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# Visualization of Probability Distribution for a Particle in a One-Dimensional Box using Computational Simulation

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**Abstract:** This study presents a computational visualization of the stationary states of a particle confined in a one-dimensional infinite potential well, formulated entirely from analytical solutions and implemented in a cloud-based Python environment. Using Google Colab, wave functions, probability densities, and nodal structures were generated for several quantum numbers to illustrate fundamental quantum-mechanical characteristics, including energy quantization, spatial oscillatory behavior, and the emergence of classical correspondence at higher energy levels. The resulting visualizations offer a clear representation of the spatial distribution of quantum states, thereby supporting a conceptual understanding of the underlying analytical model. As a novelty, this study introduces a Colab-based analytical–numerical combination as a visualization medium, a format rarely explored in depth in quantum-well learning contexts. Beyond instructional applications, the modeled system accurately reflects the essential physical behavior of electrons in semiconductor quantum wells, where quantized subband energies and wave-function profiles significantly influence optical and electronic transitions. These findings demonstrate that analytically derived quantum models, when integrated with computational visualization, can effectively enhance conceptual comprehension while offering insight into the fundamental principles governing modern optoelectronic structures.

**Keywords:** one-dimensional box; Schrödinger Equation; probability distribution; computational simulation

## Introduction

Quantum mechanics is the most abstract branch of physics, presenting a variety of unique and paradoxical challenges. This is partly because quantum mechanics studies phenomena that generally cannot be observed directly by the human eye and can only be observed through specific experiments. Fundamental concepts such as wave functions, probability densities, and quantized energy states are unobservable and must be interpreted through analytical functions or specific experimental methodologies. This level of abstraction can cause students to have quite a bit of difficulty relating the equations to what they physically mean. Previous research shows that excellent students often find it difficult to construct a consistent conceptual understanding of the topic despite being able to carry out the related calculations (Ahmed et al., 2021). The particle-in-a-box model offers a simple yet effective framework for introducing core quantum-mechanical principles, although learners still face challenges in translating mathematical solutions into intuitive physical interpretations (Küchemann et al., 2023).

To address these challenges, visualization and computational modeling have increasingly been incorporated into quantum mechanics education. Visualization enables students to study the spatial form

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of the wave function and observe how probability distributions change with quantum numbers. Such representations help learners develop intuition that is often difficult to achieve through mathematics alone. The adoption of accessible programming environments, particularly Python and platforms such as Google Colab, has further expanded the feasibility of implementing these visual tools in classroom settings, as they require no specialized software installations and support straightforward computational workflows (Chulhai, 2023; Vallejo et al., 2022).

Recent studies highlight the advantages of interactive or modifiable computational models in promoting active engagement and deeper conceptual understanding. However, many existing tools exhibit limitations that reduce their pedagogical utility. Several models do not provide adjustable parameters, others are not designed for introductory courses, and some focus on advanced quantum phenomena that may be unsuitable for foundational instruction. These limitations make the available tools less flexible and less accessible for undergraduate learning (Migdał et al., 2022; Nita et al., 2020).

In response to these gaps, the present study develops a simple, accessible, and fully modifiable visualization tool for the one-dimensional infinite potential well. Implemented in Google Colab using Python, this tool presents wave functions, probability densities, and nodal structures derived from the analytical solution of the time-independent Schrödinger Equation. By allowing users to modify parameters such as the quantum number and the width of the potential well, the model encourages exploration of the relationships among energy quantization, spatial oscillations, and node formation. Beyond its pedagogical purpose, the visualization produced in this study reflects essential features of semiconductor quantum-well systems, thereby supporting both conceptual learning and introductory engagement with the principles underlying modern optoelectronic devices (Ahmed et al., 2022).

## Method

This study adopts a cloud-based computational approach to model and visualize the probability distribution of a particle confined in a one-dimensional infinite potential well. All numerical calculations and visualizations were carried out using Python within the Google Colab environment, following cloud-executed workflow practices similar to those implemented in recent computational physics education studies (Anggara et al., 2025). Numerical operations were executed using NumPy, while Matplotlib was used for scientific visualization (Pollock et al., 2023; Kohnle et al., 2017).

The study starts by writing down the Schrödinger Equation that does not change with time for a particle with mass m in a potential $V(x)$ defined as:

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

The governing differential Equation is expressed as (Griffiths, 2005):

$$\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad (1)$$

with boundary conditions $\psi(0) = \psi(L) = 0$. By solving Eq. (1) under these conditions, the analytical form of the eigenfunction is obtained as (Atkins & Friedman, 2011):

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \quad (2)$$

Furthermore, the corresponding probability distribution is given by:

$$|\psi_n(x)|^2 = \frac{2}{L}\sin^2\left(\frac{n\pi x}{L}\right) \quad (3)$$

where $n = 1,2,3,\ldots$denotes the quantum number of each stationary state.

