8.2 THE SQUARE POTENTIAL BARRIER

We now consider a one-dimensional potential barrier of finite width and height given by

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 < x < a \\ 0 & x > a \end{cases} \tag{8.20}$$

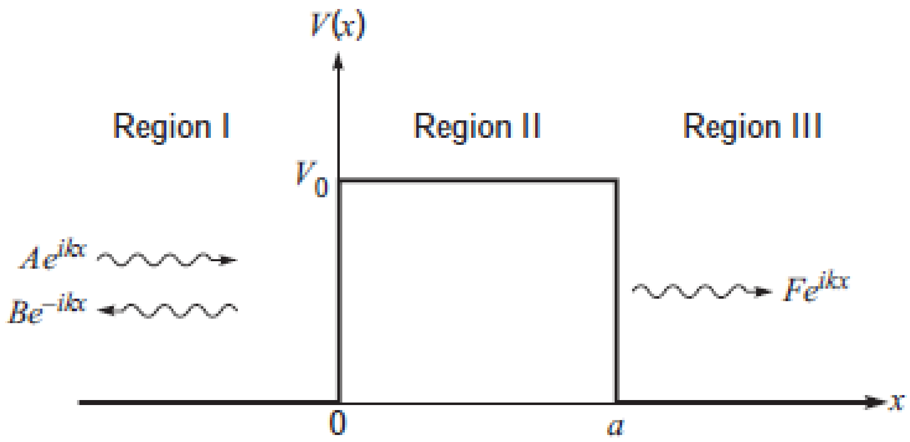

Figure 8.4 The square potential barrier.

Such a barrier is called a *square* or a *rectangular* barrier and is shown in Figure 8.4. Although the potential barriers in the real world do not have such simple shapes, this idealized treatment forms the basis for the understanding of more complicated systems and often provides a fairly good order-of-magnitude estimate.

As in the previous section, we consider a particle of mass m incident on the barrier from the left with energy E. As mentioned therein, according to classical mechanics, the particle would always be reflected back if $E < V_0$ and would always be transmitted if $E > V_0$. We shall show that, quantum mechanically, both reflection and transmission occur with finite probability for all values of E except in some special cases.

We shall discuss the two cases, $E > V_0$ and $E < V_0$, separately.

Case 1: $E > V_0$

Let us divide the whole space into three regions: Region I ($x < 0$), Region II ($0 < x < a$) and Region III ($x > a$). In regions I and III the particle is free and so the time-independent Schrödinger equation is

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

or
$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0, \quad k^2 = \frac{2mE}{\hbar^2} \tag{8.21}$$

The general solution of this equation is

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Fe^{ikx} + Ge^{-ikx} & x > a \end{cases}$$

where A, B, F, G are arbitrary constants. For $x < 0$, the term $A\exp(ikx)$ corresponds to a plane wave of amplitude A incident on the barrier from the left and the term $B\exp(-ikx)$ corresponds to a plane wave of amplitude B reflected from the barrier. For $x > a$, the term $F\exp(ikx)$ corresponds to a transmitted wave of amplitude F. Since no reflected wave is possible in this region we must set $G = 0$.

In region II the Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V_0\psi = E\psi$$

or
$$\frac{d^2\psi}{dx^2} + k'^2\psi(x) = 0, \quad k'^2 = \frac{2m(E - V_0)}{\hbar^2} \tag{8.22}$$

Since $E > V_0$, the quantity k'^2 is positive. Therefore, the general solution of this equation is

$$\psi(x) = Ce^{ik'x} + De^{-ik'x} \quad 0 < x < a$$

The complete eigenfunction is given by

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{ik'x} + De^{-ik'x} & 0 < x < a \\ Fe^{ikx} & x > a \end{cases} \tag{8.23}$$

The real part of the barrier eigenfunction for $E > V_0$ is shown schematically in Figure 8.5(a).

