b) has ψ continuous but $d\psi/dx$ discontinuous at $x = 0$,

and in

(c) both ψ and $d\psi/dx$ are continuous.

Only in case (c) can we say that ψ varies smoothly across the boundary, and this is what we require. ☞

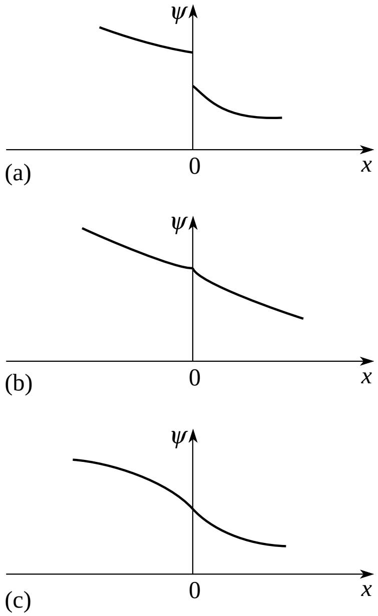

Figure 3 Boundary conditions at $x = 0$. Only (c) is allowed. (a) $\psi_1 \neq \psi_2$, (b) $\psi_1 = \psi_2$ but $d\psi_1/dx \neq d\psi_2/dx$, (c) $\psi_1 = \psi_2$ and $d\psi_1/dx = d\psi_2/dx$.

Applying the boundary conditions gives us two equations linking *A*, *B* and *C*:

Using Equations 4,

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \qquad \text{in region (I)} \qquad \text{(Eqn 4a)}$$

$$\psi_2(x) = C\exp(ik_2x) \qquad \text{in region (II)} \qquad \text{(Eqn 4b)}$$

boundary condition (1) gives:

$$\psi_1(0) = \psi_2(0)$$

so that $\quad A\exp 0 + B\exp 0 = C\exp 0$

i.e. $\quad A + B = C \qquad (5)$

Applying boundary condition (2):

$$A(ik_1)\exp 0 + B(-ik_1)\exp 0 = C(ik_2)\exp 0$$

so that $\quad Ak_1 - Bk_1 = Ck_2 \qquad (6)$

Equations 5 and 6

$$A + B = C \qquad \text{(Eqn 5)}$$

$$Ak_1 - Bk_1 = Ck_2 \qquad \text{(Eqn 6)}$$

can be used to determine the two *ratios* B/A and C/A:

$$\boxed{\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2} \qquad \frac{C}{A} = \frac{2k_1}{k_1 + k_2} \qquad (7)}$$

Question T2

Consider a string lying along the x-axis under tension F. The density per unit length of the string is ρ_1 for $x < 0$ and ρ_2 for $x \geq 0$. Considering transverse waves on the string, describe how this problem in classical mechanics might be similar to the quantum-mechanical problem of particles incident on a potential step.
(The speed of transverse waves is $\sqrt{F/\rho}$.) ❏

2.4 The wavefunctions in each region and the physical interpretation; normalization

In all our discussions of quantum mechanics so far, we have assumed that the wavefunction $\psi(x)$ is normalized to unity and represents a *single particle*, so $|\psi(x)|^2\,\Delta x$ gives the probability of finding the particle in the range x to $x + \Delta x$. Now it is convenient to modify the prescription and say that the wavefunction can represent *more than one particle*. In particular, the wavefunction $\psi(x) = A\exp(ikx)$ can represent a set of particles, moving in the x-direction, all with the same momentum $\hbar k$.

The position of any one particle is not specified (to do so violates the *Heisenberg uncertainty principle*), but we say the average number of particles per unit length is given by $|\psi(x)|^2$. In this context, 'average' means the average of a large number of observations made on particles with this wavefunction. ☞

❖ The wavefunction $\psi(x) = A\exp(ikx)$ represents a stream of particles moving in the x-direction. Show that, on average, there are $|A|^2$ particles per unit length.

Now we must examine the wavefunctions (Equations 4)

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \qquad \text{in region (I)} \qquad \text{(Eqn 4a)}$$

$$\psi_2(x) = C\exp(ik_2x) \qquad \text{in region (II)} \qquad \text{(Eqn 4b)}$$

in the potential step problem in the light of the new prescription.

In region (I), we have the wavefunction:

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \qquad \text{with} \quad k_1 = \sqrt{2mE}/\hbar$$

The first term of this single wavefunction now represents a stream of particles moving in the positive x-direction towards the step; these are the *incident particles*. The second term represents a stream of particles moving in the negative x-direction away from the step, the *reflected particles*. The average number of incident particles per unit length is $|A|^2$, and the average number of reflected particles is $|B|^2$. Notice that the single wavefunction can represent both the incident and reflected particles.

In region (II), the wavefunction is:

$$\psi_2(x) = C\exp(ik_2x) \qquad \text{with} \quad k_2 = \sqrt{2m(E-V)}/\hbar$$

This simply represents a stream of particles moving in the positive x-direction away from the step, the *transmitted particles*. The average number of transmitted particles per unit length is $|C|^2$.

A further simplification of the equations is made, with no loss of generality, if the wavefunctions are *normalized* in a special way. If the coefficient A is set equal to one, then the average number of incident particles per unit length is equal to one.

Question T3

Electrons with kinetic energy 5 eV are moving in the positive x-direction in a region of constant potential. There are on average 5×10^6 electrons per millimetre. Find a suitable wavefunction ☞ to describe them, and find A and k. ❏

2.5 Defining particle flux in the classical and quantum models

In classical mechanics, it is straightforward to define the concept of **particle flux**. We will restrict the discussion to motion in one dimension, but the extension to three dimensions is not difficult. If there are N particles per unit length and each one has speed u in the positive x-direction, then all the particles in a length $u\Delta t$ will pass a fixed point in time interval Δt. The number passing a fixed point per unit time is the particle flux F:

$$F = \frac{Nu\,\Delta t}{\Delta t} = Nu$$

In quantum mechanics, the definition of particle flux is equally simple, provided we are dealing with wavefunctions of particles with definite momentum (i.e. momentum eigenfunctions). Consider a stream of particles represented by the wavefunction $\psi(x) = A\exp(ikx)$. The average number of particles per unit length is the constant $|A|^2$, and their speed u is obtained from the momentum magnitude:

$$p = \hbar k \quad \text{and} \quad u = p/m$$

so that: $u = \hbar k/m$

Since $k > 0$, so is u.

The flux is then given by:

$$F = |A|^2 \frac{\hbar k}{m} \tag{8}$$

A word of warning is necessary here! Equation 8 can only be used when the wavefunction is a momentum eigenfunction; the momentum is then the same for all the particles, and the average number of particles per unit length is a constant, independent of position.

Question T4

What is the flux of electrons in Question T3?

[Electrons with kinetic energy 5 eV are moving in the positive x-direction in a region of constant potential. There are on average 5×10^6 electrons per millimetre.]

What is the corresponding current in amps?

(*Hint*: The current is the total charge in coulombs passing a point per second.) ❏

2.6 Reflection and transmission in the quantum model

We are now in a position to complete the quantum description of particle reflection and transmission at potential steps. Two coefficients are defined which characterize the behaviour of particles when they encounter a potential step such as that illustrated in Figure 2.

The **reflection coefficient** is defined as follows:

$$R = \frac{\text{flux of reflected particles}}{\text{flux of incident particles}}$$

The wavefunction in region (I) is:

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x)$$

The first term represents the particles incident on the step, and, using Equation 8,

$$F = |A|^2\frac{\hbar k}{m} \qquad \text{(Eqn 8)}$$

the incident flux is $|A|^2\,\hbar k_1/m$.

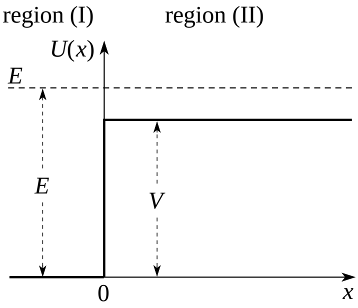

Figure 2 A schematic representation of a potential step. The distance over which the force acts is assumed to be negligible. The total energy of the particle is E.

