Chapter 3

One-dimensional potentials

3.1 Introduction to Bound States :

If the motion of a particle is confined to a limited region of space by potential energy so that the particle can move back and forth in the region, then the particle is in a bound state. The simplest example of all motions in bound state is the motion of a particle in a one-dimensional box with zero potential energy and the potential energy is assumed to be infinite at the walls of the box.

The motion of a particle in three-dimensional box, one-dimensional box, motion of a simple harmonic oscillator, motion of a particle in a one-dimensional square well potential with ($E < V_0$), motion of a particle in a one-dimensional square well potential with ($E < V_0$), motion of a particle in one-dimensional (also in three-dimensional) potential well, motion of a particle in spherically symmetric potential, etc. are the common examples of bound state. Application of Schrodinger time-independent equal to such problems leads to discrete energy values of the particles.

Properties of 1-D bound states:

(i) Energy eigenstates corresponding to one dimensional bounds states are of discrete energy and non-degenerate in nature.

(ii) The wavefunction of a particle moving under a one dimensional symmetric potential should have a definite parity i.e. it will be either even or odd parity.

(iii) The wavefunction of a particle in the n^{th} state will have n-nodes if n = 0 corresponds to the ground state of the particle and will have n-1 nodes if n = 1 corresponds to the ground state of the particles.

3.2 One-dimensional infiitely deep potential well :

Consider a particle of mass 'm' and energy 'E' is moving along x-axis, in the region from $x = 0$ to $x = a$ under the following potential i.e.

$$V(x) = 0 \qquad 0 < x < a$$
$$= \infty \qquad \text{otherwise}$$

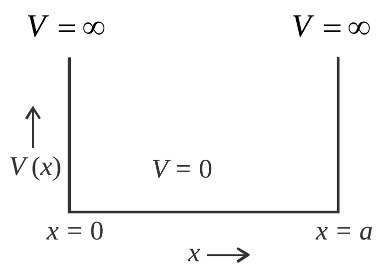


Figure : Schematic diagram of 1-D infinite potential well.

The particle experiences no force within the potential well but feels a sudden large force directed towards the origin as it reaches the points $x = 0, a$. Since, the potential is infinite outside, the particle cannot penetrate outside of the region $0 < x < a$ i.e. $\psi = 0$ for the particle outside the box.

According to 1-D time-independent Schrodinger equaion,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V\psi(x)=E\psi(x) \quad (1)$$

For the region $0<x<a$, the equation becomes,

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi \qquad \Rightarrow \frac{d^2\psi}{dx^2}+\frac{2mE}{\hbar^2}\psi=0$$

$$\Rightarrow \frac{d^2\psi}{dx^2}+k^2x=0 \text{ where } k^2=\frac{2mE}{\hbar^2} \quad (2)$$

Solution of eqn. (2) can be written as,

$$\psi(x)=A\sin kx+B\cos kx \quad (3)$$

Since, the particle remains confined within the box, then the probablity of finding the particle at $x = 0$ and $x = a$ must be zero.

Boundary conditions: $\psi(x)$ will be continuous at $x = 0$ and $x = a$

(i) Applying $\psi(x)\big|_{x=0}=0 \qquad \Rightarrow B=0$

(ii) Applying $\psi(x)\big|_{x=a}=0 \qquad \Rightarrow A\sin ka=0 \quad \Rightarrow ka=n\pi \quad \Rightarrow k=\frac{n\pi}{a}$

$$\Rightarrow \psi(x)=A\sin\left(\frac{n\pi x}{a}\right)(n=1,2,3,.........) \text{ for } 0<x<a \quad (4)$$

Note: If $n=0 \Rightarrow k=0 \Rightarrow E=0 \Rightarrow \psi(x)=0$ everywhere inside the box. Thereofore, there will be no admissible particle with zero energy within the box.

