Continuity of wavefunction

Time-independent Schrödinger equation:

\[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + V(x)\psi(x) = E\psi(x)\]

1. The wave function has to be continuous at all points, no exception.

2. The first derivative of the wave function \(\frac{\partial}{\partial x} \psi(x)\) is continuous, only if \(V(x)\) is finite.

3. If \(V(x)\) is not finite at \(x=a\):

\[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x)\psi(x) = E\psi(x)\]

\[\Rightarrow -\frac{\hbar^2}{2m} \int_a^{a+\epsilon} \frac{d}{dx} \psi(x) + \int_a^{a+\epsilon} V(x)\psi(x)dx = E\int_a^{a+\epsilon} \psi(x)dx\]

\[\Rightarrow -\frac{\hbar^2}{2m} \left[ \psi'(a + \epsilon) - \psi'(a - \epsilon) \right] + \int_a^{a+\epsilon} V(x)\psi(a)dx = 0\]

\[\Rightarrow \left[ \psi'(a + \epsilon) - \psi'(a - \epsilon) \right] = \frac{4m\psi(a)}{\hbar^2} \int_a^{a+\epsilon} V(x)dx\]
1. Particle in a box is essentially a free particle, confined to a finite region (e.g. \([0,a]\)) in space.

2. Though a simple model, it finds many real life examples, like electrons inside a good conductor.

3. The Problem:
Particle in a box II

\[ V(x) = \begin{cases} \infty & \text{if } a < x \\ 0 & \text{if } 0 \leq x \leq a \\ \infty & \text{if } x < 0 \end{cases} \]

Schrödinger equation:

In region I and III:

\[ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V \psi = E \psi \Rightarrow \frac{\partial^2 \psi}{\partial x^2} = \frac{2m}{\hbar^2} (V - E) \psi \]

\[ \Rightarrow \psi(x) = Ae^{\sqrt{\frac{2m(V-E)}{\hbar^2} x}} + Be^{-\sqrt{\frac{2m(V-E)}{\hbar^2} x}} \]

\[ \Rightarrow \psi(x) = \begin{cases} Ae^{\sqrt{\frac{2m(V-E)}{\hbar^2} x}} & \text{(for region I, } x < 0) \\ -Be^{-\sqrt{\frac{2m(V-E)}{\hbar^2} x}} & \text{(for region II, } x > a) \end{cases} \]

But \( V(x) = \infty \), \( \therefore \psi(x) = 0 \) for both cases.
Particle in a box III

Now work on region II with $V(x) = 0$

$$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + V \psi = E \psi \Rightarrow \frac{\partial^2}{\partial x^2} \psi = -\frac{2m}{\hbar^2} E \psi \quad (\because V = 0)$$

$$\Rightarrow \psi(x) = Ae^{i\frac{2mE}{\hbar^2} x} + Be^{-i\frac{2mE}{\hbar^2} x}$$

Let $k = \sqrt{\frac{2mE}{\hbar^2}}$

Continuity at $x = 0$:
$$\psi_1(0) = \psi_\| (0) \Rightarrow 0 = A + B \Rightarrow B = -A$$

Continuity at $x = a$:
$$\psi_1(a) = \psi_\| (a) \Rightarrow 0 = Ae^{ika} + Be^{-ika}$$

$$\Rightarrow 0 = Ae^{ika} - Ae^{-ika} \quad (\because B = -A)$$

$$\Rightarrow \sin ka = 0$$

$$\Rightarrow ka = n\pi \quad n = 1, 2, 3, ..., 4$$

$$\Rightarrow k_n = \frac{n\pi}{a}$$

or
$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2m} \left( \frac{n\pi}{a} \right)^2$$

$$\psi_n(x) = A \sin \frac{n\pi}{a} x$$
Now work on region II with $V(x) = 0$

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + V \psi = E \psi \Rightarrow \frac{\partial^2}{\partial x^2} \psi = -\frac{2m}{\hbar^2} E \psi$$ \hspace{1cm} (\because V = 0)

$$\Rightarrow \psi(x) = A e^{i\frac{2mE}{\hbar^2} x} + B e^{-i\frac{2mE}{\hbar^2} x}$$

Let $k = \sqrt{\frac{2mE}{\hbar^2}}$

Continuity at $x = 0$:

$$\psi_1(0) = \psi_2(0) \Rightarrow 0 = A + B \Rightarrow B = -A$$

Continuity at $x = a$:

$$\psi_1(a) = \psi_2(a) \Rightarrow 0 = A e^{ika} + B e^{-ika}$$

$$\Rightarrow 0 = A e^{ika} - A e^{-ika} \hspace{1cm} (\because B = -A)$$

$$\Rightarrow A \sin ka = 0$$

$$\Rightarrow ka = n\pi \hspace{1cm} n = 1, 2, 3, ..., 4$$

$$\Rightarrow k_n = \frac{n\pi}{a}$$

or

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2}{2m} \left( \frac{n\pi}{a} \right)^2$$

$$\psi_n(x) = A \sin \frac{n\pi x}{a}$$

1. $n \neq 0$ because $\psi(x)$ will be trivial (i.e. $\psi(x) = 0$) if $n = 0$.

2. Take only positive $n$ because negative $n$ represents the same wave function.

Some remarks

$E_1$ is the lowest energy state, so $n = 1$ is the ground state.

We require $\psi$ to be continuous at these two points, but not the first derivative $\psi'$, because $V(x)$ is not continuous at these two points.

We require $V(x)$ to be continuous at these two points, but not the first derivative $\psi'$, because $V(x)$ is not continuous at these two points.