# <u>**One-Dimensional Infinite Square Well**</u>

We consider a particle of mass m confined in a region of width 2a shown in figure (1). The potential energy of the particle is defined as below

$$V(x) = \begin{cases} 0, & |x| < a \\ \infty, & |x| \geq a \end{cases} \qquad \text{……………..} (1)$$

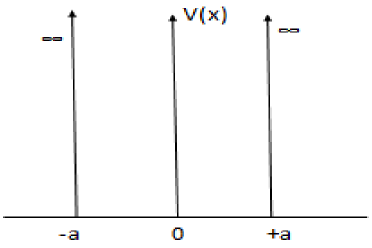


Figure 1. One-dimensional infinite square well potential

Such a system is called one dimensional box as the movement of the particle is restricted in x-dimension.

To find the eigenfunctions and energy eigenvalues for this system, we solve the time dependent Schroedinger equation

$$\frac{-\hbar^2}{2m}\frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x) \qquad \text{…………} (2)$$

Since the potential energy is infinite at x = ± a, the probability of finding the particle outside the well is zero. Therefore, the wavefunction Ψ(x) must vanish for $|x| > a$. Also the wavefunction must be continuous, it must vanish at the walls so

$$\Psi(x) = 0 \quad \text{at } x = \pm a \qquad \text{…………} (3)$$

For $|x| < a$, Eq. (2) reduces to

$$\frac{-\hbar^2}{2m}\frac{d^2\Psi}{dx^2} = E\Psi$$

Or $$\frac{-\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + k^2\Psi = 0 \quad \text{, where} \quad k^2 = \frac{2mE}{\hbar^2} \qquad \text{………………} (4)$$

The general solution of this equation is

$$\Psi(x) = A\sin kx + B\cos kx \qquad \text{………………..} (5)$$

Where A and B are constants to be determined.

Applying the boundary condition (3) at x=a, we get

$$A\sin ka + B\cos ka = 0$$

And at x= -a,

$$-A\sin ka + B\cos ka = 0$$

These equations give

A sin ka = 0, B cos ka =0 ……………….(6)

Observing eq.6, we can say that both A and B can not be equal to zero because this will give Ψ(x)=0 for all x, which is not possible. Also sin ka and cos ka can not be made zero simultaneously for a given value of k. hence we give two classes of solutions

For the first class, A =0 and cos ka=0

And for second class, B=0 and sin ka = 0

These conditions are satisfied if ka = nπ / 2, ………………..(7)

where n is odd integer for the first class and even integer for the second class. Hence the eigenfunctions for both the classes can be written as

| | |
|---|---|
| $\Psi_n(x) = B\cos\frac{n\pi x}{2a}$ | , where n = 1,3,5,…….. |
| $\Psi_n(x) = A\sin\frac{n\pi x}{2a}$ | , where n = 2,4,6,…….. |

Applying normalization condition ,

$$\int_{-a}^{a}\Psi_n^*(x)\Psi_n(x)dx = 1$$ , we get

$$A^2\int_{-a}^{a} sin^2\left(\frac{n\pi x}{2a}\right)dx = 1 \quad \text{and} \quad B^2\int_{-a}^{a} cos^2\left(\frac{n\pi x}{2a}\right)dx = 1$$

Solving these equations, we find $A = B = \frac{1}{\sqrt{a}}$ …………… (8)

Accordingly, the normalized eigenfunctions for the two classes can be written as

| | |
|---|---|
| $\Psi_n(x) = \frac{1}{\sqrt{a}}\cos\frac{n\pi x}{2a}$ | , where n = 1,3,5,…….. |
| $\Psi_n(x) = \frac{1}{\sqrt{a}}\sin\frac{n\pi x}{2a}$ | , where n = 2,4,6,…….. |

………. (9)

Eq (7) gives the allowed values of k i.e.

$$k_n = \frac{n\pi}{2a} \qquad \text{where } n = 1,2,3,\ldots\ldots \qquad \ldots\ldots\ldots\ldots (10)$$

Using eq (4) and (10), we can obtain the energy eigenvalues as follows

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{8ma^2} \qquad \text{where } n= 1,2,3,\ldots\ldots \qquad \ldots\ldots\ldots\ldots\ldots (11)$$

This equation shows that the energy is quantized. The integer n is called quantum number. The representations of energy levels, eigenfunctions and probability densities are shown in figures (2), (3) and (4) respectively.

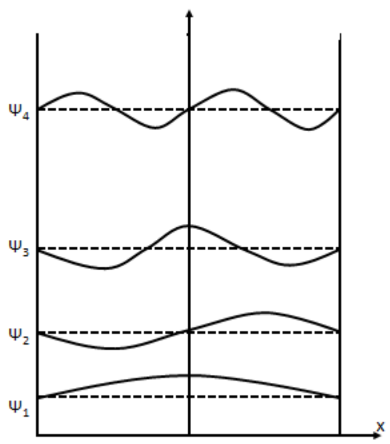


Figure (3). Wave functions

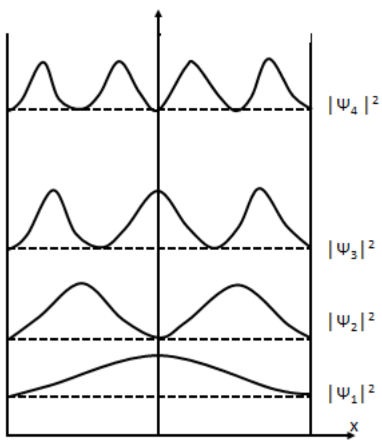


Figure (4). Probability densities