Normalization of the wave function:

The wave function ψ_n corresponding to n[th] quantum state is

$$\psi_n(x)=A\sin\frac{n\pi x}{a} \qquad 0\le x\le a$$
$$=0 \qquad \text{otherwise}$$

Since, the particle must be somewhere within the box, the total probability of finding the particle inside the box is unity i.e.

$$\int_0^a \psi_n^*(x)\psi_n(x)\,dx=1 \qquad \Rightarrow \int_0^a A^2\sin^2\frac{n\pi x}{a}dx=1$$

$$\Rightarrow A^2\int_0^a\frac{1}{2}\left[1-\cos\frac{2\pi nx}{a}\right]dx=1 \Rightarrow A=\sqrt{\frac{2}{a}}$$

Therefore, the normallized wave function will be

$$\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right) \qquad (n = 1, 2, 3, ...)$$

Energy eigenvalues:

We know that, $k=\sqrt{\frac{2mE}{\hbar^2}} \qquad \Rightarrow \frac{n^2\pi^2}{a^2}=\frac{2mE}{\hbar^2} \qquad \Rightarrow E_n=\frac{n^2\pi^2\hbar^2}{2ma^2} \qquad (n=1,2,3,.....)$

So, we get an infinite sequence of descrete energy levels that corresponds to all integral values of n, where n is called the quantum number representing the different states of the particle.

Ground state energy: $n=1 \quad \Rightarrow E_1 = \dfrac{\pi^2\hbar^2}{2ma^2}$

First excited state energy: $n=2 \quad \Rightarrow E_2 = \dfrac{4\pi^2\hbar^2}{2ma^2}$

In general, $\qquad E_n = n^2 E_1$

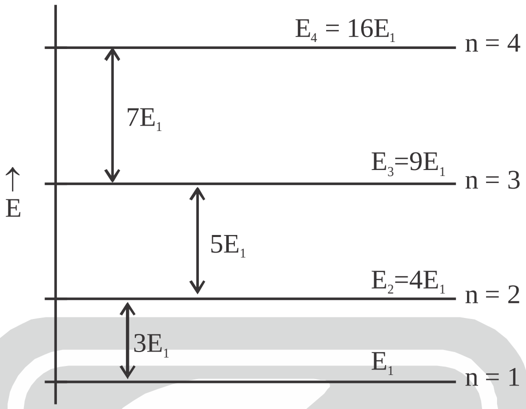


Figure : Energy levels of a particle in a 1-D infinite potential well

Difference between two consecutive energy levels

$$\Delta E_n = E_{n+1} - E_n = \frac{\pi^2\hbar^2}{2ma^2}\left[(n+1)^2 - n^2\right] = \frac{\pi^2\hbar^2}{2ma^2}(2n+1)$$

Spacing between two energy levels increases with 'n', decreases with size of the box 'a' and the mass of the particle 'm'. As $a \to \infty \Rightarrow \Delta E_n = 0$ i.e. the energy levels gets closer, forming a continuum of energy.

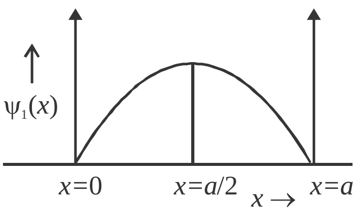
Momentum eigenvalues:

$$E_n = \frac{p_n^2}{2m} \qquad \Rightarrow P_n^2 = 2mE_n = 2m\frac{n^2\pi^2\hbar^2}{2ma^2} = \frac{n^2\pi^2\hbar^2}{a^2} \qquad \Rightarrow \quad P_n = \pm\frac{n\pi\hbar}{a}$$

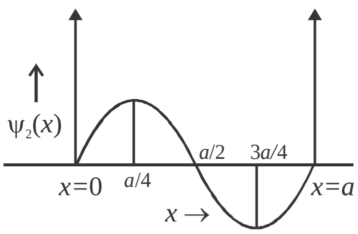
where '$\pm$' sign is due to the back and forth motion of the particle within the box.
Difference of momentum between two consecutive energy levels

$$\Delta P_n = P_{n+1} - P_n = \pm\left[\frac{(n+1)\pi\hbar}{a} - \frac{n\pi\hbar}{a}\right] = \pm\frac{\pi\hbar}{a}$$

