

Using Random Numbers to Solve Time Independent Schrödinger Equation

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1 Introduction

The wavefunction of a system is the quantity which provides us information about all the observables. Hence, to find this wavefunction is the most important task of any work. The wavefunction is obtained by solving the stationary-state Schrödinger equation $\hat{H}\psi = E\psi$ where the Hamiltonian for N particles is given by The term involving the Laplacian

$$\hat{H} = \sum_{i=1}^N \left[-\frac{\hbar^2}{2m} \nabla_i^2 + v_N(\vec{r}_i) \right] + \frac{1}{2} \sum_{i,j=1(i \neq j)}^N \frac{e^2/4\pi\epsilon_0}{|\vec{r}_i - \vec{r}_j|}$$

denotes the kinetic energy operator. The function $V_N(\mathbf{r}_i)$ represents the energy associated with the nuclear potential or any other potential perceived by individual electrons. Meanwhile, the final term signifies the potential energy interaction among electrons. It's worth noting that the kinetic energy operator operates differentially, whereas potential energy operators act multiplicatively.

In the absence of the electron-electron interaction term, the Schrödinger equation lends itself to analytical solutions for specific forms of the potential $V_N(r)$, such as those linked with one- and three-dimensional harmonic oscillators, as well as hydrogen-like atoms and ions. However, for other potentials, numerical solutions are typically pursued, or an approximate solution can be derived through the variational method for energy, as outlined below.

Nevertheless, the inclusion of the electron-electron interaction term in the Hamiltonian significantly alters the landscape. Analytical solutions for the equation become elusive, and numerical integration becomes impractical due to exponential increases in memory requirements. In such scenarios, the variational principle for energy is invoked to infer the ground-state wavefunction and its corresponding energy.

This work introduces an innovative approach to utilizing the variational principle, designed for simplicity and applicability, especially in the context of small systems. This method yields highly precise ground-state wavefunctions and energies.

1.1 Variational Principle for Energy

The principle states that the expectation value $\langle H \rangle$ of the Hamiltonian, derived from an approximate normalized wavefunction, is given by: The method consistently yields an approximate ground-state energy that is

$$\langle \hat{H} \rangle = \int \Psi_a^* \hat{H} \Psi_a dV,$$

either equal to or greater than the true ground-state energy. This approach can be effectively employed to derive an approximation of the ground-state wavefunction alongside its corresponding energy. The procedure involves selecting a functional form for the wavefunction, incorporating specific parameters, and ensuring it satisfies the appropriate boundary conditions relevant to the problem at hand. Subsequently, the expectation value of the Hamiltonian is computed and minimized with regard to these parameters. The minimum value attained for $\langle H \rangle$, along with the associated wavefunction, provides the approximation for the ground-state energy and wavefunction, respectively.

Improving the accuracy of a trial wavefunction can be achieved by incorporating a greater number of parameters, provided that the wavefunction is constructed judiciously in line with the physics of the problem. A precise calculation entails adjusting the wavefunction at numerous discrete points, ideally extending to an infinite number of points in space, treating the value at each point as a parameter, until the expectation value of the Hamiltonian is minimized. This extensive variation of the wavefunction across an infinitely large number of points essentially amounts to solving the Schrödinger equation, thereby yielding the exact ground-state wavefunction and energy. Consequently, employing a substantial number of mesh points allows us to anticipate results that closely approximate the exact ones. In this paper, we propose a method to conduct such variational calculations using random numbers. These calculations are performed numerically, employing a discrete set of mesh points to represent a trial wavefunction through random numbers assigned to each point. We subsequently evaluate $\langle H \rangle$ with this wavefunction and iteratively adjust the wavefunction freely by introducing a new set of random numbers at each mesh point until $\langle H \rangle$ reaches its minimum value.

2 Using random numbers to perform variational calculation

2.1 Single particle in one-dimension

This is the approach tailored for one-dimensional scenarios. This initial focus aims to evaluate and validate the effectiveness of the proposed method. To this end, we examine a solitary particle, with mass m ,

confined to traverse solely along the x-axis. The particle is subject to a potential energy function $V(x)$. The Hamiltonian for the problem, therefore is To conduct the calculations, we establish $(N+1)$ discrete points

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$$

x_i , where i ranges from 1 to $N+1$, along the x-axis, spaced apart by an interval Δx . This configuration yields a length $L = N\Delta x$ over which the wavefunction exists, with the wavefunction assumed to diminish beyond this interval. Subsequently, we assign a set of random numbers, one for each mesh point within the range $[0, a]$, where a lies between 1 and 0 exclusively. These numbers signify the values of the wavefunction at each respective point, denoted by ψ_i ranging from 2 to N . The choice of the interval $[0, a]$ for the random numbers aims to maintain the positivity of the ground-state wavefunction. To streamline numerical computations, we opt for two-point formulas for differentiation and integration, which consistently yield sufficiently accurate outcomes.