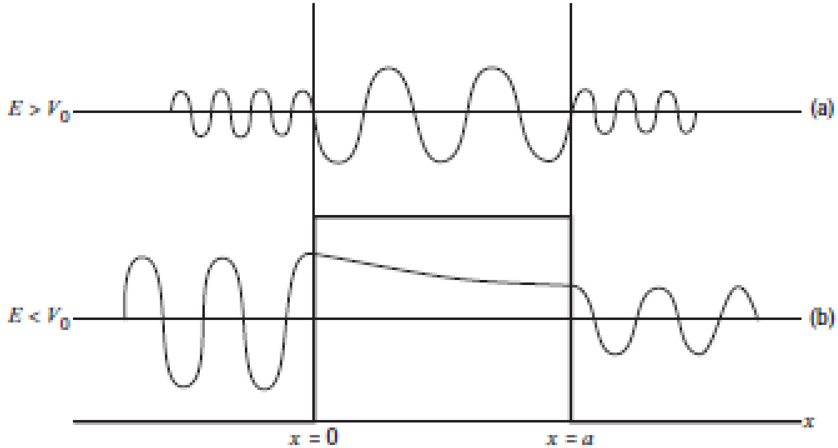

Figure 8.5 Schematic plots of the real parts of the barrier eigenfunctions for (a) $E > V_0$ and (b) $E < V_0$.

Continuity of $\psi(x)$ and $d\psi(x)/dx$ at $x = 0$ and $x = a$ gives

$$A + B = C + D \tag{8.24}$$

$$ik\,(A - B) = ik'\,(C - D) \tag{8.25}$$

$$Ce^{ik'a} + De^{-ik'a} = Fe^{ika} \tag{8.26}$$

$$ik'\,(Ce^{ik'a} - De^{-ik'a}) = ikFe^{ika} \tag{8.27}$$

From (8.24) and (8.25) we obtain

$$A = \frac{1}{2k}[C(k + k') + D(k - k')] \tag{8.28}$$

$$B = \frac{1}{2k}[C(k - k') + D(k + k')] \tag{8.29}$$

From (8.26) and (8.27) we obtain

$$C = \frac{1}{2k'}\,F(k' + k)\,e^{i(k - k')a} \tag{8.30}$$

$$D = \frac{1}{2k'}\,F(k' - k)\,e^{i(k + k')a} \tag{8.31}$$

Dividing (8.31) by (8.30)

$$\frac{D}{C} = \frac{k' - k}{k' + k}\,e^{2ik'a} \tag{8.32}$$

Dividing (8.29) by (8.28)

$$\frac{B}{A} = \frac{(k-k') + \left(\frac{D}{C}\right)(k+k')}{(k+k') + \left(\frac{D}{C}\right)(k-k')}$$

On substitution for D/C from (8.32), this becomes

$$\frac{B}{A} = \frac{(k^2-k'^2)(1-e^{2ik'a})}{(k+k')^2-(k-k')^2\,e^{2ik'a}} \tag{8.33}$$

We need a similar expression for F/A. Equations (8.24) and (8.25) yield

$$C = \frac{1}{2k'}[A(k+k') - B(k-k')]$$

Substituting in (8.30)

$$A(k+k') - B(k-k') = F(k+k')e^{i(k-k')a}$$

or

$$\frac{F}{A}\,(k+k')e^{i(k-k')a} = (k+k') - \frac{B}{A}(k-k')$$

$$= (k+k') - \left[\frac{(k^2-k'^2)(1-e^{2ik'a})}{(k+k')^2-(k-k')^2\,e^{2ik'a}}\right](k-k')$$

Simplifying, we obtain

$$\frac{F}{A} = \frac{4kk'\,e^{i(k'-k)a}}{(k+k')^2-(k-k')^2\,e^{2ik'a}} \tag{8.34}$$

The reflection and transmission coefficients are, respectively,

$$R = \left|\frac{B}{A}\right|^2 = \left[1+\frac{4k^2k'^2}{(k^2-k'^2)^2\sin^2 k'a}\right]^{-1} = \left[1+\frac{4E(E-V_0)}{V_0^2\sin^2 k'a}\right]^{-1} \tag{8.35}$$

and

$$T = \left|\frac{F}{A}\right|^2 = \left[1+\frac{(k^2-k'^2)^2\sin^2 k'a}{4k^2k'^2}\right]^{-1} = \left[1+\frac{V_0^2\sin^2 k'a}{4E(E-V_0)}\right]^{-1} \tag{8.36}$$

It can be easily shown that, as expected,

$$R + T = 1$$

Note that T is in general less than unity. This is in contradiction to the classical result that the particle always crosses the barrier when $E > V_0$. Here $T = 1$ only when $k'a = \pi, 2\pi, 3\pi, \ldots$. Now, if λ' is the de Broglie wavelength of the particle when it is passing through the barrier, then

$$k' = \frac{2\pi}{\lambda'}$$

Therefore $T = 1$ when

$$a = n\left(\frac{\lambda'}{2}\right), \quad n = 1, 2, 3, \ldots$$

Thus, there is *perfect transmission* only when the thickness of the barrier is equal to an integral multiple of half the de Broglie wavelength in the internal region. This is analogous to the interference phenomena in the transmission of light through thin refracting layers.