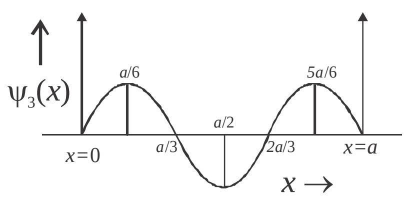
Various eigenstates of the particle inside a 1-D box :



Ground state



First excited state



Second excited state

Note: $\psi_n(x)$ has (n–1) nodes (excluding the boundary at $x = 0$ and $x = a$)

Variation of probability density corresponding to various eigenstates of the particle:

Probability density of finding the particle in the n^{th} quantum state is given by,

$$P_n(x) = |\psi_n(x)|^2 = \frac{2}{a}\sin^2\frac{n\pi x}{a}$$

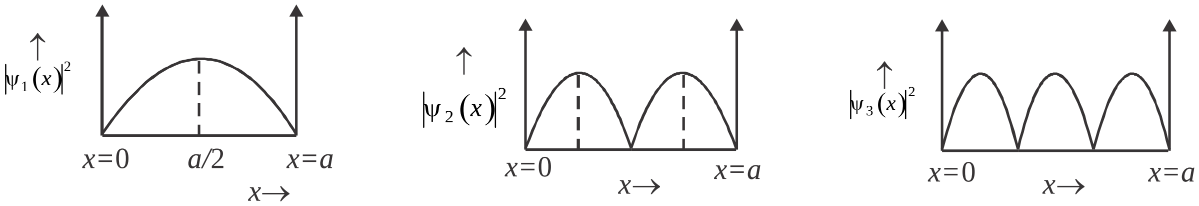


Figure : Variation of probability density corresponding to ground, first excited and second excited state respectively

Note:
(1) Probability of finding the particle in the left half of the well = Probability of finding the particle in the left half of the well = 1/2, for any state n.

(2) Probability of finding the particle between $\frac{a}{4} < x < \frac{3a}{4}$ is 1/2 for $n = 2, 4, 6, ...$

- The energy eigenfunctions of the particle confined in a 1-D box, satisfies the orthonormality condition i.e.

$$\int_0^a \psi_m^*(x)\psi_n(x)\,dx = \delta_{mn}$$

- As the energy eigenfunctions form a complete set, an arbitary function $\psi(x)$ (which is well behaved and satisfy the same boundary conditions) can be expanded in terms of these eigenfunctions as

$$\psi(x) = \sum_{n=1}^{\infty} c_n\psi_n(x) = \sum_{n=1}^{\infty} c_n\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$

Expectation values of $\hat{x}, \hat{p}_x, \hat{x}^2, \hat{p}_x^2$:

$$\langle x\rangle = \int_0^a \psi^* x\psi\,dx = \int_0^a \frac{2}{a}x\sin^2\left(\frac{n\pi x}{a}\right)dx = \frac{2}{a}\int_0^a \frac{x}{2}\left[1-\cos\frac{(2n\pi x)}{a}\right]dx$$

$$= \frac{2}{a}\frac{1}{2}\left[\frac{x^2}{2} - x\frac{\sin\frac{2\pi nx}{a}}{\frac{2\pi n}{a}} - \cos\frac{2n\pi x}{a}\right]_0^a = \frac{1}{a}\left[\frac{a^2}{2} - 1 + 1\right] = \frac{a}{2}$$

$$\langle p\rangle = \int_0^a \psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\psi\,dx = \frac{2}{a}(-i\hbar)\int_0^a \sin\left(\frac{n\pi x}{a}\right)\frac{n\pi}{a}\cos\left(\frac{n\pi x}{a}\right)dx = 0$$

Note: Expectation value of momentum for a real wave function is always zero.

