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CLASSICAL VS. QUANTUM BEHAVIOR IN THE PARTICLE-IN-A-BOX MODEL

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Abstract

This paper examines the particle-in-a-box model as a simple but powerful example that highlights the fundamental differences between classical and quantum physics. In classical mechanics, a particle confined between two rigid walls moves with constant velocity and has a uniform probability of being found anywhere in the box; its energy can take any continuous value. In contrast, solving the Schrödinger equation for an infinite potential well yields standing-wave solutions whose wavelengths must satisfy fixed boundary conditions. These constraints produce discrete, quantized energy levels and non-uniform probability distributions, features with no classical analog. Through analytical derivations and numerical simulations using Python, we visualize wave functions, probability densities, and the statistical convergence of random samples toward the theoretical quantum distributions. Comparisons with the classical uniform distribution emphasize how quantum mechanics replaces certainty with probability and continuity with quantization. Finally, we connect the model to real physical systems—such as electrons confined

in atoms—to show how this idealized system provides essential insight into the structure and stability of matter.

Keywords:
Particle-in-a-Box Model, Quantum Confinement, Standing Waves, Wavefunction, Quantum vs. Classical Behavior, Spatial Distribution

1. Introduction

1.1 General Background

For the past few hundred years, classical physics–based on Newtonian mechanics and Maxwellian electromagnetism–has been our primary tool for understanding the macroscopic world and explaining phenomena in our daily life such as the orbits of planets, the falling of objects, and the motion of vehicles. However, scientists gradually discovered that classical physics could not explain phenomena in the atomic and microscopic world, meaning that the rules of classical physics do not apply in this microscopic area. Thus, in the early 20th century, quantum mechanics was proposed (Golub & Lamoreaux, 2023).

One of the most important aspects of quantum mechanics, and its biggest difference from classical mechanics, is that even with perfect knowledge of the system under study, it is generally impossible to calculate the exact position and velocity of a particle. Instead, we can only calculate the probability that the particle has a given position and velocity. In quantum mechanics, a particle is described by a wave function ψ(x), which obeys a core equation known as the Schrödinger equation. The wave function itself cannot be directly measured, but its square $|\psi(x)|^2$ tells us the probability of a quantum appearing at a certain location. This interpretation, proposed by Max Born, states that we cannot precisely predict where a particle will be, but only where it is likely to appear (Baggott, 2020).

On the other hand, another important result in quantum mechanics is the quantization of energy (Golub & Lamoreaux, 2023) . For particles bound in a system, the energy can only take on specific, discrete values, rather than being continuous. This is completely different from classical mechanics, where, for example, energy in the motion of a ping-pong ball or a car can continuously change to any value at any time. In quantum mechanics, energy changes in jumps and cannot take on arbitrary values as we explain in the theoretical section of this paper.

This is precisely why quantum mechanics is difficult to understand: it introduces phenomena that do not exist in the classical world. Take, for example, interference between matter particles (the electron double-slit experiment) or the quantization of energy (at the atomic level). To help people better understand these abstract concepts, physicists often use the "particle in a box" model, which is a case where a single particle of mass m is trapped in a region of space. Inside that region (the box), it feels no force. This model clearly demonstrates the quantization of energy, wave-particle duality, and the probability of particle appearance in quantum mechanics through the wave function solution of the Schrödinger equation in a "one-dimensional infinite potential well." This paper focuses on the one-dimensional case, where particles can only move between x=0 and x=L, assuming in our illustration the L=3.

1.2 Historical Background

To truly understand the significance of quantum mechanics, we need to understand some theoretical challenges that classical physics couldn't resolve and the process by which physicists gradually discovered quantum mechanics. These progresses in the history of physics laid the foundation for the birth of quantum mechanics (Küçük, 2025; Darrigol, 2009).

In the late 19th century, scientists studying the radiation of objects encountered a problem that defied classical physics. If an ideal object (the black body) that absorbs and radiates all frequencies is heated, it will radiate electromagnetic waves of varying wavelengths. In experiments, the radiation intensity of the black body in the long-wavelength (low-frequency) region gradually increases as the wavelength decreases, then reaches a peak. Finally, the intensity rapidly decreases towards shorter wavelengths. However, the Rayleigh-Jeans equation, derived from classical electromagnetic theory and thermodynamics, predicts that the radiation intensity at short wavelengths will increase infinitely. This contradictory result is known as the ultraviolet catastrophe (Norton, 1987; Mavani, 2022).

