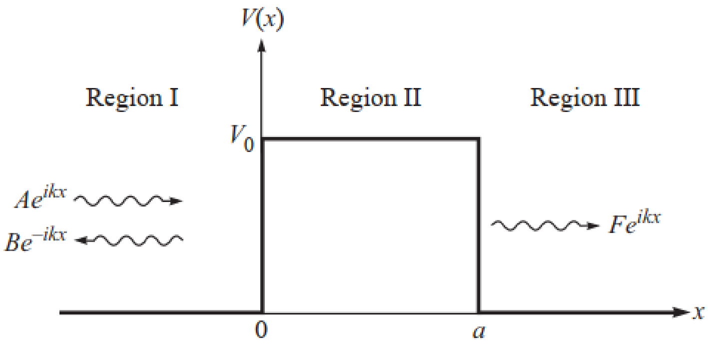
5.2 The Square Potential Barrier

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



$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 < x < a \\ 0 & x > a \end{cases} \quad \ldots(5.20)$$

We have a particle of mass m incident on the barrier from the left with energy E. According to classical mechanics, the particle would always be reflected back if $E < V_0$ and would always be transmitted if $E \geq V_0$.

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 andso the time-independent Schrödinger equation is

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

or

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0, \quad k^2 = \frac{2mE}{\hbar^2} \quad \ldots(5.21)$$

The general solution of this equation is

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

For $x < 0$,

- Ae^{ikx} corresponds to a plane wave of amplitude A incident on the barrier from the left
- Be^{-ikx}corresponds to a plane wave of amplitude B reflected from the barrier.

For $x < a$,

- Fe^{ikx} corresponds to a transmitted wave of amplitude F.
- $G = 0$ because no reflected wave is possible in this region.

In region *II*: the Schrödinger equation is

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

or

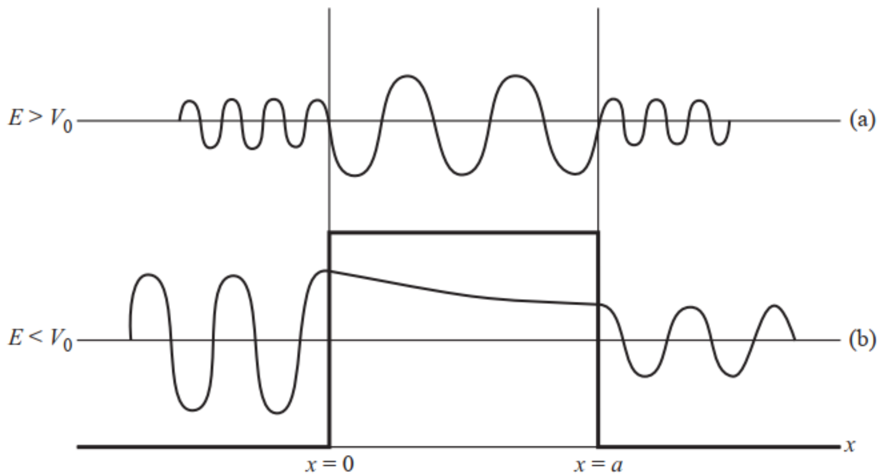
$$\frac{d^2\psi}{dx^2} + k'^2\psi(x) = 0, \quad k'^2 = \frac{2m(E - V_0)}{\hbar^2} \qquad \ldots(5.22)$$

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

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{ik'x} + De^{-ik'x} & 0 < x < a \\ Fe^{ikx} & x > a \end{cases} \qquad \ldots(5.23)$$



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

$$A + B = C + D \qquad \ldots(5.24)$$

$$ik\,(A - B) = ik'\,(C - D) \qquad \ldots(5.25)$$

$$Ce^{ik'a} + De^{-ik'a} = Fe^{ika} \qquad \ldots(5.26)$$

$$ik'\,(Ce^{ik'a} - De^{-ik'a}) = ikFe^{ika} \qquad \ldots(5.27)$$

From (5.24) and (5.25) we obtain

$$A = \frac{1}{2k}[C(k + k') + D(k - k')] \qquad \ldots(5.28)$$

$$B = \frac{1}{2k}[C(k - k') + D(k + k')] \qquad \ldots(5.29)$$

From (5.26) and (5.27) we obtain

$$C = \frac{1}{2k'} F(k' + k)\, e^{i(k - k')a} \qquad \ldots(5.30)$$

$$D = \frac{1}{2k'} F(k' - k)\, e^{i(k + k')a} \qquad \ldots(5.31)$$

Dividing (5.31) by (5.30)

$$\frac{D}{C} = \frac{k' - k}{k' + k}\, e^{2ik'a} \qquad \ldots(5.32)$$

Dividing (5.29) by (5.28)