The second term

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x)$$

represents the reflected particles which have average density $|B|^2$ per unit length and the reflected flux is $|B|^2\,\hbar k_1/m$. The reflection coefficient is therefore:

$$R = \frac{|B|^2\,\hbar k_1/m}{|A|^2\,\hbar k_1/m} = \frac{|B|^2}{|A|^2}$$

Using Equations 7,

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2} \qquad \text{(Eqn 7)}$$

we get the result:

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \qquad (9)$$

The reflection coefficient at a potential step with $E > V$

The **transmission coefficient** is defined as:

$$T = \frac{\text{flux of transmitted particles}}{\text{flux of incident particles}}$$

The wavefunction in region (II) is $\psi_2(x) = C\exp(ik_2x)$, and this represents the particles transmitted across the step. The transmitted flux is given by $|C|^2\hbar k_2/m$ and hence the transmission coefficient is:

$$T = \frac{|C|^2\hbar k_2/m}{|A|^2\hbar k_1/m} = \frac{|C|^2 k_2}{|A|^2 k_1}$$

Using Equations 7 again:

$$\frac{C}{A} = \frac{2k_1}{k_1 + k_2} \qquad \text{(Eqn 7)}$$

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2} \qquad (10)$$

The transmission coefficient at a potential step with $E > V$

In order to check that our equations for R and T are self-consistent, we must show that particles are not 'lost' at the step. The number of particles crossing the step per second (the transmitted flux) added to the number reflected per second (the reflected flux) must be equal to the incident flux. From the definitions of R and T, this means that $R + T = 1$. This is indeed the case!

Question T5

Use Equation 9 and Equation 10

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \qquad \text{(Eqn 9)}$$

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2} \qquad \text{(Eqn 10)}$$

to show that $R + T = 1$. ❏

Remember that R and T are both *ratios of fluxes*; this means that the formulae for R and T are *unchanged* whatever the value of A. It is also legitimate to regard R and T as reflection and transmission *probabilities* if you are dealing with the behaviour of a single particle at the step.

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \qquad \text{(Eqn 9)}$$

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2} \qquad \text{(Eqn 10)}$$

Notice that the reflection coefficient approaches the limit $R = 1$ and the transmission coefficient goes to zero, when $k_2 \to 0$. This happens when V is equal to the incident particle energy E.

The function $P(x) = |\,\psi(x)|^2$ represents the *probability density* when ψ is the wavefunction for a single particle. However, when ψ represents a set of particles, the function $P(x) = |\,\psi(x)|^2$ gives the average particle density at the position x. $P(x)$ is then the **particle density function** and it is interesting to plot a graph of $P(x)$ across the potential step.

This is shown in Figure 4 for the case when A, B and C are real. In region (I), we have to use the full expression for $\psi_1(x)$ (Equation 4):

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \qquad \text{in region (I)} \qquad \text{(Eqn 4a)}$$

$$\psi_2(x) = C\exp(ik_2x) \qquad \text{in region (II)} \qquad \text{(Eqn 4b)}$$

$$P_1(x) = \psi_1^*(x)\,\psi_1(x) = A^2 + B^2 + 2AB\cos(2k_1x) \tag{11}$$

In region (II)

$$P_2(x) = \psi_2^*(x)\,\psi_2(x) = C^2 \tag{12}$$

$P_1(x)$ and $P_2(x)$ join smoothly at $x = 0$ because of the boundary conditions (Equations 5 and 6).

$$A + B = C \qquad \text{(Eqn 5)}$$

$$Ak_1 - Bk_1 = Ck_2 \qquad \text{(Eqn 6)}$$

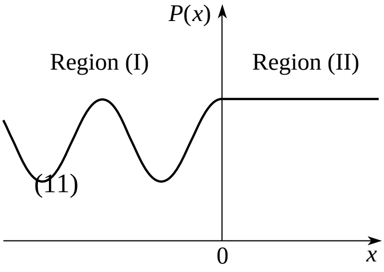

Figure 4 The particle density function $P(x)$ in the region of a potential step ($E > V$). In region (I), $P(x)$ shows a pattern of alternating maxima and minima caused by the interference of the incident and reflected waves.

In region (I), $P(x)$ has a cosine component due to the *interference* between the incident and reflected waves.

This example of quantum-mechanical interference with material particles is analogous to the interference of light beams reflected from boundaries between materials with different optical properties. The interference minima are not at zero because the amplitude of the reflected wave is less than the amplitude of the incident wave.

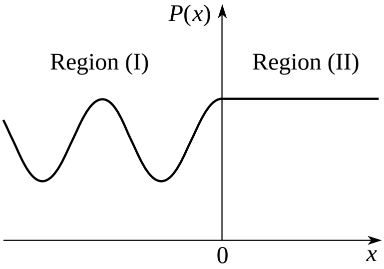

Figure 4 The particle density function $P(x)$ in the region of a potential step ($E > V$). In region (I), $P(x)$ shows a pattern of alternating maxima and minima caused by the interference of the incident and reflected waves.

Question T6

Starting from Equations 4,

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \qquad \text{in region (I)} \qquad \text{(Eqn 4a)}$$

$$\psi_2(x) = C\exp(ik_2x) \qquad \text{in region (II)} \qquad \text{(Eqn 4b)}$$

verify Equations 11 and 12.

$$P_1(x) = \psi_1^*(x)\,\psi_1(x) = A^2 + B^2 + 2AB\cos(2k_1x) \qquad \text{(Eqn 11)}$$

In region (II)

$$P_2(x) = \psi_2^*(x)\,\psi_2(x) = C^2 \qquad \text{(Eqn 12)}$$

Show that $P_1(0) = P_2(0)$. (Remember Equations 11 and 12 assume A, B and C are real.) ❏

Question T7

Figure 4 shows clearly that the probability per unit length of finding a particle in region (II) is greater, on average, than the probability in region (I). How can that be when a fraction of the incident particles is reflected? ❏

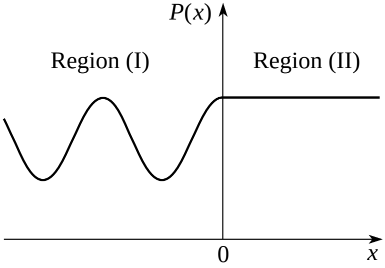

Figure 4 The particle density function $P(x)$ in the region of a potential step ($E > V$). In region (I), $P(x)$ shows a pattern of alternating maxima and minima caused by the interference of the incident and reflected waves.

3 Reflection and transmission at a potential step when $E < V$

3.1 Classical description of the problem

A particle travelling in the positive x-direction encounters a step where the potential energy $U(x)$ increases by an amount V greater than the particle energy. The physical situation is modelled by the illustration in Figure 5 and the total energy of a particle is represented by the horizontal dashed line. Applying the law of energy conservation to solve for the speed of the particle, we get:

$$\tfrac{1}{2}mv^2 = E - U(x)$$

$$v = \sqrt{\frac{2\big(E - U(x)\big)}{m}}$$

P marks the point where the total energy and the potential energy are equal, $E = U(x)$ and $v = 0$. There is no real-number solution to the speed equation anywhere to the right of P. According to classical mechanics, each particle will reach the point P and then be reflected back. The classical reflection coefficient is one.

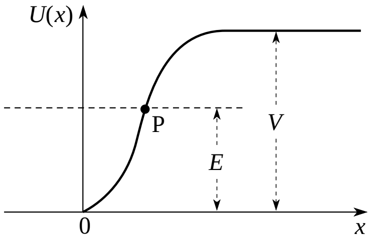

Figure 5 The function $U(x)$ at a potential step. The height of the step V is greater than the energy E of each incident particle. According to classical mechanics, the particles reach the point P and are then reflected back.

3.2 The Schrödinger equation and the solutions in each region

For the quantum mechanical problem we again make the assumption that the distance over which the potential is increasing is small compared with the de Broglie wavelength of the incident particles. The situation is illustrated schematically in Figure 6 with the region $x < 0$ designated (I) and $x \geq 0$ designated (II). The solution of the Schrödinger equation follows exactly as in Subsection 2.2, and we can write the solutions by referring to Equations 4:

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \qquad \text{in region (I)} \qquad \text{(Eqn 4a)}$$

$$\psi_2(x) = C\exp(ik_2x) \qquad \text{in region (II)} \qquad \text{(Eqn 4b)}$$

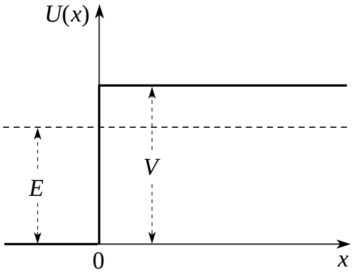

Figure 6 A schematic representation of a potential step with $E < V$. Particles are incident from the left.

The angular wavenumbers k_1 and k_2 are given by:

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \quad \text{and} \quad k_2 = \frac{\sqrt{2m(E-V)}}{\hbar}$$

In this case it is clear that k_2 is a purely imaginary number since $E < V$, but we cannot abandon this solution.