For normalization, the wavefunction is now integrated over the length L and gives Next the kinetic and potential energies are calculated and

$$C_N = \int_0^L \psi^* \psi dx = \Delta x \sum_{i=2}^N |\psi_i|^2$$

added to get the expectation value of the Hamiltonian. The expectation value of the Hamiltonian after each iteration is Following each calcu-

$$\begin{aligned} \langle \hat{H} \rangle &= \frac{1}{C_N} \left[\frac{1}{2} \int_0^L \left| \frac{d\psi}{dx} \right|^2 dx + \int_0^L V(x) |\psi|^2 dx \right] \\ &= \frac{1}{C_N} \left[\frac{1}{2\Delta x} \sum_{i=1}^N |\psi_{i+1} - \psi_i|^2 + \Delta x \sum_{i=2}^N V(x_i) |\psi_i|^2 \right] \end{aligned}$$

lation of the expectation value mentioned earlier, we proceed to create the updated wavefunction for the subsequent iteration. This involves augmenting random numbers within the range $[0, a]$ to the normalized wavefunction from the preceding iteration. Subsequently, we compute $\langle H \rangle$ using the newly generated wavefunction. If this expectation value

proves to be lower than the previous one, we adopt the new function as the revised wavefunction and commence the subsequent iteration. Conversely, if the expectation value does not decrease, we initiate a new iteration by introducing another set of random numbers to the existing wavefunction, repeating the aforementioned process.

After several iterations, the trial wavefunction begins to assume the anticipated shape for the ground state of the considered Hamiltonian. At this juncture, the refinement of the wavefunction continues by incorporating random numbers within the interval $[-a/2, a/2]$. This inclusion enables the wavefunction to encompass both positive and negative values, facilitating its potential increase or decrease at any given point.

3 Results

We can see that with an increasing number of iterations, the wavefunction gets more and more refined and finally the wavefunction is almost (because of finite number of mesh points) the same as the exact solution.

