Particle in an infinite box

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1 Conventional solution

We set $\hbar = 2m = L = 1$, therefore the Shordinger equation writes:

$$-\frac{d^2}{x^2}\psi(x) = E\psi(x) \tag{1}$$

The numerical solution procedure is:

1. Guess a value of energy E
2. set $\psi(0) = 0$ and $\psi'(0) = 1$. Setting $\psi'(0)$ to other nonzero value are OK, because it just change the normalization constant.
3. advance a step using $\psi(x + \Delta x) = \psi'(x)\Delta x + \psi(x)$, and $\psi'(x + \Delta x) = \psi'(x) - E\psi(x)\Delta x$
4. advance until $x = 1$ and check if $\psi(L) = 0$, if not, guess another value of E.
5. if yes, normalize the wavefunction and print E.

Some details:

1. store $\psi(x)$ and $\psi'(x)$ in a array, with length $N+1$, make sure $\psi[0] = 0$. The i-th step will rewrite $\psi[i+1]$ and $\psi'[i+1]$
2. note the normalization conditon is $c^2\Delta x\sum_i \psi[i]^2 = 1$.

Reference:

1. You Can Solve Quantum Mechanics' Classic Particle in a Box Problem With Code
2. Numerically solving a particle in a box problem