Remember that in quantum mechanics, the solutions make sense if the *predictions* for the values of physical observable quantities are real. We will continue the analysis and examine the form of the solution in region (II). If we replace k_2 by $i\alpha$, then α is a real number and we find:

$$\psi_2(x) = C\exp[i(i\alpha)x]$$

$$= C\exp(-\alpha x) \quad \text{since } i^2 = -1$$

The real constant α may be written in terms of E and V as follows:

$$\alpha = k_2/i = -ik_2$$

However $$k_2 = \frac{\sqrt{2m(E-V)}}{\hbar} = \frac{i\sqrt{2m(V-E)}}{\hbar}$$

so that $$\alpha = \frac{\sqrt{2m(V-E)}}{\hbar}$$

In fact, there is a second part of the general solution in region (II) corresponding to a *rising* exponential rather than a falling exponential: $\psi_2(x) = C\exp(-\alpha x) + D\exp(+\alpha x)$. ☞ The second term is ruled out as unphysical here because it predicts that the probability of observing the particles increases without limit as $x \to \infty$.

In summary, we have:

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \quad \text{in region (I)}$$

$$\psi_2(x) = C\exp(-\alpha x) \quad \text{in region (II)} \qquad (13)$$

with $k_1 = \dfrac{\sqrt{2mE}}{\hbar}$ and $\alpha = \dfrac{\sqrt{2m(V-E)}}{\hbar}$

3.3 Relationships imposed by the boundary conditions

The general requirements discussed in Subsection 2.3 that the wavefunction and its first derivative must both be continuous everywhere apply in this example. The relations between the arbitrary constants A, B and C are exactly the same as in Equations 7:

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2} \quad \text{and} \quad \frac{C}{A} = \frac{2k_1}{k_1 + k_2}$$

However now k_2 is a purely imaginary number, and we have equated it to $i\alpha$ so:

$$\frac{B}{A} = \frac{k_1 - i\alpha}{k_1 + i\alpha} \quad \text{and} \quad \frac{C}{A} = \frac{2k_1}{k_1 + i\alpha}$$

✦ Show that the complex number B/A can be written in the form: $B/A = \exp(-2i\phi)$ where $\tan\phi = \alpha/k_1$. Show also that $|B| = |A|$.

Question T8

Show that the complex number C/A can be written in the form: $C/A = 2\cos\phi\,\exp(-i\phi)$ and $|C| = 2|A|\cos\phi$. ❏

In summary, we have the following relations for the ratios of the constants:

$$\frac{B}{A} = \frac{k_1 - i\alpha}{k_1 + i\alpha} = \exp(-2i\phi) \qquad \text{so that} \qquad \frac{|B|}{|A|} = 1$$

$$\frac{C}{A} = \frac{2k_1}{k_1 + i\alpha} = 2\cos\phi\exp(-i\phi) \qquad \text{so that} \qquad \frac{|C|}{|A|} = 2\cos\phi \tag{14}$$

$$\text{with } \phi = \arctan\left(\frac{\alpha}{k_1}\right)$$

3.4 The wavefunctions in each region and the physical interpretation

The wavefunctions for particles in regions (I) and (II) are given by Equations 13,

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \qquad \text{in region (I)}$$

$$\psi_2(x) = C\exp(-\alpha x) \qquad \text{in region (II)} \qquad \text{(Eqn 13)}$$

and the ratios of the constants B/A and C/A by Equations 14.

$$\frac{B}{A} = \frac{k_1 - i\alpha}{k_1 + i\alpha} = \exp(-2i\phi) \qquad \text{so that} \qquad \frac{|B|}{|A|} = 1$$

$$\frac{C}{A} = \frac{2k_1}{k_1 + i\alpha} = 2\cos\phi\exp(-i\phi) \qquad \text{so that} \qquad \frac{|C|}{|A|} = 2\cos\phi \qquad \text{(Eqn 14)}$$

The incident beam $A\exp(ik_1x)$ has an average density of $|A|^2$ particles per unit length and the reflected beam $B\exp(-ik_1x)$ has an average density $|B|^2$. Our analysis showed that $|B|^2 = |A|^2$ (Equation 14), and the densities of the reflected and incident particles are equal.

The transmitted particles are represented by the wavefunction in region (II):

$$\psi_2(x) = C\exp(-\alpha x)$$

The density of transmitted particles is given by

$$|\psi_2(x)|^2 = |C|^2 \exp(-2\alpha x)$$

This is a most important result: quantum mechanics makes the clear prediction that particles can be observed *inside region (II)*. The particle density decreases exponentially with distance from the step. The scale of the penetration is set by the constant $\alpha = \sqrt{2m(V - E)}/\hbar$. In interesting cases, this is usually of the same order of magnitude as the angular wavenumber $k_1 = \sqrt{2mE}/\hbar$ in region (I).

It is helpful to visualize the situation by plotting a graph of the density function $P(x)$ as we did at the end of Subsection 2.6.

We can simplify the algebra by setting $A = 1$ so that there is one incident particle per unit length. In region (I), we have with the help of Equations 14:

$$\frac{B}{A} = \frac{k_1 - i\alpha}{k_1 + i\alpha} = \exp(-2i\phi) \qquad \text{so that} \qquad \frac{|B|}{|A|} = 1$$

$$\frac{C}{A} = \frac{2k_1}{k_1 + i\alpha} = 2\cos\phi\exp(-i\phi) \qquad \text{so that} \qquad \frac{|C|}{|A|} = 2\cos\phi \qquad \text{(Eqn 14)}$$

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \qquad \text{in region (I)} \qquad \text{(Eqn 4a)}$$

and, since $B = \exp(-2i\phi)$:

$$\psi_1(x) = \exp(ik_1x) + \exp[-i(2\phi + k_1x)]$$

Now $\quad P_1(x) = \psi_1^*(x)\,\psi_1(x)$

so that $\quad P_1(x) = 2 + \exp[i(2\phi + 2k_1x)] + \exp[-i(2\phi + 2k_1x)]$

$$= 2 + 2\cos(2k_1x + 2\phi) \qquad (15)$$

In region (II), we have with the help of Question T8:

$$\psi_2(x) = C\exp(-\alpha x)$$

$$P_2(x) = \psi_2^*(x)\,\psi_2(x) = |C|^2\exp(-2\alpha x)$$

and since $C = 2\cos\phi\,\exp(-i\phi)$

$$P_2(x) = 4\cos^2\phi\;\exp(-2\alpha x) \tag{16}$$

$$P_1(x) = 2 + 2\cos(2k_1x + 2\phi) \qquad \text{(Eqn 15)}$$

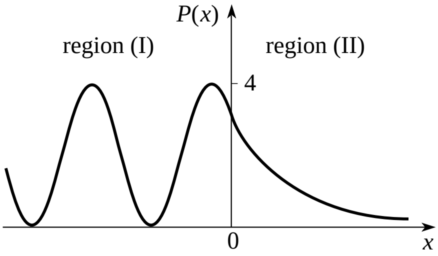

Figure 7 The density function $P(x)$ in the region of a potential step at $x = 0$. The incident beam is from the left. The energy E of each particle is less than the height of the step V. In region (I), there is a pattern of maxima and minima due to the interference between incident and reflected waves of equal amplitude. In region (II), the density decreases exponentially.

The density function is drawn in Figure 7 using Equations 15 and 16. You can see a perfect interference pattern in region (I) with the regular array of maxima and minima. The amplitudes of the incident and reflected waves are equal so the maximum value of $P_1(x)$ is 4 and the minimum 0. At the boundary, $P_1(0) = P_2(0) = 4\cos^2\phi$, and the density function passes smoothly to the decreasing exponential in region (II).

Question T9

Why does the density function have a maximum of four particles per unit length in region (I) when the incident particle density is one per unit length? ❏

We can characterize the penetration of particles into region (II) by a distance $D = 1/(2\alpha)$. At this distance, the density, given by Equation 16,

$$P_2(x) = 4\cos^2\phi\ \exp(-2\alpha x) \qquad \text{(Eqn 16)}$$

falls to 1/e of its value at $x = 0$:

$$P_2(D) = P_2(0)\exp(-2\alpha D) = P_2(0)\exp(-1) = P_2(0)/\mathrm{e}$$

The **penetration depth** is given in terms of E and V using Equations 13:

$\psi_2(x) = C\exp(-\alpha x)$ in region (II) (Eqn 13)

$$D = \frac{1}{2\alpha} = \frac{\hbar}{2\sqrt{2m(V-E)}} \tag{17}$$

The penetration depth for particles incident on a potential step with $E < V$

Question T10

A beam of electrons of energy 5 eV approaches a potential step of height 10 eV. Assume there is on average one incident particle per unit length. Calculate the following: (a) the average particle density at $x = 0$; (b) the point nearest the step where $P_1(x)$ is minimum; (c) the penetration depth D. ❏

In this subsection, we have obtained two remarkable predictions of quantum mechanics. The predictions seem to defy common sense but they have been verified experimentally in many situations.