Equation (8.36) shows that

$$T \to \left[1 + \frac{mV_0 a^2}{2\hbar^2}\right]^{-1} \text{ as } E \to V_0 \text{ (from above)} \tag{8.37}$$

As E increases, T oscillates between a steadily increasing lower envelope and unity, as shown in Figure 8.6. The dimensionless parameter $mV_0a^2/\hbar^2$ is considered as a measure of the 'opacity' of the barrier.

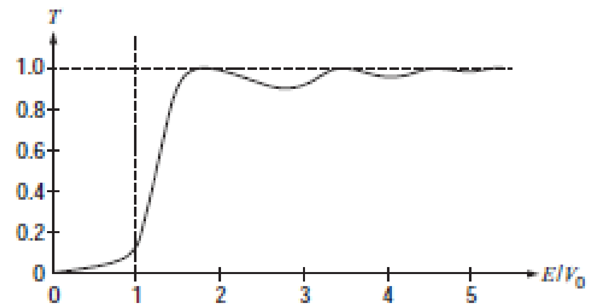

Figure 8.6 Variation of transmission coefficient for a square potential barrier as a function of E/V_0 for $mV_0a^2/\hbar^2 = 10$.

Case 2: $E < V_0$

In region I ($x < 0$) and III ($x > a$), the Schrödinger equation and its solution remain the same as in case 1. In region II ($0 < x < a$) the Schrödinger equation is

$$\frac{d^2\psi}{dx^2} - K^2\psi(x) = 0, \quad K^2 = \frac{2m(V_0 - E)}{\hbar^2} \tag{8.38}$$

Therefore, the eigenfunction in region II is

$$\psi(x) = Ce^{-Kx} + De^{Kx} \quad 0 < x < a \tag{8.39}$$

The real part of the complete eigenfunction for $E < V_0$ is shown schematically in Figure 8.5(b).

The reflection and transmission coefficients can be immediately obtained if we replace k' by iK in (8.35) and (8.36). Remembering that $\sin ix = i \sinh x$, we obtain and

$$R = \left[1 + \frac{4k^2K^2}{(k^2+K^2)^2\sinh^2(Ka)}\right]^{-1} = \left[1 + \frac{4E(V_0-E)}{V_0^2\sinh^2(Ka)}\right]^{-1} \tag{8.40}$$

$$T = \left[1 + \frac{(k^2+K^2)^2\sinh^2(Ka)}{4k^2K^2}\right]^{-1} = \left[1 + \frac{V_0^2\sinh^2(Ka)}{4E(V_0-E)}\right]^{-1} \tag{8.41}$$

It is again readily verified that $R + T = 1$. We note that $T \to 0$ in the limit $E \to 0$. Further, T is a monotonically increasing function of E and approaches

$$\left[1 + \frac{mV_0a^2}{2\hbar^2}\right]^{-1} \text{ as } E \to V_0 \text{ (from below)} \tag{8.42}$$

Thus T joins smoothly to the value given in (8.37) for the case $E \to V_0$ from above (see Figure 8.6).

For a broad high barrier, $Ka >> 1$. This is true for most cases of practical interest. We may take $\sinh Ka \approx \exp(Ka)/2$. In that case,

$$T \approx \left(\frac{4kK}{k^2+K^2}\right)^2 e^{-2Ka} = \frac{16E(V_0-E)}{V_0^2}\, e^{-2Ka} \tag{8.43}$$

and is very small.

Further, the factor $16E(V_0 - E)/V_0^2$ varies slowly with V_0 and E and is of order unity in most cases. The exponential factor is the dominant one and varies rapidly with V_0 and E. Therefore, for order of magnitude calculation, we can take

$$T \approx e^{-2Ka} \tag{8.44}$$