To address this issue, German physicist Max Planck proposed a new hypothesis in 1900: that energy emission and absorption occur not continuously but in discrete quanta(Studart, 2001; Nauenberg, 2016). The energy of each quantum is proportional to the frequency of the radiation: $E = h\nu$. Where h is Planck's constant and ν is the frequency of the radiation. Assuming that the energy of electromagnetic waves can only take on these discrete values, Planck successfully

derived a formula for blackbody radiation that matched experimental results. This idea introduced the concept of quantization and became the starting point of quantum theory.

Followed by this, Einstein proposed an innovative explanation to the photoelectric effect in 1905 (Pais, 1979; Brush, c. 1905/1935). In this experiment, light is shone on a metal surface and it is found that when the frequency of the light is below a certain value, no electrons could be ejected, even at high light intensity. However, when the frequency of the light is above a certain value, electrons are ejected, even at very low light intensity. In contrast, classical electromagnetism holds that whether electrons can be ejected depends on the intensity of the light. Einstein explained that light is composed of many particles, each with an energy of $E = h\nu$. Only when the energy of a single particle is sufficiently high can an electron be ejected.

In 1913, Niels Bohr, building on Planck's quantization ideas, proposed a model of the hydrogen atom(Nanni, 2015). This model states that electrons can only exist in certain fixed orbits, each associated with a specific energy. When an electron transitions from a higher-energy orbit to a lower-energy orbit, it releases a photon of constant frequency whose energy is equal to the energy difference between the two orbits.

In 1924, Louis de Broglie proposed that all particles, like electrons, can behave like waves, with a wavelength given by $\lambda = h/p$, where p is the particle's momentum (Darrigol, 2009; Drezet, 2024). This means slower particles have longer, easier-to-see wavelengths, which was later confirmed by experiments with electrons. Because particles act like waves, they can make patterns of interference and diffraction—behaviors once thought to happen only with waves. As a result, we cannot track tiny particles along exact paths and instead we use wave functions to show the probability of where they might be.

In 1926, Austrian physicist Erwin Schrödinger proposed the famous Schrödinger equation in quantum mechanics, one of the core equations of quantum mechanics (Küçük, 2025; Nanni, 2015). It describes how a particle's wave function, $\psi(x)$, varies in space and time. The square of the wave function, $|\psi(x)|^2$, represents the probability of the particle occurring at a certain value. One application of this equation is the one-dimensional infinite potential well, often referred to as the "particle in a box" model. In this model, particles are strictly confined to the region $0 < x < L$ and cannot occur when $x < 0$ or $x > L$. Furthermore, the wave function can only take forms that satisfy integer multiples of half the wavelength, resulting in a particle's energy $En = \frac{n^2h^2}{8mL^2}$ in a given state being limited to n = 1, 2, 3, ... This is the discrete nature mentioned

earlier, in contrast to the continuous energy allowed in classical mechanics. This is the historical discovery process of quantum mechanics.

1.3 Theoretical Foundations

The "particle in a box" model is one of the most fundamental and representative models in quantum mechanics. It describes the motion of a particle of mass m confined to a one-dimensional rigid box of length L. Its potential energy function can be expressed as:

$$V(x) = \begin{cases} 0, & \text{if } 0 < x < L \\ \infty, & \text{if } x < 0 \text{ or } x > L \end{cases}$$

This means that there are not any forces within the range $0 < x < L$, while the potential energy outside the boundary is infinite, making it impossible for the particle to appear outside the box. Although this model's assumptions are extremely idealized, it can clearly illustrate the fundamental differences between quantum mechanics and classical mechanics in terms of motion, energy values, and probability distributions. It also has the advantage that it can be solved fully analytically.

In classical physics, the motion of a particle within a box is like a ping-pong ball bouncing back and forth between two rigid walls. Since there are no forces acting within the box, the particle moves uniformly in a straight line at a constant velocity v, and upon striking the wall, it undergoes elastic reflection. Its total energy is entirely kinetic energy $Ek = \frac{1}{2}mv^2$. In this case, the particle's velocity v can take on any positive value, so the energy E is continuous and unrestricted.