- Particles can penetrate into classically forbidden regions where $V > E$.
- Quantum-mechanical interference arises from a potential step and produces a regular set of points where the particle density is zero.

3.5 Reflection and transmission in the quantum model

The reflection coefficient R was defined in Subsection 2.6:

$$R = \frac{\text{flux of reflected particles}}{\text{fllux of incident particles}}$$

The wavefunction in region (I) is:

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x)$$

Equation 8 gives the incident flux $|A|^2\,\hbar k_1/m$ and the reflected flux $|B|^2\,\hbar k_1/m$. We have already demonstrated that when $E < V$, $|B|^2 = |A|^2$ (Equation 14), so that the reflected flux is equal to the incident flux and the reflection coefficient is one.

$$R = 1 \tag{18}$$

The reflection coefficient at a potential step with $E < V$

This result agrees with the prediction of classical mechanics, but what can we say about the transmission coefficient? Particles can be observed across the step in the classically 'forbidden' region, but is there any flux? If particles are not to be created or destroyed at the boundary, then $R + T = 1$, and if $R = 1$, then $T = 0$. Even though particles are observed in region (II), there is no flux. Remember that the wavefunction $\psi_2(x) = C\exp(-\alpha x)$ is not an eigenfunction of momentum, and so does not represent a travelling wave with an associated momentum and an associated flux. Equation 8

$$F = |A|^2\,\hbar k/m \qquad \text{(Eqn 8)}$$

cannot be used to calculate flux since k is not defined.

$$T = 0 \qquad (19)$$

The transmission coefficient at a potential step with $E < V$

3.6 Summary of Sections 2 and 3

At a step where the potential energy increases by an amount V, classical mechanics makes definite predictions for the transmission and reflection of particles. If the total energy E of the incident particles is greater than V, then the particles are always transmitted across the step and are never reflected. If E is less than V, then the particles are always reflected and never transmitted.

When the distance over which the potential is changing is of the same order as, or smaller than, the de Broglie wavelength of the incident particles, then it is inappropriate to use classical mechanics. A quantum-mechanical treatment is required. Quantum mechanics makes some unexpected predictions which reveal the wave nature of particles in an interesting way. In the case $E > V$, there is always a finite probability that a particle will be reflected and the theory allows a calculation of the reflection and transmission coefficients, R and T (Equations 9 and 10).

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \qquad \text{(Eqn 9)}$$

$$T = \frac{4k_1k_2}{(k_1 + k_2)^2} \qquad \text{(Eqn 10)}$$

In the case $E < V$, the quantum predictions for R and T agree with the classical predictions but there are important new features. There is always a finite probability of particles being found in the *classically forbidden* region beyond the step where the wavefunction has an exponential shape and the particle has no defined momentum. The theory allows a calculation of the penetration depth D in terms of E and V (Equation 17).

$$D = \frac{1}{2\alpha} = \frac{\hbar}{2\sqrt{2m(V-E)}} \qquad \text{(Eqn 17)}$$

The penetration depth for particles incident on a potential step with $E < V$

Critical elements in the theory are the selection of appropriate solutions of the Schrödinger equation in the regions before and after the potential step and the matching of the solutions at the boundary with both $\psi(x)$ and $d\psi(x)/dx$ being continuous at the boundary.

The wave nature of material particles is made very clear by the appearance of 'fringes' caused by the interference of the incident and reflected waves. There is a regular pattern of points where the particle density is a minimum separated by points where the density is maximum (Figure 4 and Figure 7).

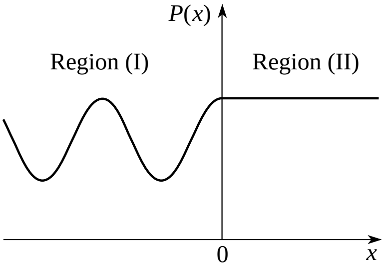

Figure 4 The particle density function $P(x)$ in the region of a potential step ($E > V$). In region (I), $P(x)$ shows a pattern of alternating maxima and minima caused by the interference of the incident and reflected waves.

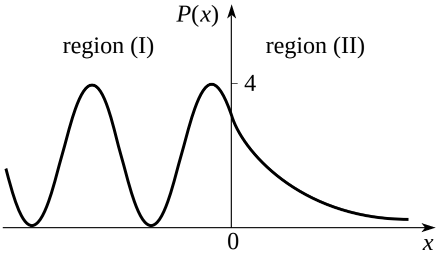

Figure 7 The density function $P(x)$ in the region of a potential step at $x = 0$. The incident beam is from the left. The energy E of each particle is less than the height of the step V. In region (I), there is a pattern of maxima and minima due to the interference between incident and reflected waves of equal amplitude. In region (II), the density decreases exponentially.

4 Reflection and transmission at a barrier when $E < V$

4.1 Classical description of the problem

We can now model a slightly more complicated physical situation by forming a **potential barrier** from two closely spaced steps. This is shown in Figure 8. The particles approach from the left and encounter first a negative force from point A to point B; from B to C there is no force, and from C to D there is a positive force. Particles with energy $E < V$ will reach point P, according to classical mechanics, before being reflected back. The classical reflection coefficient for a barrier of this nature is one.

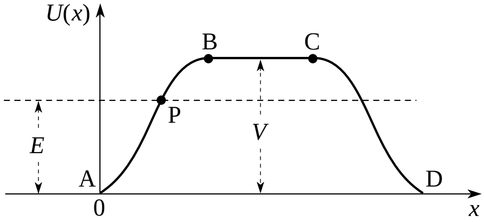

Figure 8 A potential barrier with height V. Particles with energy E are incident from the left and, according to classical theory, are reflected at the point P.

4.2 The Schrödinger equation and the solutions in each region

A quantum treatment of this barrier problem is required if any of the distances AB, BC, CD in Figure 8 are of the same order as, or less than, the de Broglie wavelength of the incident particles. We will assume that the distances AB and CD are the 'small' ones and the barrier is then drawn schematically as in Figure 9.

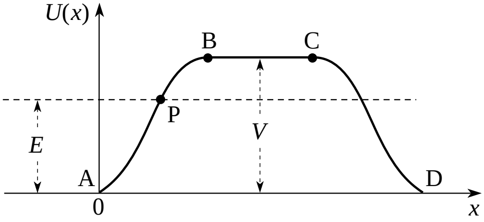

Figure 8 A potential barrier with height V. Particles with energy E are incident from the left and, according to classical theory, are reflected at the point P.

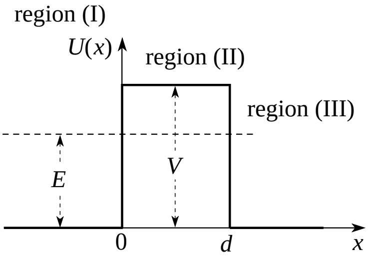

Figure 9 A schematic representation of a potential barrier width d. The energy E of each particle is less than the height of the barrier V.

In most physical situations, the width of the barrier, d, is greater than the de Broglie wavelength. The region $x < 0$ is designated (I), the region $0 \le x < d$ designated (II) and the region $x \ge d$ designated (III).

As usual, particles are incident on the barrier from the left with energy E. The solutions of the Schrödinger equation in regions (I) and (III), where the potential is zero, have the same form. You can refer back to Subsection 2.2 and Equation 2:

$$\psi_1(x) = A\exp(ikx) + B\exp(-ikx) \quad \text{in region (I)} \qquad \text{(Eqn 2)}$$

$$\psi_3(x) = G\exp(ikx) + H\exp(-ikx) \quad \text{in region (III)}$$

with $$k = \frac{\sqrt{2mE}}{\hbar}$$

We can immediately put $H = 0$ because particles cannot return from infinity. The general solution to the Schrödinger equation in region (II), where $E < V$, was derived in Subsection 3.2:

$$\psi_2(x) = C\exp(-\alpha x) + D\exp(\alpha x)$$

with $$\alpha = \frac{\sqrt{2m(V-E)}}{\hbar}$$

Notice that we have included the rising exponential term here because region (II) does not extend to infinity.

