Infinite potential well problem using Numerical solution

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The schrodinger equation is like this :

$$\frac{\hbar}{2m}\nabla^2\psi + V\psi = E\psi$$

For the 1-D infinite potentail well problem, we assume that the potential in the box is 0.

So, for the region in the potential well, the equation becomes like this :

$$\frac{\hbar}{2m}\nabla^2\psi = E\psi$$

By using boundary condition $\psi(0) = \psi(a) = 0$, and solving the differential equation, the result becomes like this:

$$\psi = \sin(kx), k^2 = \frac{2mE}{\hbar^2},$$

$$\frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2} \quad \rightarrow E = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

The energy level of a=5nm, m=0.19m_0, the energy is E=0.0793eV

Let's compare this value with the solution with numerical value

N	Energy (EV)	Error (%)
5	0.0752	5.033
50	0.0791	0.0312
500	0.0792	0.0028

As we choose larger n points, the result become more exact.