Second year quantum mechanics: the square potential barrier

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Overview

These notes are a sample of what might be used to teach the square barrier potential. They assume the students have seen the Schrödinger equation before as well as other relevant background. The notes begin with the slightly simpler problem of the step potential, and include reference to the square potential well, as there are many similarities. There are questions throughout that the students should attempt before coming to the interactive workshop.

1 The potential step

In this part of the course we will investigate solutions to the Schrödinger equation in various situations. The first is relatively straightforward: we will imagine our space has only two regions, for all $x < 0$ there is no potential $V(x) = 0$ and for $x \geq 0$ there is a constant, finite potential $V(x) = V_0$. This is shown in the diagram in Fig. 1.

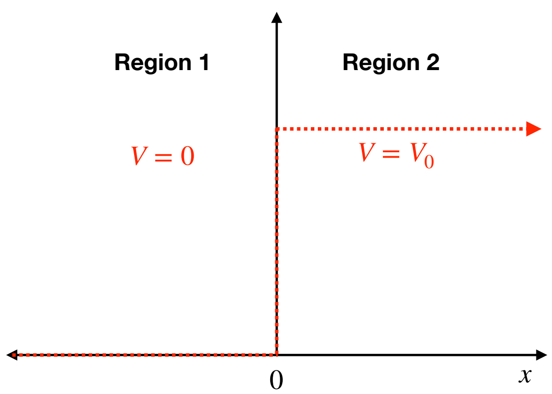

Figure 1: The step potential

We will try to solve the Schrödinger equation for this situation to determine the wavefunction for a particle of mass m in the two regions. We will only be using the time-independent Schrödinger equation for these problems. This assumes that the particle is in an energy eigenstate with eigenvalue E.

$$\Psi(x,t) = \psi(x)e^{-i\frac{Et}{\hbar}} \tag{1}$$

Task 1: [2 marks] Using the *time-dependent* Schrödinger equation, verify that the expression in Eq. 1 is indeed a solution.

The time-indepdendent Schrödinger equation for a particle of mass m is given by

$$\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{d^2x} + V(x)\psi(x) = E\psi(x) \tag{2}$$

where the potential is represented by $V(x)$. Given the simple form of $V(x)$ we can easily write out the equations for the wave functions ψ_1 and ψ_2 in the two regions

$$\frac{-\hbar^2}{2m}\frac{d^2\psi_1(x)}{d^2x} = E\psi_1(x) \tag{3}$$

$$\frac{-\hbar^2}{2m}\frac{d^2\psi_2(x)}{d^2x} + V_0\psi_2(x) = E\psi_2(x) \tag{4}$$

We want to find solutions for the wavefunctions ψ_1 and ψ_2, but luckily these are both equations that we have seen and solved before:

$$\frac{d^2\psi_1(x)}{d^2x} = -\frac{2mE}{\hbar^2}\psi_1(x) = -k_1^2\psi_1(x) \tag{5}$$

$$\frac{d^2\psi_2(x)}{d^2x} = -\frac{2m(E-V_0)}{\hbar^2}\psi_2(x) = -k_2^2\psi_2(x) \tag{6}$$

The general solutions to these equations are given by

$$\psi_1(x) = Ae^{+ik_1x} + Be^{-ik_1x} \tag{7}$$

$$\psi_2(x) = Ce^{+ik_2x} + De^{-ik_2x}. \tag{8}$$

These can be thought of as a forwards and backwards propagating wave with arbitrary amplitudes.
Task 2: [2 marks] Verify these are solutions of the time-indepdendent Schrödinger equation

1.1 The general solution

Now we have the general form of the wavefunction we need to impose the physical constraints of the system to understand how the four parameters A, B, C and D relate to one another. The parameter A corresponds to the amplitude of the incoming wave in region 1. In an experiment this would be the parameter that we specify, as it relates to how many particles are being fired a the potential step. We will set this quantity equal to 1, such that we can determine the reflected and transmitted wave relative to this component. The parameter B accordingly becomes the size of the *reflected* wave, i.e. that which ends up coming back towards us, so we will rename it r. Similarly, C is the transmitted wave that we will call t. The parameter D dictates the size of the wave coming into the system from the right. In our setup there would not be any particle source on this side, so this component is zero. This gives us

$$\psi_1(x) = e^{+ik_1x} + re^{-ik_1x} \tag{9}$$

$$\psi_2(x) = te^{+ik_2x}. \tag{10}$$

At the boundary the wavefunction must obey certain behaviours. It must be *continuous* and *smooth*. This means that the value of the wavefunction at $x = 0$ must be the same for both region 1 and region 2, and the similarly the first derivative must be the same. These conditions arise because the chance of finding a particle at a given point (the square modulus of the wavefunction) mustn't have any discontinuities, and the derivative which represents the change in probability (or current) must also not have any discontinuities.