In summary, we have the general forms of the wavefunctions in the three regions:

$$\begin{aligned}
\psi_1(x) &= A\exp(ikx) + B\exp(-ikx) && \text{in region (I)} \\
\psi_2(x) &= C\exp(-\alpha x) + D\exp(\alpha x) && \text{in region (II)} \qquad (20) \\
\psi_3(x) &= G\exp(ikx) && \text{in region (III)}
\end{aligned}$$

with $k = \dfrac{\sqrt{2mE}}{\hbar}$ and $\alpha = \dfrac{\sqrt{2m(V-E)}}{\hbar}$

4.3 Relationships imposed by the boundary conditions

The situation now seems to be getting out of hand with five arbitrary complex constants and the boundary conditions to be applied at $x = 0$ and $x = d$. Matching the wavefunctions and their derivatives at the boundaries gives us four independent simultaneous equations which can, in principle, be solved for the four ratios B/A, C/A, D/A, and G/A. This piece of algebraic manipulation is extremely tedious, and we will not bore you with the details. We are interested mainly in the constant G because this tells us what the transmission coefficient is. We will quote the result and not even ask you to confirm it!

$$\frac{G}{A} = \frac{4k\alpha\exp(-\alpha d)}{(k+i\alpha)^2 - (k-i\alpha)^2\exp(-2\alpha d)}$$

Now look closely at the denominator of this expression. We have already stated that the width of the barrier d is usually much greater than the de Broglie wavelength of the incident particles. This in turn makes the argument of the exponential large and the second term in the denominator negligibly small compared with the first term. To a very good approximation, we have the following expression:

$$\frac{G}{A} = \frac{4k\alpha\exp(-\alpha d)}{(k+i\alpha)^2} \tag{21}$$

This can be rewritten more conveniently as:

$$\frac{G}{A} = \frac{4\exp(-\alpha d)\exp(-2i\phi)}{k/\alpha + \alpha/k} \tag{22}$$

Question T11

Show that Equation 21

$$\frac{G}{A} = \frac{4k\alpha\exp(-\alpha d)}{(k+i\alpha)^2} \qquad \text{(Eqn 21)}$$

can be written in the form of Equation 22.

What is the modulus of G/A when $\alpha = k$? ❏

The presence of the exponential factor $\exp(-\alpha d)$ in the numerator of Equation 22 ensures that $|G|/|A|$ is very small and very sensitive to the value of d.

We can now make similar approximations in region (II), and we find that the wavefunction is dominated by the falling exponential term, $\psi_2(x) = C\exp(-\alpha x)$, and the rising exponential makes a negligible contribution. The ratios B/A and C/A are then to a good approximation the same as for the potential step (Equation 14 in Subsection 3.3). In summary, we have the following results:

$$\frac{B}{A} \approx \frac{k - i\alpha}{k + i\alpha} = \exp(-2i\phi) \qquad \text{and} \qquad \frac{|B|}{|A|} \approx 1$$

$$\frac{C}{A} \approx \frac{2k}{k + i\alpha} = 2\cos\phi\exp(-i\phi) \qquad \text{and} \qquad \frac{|C|}{|A|} \approx 2\cos\phi$$

$$\frac{D}{A} \approx 0 \tag{23}$$

$$\frac{G}{A} \approx \frac{4\exp(-\alpha d)}{k/\alpha + \alpha/k}\exp(-2i\phi) \qquad \text{and} \qquad \frac{|G|}{|A|} \approx \frac{4\exp(-\alpha d)}{k/\alpha + \alpha/k}$$

$$\text{with} \qquad \tan\phi = \frac{\alpha}{k}$$

4.4 The wavefunctions in each region and the physical interpretation

The wavefunctions in the three regions are given by Equations 20, with the ratios of the constants given by Equations 23. Remember that we have made the assumption that the width of the barrier is much greater than the de Broglie wavelength. In region (I), the particles are represented by travelling waves, the incident particles by $A\exp(ikx)$ and the reflected particles by $B\exp(-ikx)$. The density of the reflected particles, $|B|^2$, is almost equal to the density of the incident particles, $|A|^2$, since $|B/A| \approx 1$. In the classically forbidden region (II), the wavefunction is dominated by the falling exponential so that the density of particles is given approximately by $|\psi_2(x)|^2 = |C|^2\exp(-2\alpha x)$. Finally, in region (III), the transmitted particles are represented by the travelling wave $G\exp(ikx)$, where $|G|$ is much smaller than $|A|$. The density of the transmitted particles is consequently very much smaller than the density of the incident particles.

Quantum mechanics unambiguously predicts that particles can tunnel through a potential barrier and can be observed with reduced density but with their original momentum. This process is known as **quantum tunnelling**.

Question T12

Show that the density of particles in region (III) is constant and is given by $16 \times |A|^2 \dfrac{\exp(-2\alpha d)}{(k/\alpha + \alpha/k)^2}$. ❑

All these facts can be neatly represented by the graph of the density function $P(x) = |\psi(x)|^2$ shown in Figure 10. The form of $P(x)$ in regions (I) and (II) is very similar to that shown in Figure 7 for the potential step, because of the realistic approximations described in Subsection 4.3, so there is no need to repeat the calculations. In region (I), there is an almost perfect pattern due to the interference between incident and reflected waves of almost equal amplitude. At the boundary, $x = d$, $P(x)$ has not quite fallen to zero and joins smoothly to its constant value in region (III). ☞

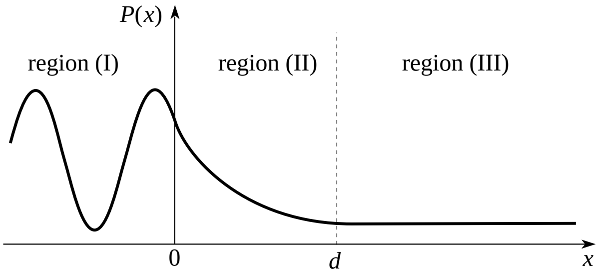

Figure 10 The particle density function $P(x)$ near a potential barrier of height V. Particles are incident from the left, each with energy E less than V.

4.5 Transmission in the quantum model

The method for finding the particle fluxes and hence the reflection and transmission coefficients follows from Equation 8

$$F = |A|^2 \frac{\hbar k}{m} \qquad \text{(Eqn 8)}$$

and the pattern set in Subsections 2.6 and 3.5. The transmission coefficient for the potential barrier illustrated in Figure 9 is given by:

$$T = \frac{\text{flux of transmitted particles}}{\text{flux of incident particles}}$$

The incident flux in region (I) is given by $|A|^2\,\hbar k/m$ and the transmitted flux in region (III) by $|\,G\,|^2\,\hbar k/m$. Consequently:

$$T = \frac{|G|^2}{|A|^2}$$

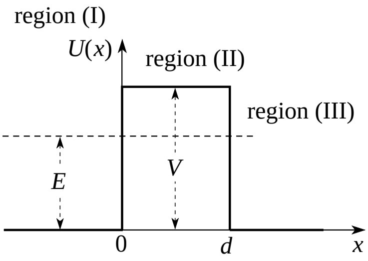

Figure 9 A schematic representation of a potential barrier width d. The energy E of each particle is less than the height of the barrier V.

Equation 21

$$\frac{G}{A} = \frac{4k\alpha\exp(-\alpha d)}{(k+i\alpha)^2} \qquad \text{(Eqn 21)}$$

gives the constant G in terms of A, and from this we can get the square modulus of G (see, for example, Question T12):

$$|G|^2 \approx \frac{|A|^2\,16\exp(-2\alpha d)}{\left(k/\alpha + \alpha/k\right)^2}$$

It follows immediately that:

$$T \approx \frac{16\exp(-2\alpha d)}{\left(k/\alpha + \alpha/k\right)^2} \qquad (24)$$

The transmission coefficient for a potential barrier

In many applications, the incident particle angular wavenumber k, and the factor α which characterizes the wavefunction inside the barrier, are the same order of magnitude. The denominator then takes a value of about 4, and the transmission coefficient has the approximate value:

$$T \approx 4\exp(-2\alpha d) \tag{25}$$

where $\alpha = \dfrac{\sqrt{2m(V-E)}}{\hbar}$ and d is the barrier width.

An approximate value for the transmission coefficient when $k \approx \alpha$

This is a good equation to remember, because it usually gives a good estimate of the transmission coefficient of a barrier. The most important factor in calculating T is the exponential; remember that exponential functions can change by orders of magnitude for relatively small changes in the argument.

The reflection coefficient of the barrier R is of course very close to one because T is small with the approximations we have used. Application of the approximate formulae for $|B|/|A|$ given in Equations 23, also gives $R \approx 1$; a better approxi-mation is obtained by using Equation 25 and putting $R = 1 - T$.

We can show that the phenomenon of barrier penetration is consistent with the Heisenberg uncertainty principle $\Delta E\ \Delta t \approx \hbar$.

