Particle in an infinite square well (Particle in 1D box)

The potential in the form of a square well serves as a good model/approximation for more realistic interaction. The importance of the square well potential also stems from the fact that this potential allows an analytic solution. There are only a few cases/potentials for which the 1D Schrödinger equation can be solved analytically and the solutions can be written in a simple compact form.

The square well potential has the following simple form:

\[ V(x) = \begin{cases} V_0, & 0 \leq x \leq a \\ 0, & \text{otherwise} \end{cases} \]

The time-independent Schrödinger equation is

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

Our task is to find the allowed values of \( E \) and the corresponding wave functions, \( \psi \). For simplicity we will be concerned with the limiting case when \( V_0 \to \infty \). In this case
\( \psi(x) \) must vanish everywhere outside \( [0,a] \) interval. That is we must require that

\[
\psi(0) = \psi(a) = 0
\]

Within interval \( [0,a] \) the Schrödinger equation (SE) takes a particularly simple form in this interval:

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

or

\[
\psi'' + \kappa^2 \psi = 0 \quad \text{where} \quad \kappa = \sqrt{\frac{\sqrt{2mE}}{\hbar^2}}
\]

The latter is a well known harmonic oscillator equation. The general solution of this equation is

\[
\psi(x) = Fe^{i\kappa x} + Ge^{-i\kappa x} = C \cos(\kappa x + \phi) = A \sin \kappa x + B \cos \kappa x
\]

Where \( F, G, C, \phi, A, \) and \( B \) are some integration constants. We will stick to the last form as it is more convenient for our purposes:

\[
\psi(x) = A \sin \kappa x + B \cos \kappa x
\]

Since \( \psi(0) = 0 \) we must set \( B \) to zero. Then

\[
\psi(a) = A \sin ka = 0 \implies ka = n\pi \quad n = 0, 1, 2, \ldots
\]

If \( n = 0 \) then we are left with a trivial solution \( \psi = 0 \), so we discard this case as physically meaningless. For \( \kappa \) we have the relation
\[ k = \frac{n\pi}{a} \quad n = 1, 2, 3 \]

If only certain \( k_n \) values are allowed then the energy is also "quantized":

\[ E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2ma^2} \]

Now let us turn our attention to the wave function

\[ \psi_n(x) = A_n \sin \left( \frac{n\pi x}{a} \right) \]

To find \( A_n \) we use the normalization condition:

\[
1 = \int_{-\infty}^{+\infty} |\psi(x)|^2 \, dx = \int_{0}^{a} |A_n|^2 \sin^2 (k_n x) \, dx = \\
= \int_{0}^{a} |A_n|^2 \left( 1 - \cos \left[ 2k_n x \right] \right) \, dx = |A_n|^2 \frac{a}{2}
\]

So

\[ A_n = \sqrt{\frac{2}{a}} \]

It turns out that \( A_n \) is independent of \( n \) (usually the normalization constant for the solution of the SE does depend on the quantum number \( n \)).

There are important properties of eigenfunctions \( \psi_n \) that should be outlined. Some of these properties are general and hold for any form of potential \( V(x) \):

1) \( \psi_n(x) \) are either symmetric or antisymmetric with respect to the middle point of the potential well. This results from the symmetry of \( V(x) \).
2) $\psi_{n+1}$ has one more node than $\psi_n$. This is related to property 3).

3) Functions $\psi_n$ and $\psi_m$ are orthogonal when $n \neq m$. Indeed,

$$\int_0^a \psi_n^*(x) \psi_m(x) \, dx = \frac{2}{a} \int_0^a \sin \left( \frac{m \pi x}{a} \right) \sin \left( \frac{n \pi x}{a} \right) \, dx =$$

$$= \frac{2}{a} \int_0^a \frac{1}{2} \left[ \cos \left( \frac{m-n \pi x}{a} \right) - \cos \left( \frac{m+n \pi x}{a} \right) \right] \, dx =$$

$$= \left[ \frac{1}{(m-n)\pi} \sin \left( \frac{m-n \pi x}{a} \right) - \frac{1}{(m+n)\pi} \sin \left( \frac{m+n \pi x}{a} \right) \right]_0^a = 0 \text{ if } m \neq n.$$

For $m = n$ we get 1. Therefore we can write

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

4) Set of functions $\psi_n$ is called complete because any function $f(x)$ (at least those that have proper physical behavior and are relevant to quantum mechanics) can be expanded as a linear combination in terms of $\psi_n$.

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

In our particular case of the infinite square well potential we basically get a Fourier series coefficients $c_n$ are found as follows:

$$c_n = \int_0^a \psi_n^*(x) f(x) \, dx$$
If we need to write an arbitrary time-dependent solution to the SE we must specify the initial state, \( \psi(x, t=0) \). Then

\[
C_h = \sqrt{\frac{2}{a}} \int_0^a \sin \left( \frac{\pi n}{a} x \right) \psi(x, 0) \, dx
\]

and

\[
\psi(x, t) = \sum_{h=1}^{\infty} C_h \sqrt{\frac{2}{a}} \sin \left( \frac{\pi h}{a} x \right) e^{-\frac{i E_h t}{\hbar}}
\]

5) \[ \sum_{h=1}^{\infty} |C_h|^2 = 1 \quad \text{Indeed,} \]

\[
1 = \int |\psi(x, 0)|^2 \, dx = \int (\sum_{w=1}^{\infty} c_w^* \psi_w(x))(\sum_{h=1}^{\infty} c_h \psi_h(x)) \, dx = \\
= \sum_{h, k=1}^{\infty} c_w^* c_h \int \psi_w^*(x) \psi_h(x) \, dx = \sum_{w, h=1}^{\infty} c_w^* c_h \delta_{wh} = \sum_{h=1}^{\infty} |C_h|^2
\]
Wave functions and probability densities for the lowest four states of a particle in an infinite potential well.