$$\langle x^2\rangle = \int_0^a \psi^* x^2\,\psi\,dx = \frac{2}{a}\int_0^a x^2\sin^2\frac{n\pi x}{a}\,dx$$

$$=\frac{1}{a}\left[\left(\frac{x^3}{3}\right)_0^a-\left(x^2\frac{\sin 2n\pi x/a}{2n\pi/a}\right)_0^a+\int_0^a 2x.\sin\frac{2n\pi x/a}{2n\pi/a}dx\right]$$

$$=\frac{1}{a}\left[\frac{a^3}{3}-0+2\left\{-x\frac{\cos\frac{2n\pi x}{a}}{\left(\frac{2n\pi}{a}\right)^2}+\frac{\sin\frac{2n\pi x}{a}}{\left(\frac{2n\pi}{a}\right)^2}\right\}_0^a\right]=\frac{1}{a}\left[\frac{a^3}{3}-\frac{a^3}{2(n\pi)^2}\right]=\frac{a^2}{3}-\frac{a^2}{2n^2\pi^2}$$

$$\left\langle p^2\right\rangle=\frac{2}{a}\int_0^a\sin\left(\frac{n\pi x}{a}\right)\left(-\hbar^2\frac{\partial^2}{\partial x^2}\right)\sin\left(\frac{n\pi x}{a}\right)dx=\frac{2}{a}\left(-\hbar^2\right)\left(\frac{n\pi}{a}\right)^2(-1)\int_0^a\sin^2\left(\frac{n\pi x}{a}\right)dx$$

$$=\frac{2}{a}\left(-\hbar^2\right)\left(\frac{n\pi}{a}\right)^2(-1)\int_0^a\sin^2\left(\frac{n\pi x}{a}\right)dx$$

$$=\frac{n^2\pi^2\hbar^2}{a^2}\int_0^a\left[1-\cos\left(\frac{2n\pi x}{a}\right)\right]dx=\frac{n^2\pi^2\hbar^2}{a^3}\left[x-\frac{\sin\frac{2n\pi x}{a}}{\frac{2n\pi}{a}}\right]_0^a=\frac{n^2\pi^2\hbar^2}{a^2}$$

Uncertainity in the position of the particle is

$$\Delta x=\left[\left\langle x^2\right\rangle-\left\langle x\right\rangle^2\right]^{1/2}=\left[\frac{a^2}{3}-\frac{a^2}{2n^2\pi^2}-\frac{a^2}{4}\right]^{1/2}=\left[\frac{a^2}{12}-\frac{a^2}{2n^2\pi^2}\right]^{1/2}$$

Uncertainity in the momentum of the particle is

$$\Delta p=\left[\left\langle p^2\right\rangle-\left\langle p\right\rangle^2\right]^{1/2}=\frac{n\pi\hbar}{a}$$

Therefore, the uncertainity product $\Delta x\Delta p=n\pi\hbar\left[\frac{1}{12}-\frac{1}{2n^2\pi^2}\right]^{1/2}$

Example 1: A particle in a deep square well potential extending from $x=0$ to $x=L$ has a wave function $\psi(x)=\frac{1}{\sqrt{5}}\left[|\phi_1\rangle+2|\phi_2\rangle\right]$ where $|\phi_1\rangle$ and $|\phi_2\rangle$ denote the ground state and the first excited state wave functions. Find the expectation of '*x*' in this state.

Soln. $\langle x\rangle=\langle\psi|x|\psi\rangle=\frac{1}{\sqrt{5}}\left(\langle\phi_1|+2\langle\phi_2|\right)x\frac{1}{\sqrt{5}}\left(|\phi_1\rangle+2|\phi_2\rangle\right)$

$$=\frac{1}{5}\left[\langle\phi_1|x|\phi_1\rangle+2\langle\phi_1|x|\phi_2\rangle+2\langle\phi_2|x|\phi_1\rangle+4\langle\phi_2|x|\phi_2\rangle\right]$$