The Heisenberg uncertainty principle tells us that a particle can 'borrow' energy ΔE sufficient to surmount the barrier provided it 'repays' the debt in a time Δt of order $\hbar/\Delta E$. The value of ΔE is given by $V - E$.
Let us assume a typical barrier of width $d = 2/\alpha$ so that $T \approx 4\exp(-4) = 0.07$ (using Equation 25).

$$T \approx 4\exp(-2\alpha d) \qquad \text{(Eqn 25)}$$

where $\alpha = \dfrac{\sqrt{2m(V-E)}}{\hbar}$ and d is the barrier width.

We estimate Δt from the speed of the particle:

$$\Delta t \approx \frac{d}{v} \quad \text{and} \quad v = \frac{p}{m} = \frac{\hbar k}{m}$$

Hence $$\Delta t \approx \frac{2/\alpha}{\hbar k/m} = \frac{2m}{\hbar k\alpha}$$

However $\qquad \alpha = \dfrac{\sqrt{2m(E-V)}}{\hbar}$ and $\quad k = \dfrac{\sqrt{2mE}}{\hbar}$

Substituting these gives $\qquad \Delta t \approx \dfrac{\hbar}{\sqrt{E(V-E)}}$

Both E and $V - E$ are of the same order of magnitude, so that:

$$\Delta t \approx \frac{\hbar}{V-E} \approx \frac{\hbar}{\Delta E}$$

which is the required relation. ❑

4.6 Examples of quantum tunnelling

The idea of tunnelling was first used to explain α-decay in radioactive nuclei. α-particles may be formed within a nucleus. In heavy nuclei they may be formed with enough energy to escape. ☞ They are held within the nucleus by a potential barrier which consists of an attractive part (due to nuclear forces), and a repulsive part (due to the electrostatic repulsion between the α-particle and the residual nucleus), as shown schematically in Figure 11.

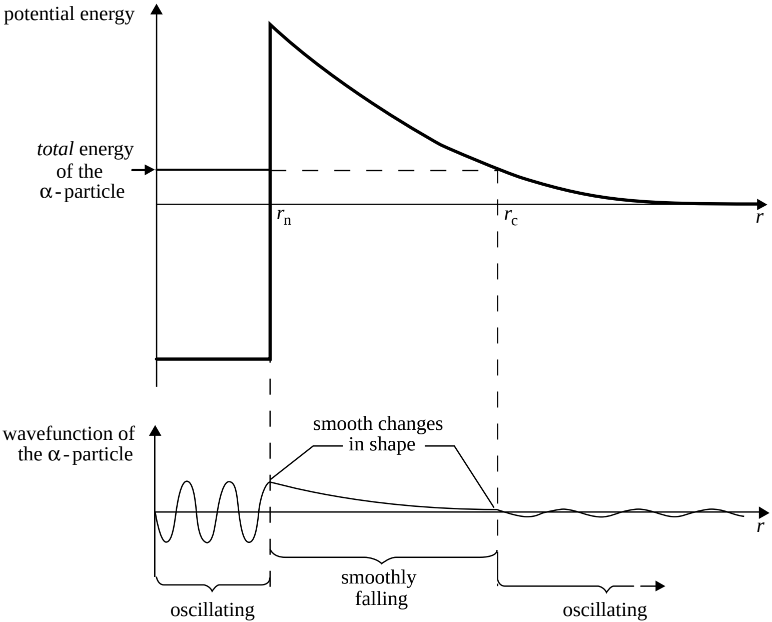

Figure 11 The potential barrier 'seen' by an α-particle in a radioactive nucleus.

This combination produces a **potential well** in which in which the α-particle is trapped. Notice that the energy is positive and states of this same energy exist outside the potential well of the nucleus, so the α-particle can tunnel out of its potential well and escape from the nucleus. This is *α-decay*.

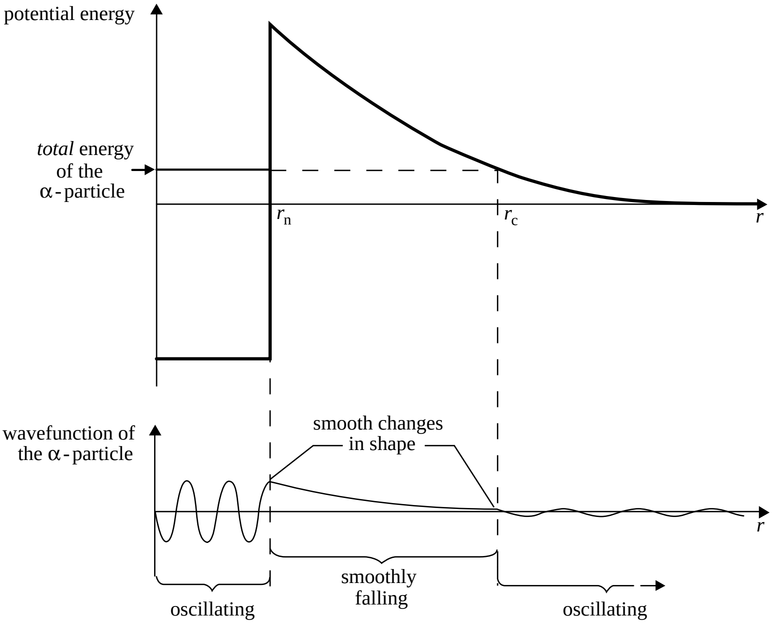

Figure 11 The potential barrier 'seen' by an α-particle in a radioactive nucleus.

The shape of the barrier is more complex than we have envisaged so far, but it should be clear that the higher the energy of the α-particle, the more likely it will be to penetrate the barrier, both directly because of the increased energy, and indirectly because of the decreased width of the barrier. These two effects lead to an extremely wide variation in decay rates for a relatively small change in energy. Figure 12 shows a variation of a factor 10^{24} in decay rates λ for a change of a factor 2 in energy. ☞

This same idea, used in reverse, suggested to Cockcroft and Walton that it would be possible to induce nuclear reactions using low-energy protons (about 0.5 MeV) without sufficient energy to overcome the electrostatic repulsion. This began the whole study of nuclear physics using particle accelerators.

The same process is involved in the nuclear reactions that supply the Sun's energy. The principal reaction here involves the eventual formation of helium by the fusion of hydrogen nuclei (protons). It is essential to take tunnelling into account to be able to explain the rate of energy production. In laboratory fusion experiments the same principle allows nuclear fusion at attainable temperatures.

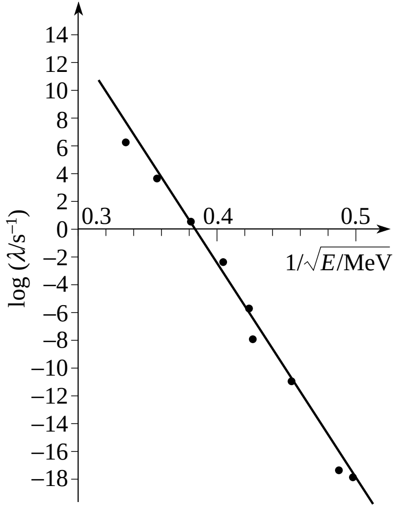

Figure 12 The variation in decay rate with α-particle energy for a number of radioactive nuclei.

An example of quantum tunnelling occurs when an electric current passes through a junction made by twisting two copper wires together. The surface of the copper, unless it is newly cleaned, is always covered with a thin layer of oxide — an insulator — so that in classical physics no current would flow; the potential energy of the electrons varies in the same way as in Figure 9. However, since the oxide layer is very thin, it is possible for electrons to tunnel through the barrier.

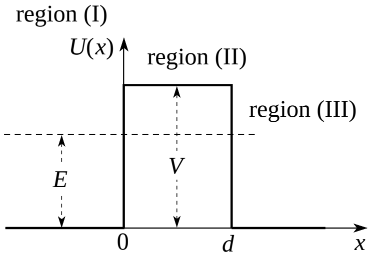

Figure 9 A schematic representation of a potential barrier width d. The energy E of each particle is less than the height of the barrier V.

A development of this idea is the **tunnel diode**; in this device, the height of the potential barrier between two semiconductors is controlled externally, and the physical size of the junction is so small that the flow of electrons can be turned on or off very rapidly, within a few picoseconds. Further developments using **superconductors** have led to the **Josephson junction** and the **SQUID** (semiconducting quantum interference device), which can measure magnetic fields as small as 10^{-15} T.

The scanning tunnelling electron microscope was developed recently by Binnig and Rohrer, who were awarded the Nobel Prize in 1986. This remarkable device works by the tunnelling of electrons from the surface of a sample to the tip of a very fine needle. It is so sensitive that the detail of the surface can be resolved to distances much less than an atomic radius.