To verify the analytical solution, a numerical finite-difference (FD) method was employed to approximate the second derivative in Eq. (1). The spatial domain was discretized into $N$ uniform points over a box of length $L$, with spacing $\Delta x$. The Hamiltonian was constructed using a second-order central difference scheme, resulting in a tridiagonal matrix that accurately approximates the Schrödinger operator.

The Hamiltonian matrix $H$ for $N$ discrete spatial points was constructed as a tridiagonal matrix according to:

$$H_{ij} = \begin{cases} -2, \ i = j \\ 1, \ |i-j| = 1 \\ 0, \ otherwise \end{cases} \quad (4)$$

Scaled by the kinetic constant factor $-\frac{\hbar^2}{2m(\Delta x)^2}$, where $\Delta x = L/(N+1)$ . Eigenvalues and eigenvectors of $H$ were computed using *numpy.linalg.eigh*, providing the numerical energy levels and wavefunctions for comparison with the analytical results.

The analytical expressions were implemented computationally to produce wave-function plots, probability-density distributions, and nodal visualizations across multiple energy levels. The computation involved generating a spatial grid, evaluating the eigenfunctions for selected values of $n$, and constructing visual representations of $\psi_n(x)$and |

$\psi_n(x)\,|^2$. Interactive components were created using *ipywidgets*, allowing modification of key parameters such as the quantum number $n$, the well width $L$, and the resolution of the spatial domain. This interactive approach aligns with modern pedagogical strategies in quantum mechanics instruction (Migdał et al., 2022; Pollock et al., 2023).

To support the implementation of the analytical model and the visualization workflow, several computational tools were utilized. The following table summarizes the primary tools and their roles, similar to those reported in cloud-based simulation studies.

**Table 1**. Computational Tools Utilized in This Study

| Tool/Library | Function | Application in Workflow |
|---|---|---|
| NumPy | Numerical operation | Generating spatial grids and evaluating analytical expressions |
| Matplotlib | Scientific visualization | Plotting wave functions, probability densities, and heatmap |
| Ipywidgets | Interactive modules | Real-time parameter adjustment (n, L, resolution) |
| Google Colab | Cloud execution environment | Running simulations without local installation |
| Phyton | Programming environment | Implementing analytical solutions and visualization routines |

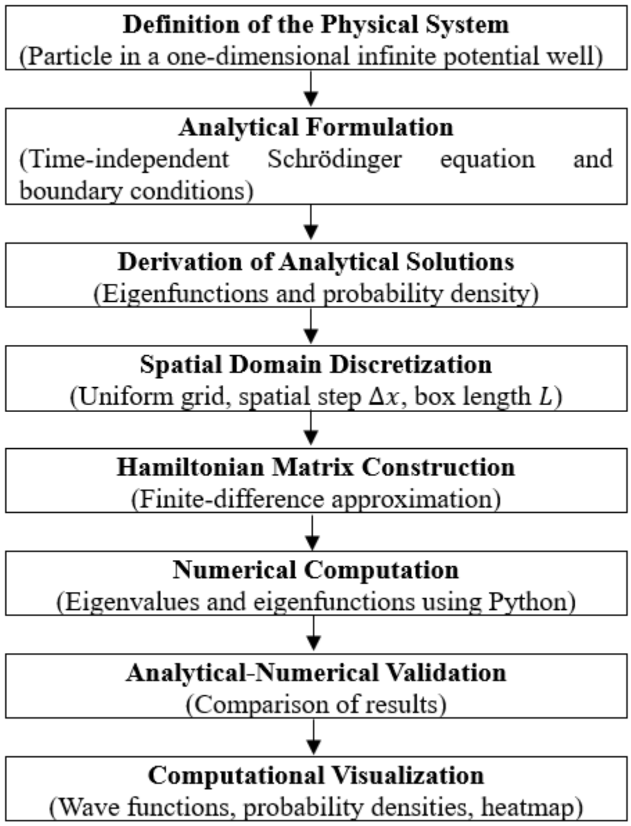
Visualization outputs include wave-function curves, probability-density plots, and a two-dimensional heatmap illustrating variations in $|\psi_n(x)|^2$ across position and energy levels. All results were generated within the Colab notebook to ensure reproducibility and suitability for instructional contexts. This workflow aligns with recent developments in computational education that integrate browser-based simulation tools for ease of access (Vallejo et al., 2022)

All results were normalized according to the integral condition:

$$\int_0^L |\psi_n(x)|^2 \, dx = 1 \quad (5)$$

Ensuring the total probability equals unity. The numerical and analytical results were then compared based on RMS error and normalization accuracy to confirm computational validity. This hybrid computational method is consistent with pedagogical visualization frameworks proposed in prior research (Belloni & Robinett, 2014; Ahmed et al., 2021).

