Infinite Square Well
Infinite Square Well

- We can use the time independent Schrödinger equation
- Outside the well
  \[ \psi(x) = 0 \]
- Inside the well
  \[ -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \]
  \[ \frac{d^2\psi}{dx^2} = -k^2\psi \text{ where } k = \frac{\sqrt{2mE}}{\hbar} \]
  Try solutions \[ \psi(x) = A\sin kx + B\cos kx \]
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- Typically the constants are determined by the boundary conditions (and normalization)
- In this case the boundary conditions needed to ensure continuity of $\psi$ are

$$\psi(0) = \psi(L) = 0$$

- Thus

Since $\psi(0) = A \sin 0 + B \cos 0 = 0, \ B = 0$
Since $\psi(L) = A \sin kL = 0$, then $kL = 0, \pm \pi, \pm 2\pi, ...$

$k$ cannot be 0, so solutions have $k_n = \frac{n\pi}{L}, \ n = 1,2,3,...$

$$E_n = \frac{\hbar^2 k_n^2}{2m} = n^2 \frac{\pi^2 \hbar^2}{2mL^2}; \ \text{energy is quantized!!}$$
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What about the normalization of $\psi_n$?

$$\int_0^L dx |\psi_n|^2 = \int_0^L dx |A|^2 \sin^2 kx$$

$$= |A|^2 \left( \frac{x}{2} - \frac{\sin 2kx}{4k} \right)_{x=0}^{x=L}$$

$$= |A|^2 \frac{L}{2} = 1$$

thus $A = \sqrt{\frac{2}{L}}$

so the solutions are $\psi_n = \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi x}{L} \right)$
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\[ \psi_1, \psi_2, \psi_3 \]

\[ |\psi_1|^2, |\psi_2|^2, |\psi_3|^2 \]

\[ 0 \quad L \quad 0 \quad L \]

\[ \rightarrow \text{Energy} \]

\[ 25 \ E_1, 16 \ E_1, 9 \ E_1, 4 \ E_1, E_1 \]
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Comments

- $\Psi$ and $d\Psi/dx$ must be continuous at all boundaries except where the potential is infinite.
- As $n$ increases, $\lambda$ decreases, $E$ increases.

\[
\begin{align*}
k_n &= \frac{n\pi}{L} = \frac{2\pi}{\lambda} \\
\lambda &= \frac{2L}{n}
\end{align*}
\]

- Number of nodes in the $n$’th eigenfunction = $n-1$
- The eigenfunctions are alternating even and odd functions about the symmetry axis.
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Comments

- Energy states are

\[ E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} = n^2 E_1 \]

- The lowest energy bound state has non-zero energy (zero point energy)
- The excitation/de-excitation energy is \( E_{\text{final}} - E_{\text{initial}} \)
Infinite Square Well

Comments

- The eigenfunctions $\psi$ are mutually orthogonal (recall postulate #4)

$$\int_0^a dx \psi_i^* \psi_j = \frac{2}{L} \int_0^L dx \sin \frac{i \pi x}{L} \sin \frac{j \pi x}{L} = \delta_{ij}$$

- Please look at the calculation of expectation values in Thornton-Rex (Example 6.8)
  - What would you expect for $<x>$?, $<p>$?, $<p^2>$?
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Comments

- What are the possible momentum states?

Look at the eigenvalue equation

$$-i\hbar \frac{\partial f_n(x)}{\partial x} = p_n f_n(x) = \pm \hbar k_n f_n(x)$$

Solutions are $f_n(x) = Ae^{\pm ik_n x}$

Makes sense since our energy eigenfunctions can be written as

$$\sin k_n x = \frac{1}{2i} \left( e^{ik_n x} - e^{-ik_n x} \right)$$
The stationary states of the infinite well are

\[ \Psi_n(x, t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n \pi x}{L}\right) e^{-iE_n t / \hbar} \text{ where } E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \]

A general solution to the time dependent Schrödinger equation (see postulate #4) is

\[ \Psi(x, t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{L}} \sin\left(\frac{n \pi x}{L}\right) e^{-iE_n t / \hbar} \]

Given an initial condition the coefficients \( c_n \) can be determined

\[ c_n = \sqrt{\frac{2}{L}} \int_0^L dx \sin\left(\frac{n \pi x}{L}\right) \Psi(x, 0) \]
Problem

- Let
  \[ \psi(x) = \frac{1}{\sqrt{5L}} \sin \frac{\pi x}{L} + \frac{3}{\sqrt{5L}} \sin \frac{3\pi x}{L} \]

- What are the possible results of an energy measurement?
- What are the probabilities?
- What is the form of the wave function immediately after an energy measurement?
Problem

- What is the ratio of probabilities for the particle to be at $x=L/3$ to $x=L/4$?
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Problem

Let

$$\Psi(x,0) = A\{\psi_1(x) + \psi_2(x)\}$$

- Normalize $\psi$
- Calculate $|\psi(x,t)|^2$
- Calculate $\langle x \rangle$
- Calculate $\langle H \rangle$
Infinite Square Well

➢ Note to myself
  - www.phys.uri.edu/~yoon/deepwellmain.html
In three dimensions, Schrodinger’s equation becomes

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}, \hat{p}_y = -i\hbar \frac{\partial}{\partial y}, \hat{p}_z = -i\hbar \frac{\partial}{\partial z}$$

$$\hat{p} = -i\hbar \vec{\nabla} \text{ and } \hat{p}^2 = -\hbar^2 \nabla^2$$

where $$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V \Psi$$

and $$\Psi(x, t) \rightarrow \Psi(\vec{r}, t)$$
Infinite Square Well

- Free particle in a box
  - An infinite well in 3 dimensions

\[ -\frac{\hbar^2}{2m} \nabla^2 \psi = E \psi \quad (1) \]

Try \( \psi = A \sin k_1 x \sin k_2 y \sin k_3 z \)

Boundary conditions give

\[ k_1 = \frac{n_1 \pi}{L_1} \quad k_2 = \frac{n_2 \pi}{L_2} \quad k_3 = \frac{n_3 \pi}{L_3} \]

Since \( \frac{\partial^2 \psi}{\partial x^2} = -k_1^2 \psi \quad (1) \) becomes

\[ \frac{\hbar^2}{2m} \left( k_1^2 + k_2^2 + k_3^2 \right) \psi = E \psi \]
Infinite Square Well

- Free particle in box
  - Continuing

\[ E = \frac{\hbar^2}{2m} \left( k_1^2 + k_2^2 + k_3^2 \right) \]

\[ E = \frac{\pi^2 \hbar^2}{2m} \left( \frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2} \right) \]

for \( L_1 = L_2 = L_3 = L \)

\[ E = \frac{\pi^2 \hbar^2}{2mL^2} \left( n_1^2 + n_2^2 + n_3^2 \right) \]

- States with different quantum numbers but the same energy are called degenerate
Quantum Dots

- Quantum dots are semiconductor nanostructures that confine 1-1000 conduction electrons in all three dimensions (just like the particle in a box)
Quantum Dots

- CdSe quantum dots in solution under exposure to UV light
- Which sample has the largest quantum dots?
Quantum Corrals

- Electron in a corral of iron atoms on copper
Quantum Corrals

- Electron in a corral of iron atoms
Quantum Corrals