4.7 Summary of Section 4

This section describes one of the most powerful predictions of quantum mechanics. We have seen that material particles can penetrate into classically forbidden regions due to their wave nature. Here we go further and show that particles can penetrate through classically forbidden barriers (Figures 8 and 9). In most realistic situations, the width of the barrier is such that the transmission coefficient is small and considerable simplifications can be made in the theory. The nature of the particle wavefunctions is described in the regions before the barrier, inside the barrier and after the barrier. Matching the wavefunctions at the two boundaries allows the particle density ratios to be calculated. A graph of the particle density function near the barrier is given in Figure 10. Three features are important:

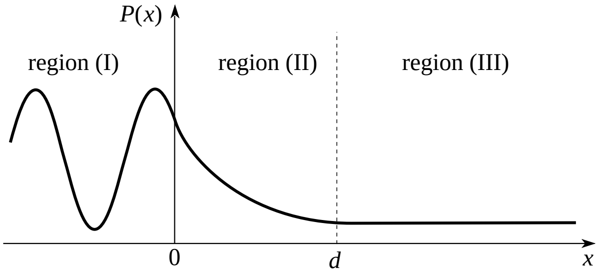

Figure 10 The particle density function $P(x)$ near a potential barrier of height V. Particles are incident from the left, each with energy E less than V.

- The interference pattern due to the incident and reflected waves;
- The exponential decay within the barrier;
- The constant density beyond the barrier.

Finally, good approximations are derived for the transmission coefficient T. In our approximation, T is dominated by the exponential factor $\exp(-2\alpha d)$.

5 Closing items

5.1 Module summary

1 A particle with kinetic energy E approaches a step where the potential increases by V. Classical mechanics predicts that if $E > V$ then the particle will always pass over the step.

2 If the dimensions of the step are of the same order or less than the de Broglie wavelength of the incident particle, then quantum mechanics rather than classical mechanics must be used.

3 A *potential step* where $E > V$ is shown in Figure 2. The solutions of the Schrödinger equation are:

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \quad \text{in region (I)} \qquad \text{(Eqn 4a)}$$

$$\psi_2(x) = C\exp(ik_2x) \quad \text{in region (II)} \qquad \text{(Eqn 4b)}$$

with $k_1 = \dfrac{\sqrt{2mE}}{\hbar}$ and $k_2 = \dfrac{\sqrt{2m(E-V)}}{\hbar}$

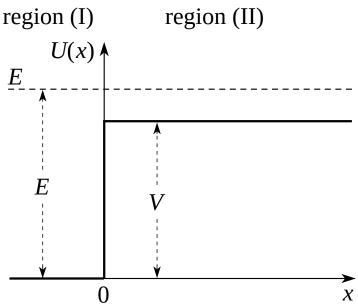

Figure 2 A schematic representation of a potential step. The distance over which the force acts is assumed to be negligible. The total energy of the particle is E.

The ratios of the coefficients are determined by *boundary conditions*. The wavefunction ☞ and its slope must both be continuous at $x = 0$. This gives:

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2} \quad \text{and} \quad \frac{C}{A} = \frac{2k_1}{k_1 + k_2} \qquad \text{(Eqn 7)}$$

4 The wavefunction $\psi_1(x)$ represents the incident particles, with density $|A|^2$ per unit length, moving with momentum $\hbar k_1$ in the positive x-direction, and the reflected particles, with density $|B|^2$ moving with momentum $-\hbar k_1$. The wavefunction $\psi_2(x)$ represents the transmitted particles, of density $|C|^2$, moving with momentum $\hbar k_2$.

5 For a wavefunction $\psi(x) = A\exp(ikx)$, which is a momentum eigenfunction, the *flux* of particles is given by

$$F = |A|^2\,\hbar k/m \qquad \text{(Eqn 8)}$$

6 At a potential step, the *reflection coefficient* R and the *transmission coefficient* T are defined:

$$R = \frac{\text{flux of reflected particles}}{\text{flux of incident particles}} \quad \text{and} \quad T = \frac{\text{flux of transmitted particles}}{\text{flux of incident particles}}$$

If $E > V$, quantum mechanics predicts:

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2 \quad \text{and} \quad T = \frac{4k_1k_2}{(k_1 + k_2)^2} \qquad \text{(Eqns 9 and 10)}$$

As expected $R + T = 1$. The prediction that $R > 0$ when $E > V$ is a direct contradiction of classical mechanics.

7 The wave nature of particles is demonstrated by the *particle density function* $P(x)$ in region (I), which shows the interference between the incident and reflected waves (Figure 4).

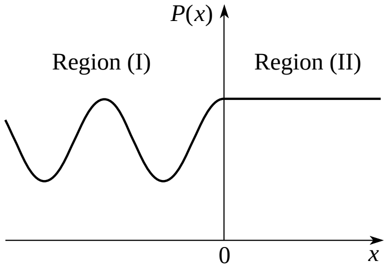

Figure 4 The particle density function $P(x)$ in the region of a potential step ($E > V$). In region (I), $P(x)$ shows a pattern of alternating maxima and minima caused by the interference of the incident and reflected waves.

8 A potential step where $E < V$ is shown in Figure 5. The solutions of the Schrödinger equation are:

$$\psi_1(x) = A\exp(ik_1x) + B\exp(-ik_1x) \quad \text{in region (I)}$$

$$\psi_2(x) = C\exp(-\alpha x) \quad \text{in region (II)} \qquad \text{(Eqn 13)}$$

with $\quad k_1 = \dfrac{\sqrt{2mE}}{\hbar} \quad$ and $\quad \alpha = \dfrac{\sqrt{2m(V-E)}}{\hbar}$

The ratios of the constants are given by the boundary conditions at $x = 0$:

$$\frac{B}{A} = \frac{k_1 - i\alpha}{k_1 + i\alpha} = \exp(-2i\phi) \quad \text{so that} \quad \frac{|B|}{|A|} = 1$$

$$\frac{C}{A} = \frac{2k_1}{k_1 + i\alpha} = 2\cos\phi\exp(-i\phi) \quad \text{so that} \quad \frac{|C|}{|A|} = 2\cos\phi \qquad \text{(Eqn 14)}$$

with $\quad \phi = \arctan\left(\dfrac{\alpha}{k_1}\right)$

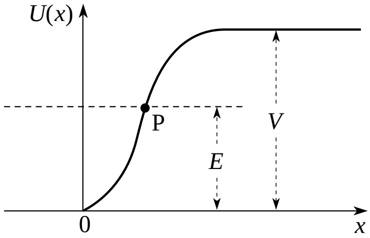

Figure 5 The function $U(x)$ at a potential step. The height of the step V is greater than the energy E of each incident particle. According to classical mechanics, the particles reach the point P and are then reflected back.

9 In region (I), the wavefunction $\psi_1(x)$ represents the incident and reflected particles with the same density, $|B|^2 = |A|^2$.

In region (II), the wavefunction $\psi_2(x)$ is not a momentum eigenfunction and there is no flux of particles. The particle density function $P(x)$ (Figure 7) shows a perfect interference pattern in region (I) and joins smoothly to the falling exponential in region (II). There is a finite probability of particles being observed in the classically forbidden region: $P_2(x) = 4\cos^2\phi\,\exp(-2\alpha x)$. At the penetration depth $D = 1/(2\alpha)$, the particle density is 1/e of its value at $x = 0$.

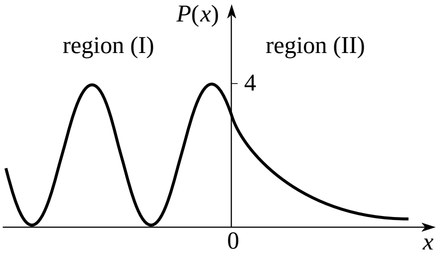

Figure 7 The density function $P(x)$ in the region of a potential step at $x = 0$. The incident beam is from the left. The energy E of each particle is less than the height of the step V. In region (I), there is a pattern of maxima and minima due to the interference between incident and reflected waves of equal amplitude. In region (II), the density decreases exponentially.

10 The reflection coefficient at the step where $E < V$ is given by:

$$R = \frac{|B|^2}{|A|^2} = 1 \qquad \text{(Eqn 18)}$$

This agrees with the classical prediction.

11 A *potential barrier* with width d and $V > E$ is shown schematically in Figure 9. The distances over which the potential is increasing or decreasing are assumed to be smaller than the de Broglie wavelength of the incident particles. The solutions of the Schrödinger equation are

$$\psi_1(x) = A\exp(ikx) + B\exp(-ikx) \qquad \text{in region (I)}$$

$$\psi_2(x) = C\exp(-\alpha x) + D\exp(\alpha x) \qquad \text{in region (II)} \qquad \text{(Eqn 20)}$$

$$\psi_3(x) = G\exp(ikx) \qquad \text{in region (III)}$$

with $\quad k = \dfrac{\sqrt{2mE}}{\hbar}$ and $\alpha = \dfrac{\sqrt{2m(V-E)}}{\hbar}$

The ratios of the constants are given by matching the wavefunctions and their slopes at the two boundaries.

