

Functions for potentials:

Step potential

$$\begin{aligned}\text{step}(a) &= 0 \text{ for } x < a \\ &= 1 \text{ for } x > a\end{aligned}$$

Barrier

$$\begin{aligned}\text{box}(a,b) &= 0 \text{ for } x < a \text{ \& } x > b \\ &= 1 \text{ for } a < x < b\end{aligned}$$

Finite Wells:

$$\begin{aligned}\text{finite}(a,b) &= 1 \text{ for } x < a \text{ \& } x > b \\ &= 0 \text{ for } a < x < b\end{aligned}$$

$$\begin{aligned}\text{well}(a,b) &= 0 \text{ for } x < a \text{ \& } x > b \\ &= -1 \text{ for } a < x < b\end{aligned}$$

Infinite well:

$$\begin{aligned}\text{infinite}(a,b) &= \infty \text{ for } x < a \text{ \& } x > \\ &= 0 \text{ for } a < x < b\end{aligned}$$

Numerical simulations tend to dislike hard bounds. Sometimes we use soft versions of the above potentials.

For example: A softer version of the box potential: $\text{sbox}(a,b,h)$ where h is the hardness of the box. You could try out different values of h to be 10, 50, 100.. to see what happens to the box potential.

You can also try out:

$\text{swell}(a,b,h)$

$\text{sstep}(a,h)$

Basic functions:

Absolute value of any number: `abs(x)`

Square root: `sqrt(a)`

Power of a number, x^a : `pow(x,a)`

Exponential of x : `exp(x)`

Trigonometric functions

`sin(x)`, `cos(x)`, `tan(x)`

`sinh(x)`, `cosh(x)`, `tanh(x)`

Arithmetic operators:

`+`, `-`, `*`, `/`

Constants

`pi = 3.14159265358979323846`

`i = 0+1i`

`m= 1`, `ħ= 1`

You are free to write any arbitrary potential or wave function using the above functions, constants and arithmetic operators.

For example:

- The harmonic potential is written as: `0.5*a*x^2`
- The gaussian wave function is written as: `sqrt(sqrt(a/pi))*exp(-0.5*a*x^2)`
- A combination of potentials to design your own potential : `-box(0,1)+step(2)-step(4)`