6.3: Square Barrier

A slightly more involved example is the square potential barrier, an inverted square well, see Figure $6.3.1$.

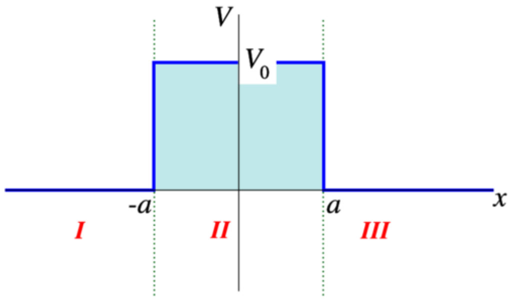

Figure* $6.3.1$*: The square barrier.

We are interested in the case that the energy is below the barrier height, $0 < E < V_0$. If we once again assume an incoming beam of particles from the right, it is clear that the solutions in the three regions are

$$\phi_I(x) = A_1 e^{ikx} + B_1 e^{-ikx} \tag{6.3.1}$$

$$\phi_{II}(x) = A_2 \cosh(\kappa x) + B_2 \sinh(\kappa x) \tag{6.3.2}$$

$$\phi_{III}(x) = A_3 e^{ikx}. \tag{6.3.3}$$

Here

$$k = \sqrt{\frac{2m}{\hbar^2}E} \tag{6.3.4}$$

and

$$\kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}. \tag{6.3.5}$$

Matching ϕ_I and ϕ_{II} at $x = -a$ and ϕ_{II} and ϕ_{III} at $x = a$ gives (use $\sinh(-x) = -\sinh x$ and $\cosh(-x) = \cosh x$).

$$A_1 e^{-ika} + B_1 e^{ika} = A_2 \cosh \kappa a - B_2 \sinh \kappa a \tag{6.3.6}$$

$$ik(A_1 e^{-ika} - B_1 e^{ika}) = \kappa(-A_2 \sinh \kappa a + B_2 \cosh \kappa a) \tag{6.3.7}$$

$$A_3 e^{ika} = A_2 \cosh \kappa a + B_2 \sinh \kappa a \tag{6.3.8}$$

$$ik(A_3 e^{ika}) = \kappa(A_2 \sinh \kappa a + B_2 \cosh \kappa a) \tag{6.3.9}$$

These are four equations with five unknowns. We can thus express for of the unknown quantities in one other. Let us choose that one to be A_1, since that describes the intensity of the incoming beam. We are not interested in A_2 and B_2, which describe the wave function in the middle. We can combine the equation above so that they either have A_2 or B_2 on the right hand side, which allows us to eliminate these two variables, leading to two equations with the three interesting unknowns A_3, B_1 and A_1. These can then be solved for A_3 and B_1 in terms of A_1:

The way we proceed is to add Equations 6.3.6 and 6.3.8, subtract Equations 6.3.7 from 6.3.9, subtract 6.3.8 from 6.3.6, and add 6.3.7 and 6.3.9. We find

$$A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika} = 2A_2 \cosh \kappa a \tag{6.3.10}$$

$$ik(-A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika}) = 2\kappa A_2 \sinh \kappa a \tag{6.3.11}$$

$$A_1 e^{-ika} + B_1 e^{ika} - A_3 e^{ika} = -2B_2 \sinh \kappa a \tag{6.3.12}$$

$$ik(A_1 e^{-ika} - B_1 e^{ika} + A_3 e^{ika}) = 2\kappa B_2 \cosh \kappa a \tag{6.3.13}$$

We now take the ratio of equations 6.3.10 and 6.3.11 and of 6.3.12 and 6.3.13, and find (i.e., we take ratios of left- and right hand sides, and equate those)

$$\frac{A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika}}{ik(-A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika})} = \frac{1}{\kappa \tanh \kappa a} \tag{6.3.14}$$

$$\frac{A_1 e^{-ika} + B_1 e^{ika} - A_3 e^{ika}}{ik(-A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika})} = -\frac{\tanh \kappa a}{\kappa} \tag{6.3.15}$$

These equations can be rewritten as (multiplying out the denominators, and collecting terms with A_1, B_3 and A_3)

$$A_1 e^{-ika}(\kappa \tanh \kappa a + ik) + B_1 e^{ika}(\kappa \tanh \kappa a - ik) + A_3 e^{ika}(\kappa \tanh \kappa a - ik) = 0 \tag{6.3.16}$$

$$A_1 e^{-ika}(\kappa - ik \tanh \kappa a) + B_1 e^{ika}(\kappa + ik \tanh \kappa a) + A_3 e^{ika}(-\kappa + ik \tanh \kappa a) = 0 \tag{6.3.17}$$

