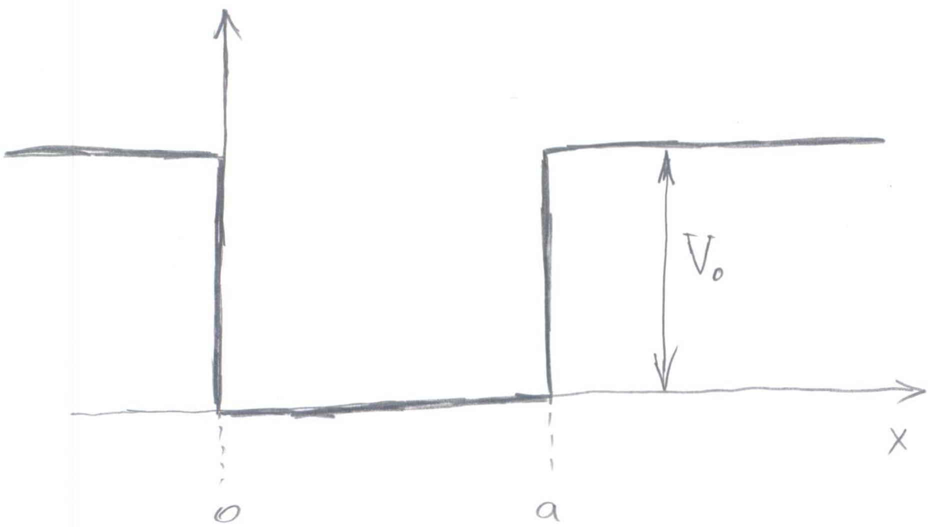
Particle in an infinite square well (particle in 1D box)

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

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

Our task is to find the allowed values of E and the corresponding wave functions, ψ.

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

$$\psi'' + k^2\psi = 0 \qquad \text{where} \qquad k \equiv \sqrt{\frac{2mE}{\hbar^2}}$$

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

$$\psi(x) = Fe^{ikx} + Ge^{-ikx} = C\cos(kx+\alpha) =$$

$$= A\sin kx + B\cos kx$$

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

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

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

$$\psi(a) = A\sin ka = 0 \Rightarrow ka = n\pi \qquad n = 0, 1, 2, \ldots$$

If $n=0$ then we are left with a trivial solution $\psi = 0$, so we discard this case as physically meaningless. For k we have the relation

$$k = \frac{n\pi}{a} \qquad n = 1, 2, 3$$

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

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

Now let us turn our attention to the wave function

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

To find A_n we use the normalization condition:

$$1 = \int_{-\infty}^{+\infty} |\psi(x)|^2 dx = \int_0^a |A_n|^2 \sin^2(k_n x)\, dx =$$

$$= \int_0^a |A_n|^2 \left(\frac{1 - \cos[2k_n x]}{2}\right) dx = |A_n|^2 \frac{a}{2}$$

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 ψ_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) ψ_{n+1} has one more node than ψ_n. This is related to property 3)

3) Functions ψ_n and ψ_m are orthogonal when $n \neq m$. Indeed,

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

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

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

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

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

4) Set of functions ψ_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 ψ_n:

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

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

$$c_n = \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a}x\right) \Psi(x,0)\, dx$$

and

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

5) $\sum_{n=1}^{\infty} |c_n|^2 = 1$ Indeed,

$$1 = \int |\Psi(x,0)|^2 dx = \int \left(\sum_{m=1}^{\infty} c_m^* \psi_m(x)\right)\left(\sum_{n=1}^{\infty} c_n \psi_n(x)\right) dx =$$

$$= \sum_{m,n=1}^{\infty} c_m^* c_n \int \psi_m^*(x)\, \psi_n(x)\, dx = \sum_{m,n=1}^{\infty} c_m^* c_n \delta_{mn} = \sum_{n=1}^{\infty} |c_n|^2$$