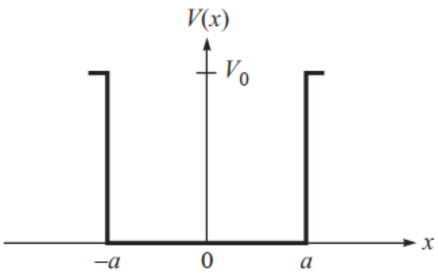
4.3 One-Dimensional Finite Square Well (First Type)



$$V(x) = \begin{cases} 0 & |x| < a \\ V_0 & |x| > a \end{cases} \qquad \ldots(4.44)$$

Consider a particle of mass m moving in this potential with energy E.

Case One: When $E < V_0$. The particle is confined in a bound state.

Inside the well the time-independent Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \qquad |x| < a$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0, \qquad k^2 = \frac{2mE}{\hbar^2} \qquad \ldots(4.45)$$

The general solution of this equation is

$$\psi(x) = A \sin kx + B \cos kx \qquad \ldots(4.46)$$

Outside the well the equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi, \qquad |x| > a$$

or

$$\frac{d^2\psi}{dx^2} - K^2\psi = 0, \quad K^2 = \frac{2m(V_0 - E)}{\hbar^2} \qquad \ldots(4.47)$$

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

$$\psi(x) = Ce^{-Kx} + De^{Kx} \qquad \ldots(4.48)$$

The wave function should not become infinite as $x \longrightarrow \pm\infty$. Therefore, we must take $C = 0$ for $x < -a$ and $D = 0$ for $x > a$. So, the wave function can be written as

$$\psi(x) = \begin{cases} De^{Kx} & x < -a \\ A \sin kx + B \cos kx & -a < x < a \\ Ce^{-Kx} & x > a \end{cases} \qquad \ldots(4.49)$$

The requirement that $\psi(x)$ and $\frac{d\psi}{dx}$ be continuous at$x = -a$ gives

$\ldots(4.50)$

$$-A\sin ka + B\cos ka = De^{-Ka}$$

and

$$kA\cos ka + kB\sin ka = KDe^{-Ka} \quad \ldots(4.51)$$

Similarly, the continuity of $\psi(x)$ and $d\psi/dx$ at $x = a$ gives

$$A\sin ka + B\cos ka = Ce^{-Ka} \quad \ldots(4.52)$$

and

$$kA\cos ka - kB\sin ka = -KCe^{-Ka} \quad \ldots(4.53)$$

Equations (4.50) and (4.52) give

$$2A\sin ka = (C - D)\,e^{-Ka} \quad \ldots(4.54)$$

$$2B\cos ka = (C + D)\,e^{-Ka} \quad \ldots(4.55)$$

Equations (4.51) and (4.53) give

$$2kA\cos ka = -K\,(C - D)\,e^{-Ka} \quad \ldots(4.56)$$

$$2kB\sin ka = K\,(C + D)\,e^{-Ka} \quad \ldots(4.57)$$

Equations (4.54) and (4.56) yield

$$k\cot ka = -K \quad \ldots(4.58)$$

unless $A = 0$ and $C = D$. Similarly, Equations (4.55) and (4.57) yield

$$k\tan ka = K \quad \ldots(4.59)$$

unless $B = 0$ and $C = -D$.

Eliminating K from (4.58) and (4.59) leads to $tan^2 ka = -1$ which is not possible because both k and a are real. Therefore, these two equations cannot be valid simultaneously.

We have two classes of solutions:

For the *first class*

$$A = 0,\ C = D \quad \text{and} \quad k\tan ka = K \quad \ldots(4.60)$$

and for the *second class*

$$B = 0,\ C = -D \quad \text{and} \quad k\cot ka = -K \quad \ldots(4.61)$$

Eigenfunctions

The *eigenfunctions* of the *first class* are given by

$$\psi(x) = \begin{cases} Ce^{Kx} & x < -a \\ B\cos kx & -a < x < a \\ Ce^{-Kx} & x > a \end{cases} \quad \ldots(4.62)$$

The *eigenfunctions* of the *second class* are given by

$$\psi(x) = \begin{cases} Ce^{Kx} & x < -a \\ A\sin kx & -a < x < a \\ -Ce^{-Kx} & x > a \end{cases} \qquad \ldots(4.63)$$

It is interesting to note that the eigenfunctions extend into the classically forbidden region $|x| > a$. The distance through which they extend is roughly $K^{-1} = \hbar/[2m(V_0 - E)]^{1/2}$, which increases as the energy E of the particle increases.

Parity

It may be noted, as in the case of the infinite square well, that the eigenfunctions of the first class have ***even*** parity, satisfying

$$\psi(-x) = \psi(x)$$

and the eigenfunctions of the second class have ***odd*** parity, satisfying

$$\psi(-x) = -\psi(x)$$

This division of eigenfunctions into even and odd types is due to the fact that the potential energy is symmetric about the origin, that is, $V(-x) = V(x)$.