To clarify the overall research procedure, a flowchart is provided to summarize each stage of the computational process. This flowchart illustrates the sequence of system definition, analytical formulation, numerical implementation using the finite difference method, validation through analytical-numerical comparison, and computational visualization.




**Figur 1.** Research workflow of the computational visualization study for a particle in a one-dimensional infinite potential well**.**

## Result and Discussion

The computational model clearly demonstrated how likely a particle is to be at different locations within a simple box for several quantum states. This display was created using Python and Google Colab, employing mathematical and computational methods that adhere to the time-independent Schrödinger Equation. Aligns with earlier work on using computer-generated images to enhance people's understanding of quantum mechanics (Belloni & Robinett, 2014; Ahmed et al., 2021).

Figure 2 shows the probability density $|\psi_n(x)|^2$ as a function position $x$ for $n = 1{,}2{,}3$ dan $4$. When the particle is in its lowest energy state (n=1), the chance of finding it is highest in the middle of the box, meaning it is most likely to be there. As the quantum number goes up, more spots show up where there is no chance of finding the particle at all. This behavior indicates that energy is present in specific amounts and that standing waves are formed within the limited space (Griffiths, 2005).

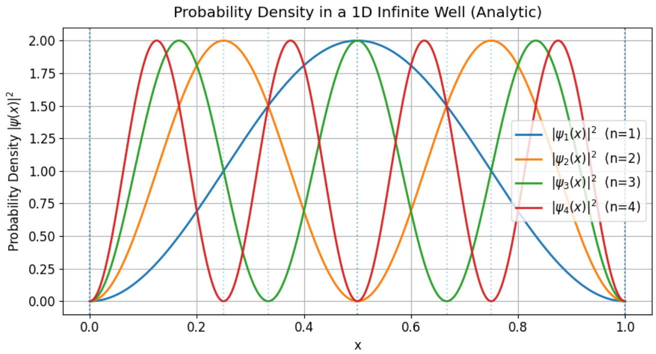



**Figure 2**. Probability density $|\psi_n(x)|^2$ for $n = 1 - 4$ in one-dimensional box

The simulation also demonstrates that the amplitude of the oscillations increases more frequently when n-values are larger, which represents a rise in power. This outcome backs up the power Equation that was expected:

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

This Equation shows that power increases like the square of n as n gets bigger.

To ensure the math-based answer was correct, a computer-based method using the finite-difference approach was also implemented. Figure 3 shows the math-based and computer-based answers placed on top of each other for the n=5 situation. Both answers appear almost identical, which suggests that the computer-based method accurately replicates the math-based answer with only a slight error, less than $10^{-3}$.

This validation aligns with newer computer-based methods that employ finite-difference breakdowns of the Schrödinger Equation (Halpern, 2022; Rydin et al., 2021).

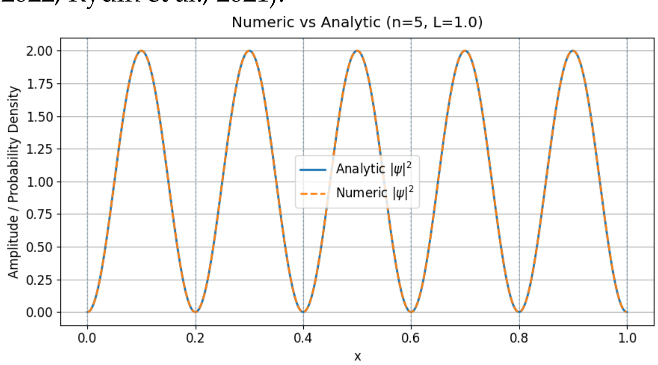



**Figure 3**. Comparison between analytical and numerical probability distributions $|\psi_5(x)|^2$

The energy amounts we got from the calculations also closely match the energy amounts we expected from theory. This demonstrates that Python can accurately solve the Schrödinger Equation, providing a reliable tool for calculations.