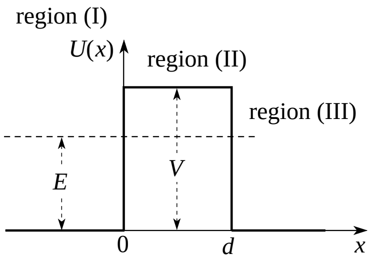

Figure 9 A schematic representation of a potential barrier width d. The energy E of each particle is less than the height of the barrier V.

With the assumption that $d >> 1/\alpha$, the following approximations are valid:

$$\frac{B}{A} \approx \frac{k - i\alpha}{k + i\alpha} = \exp(-2i\phi) \qquad \text{and} \qquad \frac{|B|}{|A|} \approx 1$$

$$\frac{C}{A} \approx \frac{2k}{k + i\alpha} = 2\cos\phi\exp(-i\phi) \qquad \text{and} \qquad \frac{|C|}{|A|} \approx 2\cos\phi$$

$$\frac{D}{A} \approx 0 \qquad \text{(Eqn 23)}$$

$$\frac{G}{A} \approx \frac{4\exp(-\alpha d)}{k/\alpha + \alpha/k}\exp(-2i\phi) \qquad \text{and} \qquad \frac{|G|}{|A|} \approx \frac{4\exp(-\alpha d)}{k/\alpha + \alpha/k}$$

with $\quad \tan\phi = \dfrac{\alpha}{k}$

12 In region (I), the wavefunction $\psi_1(x)$ represents both the incident and reflected particles with approximately the same density. In region (II), the wavefunction $\psi_2(x)$ is not a momentum eigenfunction. In region (III), the wavefunction $\psi_3(x)$ represents the transmitted particles. The density function $P(x)$ (Figure 10) shows a typical interference pattern in region (I), falls exponentially in region (II) and joins smoothly to the constant value $|G|^2$ in region (III).

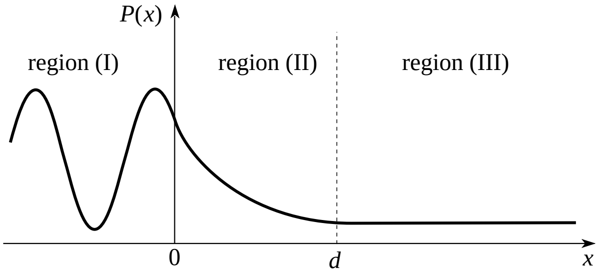

Figure 10 The particle density function $P(x)$ near a potential barrier of height V. Particles are incident from the left, each with energy E less than V.

13 The transmission coefficient at a barrier where $V > E$ is given by $T = |G|^2/|A|^2$ so that:

$$T \approx \frac{16\exp(-2\alpha d)}{(k/\alpha + \alpha/k)^2} \qquad \text{(Eqn 24)}$$

When α and k are of the same order of magnitude, a good approximation is $T \approx 4\exp(-2\alpha d)$. The transmission coefficient is normally much less than one so that the reflection coefficient $R \approx 1$.

14 *Quantum tunnelling* also allows particles to tunnel into or out of a *potential well*. Such processes are responsible for nuclear fusion and also allow many technological developments.

5.2 Achievements

Having completed this module, you should be able to:

A1 Define the terms that are emboldened and flagged in the margins of the module.

A2 Describe the motion of a particle at a potential step using classical mechanics. Identify the circumstances when quantum mechanics should be used rather than classical mechanics.

A3 Recall the form of the solutions of the Schrödinger equation for particles of energy E encountering an idealized potential step when $E > V$. Interpret the solutions in terms of the density and flux of the incident, reflected and transmitted particles.

A4 Recall conditions on the wavefunctions at a boundary, and use the conditions to determine the relations between the constants appearing in the wavefunctions.

A5 Derive expressions for the transmission and reflection coefficients at a potential step when $E > V$. Compare and contrast the predictions of quantum and classical mechanics.

A6 Recall the form of the solutions of the Schrödinger equation for particles of energy E encountering an idealized potential step when $E < V$. Interpret the solutions in terms of the density and flux of the incident and reflected particles. Explain how these solutions predict that particles can penetrate into the classically forbidden region.

A7 Use the theory to confirm that the reflection coefficient for a step is unity when $E < V$, in agreement with classical theory.

A8 Recall the form of the solutions of the Schrödinger equation for particles of energy $E < V$ encountering an idealized potential barrier of width d. Interpret the solutions in terms of the density and flux of the incident, reflected and transmitted particles.

A9 Use the approximate formula for the transmission coefficient through a potential barrier.

A10 Use the quantum theory results to calculate fluxes of particles transmitted by, and reflected from, specified steps and barriers.

A11 Outline the use of barrier penetration, or tunnelling, in different physical situations.

Study comment You may now wish to take the *Exit test* for this module which tests these Achievements. If you prefer to study the module further before taking this test then return to the *Module contents* to review some of the topics.

5.3 Exit test

Study comment Having completed this module, you should be able to answer the following questions, each of which tests one or more of the Achievements.

Note We have used electron beams with energies in the eV region to illustrate the general principles of quantum mechanics applied to steps and barriers. This is an attempt to keep to a minimum the amount of repetitive arithmetic in the questions. You should be fully aware that similar examples can be generated using nuclear particles (e.g. protons or α-particles) with energies in the MeV region and lengths of the order of 10^{-15} m.

Question E1

(*A2* and *A10*) A beam of electrons, each with kinetic energy 5 eV, is incident on a step where the potential energy *decreases* by 2.5 eV. Calculate the transmission and reflection coefficients in the quantum model. What does classical mechanics predict? How can you decide which theory of mechanics to use?

Question E2

(*A4*, *A5* and *A7*) Explain qualitatively how the boundary conditions on wavefunctions lead to Equations 5 and 6.

$$A + B = C \qquad \text{(Eqn 5)}$$

$$Ak_1 - Bk_1 = Ck_2 \qquad \text{(Eqn 6)}$$

Verify Equations 7

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2} \quad \text{and} \quad \frac{C}{A} = \frac{2k_1}{k_1 + k_2} \qquad \text{(Eqn 7)}$$

from Equations 5 and 6. Derive expressions for the transmission and reflection coefficients when $V < E$.

Show that for a potential step with $V > E$ the ratio

$$\frac{B}{A} = \frac{k_1 - i\alpha}{k_1 + i\alpha} \quad \text{where} \quad \alpha = \frac{\sqrt{2m(V - E)}}{\hbar}$$

Hence show that $|B| = |A|$ and the reflection coefficient is one.

Question E3

(*A3*) Find a suitable wavefunction to describe the *incident* electrons in Question E1 if the current is 10 μA.

[A beam of electrons, each with kinetic energy 5 eV, is incident on a step where the potential energy *decreases* by 2.5 eV.]

What is the current after the step?

Question E4

(*A6*) At the junction between copper and an insulator, the potential energy of a conduction electron increases by 11.1 eV. Find the penetration depth, into the insulator, of a typical conduction electron with kinetic energy 7.0 eV.

Sketch the graph of the density function and account for the series of maxima and minima inside the copper.

Question E5

(*A8*, *A9* and *A10*) A beam of electrons with kinetic energy 5 eV approaches a potential barrier of height 10 eV and width 1 nm. Sketch the graph of the density function near the barrier.

Calculate the transmission coefficient, T, according to Equation 24.

$$T \approx \frac{16\exp(-2\alpha d)}{\left(k/\alpha + \alpha/k\right)^2} \qquad \text{(Eqn 24)}$$

Are the approximations made to derive the formula valid in this case?

What is the value of T when the barrier potential is reduced to 6 eV?

Is Equation 25 also a good approximation?

$$T \approx 4\exp(-2\alpha d) \qquad \text{(Eqn 25)}$$

Question E6

(*A9*, *A10* and *A11*) In a modern scanning tunnelling microscope, the tip of a fine needle is 1 nm from a metal surface. The needle to metal gap behaves like a potential barrier of height 5 eV. Calculate the transmission coefficient T for electrons of energy 2.5 eV.

By what factor does T change when the gap increases to 1.1 nm? What is the significance of this result?

Study comment This is the final *Exit test* question. When you have completed the *Exit test* go back to Subsection 1.2 and try the *Fast track questions* if you have not already done so.

If you have completed **both** the *Fast track questions* and the *Exit test*, then you have finished the module and may leave it here.