These requirements give us the following conditions

$$1 + r = t \tag{11}$$

$$k_1(1 - r) = k_2 t. \tag{12}$$

Task 3: [2 marks] Use Equation 11 and 12 to show that the probability density for reflected waves is given by

$$R = |r|^2 = \left| \frac{(k_1 - k_2)}{(k_1 + k_2)} \right|^2 \tag{13}$$

1.2 Quantum mechanics solution when $E > V_0$

In classical physics, a particle that passes over a potential step with more kinetic energy that the step ($E > V_0$) would simply keep going. However this is not always the case in quantum mechanics. The value of R is non zero, which means there is a probability that the particle reflects when it passes over the barrier. We can note that $K_1 \propto \sqrt{E}$ and $K_2 \propto \sqrt{E - V_0}$. In doing so, we can rewrite the reflection probability as

$$R = |r|^2 = \left| \frac{1 - \sqrt{1 - \frac{V_0}{E}}}{1 + \sqrt{1 - \frac{V_0}{E}}} \right|^2 \tag{14}$$

Task 4: [4 marks] Expand equation 14 to find an approximate expression for R in the limit $E >> V_0$.

1.3 Quantum mechanics solution when $E < V_0$

Classically a particle whose energy is less than the barrier height would just reflect off the barrier. However, quantum mechanically, the wavefunction extends into the potential. If $E < V_0$ the wavenumber k_2 becomes imaginary as the term inside the square root becomes negative. It is therefore possible to rewrite the wave number as $k_2 = iq$ where q is some real quantity. The wave function in region 2 now becomes

$$\psi_2(x) = te^{+ik_2x} = te^{-qx}. \tag{15}$$

It can be seen that rather than a propagating wave, this now becomes a falling exponential. This means the wave function extends into the barrier, and there is a non-zero chance of finding the particle there.

It is important to note, however, that because the barrier is infinite, there is no region beyond the barrier. Therefore although the wavefunction extends into the barrier, there is no current of particles through it. This can be seen by calculating the reflection probability:

$$R = \left| \frac{(k_1 - iq)}{(k_1 + iq)} \right|^2 = \frac{(k_1 - iq)}{(k_1 + iq)} \frac{(k_1 + iq)}{(k_1 - iq)} = 1, \tag{16}$$

which tells us that all particles reflect off the barrier. In order to allow particles to realise their non-zero wave function, we must make region 2 finite...

2 The square barrier potential

The square barrier potential is very similar to the step potential, but in this example we make the region in which the potential increases finite. This can be seen in Fig. 2 where the new potential is shown. We have introduced a third region in which the potential goes back to $V(x) = 0$ such that the barrier has a finite width of a.

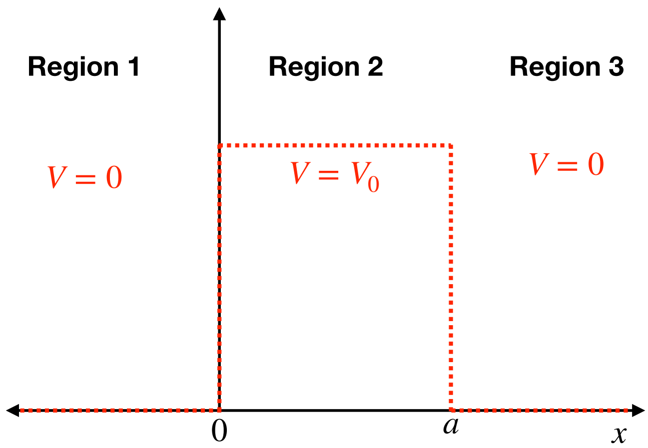

Figure 2: The square barrier potential

The procedure to find the wavefunctions is same as what we've already seen. First we take the general solutions in the three regions

$$\psi_1(x) = Ae^{+ik_1x} + Be^{-ik_1x} \tag{17}$$
$$\psi_2(x) = Ce^{+ik_2x} + De^{-ik_2x} \tag{18}$$
$$\psi_3(x) = Ee^{+ik_1x} + Fe^{-ik_1x}, \tag{19}$$

note that here in region three we have used k_1 again as the potential is the same as region 1. Next we use the same arguments as before to set some of the parameters $A...F$ to specific values. Firstly we are interested in the size fo the transmitted and reflected waves relative to our input wave, so we can set $A = 1$, $B = r$ and $E = t$. As before there is no incoming wave from the right so $F = 0$. This leaves us with

$$\psi_1(x) = e^{+ik_1x} + re^{-ik_1x} \tag{20}$$
$$\psi_2(x) = Ce^{+ik_2x} + De^{-ik_2x} \tag{21}$$
$$\psi_3(x) = te^{+ik_1x}. \tag{22}$$

We now have two positions where the wavefunction must be smooth and continuous, $x = 0$ and $x = a$. This will give us four equations and four unknown parameters.