Furthermore, since the particle spends the same amount of time at each location during its motion, the probability of the particle being at any location within the box is also the same. This means that the probability distribution in the classical case is a horizontal line, uniformly distributed throughout the box. Consider a small region of space inside the box at position x (such that $0 < x < L$), the probability dP that the particle is within dx around x is vdx. So dP is constant within the box. Also, when L = 3 m, the ping-pong ball could move at 1 m/s, 10 m/s, 100 m/s, or 1000 m/s. The energy value is entirely determined by the velocity, with no limited range.

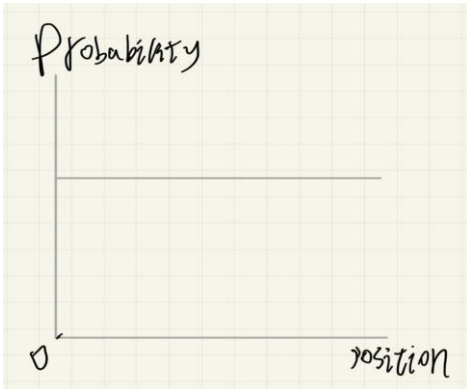


Figure 1. *Probability Distribution of Ping-Pong Ball Positions*

In quantum mechanics, the state of a particle is described by a wave function ψ(x), whose behavior must satisfy the stationary Schrödinger equation $\frac{-h^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x)$. For a one-dimensional infinite potential well, outside the box, V(x) = ∞, so ψ(x) = 0. Inside the box, 0 < x < L, V(x) = 0. The equation inside the box can be simplified to $\frac{-h^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x)$, and its general solution is sine form $\psi n(x) = \sqrt{\frac{2}{L}}sin(\frac{n\pi x}{L})$, n is quantum numbers, n =1,2,3….

On the other hand, $En = \frac{n^2h^2}{8mL^2}$ are the allowed energy levels. The energy of the particle in a box is quantified: it can be $\frac{1^2h^2}{8mL^2}$, $\frac{2^2h^2}{8mL^2}$ or $\frac{4^2h^2}{8mL^2}$…, but (for instance) E=$\frac{1.5^2h^2}{8mL^2}$ is forbidden. This discrete energy behavior is a purely quantum phenomenon with no equivalent in classical physics.

2. Result

2.1 Visualization of the Wave Function and Probability Distribution

Previously, we introduced the theoretical foundations and derived the solutions to the stationary Schrödinger equation for the "infinite potential well" model and the conclusions about energy quantization. This section will use a numerical Python script to visualize the distribution of wave functions and probability densities, providing a more intuitive understanding of the characteristics of quantum states. The simulations used the Google Colab and Matplotlib libraries. The potential well width is set to L = 3 (consistent with the previous section), and the wave functions and probability densities are plotted for quantum numbers n = 1, 2, and 3, respectively.

When n=1:

```
import numpy as np
import matplotlib.pyplot as plt
```

```
L = 3 # Box length is fixed at L = 3
n_max = 1 # n can be changed to 1,2 or 3

x = np.linspace(0, L, 200) # Generate 200 points in the interval [0, L]

fig, (ax1, ax2) = plt.subplots(2, 1, figsize=(8, 8)) #  Create two vertically
stacked subplots

#if x < 0:
 #fx = 0
#if x>=0 and x<=L:
 #fx = np.sin(x/L)
#if x > L:
 #fx = 0

# Design the title of first graph for wave functions
ax1.set_title('Wave function')
ax1.set_xlabel('Position (x)')
ax1.set_ylabel('Wave function')
ax1.grid(True)

# Define the quantum number
n = 1 # n can be changed to 1,2 or 3
psi_n = np.sin( n * np.pi * x / L) # Wave function formula ψ_n(x) = sin(nπx/L)
ax1.plot(x, psi_n, label=f'n = {n}') #  Plot the wave function curve
ax1.legend()

# Design the second graph for probability density
ax2.set_title('Particle in a Box Probability Density')
ax2.set_xlabel('Position (x)')
ax2.set_ylabel('Probability Density')
ax2.grid(True)

n = 1
psi_n_squared = (np.sin(np.pi * x / L))**2
ax2.plot(x, psi_n_squared, label=f'n = {n}')
ax2.legend()

#  Display the two plots
plt.tight_layout()
plt.show()
```

