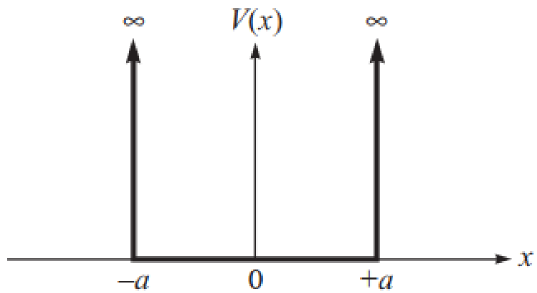
4.2 One-Dimensional Infinite Square Well Potential

Let us consider a particle of mass m confined in a region of width $2a$ from $x = -a \ to \ x = +a$ by impenetrable walls. Such a system is also called a one-dimensional box.



The one-dimensional infinite square well potential.

Inside the box, the particle is free but experiences a sudden large force directed towards the origin as it reaches the points $x = \pm a$. Therefore, the potential energy for this problem is,

$$V(x) = \begin{cases} 0 & |x| < a \\ \infty & |x| > a \end{cases} \qquad \text{...(4.12)}$$

To find the eigenfunctions and energy eigenvalues for this system, we have to solve the time-independent Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\,\psi(x) \qquad \text{...(4.13)}$$

Since the potential energy is infinite at $x = \pm a$, the probability of finding the particle outside the well is zero. Therefore, the wave function $\psi(x)$ must vanish for $|x| > a$.

Since the wave function must be continuous, it must vanish at the walls:

$$\psi(x) = 0 \qquad \text{at} \qquad x = \pm a \qquad \text{...(4.14)}$$

For $|x| < a$, the Schrödinger equation reduces to

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

or
$$\frac{d^2\psi}{dx^2} + k^2\psi = 0; \quad k^2 = \frac{2mE}{\hbar^2} \qquad \text{...(4.15)}$$

The general solution of this equation is,

$$\psi(x) = A \sin kx + B \cos kx \qquad \ldots(4.16)$$

Applying the boundary condition

1) at $x = a$, we obtain

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

2) at $x = -a$, we obtain

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

By *addition* these two equations we get,

$$B\, cos\, ka = 0 \qquad \ldots(4.17\text{-a})$$

By *subtraction* these two equations we get

$$A\, sin\, ka = 0 \qquad \ldots(4.17\text{-b})$$

- We cannot allow both *A* and *B* to be zero because this would give the physically uninteresting trivial solution $\boldsymbol{\psi(x) = 0}$ for all *x*.
- We cannot make both ***sin ka*** and ***cos ka*** zero for a given value of *k*.
- Hence, there are *two* possible classes of solutions:

First-class: $A = 0 \quad and \quad \cos ka = 0$

Second class: $B = 0 \quad and \quad \sin ka = 0$

The conditions are satisfied if

$$ka = \frac{n\pi}{2} \qquad \ldots(4.18)$$

Where *n* is *odd* integer for the first class and an *even* integer for the second class. Thus, the eigenfunctions for the two classes are, respectively,

$$\boxed{\psi_n(x) = B \cos \frac{n\pi x}{2a}, \qquad n = 1,3,5,\ldots}$$

$$\boxed{\psi_n(x) = A \sin \frac{n\pi x}{2a}, \qquad n = 2,4,6,\ldots}$$

In order to normalize the eigenfunctions, we apply the condition

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

This gives,

$$A^2\int_{-a}^{a} \sin^2\frac{n\pi x}{2a}\,dx = B^2\int_{-a}^{a} \cos^2\frac{n\pi x}{2a}\,dx = 1$$

Solving these integrals we obtain

$$\boxed{A = B = 1/\sqrt{a}} \qquad \ldots(4.19)$$

Thus, the **normalized eigenfunctions** for the two classes are, respectively,

$$\psi_n(x) = \frac{1}{\sqrt{a}}\cos\frac{n\pi x}{2a}, \qquad n = 1,3,5,\ldots \qquad \ldots(4.20)$$

$$\psi_n(x) = \frac{1}{\sqrt{a}}\sin\frac{n\pi x}{2a}, \qquad n = 2,4,6,\ldots \qquad \ldots(4.21)$$

From the equation (4.18), the only allowed values of k are,

$$k_n = \frac{n\pi}{2a} \qquad n = 1,2,3,\ldots \qquad \ldots(4.22)$$

From (4.15) and (4.22) the energy eigenvalues for both classes are,

$$\boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{8ma^2}, \qquad n = 1,2,3,\ldots} \qquad \ldots(4.23)$$

Conclusion: from equation (4.23)

- The energy is quantized.
- The integer n is called a quantum number.
- There is an infinite sequence of discrete energy levels.
- There is only one eigenfunction for each level.
- The energy levels are nondegenerate.
- The eigenfunctions $\psi_n(x)$ and $\psi_m(x)$ corresponding to different eigenvalues are orthogonal.