First, at $x = 0$

$$\psi_1(0) = \psi_2(0) \tag{23}$$
$$\frac{d\psi_1(0)}{dx} = \frac{d\psi_2(0)}{dx} \tag{24}$$

and second at $x = a$

$$\psi_2(a) = \psi_3(a) \tag{25}$$
$$\frac{d\psi_2(a)}{dx} = \frac{d\psi_3(a)}{dx} \tag{26}$$

Task 4: [4 marks] Use Equations 23, 24, 25 and 26 to determine the four conditions:

$$1 + r = C + D \tag{27}$$
$$k_1(1 - r) = k_2(C - D) \tag{28}$$
$$Ce^{+ik_2a} + De^{-ik_2a} = te^{+ik_1a} \tag{29}$$
$$k_2(Ce^{+ik_2a} - De^{-ik_2a}) = k_1te^{+ik_1a} \tag{30}$$

Ideally we would like to solve these equations to determine the each of the parameters only in terms of k_1, k_2 and a. This is algebraically quite tedious. One approach is to rearrange the equations by hand:

- First, we can use Equations 27 and 28 to determine expressions for C and D in terms of r, k_1 and k_2.
- Second we can use Equations 29 and 30 to cancel t, and then substitute in our previous expressions for C and D to leave only r, k_1, k_2 and a remaining. After significant rearranging we can determine the expression for r (and hence C and D).

Another approach is to observe this these four coupled equations can be written as a matrix equation:

$$\begin{pmatrix} 1 & -1 & -1 & 0 \\ -k_1 & -k_2 & k_2 & 0 \\ 0 & e^{+ik_2a} & e^{-ik_2a} & -e^{+ik_1a} \\ 0 & k_2e^{+ik_2a} & -k_2e^{-ik_2a} & -k_1e^{+ik_1a} \end{pmatrix} \times \begin{pmatrix} r \\ C \\ D \\ t \end{pmatrix} = \begin{pmatrix} -1 \\ -k_1 \\ 0 \\ 0 \end{pmatrix} \tag{31}$$

This can be solved in a number of ways. Eventually you will arrive at solutions of the form

$$r = \frac{(k_1^2 - k_2^2)\sin(k_2a)}{2ik_1k_2\cos(k_2a) + (k_1^2 + k_2^2)\sin(k_2a)} \tag{32}$$
$$t = \frac{4k_2k_1e^{-ia(k_1-k_2)}}{(k_1 + k_2)^2 - e^{2iak_2}(k_1 - k_2)^2} \tag{33}$$

Task 5: [4 marks] Show that the reflection and transmission probabilities $R = |r|^2$ and $T = |t|^2$ are given by

$$R = \frac{(k_1^2 - k_2^2)\sin^2(k_2a)}{4k_1^2k_2^2 + (k_1^2 - k_2^2)^2\sin^2(k_2a)} \tag{34}$$
$$T = \frac{4k_1^2k_2^2}{4k_1^2k_2^2 + (k_1^2 - k_2^2)^2\sin^2(k_2a)} \tag{35}$$

2.1 Solutions when $E > V_0$

When the energy is greater than the potential the wave numbers are purely real and we can see that the transmission and reflection coefficients depend on oscillating terms.
Task 6: [2 marks] What condition determines when $T = 0$?

2.2 Solutions when $E < V_0$

If the energy is less than the barrier, wave number k_2 becomes imaginary. We can rewrite $k_2 = i\kappa$ where κ is a real number.

$$T = \frac{4k_1^2\kappa^2}{4k_1^2\kappa^2 + (k_1^2 + \kappa^2)^2 \sinh^2(\kappa a)} \tag{36}$$

where we've replaced $\sin(x) \equiv (e^{ix} - e^{-ix})/2i$ with $\sinh(x) \equiv (e^x - e^{-x})/2$.

For a large barrier, i.e. when $\kappa a >> 1$, the first exponential in the sinh function dominates, leading to the approximation

$$T \sim \frac{4k_1^2\kappa^2}{(k_1^2 + \kappa^2)} e^{-\kappa a}. \tag{37}$$

This shows us that the transmission probability is exponentially related to the barrier width, so for tunnelling probabilities to be significant, the barrier must be very thin.