When n=2:

```
import numpy as np
import matplotlib.pyplot as plt

L = 3 # Box length is fixed at L = 3
n_max = 2 # n can be changed to 1,2 or 3

x = np.linspace(0, L, 200) # Generate 200 points in the interval [0, L]

fig, (ax1, ax2) = plt.subplots(2, 1, figsize=(8, 8)) #  Create two vertically
stacked subplots

#if x < 0:
```

```
 #fx = 0
#if x>=0 and x<=L:
 #fx = np.sin(x/L)
#if x > L:
 #fx = 0

# Design the title of first graph for wave functions
ax1.set_title('Wave function')
ax1.set_xlabel('Position (x)')
ax1.set_ylabel('Wave function')
ax1.grid(True)

# Define the quantum number
n = 2 # n can be changed to 1,2 or 3
psi_n = np.sin( n * np.pi * x / L) # Wave function formula ψ_n(x) = sin(nπx/L)
ax1.plot(x, psi_n, label=f'n = {n}') #  Plot the wave function curve
ax1.legend()

# Design the second graph for probability density
ax2.set_title('Particle in a Box Probability Density')
ax2.set_xlabel('Position (x)')
ax2.set_ylabel('Probability Density')
ax2.grid(True)

n = 2
psi_n_squared = (np.sin(np.pi * x / L))**2
ax2.plot(x, psi_n_squared, label=f'n = {n}')
ax2.legend()

#  Display the two plots
plt.tight_layout()
plt.show()
```

When n=3:

```
import numpy as np
import matplotlib.pyplot as plt

L = 3 # Box length is fixed at L = 3
n_max = 3 # n can be changed to 1,2 or 3

x = np.linspace(0, L, 200) # Generate 200 points in the interval [0, L]

fig, (ax1, ax2) = plt.subplots(2, 1, figsize=(8, 8)) #  Create two vertically
stacked subplots

#if x < 0:
 #fx = 0
#if x>=0 and x<=L:
 #fx = np.sin(x/L)
#if x > L:
 #fx = 0

# Design the title of first graph for wave functions
ax1.set_title('Wave function')
ax1.set_xlabel('Position (x)')
ax1.set_ylabel('Wave function')
```

```
ax1.grid(True)

# Define the quantum number
n = 3 # n can be changed to 1,2 or 3
psi_n = np.sin( n * np.pi * x / L) # Wave function formula ψ_n(x) = sin(nπx/L)
ax1.plot(x, psi_n, label=f'n = {n}') #  Plot the wave function curve
ax1.legend()

# Design the second graph for probability density
ax2.set_title('Particle in a Box Probability Density')
ax2.set_xlabel('Position (x)')
ax2.set_ylabel('Probability Density')
ax2.grid(True)

n = 3
psi_n_squared = (np.sin(np.pi * x / L))**2
ax2.plot(x, psi_n_squared, label=f'n = {n}')
ax2.legend()

#  Display the two plots
plt.tight_layout()
plt.show()
```

2.2 Explanations and Graphs

numpy is used for numerical operations (creating arrays and evaluating sine functions).

matplotlib.pyplot is used for plotting graphs.

L = 3: Sets the length of the infinite potential well.

x = np.linspace(0, L, 200): Generates 200 points between 0 and L. These points are the positions where we evaluate the wave function.

plt.subplots(2, 1, figsize=(8, 8)): Creates a figure with two stacked subplots:

The first subplot (ax1) is for the wave function.

The second subplot (ax2) is for the probability density.

n = 1: Sets the quantum number. This value can be changed to n=1, 2 or 3.

psi_n = np.sin(n * np.pi * x / L): Implements the analytical solution for the wave function inside the infinite well.

ax1.plot(x, psi_n, label=f'n = {n}'): Plots the wave function versus position. The label shows which n value is being plotted.

ax1.legend(): Displays the legend for clarity.

psi_n_squared = (np.sin(n * np.pi * x / L))**2: Squares the wave function to obtain the probability density |ψn(x)|**2.

ax2.plot(x, psi_n_squared, label=f'n = {n}'): Plots the probability density.

