Schroedinger equation with Python 1: 1D Infinite Square-Well potential

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I. INTRODUCTION

We obtain the numerical solutions for the eigen-energies and wavefunctions of the 1D infinite square-well potential. We solve the 1D Schroedinger equation (using finite-difference method [1]),

$$\frac{d^2\psi(x)}{dx^2} + 2m[E - V(x)]\psi(x) = 0, \tag{1}$$

for the potential $V(x)$,

$$V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & otherwise \end{cases} \tag{2}$$

To obtain the eigen-energies, we integrate the wavefunction upto $x = L$ and look for energies such that $\psi(x = L) = 0$. The initial conditions for the finite-difference method are $\psi(x = 0) = 0$ and $\psi(x + h) = 1$. From the finite-difference method, we have

$$\psi(x + 2h) = -[1 + 2E\ dx^2]\psi(x) + 2\psi(x + h), \tag{3}$$

where h is the integration step. We use the atomic units in our calculations ($m_e = 1, e = 1, \hbar = 1$). Figure 1 shows the roots of $\psi(x = L)$ as a function of energy E and the eigen-energies are therefore the points where $\psi(x = L) = 0$. Note the obvious n^2 behavior of the roots.

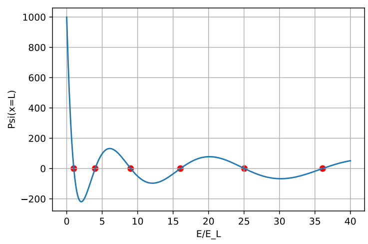

FIG. 1: $\psi(x = L)$ as a function of energy. Note that our energy is scaled to $E_L = \pi^2/2L^2$ which is the ground state energy of the 1D infinite square-well. The roots, i.e.,eigen-energies (roots of $\psi(x = L) = 0$) are marked in red circles. We have set $L = 1$

Figure 2 shows some of the wavefunctions for computed eigen-energies.They are also compared with the exact wavefunctions ($\sqrt{2/L}\sin(n\pi x/L)$).

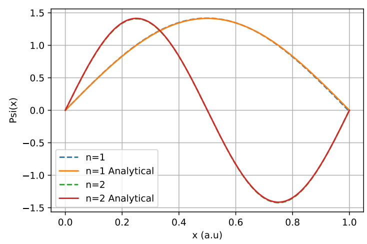

FIG. 2: First two eigenstates of the 1D square-well potential. Exact eigenstates are also shown for comparison.

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[1]

$$\psi(x)'' = \frac{\psi(x + 2h) - 2\psi(x + h) + \psi(x)}{h^2}$$