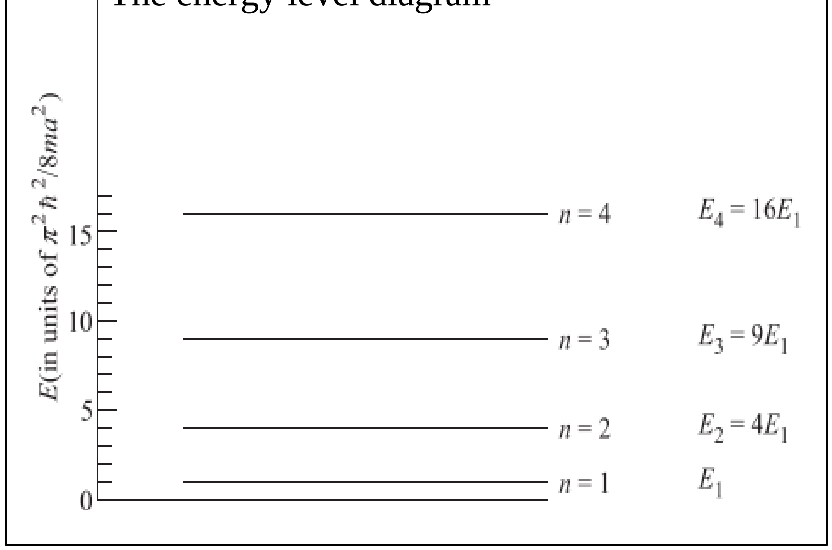
$$\int_{-a}^{a} \psi_m^*(x)\,\psi_n(x)\,dx = 0, \quad m \neq n$$

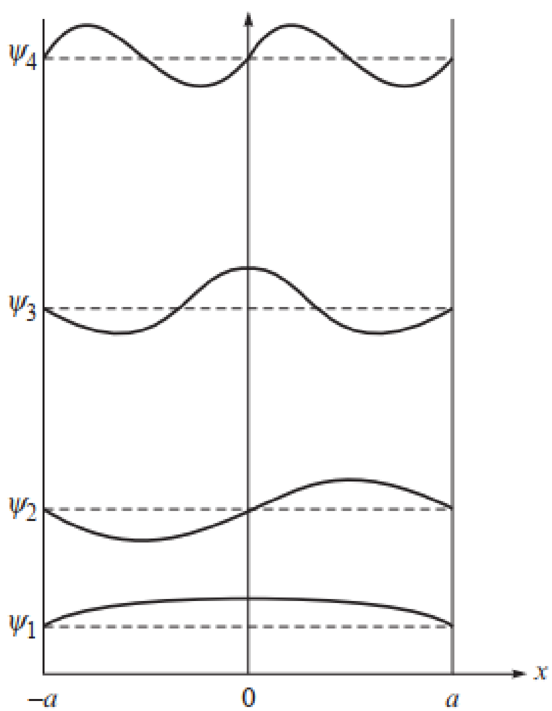
Combining orthogonality and normalization, we have the *orthonormality* condition:

…(4.24)

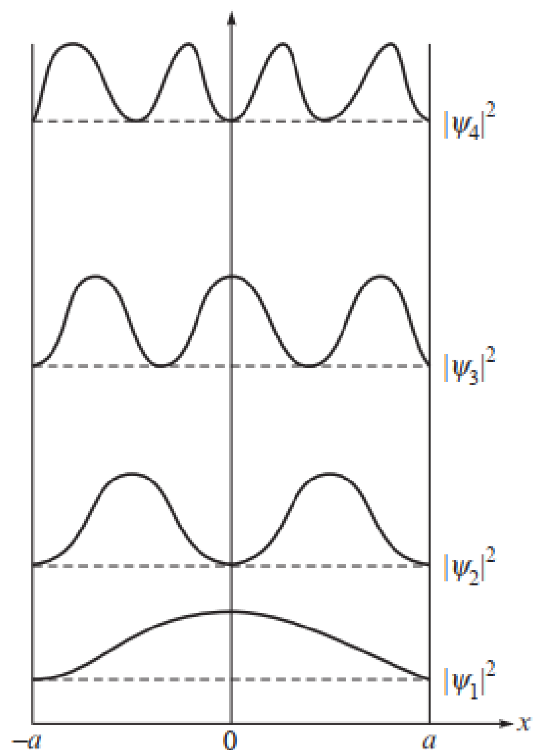
$$\int_{-a}^{a} \psi_m^*(x)\, \psi_n(x)\, dx = \delta mn$$

The energy level diagram





Wave function



Probability density

Note that the *n*th eigenfunction has (n – 1) nodes within the box. This follows from (4.20) and (4.21).

The position uncertainty is roughly given by $\Delta x \approx a$. Therefore, the minimum momentum uncertainty is $\Delta p \approx \hbar/a$. This leads to the minimum kinetic energy of order $\hbar^2/ma^2$. Equation (4.23) tells us that this agrees with the value of E_1.

It is important to note that *the lowest possible energy, also called the zero-point energy, is not zero*.

Why the lowest energy cannot be zero in a one-dimensional infinite square well?

By trapping the particle in a limited region, we get information about its position. Therefore, its momentum cannot be known with complete precision and this prevents any possibility of the particle being at rest. So, the lowest energy cannot be zero, and this fact is in agreement with the uncertainty principle.

Parity

The two classes of eigenfunctions that we have obtained have one important difference.

1- The eigenfunctions (4.20) belonging to the first class are ***even functions*** of x:

$$\psi_n(x) = \frac{1}{\sqrt{a}} \cos\left(\frac{n\pi}{2a} x\right)$$

$$\psi_n(-x) = \psi_n(x)$$

These functions are said to have ***even parity***.

2- The eigenfunctions (4.21) belonging to the second class are ***odd functions*** of x:

$$\psi_n(x) = \frac{1}{\sqrt{a}} \sin\left(\frac{n\pi}{2a} x\right)$$

$$\psi_n(-x) = -\psi_n(x)$$

These functions are said to have ***odd parity***.

This dividing of the eigenfunctions into even and odd types is a consequence of the fact that the potential is symmetric about the origin: $V(-x) = V(x)$.