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

On substitution for D/C from (5.32), this becomes

$$\frac{B}{A} = \frac{(k^2 - k'^2)(1 - e^{2ik'a})}{(k + k')^2 - (k - k')^2\, e^{2ik'a}} \qquad \ldots(5.33)$$

We need a similar expression for F/A. Equations (5.24) and (5.25) yield

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

Substituting in (5.30)

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

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

$$\frac{F}{A} = \frac{4kk'\, e^{i(k' - k)a}}{(k + k')^2 - (k - k')^2\, e^{2ik'a}} \qquad \ldots(5.34)$$

The **reflection** and **transmission coefficients** are, respectively,

$$R = \left|\frac{B}{A}\right|^2 = \left[1 + \frac{4k^2k'^2}{(k^2 - k'^2)^2 \sin^2 k'a}\right]^{-1} = \left[1 + \frac{4E(E - V_0)}{V_0^2 \sin^2 k'a}\right]^{-1} \quad \ldots(5.35)$$

and

$$T = \left|\frac{F}{A}\right|^2 = \left[1 + \frac{(k^2 - k'^2)^2 \sin^2 k'a}{4k^2k'^2}\right]^{-1} = \left[1 + \frac{V_0^2 \sin^2 k'a}{4E(E - V_0)}\right]^{-1} \quad \ldots(5.36)$$

It can be easily shown that, as expected,

$$R + T = 1$$

The perfect transmission

$$T \to \left[1 + \frac{mV_0 a^2}{2\hbar^2}\right]^{-1} \quad \text{as } E \to V_0 \text{ (from above)} \quad \ldots(5.37)$$

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

$$\frac{d^2\psi}{dx^2} - K^2\psi(x) = 0, \quad K^2 = \frac{2m(V_0 - E)}{\hbar^2} \quad \ldots(5.38)$$

Therefore, the eigenfunction in region II is

$$\psi(x) = Ce^{-Kx} + De^{Kx} \quad 0 < x < a \quad \ldots(5.39)$$

The real part of the complete eigenfunction for $E < V_0$ is shown in above Figure.

The reflection and transmission coefficients can be immediately obtained if we replace k' by iK in (5.35) and (5.36). Remembering that $\sin ix = i \sinh x$, we obtain

$$R = \left[1 + \frac{4k^2K^2}{(k^2 + K^2)^2 \sinh^2(Ka)}\right]^{-1} = \left[1 + \frac{4E(V_0 - E)}{V_0^2 \sinh^2(Ka)}\right]^{-1} \quad \ldots(5.40)$$

and

$$T = \left[1 + \frac{(k^2 + K^2)^2 \sinh^2(Ka)}{4k^2K^2}\right]^{-1} = \left[1 + \frac{V_0^2 \sinh^2(Ka)}{4E(V_0 - E)}\right]^{-1} \quad \ldots(5.41)$$

It is again readily verified that $R + T = 1$. We note that $T \to 0$ in the limit $E \to 0$.

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,

$$T \approx \left(\frac{4kK}{k^2 + K^2}\right)^2 e^{-2Ka} = \frac{16E(V_0 - E)}{V_0^2} e^{-2Ka} \quad \ldots(5.42)$$

Problem 3: Obtain Equation (5.42) from Equation (5.41).

Solution: If $Ka >> 1$, then $\sinh^2(Ka) >> 1$.