Now eliminate A_3, add Equations 6.3.16 and 6.3.17 to find

$$\begin{aligned}&A_1 e^{-ika}[(\kappa - ik\tanh\kappa a)(\kappa\tanh\kappa a + ik)+\\&(\kappa\tanh\kappa a - ik)(\kappa - ik\tanh\kappa a)]\\&+B_1 e^{ika}[(\kappa - ik\tanh\kappa a)(\kappa\tanh\kappa a - ik)+\\&(\kappa\tanh\kappa a - ik)(\kappa + ik\tanh\kappa a)] = 0\end{aligned} \tag{6.3.18}$$

Thus we find

$$B_1 = -A_1 e^{-2ika}\frac{\tanh\kappa a(k^2+\kappa^2)}{(\kappa - ik\tanh\kappa a)(\kappa\tanh\kappa a - ik)} \tag{6.3.19}$$

and we find, after using some of the angle-doubling formulas for hyperbolic functions, that the absolute value squared, i.e., the reflection coefficient, is

$$R = \frac{\sinh^2 2\kappa a\left(\kappa^2+k^2\right)^2}{4\kappa^2k^2 + \left(\kappa^2-k^2\right)^2\sinh^2 2\kappa a} \tag{6.3.20}$$

In a similar way we can express A_3 in terms of A_1 (add Equations 6.3.16 and Equation 6.3.17, or use

$$T = 1 - R! \tag{6.3.21}$$

Alternative approach

The equation can be given in matrix form as

$$\begin{pmatrix} e^{-ika} & e^{ika} \\ ike^{-ika} & -ike^{ika}\end{pmatrix}\begin{pmatrix}A_1\\B_1\end{pmatrix}\begin{pmatrix} \cosh\kappa a & -\sinh\kappa a \\ -\kappa\sinh\kappa a & \kappa\cosh\kappa a\end{pmatrix}\begin{pmatrix}A_2\\B_2\end{pmatrix}\begin{pmatrix} e^{ika} & e^{-ika} \\ ike^{-ika} & -ike^{ika}\end{pmatrix}\begin{pmatrix} \cosh\kappa a & \sinh\kappa a \\ \kappa\sinh\kappa a & \kappa\cosh\kappa a\end{pmatrix}\begin{pmatrix}A_2\\B_2\end{pmatrix} \tag{6.3.22}$$

Question: Can you invert the matrices and find the same answer as before?

Example 6.3.1: Hydrogen Atom Scattering

We now consider a particle of the mass of a hydrogen atom, $m = 1.67\times 10^{-27} kg$, and use a barrier of height 4 meV and of width $10^{-10}m$. The picture for reflection and transmission coefficients can seen in Figure $6.3.1; left$. We have also evaluated R and T for energies larger than the height of the barrier (the evaluation is straightforward).

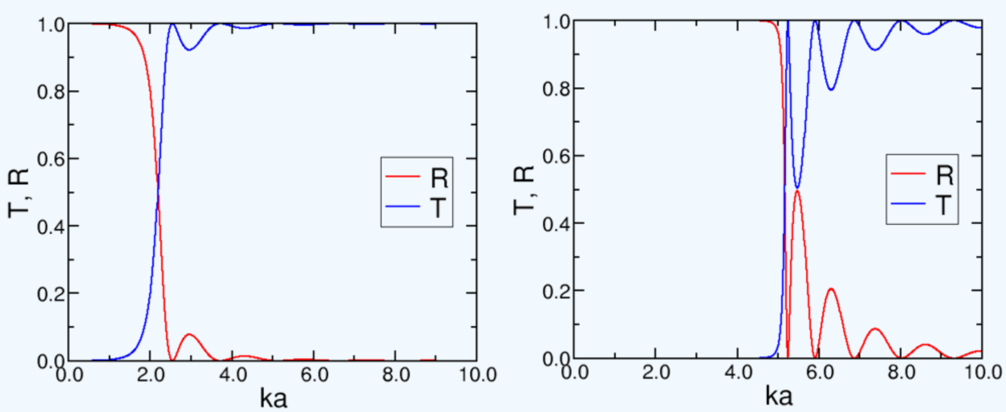

***Figure $6.3.2$**: The reflection and transmission coefficients for a square barrier of height 4 meV (left) amd 50 meV (right) and width 1 0− 1 0 m.*

If we heighten the barrier to 50 meV, we find a slightly different picture (Figure $6.3.1; right$).

Notice the oscillations (resonances) in the reflection. These are related to an integer number of oscillations fitting exactly in the width of the barrier, $\sin^2\kappa a = 0$.