Mathematics of Wave Functions for Particles in 1-D

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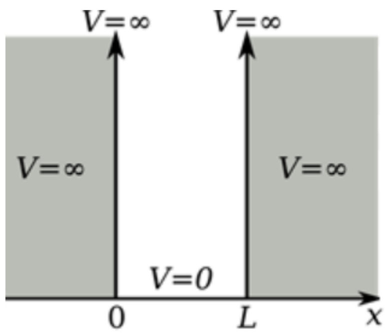
Here I will be going over the mathematics to derive the wave functions and the discrete energy levels which we will need to implement them in Python and have the program display the wave functions.

The time-independent Schrodinger equation over the one dimensional real vector space $\mathbb{R}$ (i.e. the real numbers) is given as

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0$$

where ψ is the wave function dependent on $x \in \mathbb{R}$, otherwise known as the eigenfunction, E is the total energy otherwise known as the eigenvalue, and V is the potential energy.

For simplicity, we shall assume the particle is in an infinite potential box.



At the barrier, the particle does not exist since $V = \infty$ which means

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - \infty)\psi = 0$$

For the particle's position within the barrier, i.e. for $0 < x < L,\ x \in \mathbb{R}$, then

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E - 0)\psi = 0$$

The above equation can be isolated for $E\psi$ giving us

$$\left(-\frac{h^2}{8\pi^2 m}\right)\frac{\partial^2 \psi}{\partial x^2} = E\psi \ \ (1)$$

For this type of second order differential equation, we get that the general solution is

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

for some constants $A, B, k \in \mathbb{R}$.

As established above, for $x = 0, L$, the probability amplitude for this particle should be 0, meaning we must have that $\psi(0) = 0$. This further means that $\psi(0) = A(0) + B(1) = B = 0$ so the wave function turns out to just be

$$\psi(x) = A\sin(kx)$$

for $0 \leq x \leq L$. Now all that's left is to find the constants $A, k \in \mathbb{R}$.

Differentiating the wave function w.r.t x, we get

$$\frac{\partial \psi}{\partial x} = kA\cos(kx)$$

$$\frac{\partial^2 \psi}{\partial x^2} = -k^2 A\sin(kx) = -k^2\psi(x)$$

Now we put this into equation (1) to get

$$\frac{h^2}{8\pi^2 m} \cdot k^2\psi(x) = E\psi(x)$$

$$k = \sqrt{\frac{8\pi^2 mE}{h^2}}$$

With this into the wave function ψ, we get

$$\psi(x) = A\sin\left(\sqrt{\frac{8\pi^2 mE}{h^2}}x\right)$$

Now we can apply further boundary condition, namely that $\psi(x) = 0$ for $x = 0, L.$

$$\psi(L) = A\sin\left(\sqrt{\frac{8\pi^2 mE}{h^2}}L\right) = 0$$

$$\sqrt{\frac{8\pi^2 mE}{h^2}}L = n\pi\ , \ \ (n \in \{1, 2, 3, \cdots\}) \ \ (2)$$

$$k = \sqrt{\frac{8\pi^2 mE}{h^2}} = \frac{n\pi}{L}, \ \ (n \in \{1, 2, 3, \cdots\})$$

Thus, we have that

$$\psi(x) = A\sin\left(\frac{n\pi}{L}x\right) \ \ \text{for } x \in [0, L]$$

To find A is the next step, which we can do so from the normalization principle, namely that the sum of all the probabilities must be 1. Mathematically, this is equivalent to saying

$$\int_0^L |\psi(x)|^2 dx = 1$$

where the probability of a particle appearing at some position x is given by $P(x)\delta x = |\psi(x)|^2 \delta x.$

Now to solve for this integral,

$$A^2 \int_0^L \sin^2\left(\frac{n\pi}{L}x\right) dx = 1$$

We can do so by making the substitution of $u = n\pi x/L \implies du/dx = n\pi/L$ which transforms the integral $\int \sin^2(n\pi x/L) \to (L/n\pi)\int \sin^2(u)$ where the latter integral can be solves through the use of integration by parts or applying the reduction formula with $m = 2$ (where m is the exponent on $\sin$).

Thus, applying the bounds and taking the definitive integral, we get the overall equation to be

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

which means

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \text{ for } x \in [0, L]$$

Also, from equation (2), we can solve for E by squaring both sides and rearranging for this quantity to get that the total energy is indeed discrete (i.e. quantized) with the precise mathematical form being

$$E_n = \frac{n^2 h^2}{8mL^2} \text{ for } n \in \{1, 2, 3, \cdots\}$$

We now have the formation on the structure of both the wave function $\psi(x)$ as well as the total energy E_n of a particle in a box, thus allowing us to proceed to the next step which is the implementation of Python scripting and algorithms to visualize the wave functions.