The Finite Square Well

Consider 1D motion of a particle. Assume the potential is given by

\[
U(x) = \begin{cases} 
0 & |x| < L/2 \\
U_0 & |x| \geq L/2 
\end{cases}
\]  

(1)

where \(U_0\) is a positive constant. The behaviour of the particle depends on whether \(E < U_0\) or \(E > U_0\).
Bound State

Consider first the case of $E < U_0$.

In the region $x < -L/2$

$$-rac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U_0 \psi = E \psi$$

(2)

or

$$\frac{\partial^2 \psi}{\partial x^2} - \frac{2m(U_0 - E)}{\hbar^2} \psi = 0$$

(3)

Let

$$\kappa = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$$

(4)

Eq.(3) becomes

$$\frac{\partial^2 \psi}{\partial x^2} - \kappa^2 \psi = 0$$

(5)

Solution of Eq.(5) is

$$\psi(x) = Ae^{\kappa x}$$

(6)

e$^{-\kappa x}$ is omitted since it diverges at $x \to -\infty$. 
Bound State

Similarly, in the region $x > L/2$

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + U_0 \psi = E \psi \quad (7)$$

or

$$\frac{\partial^2 \psi}{\partial x^2} - \kappa^2 \psi = 0 \quad (8)$$

where

$$\kappa = \sqrt{\frac{2m(U_0 - E')}{\hbar^2}} \quad (9)$$

Solution of Eq.(8) is

$$\psi(x) = Be^{-\kappa x} \quad (10)$$

$e^{\kappa x}$ is omitted since it diverges at $x \to \infty$. 
Bound State

In the region \(-L/2 < x < L/2, \ U(x) = 0\)

\[-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E\psi\]  \hspace{1cm} (11)

or

\[\frac{\partial^2 \psi}{\partial x^2} + \frac{2mE}{\hbar^2} \psi = 0\]  \hspace{1cm} (12)

Let

\[k = \sqrt{\frac{2mE}{\hbar^2}}\]  \hspace{1cm} (13)

Eq.(3) becomes

\[\frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0\]  \hspace{1cm} (14)

Solution of Eq.(5) is

\[\psi(x) = Ce^{ikx} + De^{-ikx}\]  \hspace{1cm} (15)
Boundary Conditions

1. \( \psi \) is continuous at \( x = L/2 \)

\[
Ce^{ikL/2} + De^{-ikL/2} = Be^{-\kappa L/2}
\]  
(16)

2. \( \psi \) is continuous at \( x = -L/2 \)

\[
Ce^{-ikL/2} + De^{ikL/2} = Ae^{-\kappa L/2}
\]  
(17)

3. \( d\psi/dx \) is continuous at \( x = L/2 \)

\[
ike^{ikL/2} - ike^{-ikL/2} = -\kappa Be^{-\kappa L/2}
\]  
(18)

4. \( d\psi/dx \) is continuous at \( x = -L/2 \)

\[
ike^{-ikL/2} - ike^{ikL/2} = \kappa Ae^{-\kappa L/2}
\]  
(19)

The constants \( A, B, C, D \) and the eigen states can be obtained by solving these equations.
Physical Consideration

1. The potential is symmetric $\implies$ the wave function
   can be either an even or an odd function of $x$.
   Since
   \[
   \frac{\partial^2 \psi}{\partial x^2} + k^2 \psi = 0
   \]
   The solution must be either $\sin(kx)$ or $\cos(kx)$.

2. For an even wave function
   \[
   \psi(x) = \begin{cases} 
   A e^{kx} & x < -L/2 \\
   C \cos(kx) & -L/2 \leq x \leq L/2 \\
   B e^{-kx} & x > L/2 
   \end{cases}
   \]
   It is required for $A = B$. Furthermore, the boundary conditions at $x = L/2$ requires
   \[
   C \cos kL/2 = B e^{-\kappa L/2}
   \]
   \[
   -Ck \sin kL/2 = -\kappa B e^{-\kappa L/2}
   \]
   The boundary conditions at $x = -L/2$ are satisfied.
Divide these two equations, we get

\[ k \tan \frac{kL}{2} = \kappa \] \hspace{1cm} (20)

and the wave function can be written as

\[ \psi(x) = \begin{cases} 
    Ce^{\kappa L/2} \cos(kL/2)e^{\kappa x} & x < -L/2 \\
    C \cos(kx) & -L/2 \leq x \leq L/2 \\
    Ce^{\kappa L/2} \cos(kL/2)e^{-\kappa x} & x > L/2 
\end{cases} \]

Finally, \( C \) is determined by normalization of the wave function.

Eq.(20) determines the energy of the particle. Note that both \( k \) and \( \kappa \) are functions of energy. The equation can be solved numerically or graphically. Let

\[ z = \frac{kL}{2} = \sqrt{\frac{mL^2E}{2\hbar^2}}, \quad z_0 = \frac{\kappa L}{2} = \sqrt{\frac{mL^2U_0}{2\hbar^2}} \]

Eq.(2) can be written as

\[ \tan z = \sqrt{\left(\frac{z_0}{z}\right)} - 1 \]
Unnormalized wave functions.
3. For the odd wave function

\[ \psi(x) = \begin{cases} 
  Ae^{\kappa x} & x < -L/2 \\
  C \sin(kx) & -L/2 \leq x \leq L/2 \\
  Be^{-\kappa x} & x > L/2 
\end{cases} \]

It is required that \( B = -A \). Furthermore, the boundary conditions at \( x = L/2 \) requires

\[ C \sin kl/2 = Be^{-kL/2} \]

\[ Ck \cos kl/2 = -\kappa Be^{-kL/2} \]

This gives

\[ k \coth \frac{kL}{2} = -\kappa \]  \hspace{1cm} (21)

or

\[ \coth z = -\sqrt{\left(\frac{z_0}{z}\right)^2 - 1} \]  \hspace{1cm} (22)

Wave function (unnormalized)

\[ \psi(x) = \begin{cases} 
  C e^{\kappa L/2} \sin(kL/2)e^{\kappa x} & x < -L/2 \\
  C \sin(kx) & -L/2 \leq x \leq L/2 \\
  -Ce^{\kappa L/2} \sin(kL/2)e^{-\kappa x} & x > L/2 
\end{cases} \]
Unnormalized wave functions.

\[ -\sqrt{\left(\frac{z_0}{z}\right)^2} - 1 \]