Now, $\langle\phi_1|x|\phi_2\rangle=\int_0^L\left(\sqrt{\frac{2}{L}}\sin\frac{\pi x}{L}\right)x\left(\sqrt{\frac{2}{L}}\sin\frac{2\pi x}{L}\right)dx$

$$=\frac{1}{L}\int_0^L x\left(\cos\frac{\pi x}{L}-\cos\frac{3\pi x}{L}\right)dx=\frac{1}{L}\left(-\frac{2L^2}{\pi^2}+\frac{2L^2}{9\pi^2}\right)=-\frac{16L}{9\pi^2}$$

Therefore, $\langle x\rangle = \frac{1}{5}\left[\frac{L}{2} - \frac{32L}{9\pi^2} - \frac{32L}{9\pi^2} + 4.\frac{L}{2}\right] = \frac{L}{2} - \frac{64L}{45\pi^2}$

Example 2: Calculate $\langle p_x\rangle$ for $\psi(x) = \frac{1}{\sqrt{2}}\left(|\phi_1\rangle + |\phi_2\rangle\right)$ where $|\phi_1\rangle$ and $|\phi_2\rangle$ are the ground state and the first excited state wave functions of a particle in a deep square well potential.

Soln. $\langle p_x\rangle = \langle\psi|p_x|\psi\rangle = \frac{1}{2}\left[\langle\phi_1|p_x|\phi_1\rangle + \langle\phi_2|p_x|\phi_1\rangle + \langle\phi_1|p_x|\phi_2\rangle + \langle\phi_2|p_x|\phi_2\rangle\right]$

$$\langle\phi_2|p_x|\phi_1\rangle = \int_{-\infty}^{\infty}\phi_2^*\left(-i\hbar\frac{d}{dx}\right)\phi_1(x)\,dx = \frac{2}{L}(-i\hbar)\int_0^L \sin\frac{2\pi x}{L}\frac{d}{dx}\left(\sin\frac{\pi x}{L}\right)dx$$

$$= \frac{-i\hbar\pi}{L^2}\int_0^L 2\sin\frac{2\pi x}{L}\cos\frac{\pi x}{L}\,dx = \frac{-i\hbar\pi}{L^2}\int_0^L\left(\sin\frac{3\pi x}{L} + \sin\frac{\pi x}{L}\right)dx = -\frac{8i\hbar}{3L}$$

Similarly, $\langle\phi_1|p_x|\phi_2\rangle = \frac{8i\hbar}{3L}$

Therefore, $\langle p_x\rangle = 0$

Example 3: The wave function of a particle in a deep square well potential extending from $x = 0$ to $x = L$ is $\psi(x) = \sqrt{30}\;x(x-L)/L^i$ (a) Find the value of i, (b) Find the average value of 'x' in this state.

Soln. (a) Any wave function of a particle in one dimension has the dimensions of $\frac{1}{\sqrt{L}}$. Thus $i = \frac{5}{2}$

(b) $\langle x\rangle = \int_{-\infty}^{\infty}\psi^*(x)\,x\psi(x)\,dx = \frac{30}{L^5}\int_0^L x^3(x-L)^2\,dx = \frac{L}{2}$

Example 4: A particle is in the ground state of a deep square well in the range $0 < x < L$. Suddenly the wall $x = L$ of the well is shifted to $x = 2L$, so as to make it a deep square well in the range $0 < x < 2L$. Immediately after this, the energy of the particle is measured. What will be the probability of getting the energy as the new ground state energy?

Soln. The wave function just before the shifting of the wall is

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\frac{\pi x}{L} \text{ for } 0 < x < L$$
$$= 0 \qquad \text{otherwise}$$

This is the energy eigenfunction corresponding to the ground state in the original well. When the wall is shifted, the new ground state wave function becomes,

$$\phi(x) = \sqrt{\frac{2}{2L}}\sin\frac{\pi x}{2L} \text{ for } 0 < x < 2L$$
$$= 0 \qquad \text{otherwise}$$

The probability of getting the ground state energy in measurements is $|\langle\phi|\psi\rangle|^2$