Energy Levels: The energy levels can be found by solving the equations (4.60) and (4.61) numerically or graphically.

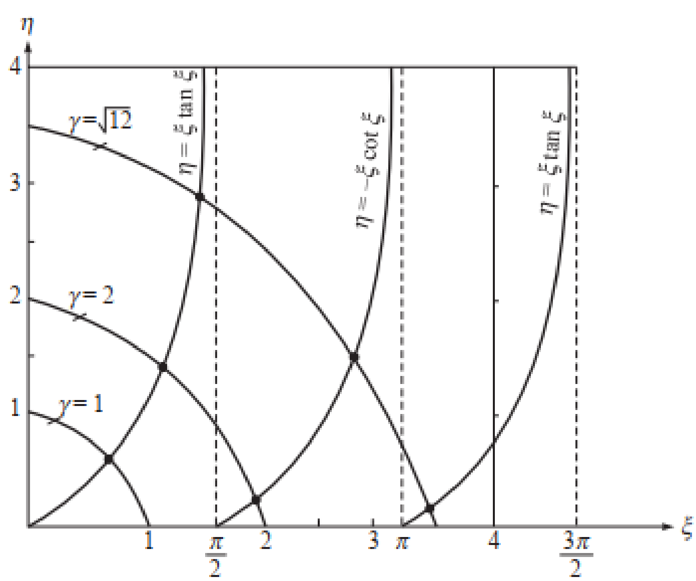
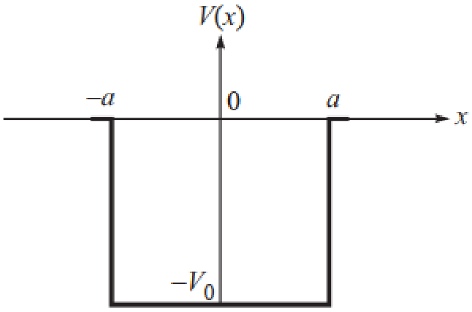


Figure: Graphical determination of the energy levels for a square well potential.

As, $\xi = ka$, $\eta = Ka$ and $\gamma = \sqrt{2mV_o a^2/\hbar^2}$

4.4 One-Dimensional Finite Square Well (Second Type)



$$V(x) = \begin{cases} -V_0 & |x| < a \\ 0 & |x| > a \end{cases} \qquad \ldots(4.64)$$

It should be noted that the potentials in *First type* and *Second type* differ only in the origin of the energy scale and are, therefore, physically equivalent.

We shall discuss the case $E < 0$ which gives rise to bound states. Inside the well the time-independent Schrödinger equation is,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi = -|E|\psi, \quad |x| < a$$

or

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0, \quad \alpha^2 = \frac{2m(V_0 - |E|)}{\hbar^2} \qquad \ldots(4.65)$$

Here $|E| = -E$ is the binding energy of the particle in the well. Since $V_0 > |E|$, the quantity α^2 is positive. Therefore, the general solution of this equation is,

$$\psi(x) = A\sin\alpha x + B\cos\alpha x \qquad \ldots(4.66)$$

Outside the well the equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi = -|E|\psi, \quad |x| > a$$

$$\frac{d^2\psi}{dx^2} - \beta^2\psi = 0, \quad \beta^2 = \frac{2m|E|}{\hbar^2} \qquad \ldots(4.67)$$

The general solution of this equation is,

$$\psi(x) = Ce^{-\beta x} + De^{\beta x} \qquad \ldots(4.68)$$

The wave function should not become infinite as $x \longrightarrow \pm\infty$. Therefore, we must take $C = 0$ for $x < -a$ and $D = 0$ for $x > a$. So the wave function can be written as,

$$\psi(x) = \begin{cases} De^{\beta x} & x < -a \\ A\sin\alpha x + B\cos\alpha x & -a < x < a \\ Ce^{-\beta x} & x > a \end{cases} \qquad \ldots(4.69)$$

Imposing that $\psi(x)$ and $d\psi/dx$ be continuous at $x \pm a$ and doing the same treatments as in the previous section, we obtain two classes of solutions:

The **eigenfunctions** of the *first class* are given by

$$\psi(x) = \begin{cases} Ce^{\beta x} & x < -a \\ B\cos\alpha x & -a < x < a \\ Ce^{-\beta x} & x > a \end{cases} \qquad \ldots(4.70)$$

The **eigenfunctions** of the *second class* are given by

$$\psi(x) = \begin{cases} Ce^{\beta x} & x < -a \\ A\sin\alpha x & -a < x < a \\ -Ce^{-\beta x} & x > a \end{cases} \qquad \ldots(4.71)$$

The **energy levels** can be found by solving the equations

$$\xi \tan \xi = \eta$$
$$\xi \cot \xi = -\eta$$

where $\xi = \alpha a$ and $\eta = \beta a$. These equations can be solved to obtain the energy levels following the same procedure as in the previous section.