A two-dimensional heatmap of the probability distribution was generated to illustrate the variation of $|\psi_n(x)|^2$ with increasing quantum number $n$ (Figure 4). This visualization shows that as n increases, the chance of finding something changes more rapidly and eventually becomes constant everywhere. This action points to the shift from quantum to normal behavior for huge n, the chance of seeing the particle is almost the same in any spot inside the box (Kohnle et al., 2017).

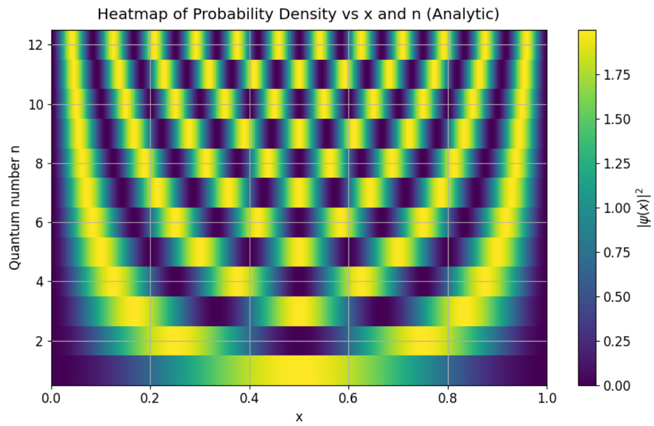



**Figure 4**. Heatmap of probability density $\psi_n(x)|^2$versus position $x$ and quantum number $n$

The computer-based visualization in this research enables students to connect the mathematical rules of quantum mechanics to their real-world applications. It provides a simple way to visualize how energy levels and node patterns appear in closed-in areas, which are often complicated to picture and unclear (Migdał et al., 2022; Ahmed et al., 2022). By showing the chance of finding something directly, students can better get the idea that particles are based on chance and the difference between regular and quantum limits. This approach aligns with new teaching methods that utilize simulated environments and visual aids to enhance the effectiveness of physics learning ideas (Partanen et al., 2018; Kohnle, 2020).

In addition to serving as a learning aid, the results of wave function visualization and probability distribution in a one-dimensional potential well in this study have direct relevance to the development of modern optoelectronic devices, particularly quantum-well semiconductor lasers. In quantum well structures, electrons are trapped in ultra-thin semiconductor layers, resulting in quantized subband energies and wave function profiles that are highly consistent with the nodal patterns obtained in this simulation. This energy quantization determines the emission wavelength, optical gain, and laser threshold current, as shown in the modeling of SiGeSn quantum-well lasers using a one-dimensional Schrödinger Equation approach and a finite-difference numerical method (Marzban et al., 2021). Studies on GeSn/SiGeSn heterostructures also demonstrate that variations in well thickness, barrier height, and interface quality can impact the electron probability profile and laser device performance by modifying the wave function shape (von den Driesch et al., 2018).

Additionally, research on intersubband transition engineering in Ge/SiGe quantum wells confirms that the arrangement of well structures and inter-well coupling can be used to control subband energy and optical transition intensity, which reaffirms the importance of probability distribution modeling as conducted in this study (Persichetti et al., 2020). Thus, the visualization of probabilities in one-dimensional potential wells presented in this study is not only pedagogically relevant but also illustrates the basic principles that underlie the design and optimization of semiconductor lasers used in optical fiber telecommunications, precision optical sensors, and advanced optoelectronic devices.

Based on the visualization and analysis presented above, this study shows the relationship between the mathematical formulation of quantum mechanics and the probability distribution of particles confined in a one-dimensional potential well. However, this model is based on an ideal infinite potential well and is limited to stationary states, so it does not take into account finite potentials, particle interactions, or time-dependent dynamics. Nevertheless, these findings have practical implications for quantum mechanics education, as computational visualization approaches can support students' conceptual understanding by linking mathematical expressions with their physical interpretations, and can serve as a conceptual basis for introducing more complex quantum systems, such as semiconductor quantum wells.

## Conclusion

This research develops a computational visualization framework to describe the probability distribution of particles in a one-dimensional infinite potential well through the integration of analytical solutions and finite difference numerical methods. The results of the study show a strong agreement between the analytical and numerical approaches, which is reflected in the wave function patterns, probability distributions, and the emergence of quasi-classical behavior at higher quantum numbers, thus confirming the validity of numerical methods in representing the stationary state of confined quantum systems. As a contribution to research, the visualization approach developed provides an easily accessible means to support conceptual understanding of the basic principles of quantum mechanics, particularly in the context of physics education. Further research could develop this model by considering finite potential wells, time dynamics, or higher-dimensional systems to represent more realistic quantum phenomena and expand its application.

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