

Q: What are the main mathematical formulas involved?

A: Here are the main mathematical formulas involved in solving the infinite quantum well with the usual boundary conditions ($\psi(0) = 0$ and $\psi(a) = 0$):

1. Time-independent Schrödinger Equation (SE):

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

- \hbar (pronounced "h-bar") is the reduced Planck constant ($\approx 1.054 \times 10^{-34}$ J s)
- m is the mass of the particle
- $\frac{d^2\psi}{dx^2}$ is the second derivative of the wave function (ψ) with respect to position (x)
- $V(x)$ is the potential energy function (0 inside the well, infinite outside)
- E is the total energy of the particle

2. Separation of Variables:

We assume the wave function can be written as a product of separate functions for the spatial ($X(x)$) and time-dependent ($T(t)$) parts (for generality, here):

$$\psi(x, t) = X(x) \cdot T(t) \quad (2)$$

In the case of the infinite well, we focus on time-independent solutions, so $T(t)$ becomes a constant. This leaves us with:

$$\psi(x) = X(x) \quad (3)$$

3. Solution for Spatial Part ($X(x)$):

Since $V(x) = 0$ inside the well, the ODE for the spatial part becomes:

$$-\frac{\hbar^2}{2m} \frac{d^2X}{dx^2} = EX \quad (4)$$

This has solutions of the form:

$$X(x) = A \sin(kx) + B \cos(kx) \quad (5)$$

- A and B are constants determined by the boundary conditions
- k is the wave number (related to the wavelength λ by $k = \frac{2\pi}{\lambda}$)

4. Applying Boundary Conditions:

The common boundary conditions for the infinite well are:

- $\psi(0) = 0$ (wave function is zero at $x = 0$)
- $\psi(a) = 0$ (wave function is zero at $x = a$, well width)

Applying these conditions leads to:

$$A \sin(0) + B \cos(0) = 0 \quad \text{implies} \quad B = 0 \quad (\text{since } \cos(0) = 1) \quad (6)$$

$$A \sin(ka) = 0 \quad \text{implies} \quad \sin(ka) = 0 \quad (A \neq 0 \text{ for non-zero wave function}) \quad (7)$$

5. Quantization of Energy Levels:

For $\sin(ka) = 0$, ka must be an integer multiple of π :

(continued)

$$ka = n\pi \quad \text{where } n \text{ is an integer}(0, 1, 2, \dots) \quad (8)$$

Relating k to λ (wavelength), we get:

$$n\lambda = 2a \quad \text{where } n \text{ is an integer}(1, 2, 3, \dots) \quad (9)$$

This equation shows that only specific wavelengths (and their corresponding wave functions) are allowed, leading to quantized energy levels.

Additional Formulas:

- Relationship between wave number (k) and momentum (p): $p = \hbar k$
- Energy-momentum relationship (for non-relativistic particles): $E = \frac{p^2}{2m}$