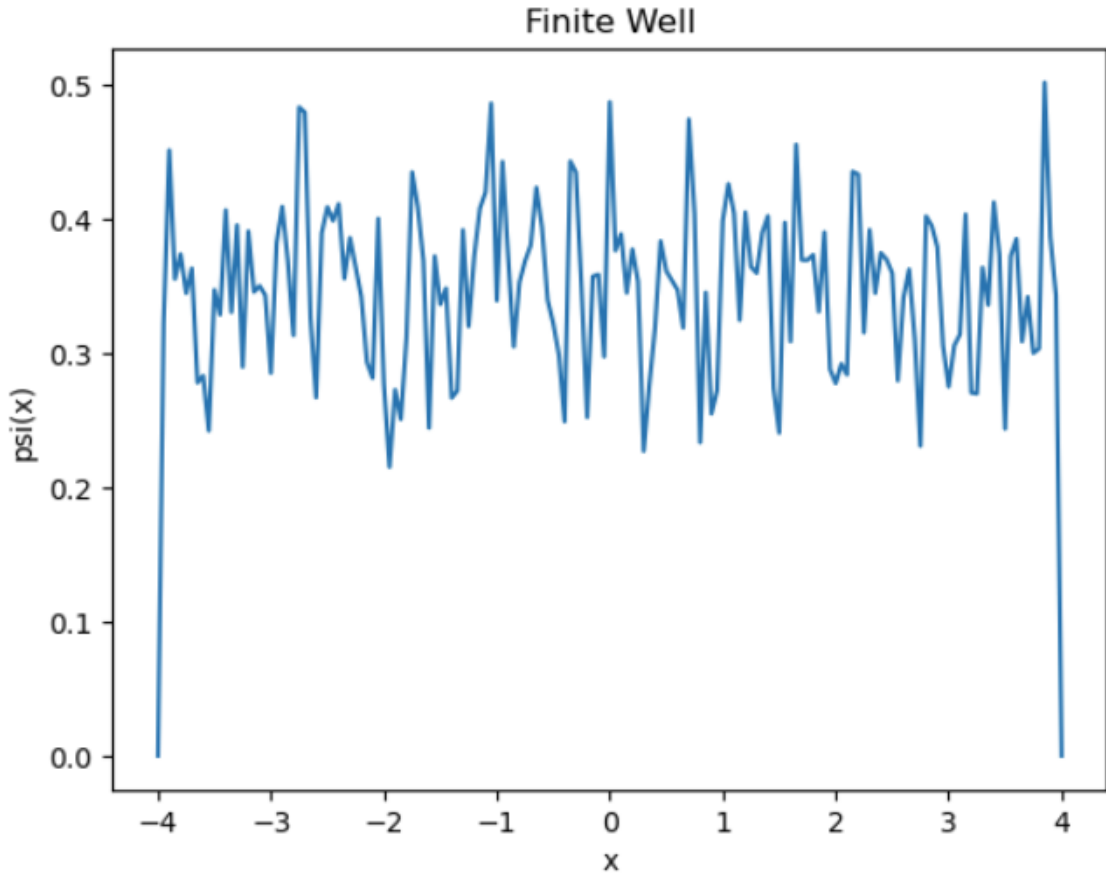


Figure 1: Wavefunction after 10 Iterartions

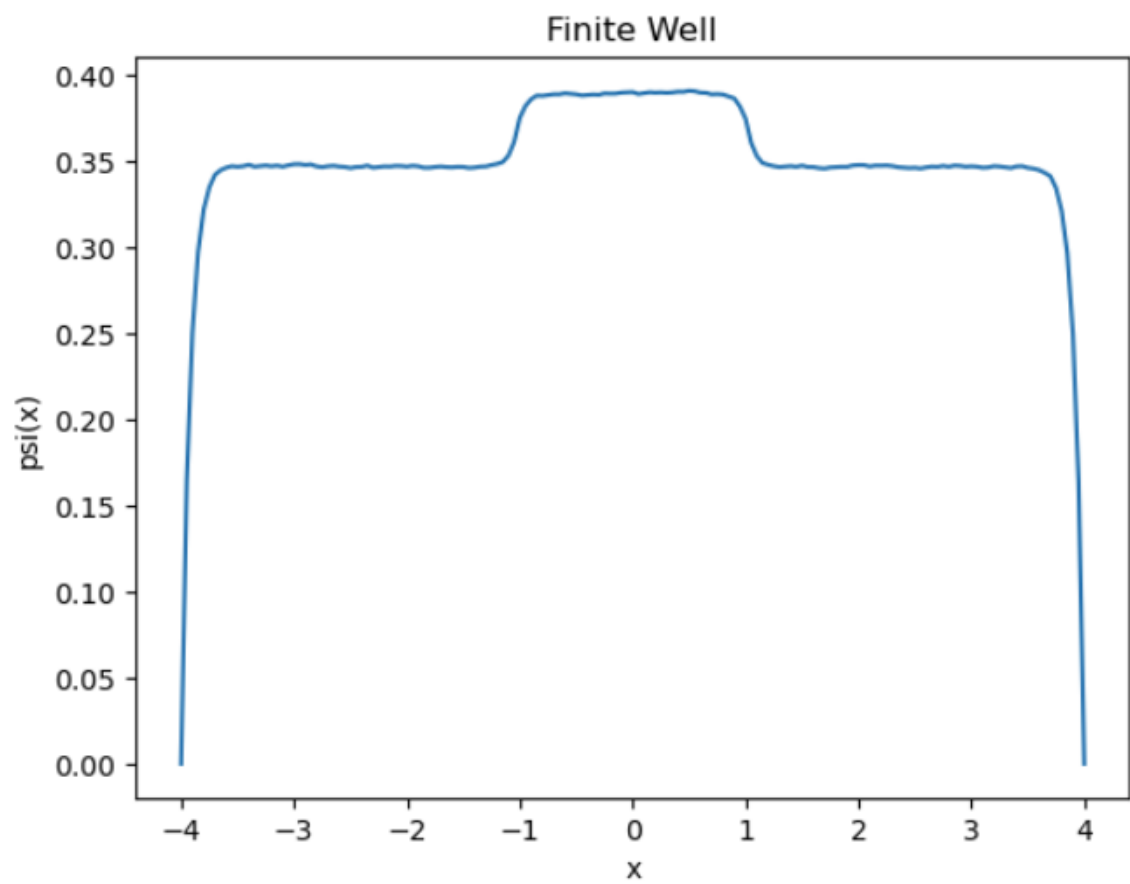


Figure 2: Wavefunction after 10000 Iterartions