Therefore, Equation (5.41) reduces to

$$T \approx \frac{4k^2K^2}{(k^2+K^2)^2 \sinh^2(Ka)} = \frac{4E(V_0-E)}{V_0^2 \sinh^2(Ka)}$$

Now,

$$\sinh(Ka) = \frac{e^{Ka}-e^{-Ka}}{2} = \frac{e^{-Ka}}{2}\left(e^{2Ka}-1\right) \approx \frac{\left(e^{-Ka}\right)\left(e^{2Ka}\right)}{2}$$

$$= \frac{e^{Ka}}{2}$$

Substituting in the above equation

$$T = \frac{4k^2K^2}{(k^2+K^2)^2}\left(\frac{2}{e^{Ka}}\right)^2 = \frac{4E(V_0-E)}{V_0^2}\left(\frac{2}{e^{Ka}}\right)^2$$

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

Problem 4: Electrons of energy *2 eV* are incident on a barrier *3 eV* high and *0.4 nm* wide. Calculate the transmission probability.

Solution: Transmission probability $T = \left[1+\frac{V_0^2\sinh^2(Ka)}{4E(V_0-E)}\right]^{-1}$

Here
$$V_0 - E = (3.0 - 2.0) = 1 \text{ eV} = 1.6 \times 10^{-19} \text{ J}$$

$$Ka = \frac{[2m(V_0-E)]^{1/2}}{\hbar}\, a$$

$$= \frac{[2\times 9\times 10^{-31}\times 1.6\times 10^{-19}]^{1/2}}{1.05\times 10^{-34}} \times 4 \times 10^{-10}$$

$$= 2.045$$

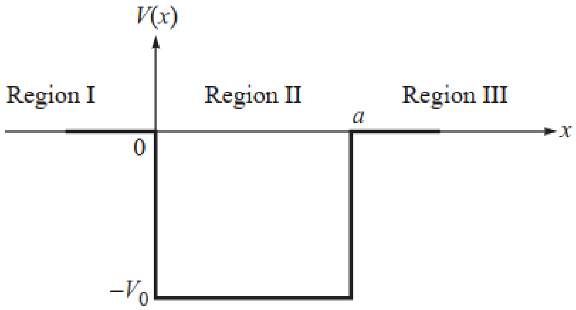
$$\sinh(2.045) = 3.805$$

$$\frac{V_0^2}{4E(V_0-E)} = \frac{(3.0)^2}{4\times 2.0\times 1.0} = \frac{9}{8} = 1.125$$

$$T = [1 + 1.125 \times (3.805)^2]^{-1}$$

$$= \boxed{0.058}$$

5.3 The Square Potential Well



One-dimensional square well of depth V_0 and range a.

$$V(x) = \begin{cases} 0 & x < 0 \\ -V_0 & 0 < x < a \\ 0 & x > a \end{cases} \qquad \ldots(5.43)$$

This potential has depth V_0 and range a. Suppose that the particle is incident upon the well from the left. Let us divide the whole space into three regions: Region I ($x < 0$), Region II ($0 < x < a$) and Region III ($x > a$). In the external regions I and III the particle is free and so the time independent Schrödinger equation is

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

or

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0, \quad k^2 = \frac{2mE}{\hbar^2} \qquad \ldots(5.44)$$

In the interior region II, the Schrödinger equation is

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

or

$$\frac{d^2\psi(x)}{dx^2} + \beta^2\psi(x) = 0, \quad \beta^2 = \frac{2m(E+V_0)}{\hbar^2} \qquad \ldots(5.45)$$

Solving Equations (5.44) and (5.45), we obtain the physically acceptable wave function

$$\psi(x) = \begin{cases} \underset{\text{(Incident)}}{Ae^{ikx}} + \underset{\text{(Reflected)}}{Be^{-ikx}} & x < 0 \\ Ce^{i\beta x} + De^{-i\beta x}, \quad \beta = \left(\frac{2m(E+V_0)}{\hbar^2}\right)^{1/2} & 0 < x < a \\ \underset{\text{(Transmitted)}}{Fe^{ikx}} & x > a \end{cases} \qquad \ldots(5.46)$$

In order to obtain the ***reflection*** and ***transmission*** coefficients, we note that the present problem of scattering by a potential well is mathematically similar to the scattering by a potential barrier.

$$R = \left[1 + \frac{4E(E+V_0)}{V_0^2 \sin^2(\beta a)}\right]^{-1} \qquad T = \left[1 + \frac{V_0^2 \sin^2(\beta a)}{4E(E+V_0)}\right]^{-1}$$