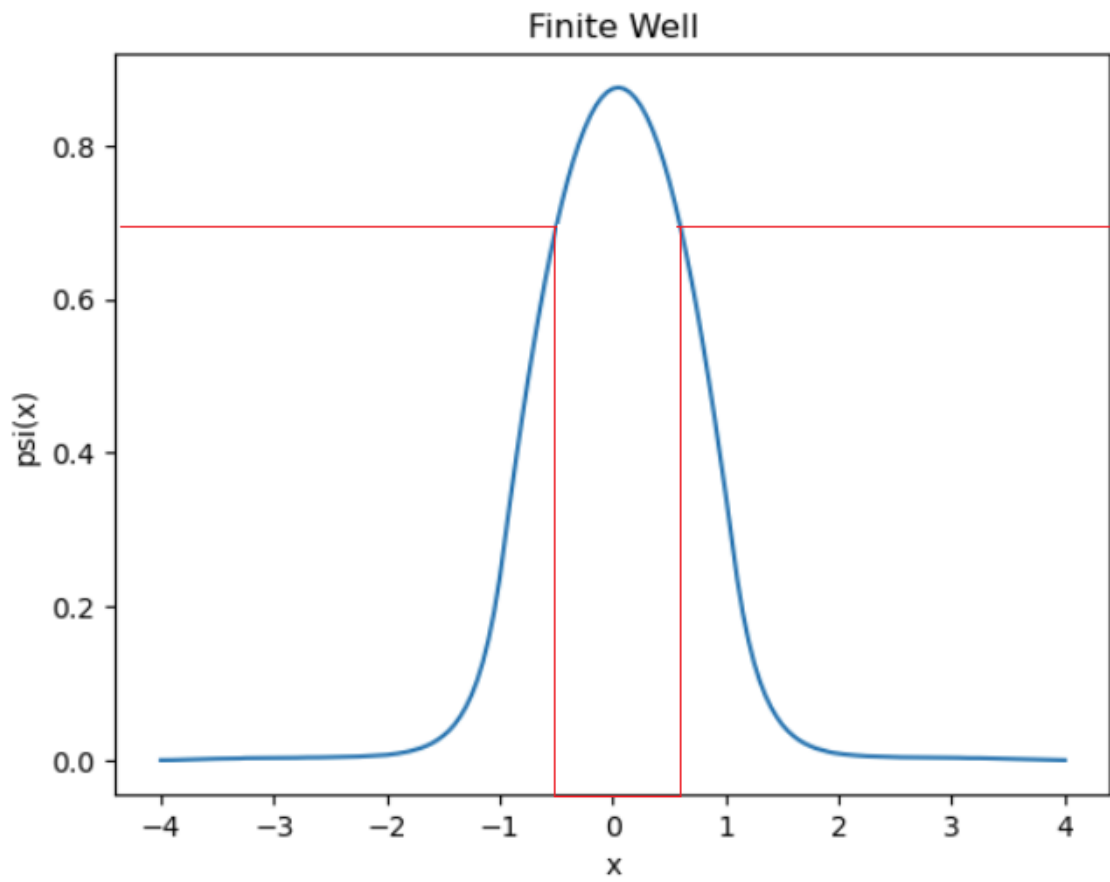


Figure 3: Wavefunction after 1000000 Iterations

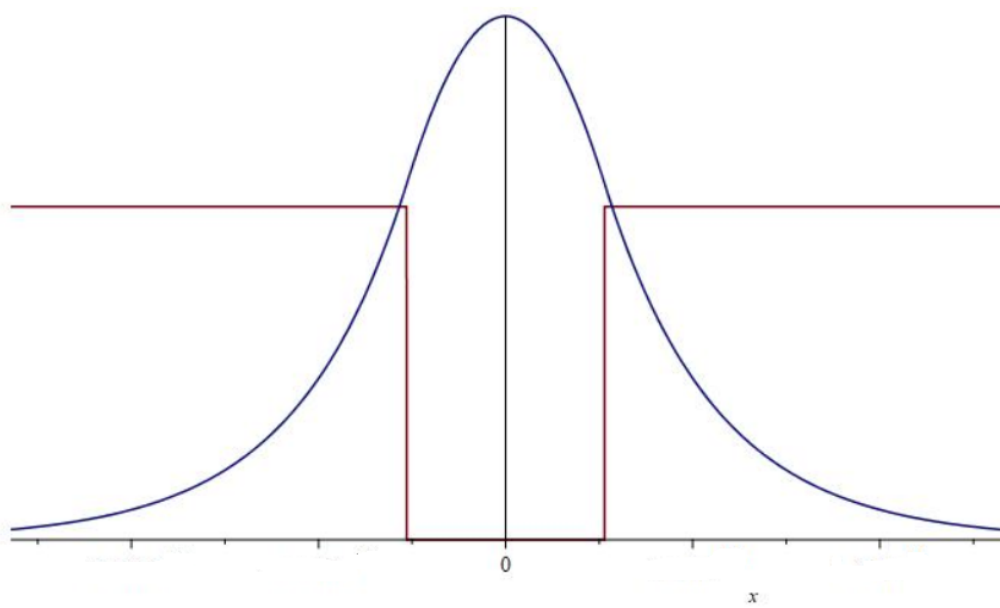


Figure 4: Theoretical Plot of the Wavefunction