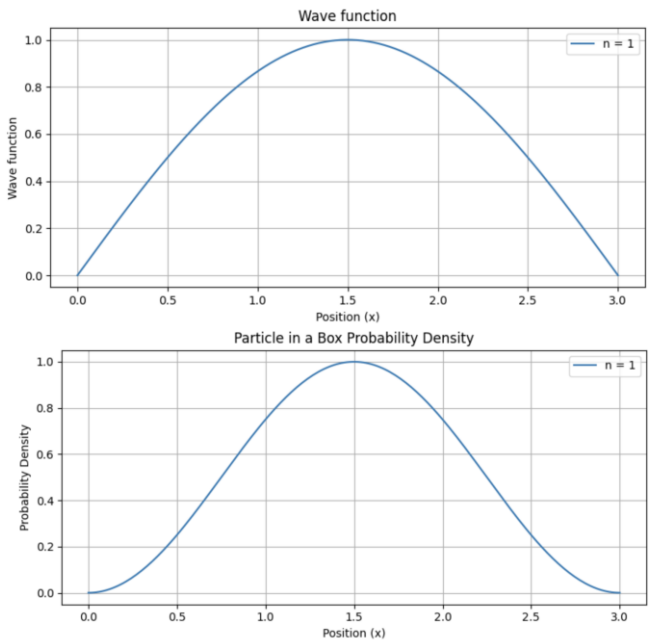
ax2.legend(): Adds the legend for clarity.

plt.tight_layout(): Prevents overlap between subplots.

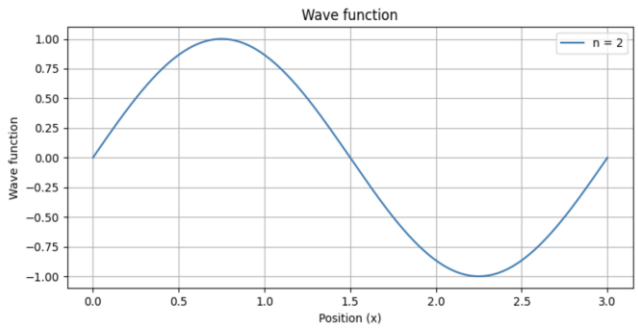
plt.show(): Renders the final figure with both subplots.

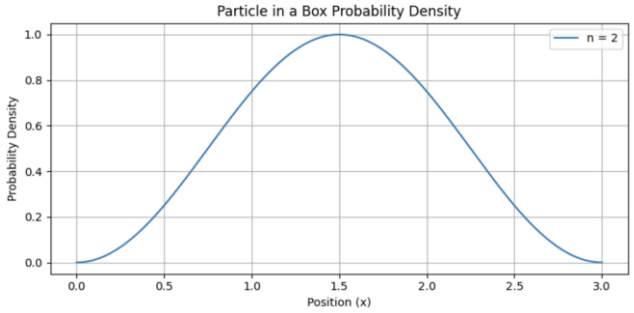
Above is the code generated by Google Colab and explanation of how the code works. Below are the wave function graph and Particle in a Box Probability Density graph when n=1, 2 or 3 respectively.

n=1:

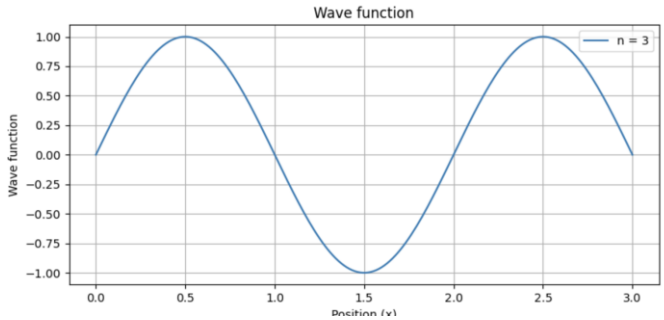


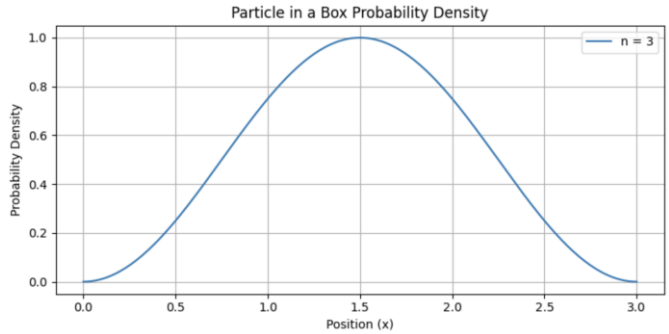
n=2:





n=3:





2.2 Graph Analysis

When n=1:

The first graph (wave function) shows the wave function ψ1. It has the form of a single half sine wave within the box (0<x<L), starting at zero at x=0, reaching a maximum at the center (x=L/2), and returning to zero at x=L. This represents the fundamental standing wave mode of the system. The fact that the wave function vanishes at the walls reflects the infinite potential barriers: the particle cannot exist outside the box.

The second graph plots $|| \psi(x) |^2$. The distribution peaks sharply at the center and decreases smoothly toward the edges. This means the particle is most likely to be found at the middle of the box and least likely near the boundaries. This is fundamentally different from the classical picture, where the particle would have a flat, uniform distribution.

When n=2:

The wave function $\psi(x)$ has one full sine wave in the box, with a node at x=L/2. The function oscillates between positive and negative values, but the sign itself has no direct physical meaning since probability depends on $|| \psi(x) |^2$.

The probability density $|| \psi(x) |^2$ now has two symmetric peaks: one between 0 and L/2, the other between L/2 and L. The center of the box becomes a forbidden point (zero probability). Thus, the particle is never found exactly at x=L/2, even though in the classical case the center is no different from other points.

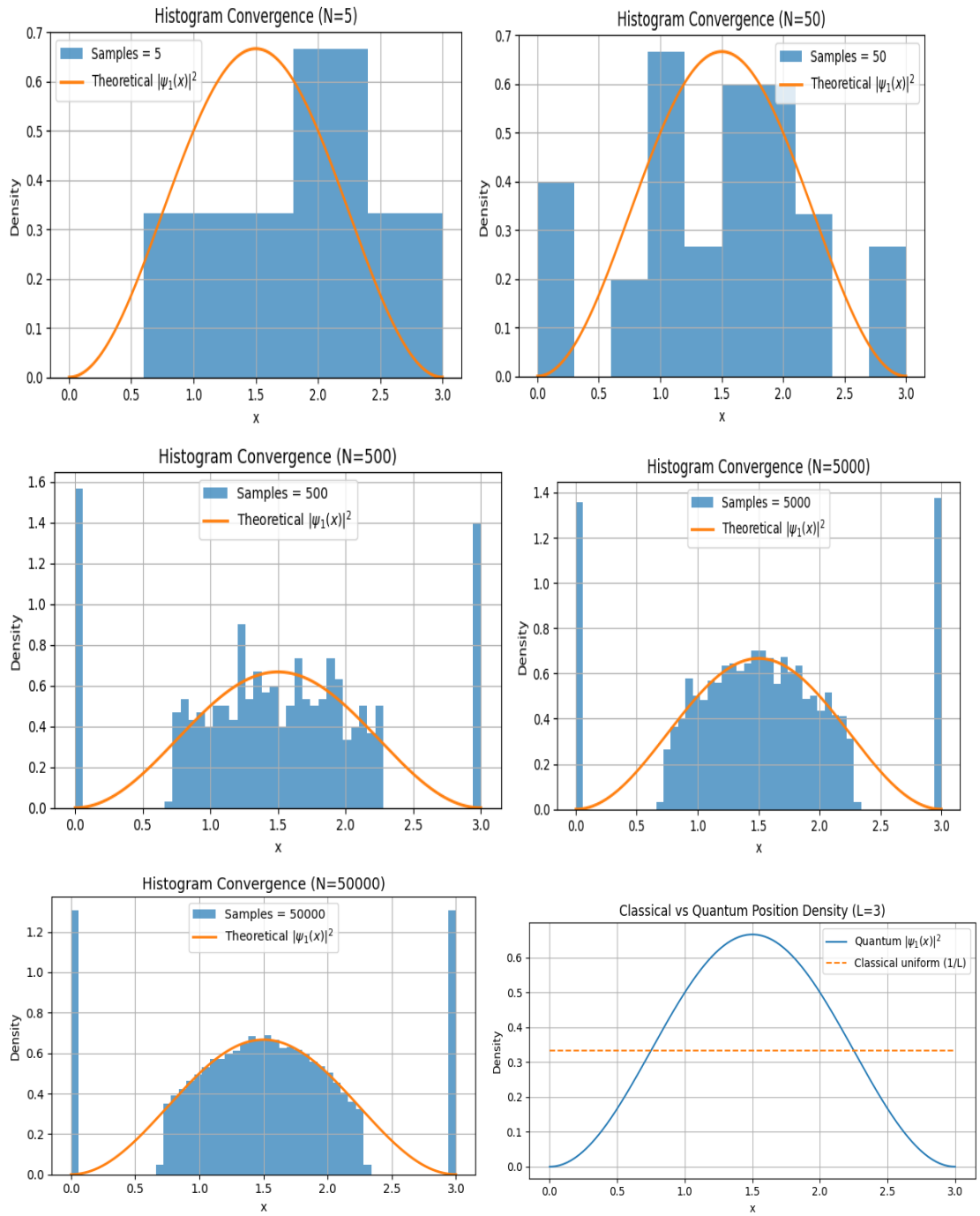
When n=3:

The wave function shows 1.5 sine oscillations within the box, with two internal nodes at x=L/3 and x=2L/3. Compared with n=1and n=2, the wave function oscillates more rapidly, indicating higher momentum components.

The probability density now exhibits three peaks: near x=L/6, x=L/2, and x=5L/6. Each peak corresponds to regions where the particle is most likely to be found, separated by nodes (zero-probability regions). The distribution is becoming increasingly structured and oscillatory.

2.3 Simulations

In this section, to illustrate the predictions of classical and quantum physics models, we simulated a one-dimensional particle-in-a-box system with L=3 by randomly drawing realizations of the particle position (for n = 1) and using histograms to show the results. The goal was to understand the two major differences in spatial distribution: in quantum mechanics, the probability of finding a particle at different positions varies, while in classical mechanics the probability distribution is uniform. Furthermore, in quantum mechanics, energy can only take discrete values, whereas in classical mechanics energy is continuous. We plotted histograms for five different scenarios, using varying sample sizes for particle positions (N=5, 50, 500, 5000, 50000). The histograms visually demonstrate the convergence of the random process toward the theoretical curve and compare it with the classical prediction.



In the classical case, the particle moves with constant velocity inside the box and bounces elastically at the walls. The probability of being in is the same everywhere, the formula should be classical(x)=$\frac{1}{L}$. This yields a flat, uniform distribution. But in the quantum case for n=1, the particle is most likely to be found at the center and least likely near the walls, as dictated by $|| \psi(x) |^2$. The distribution has a sinusoidal form, vanishing exactly at the boundaries.

These five histograms demonstrate how empirical distributions converge to the theoretical probability density as the number of samples increases

When **N = 5**: The histogram is very rough, with only a few counts. Although highly noisy, some clustering near the center is visible, hinting at the correct distribution.
When **N = 50**: The histogram begins to reveal the central preference, though fluctuations remain significant. Peaks and troughs are irregular.
When **N = 500**: The histogram becomes much smoother. The central peak and reduced edge probability are evident, closely approximating the analytic curve.
When **N = 5000**: The histogram aligns almost perfectly with the theoretical distribution. The shape is clear, with maximum probability at the box center and near-zero probability at the walls.
When **N = 50000**: The convergence is complete. The histogram and the theoretical curve are practically indistinguishable, confirming the probabilistic interpretation of the wave function.

The final graph illustrates the differences between quantum physics and classical physics. The orange dashed line represents the classical prediction, while the blue sinusoidal curve represents the quantum distribution. This comparison highlights their key differences: the orange dashed line is uniform everywhere, while the blue curve shows a structured distribution, with a higher probability density in the central region.

The second major difference is the quantization of energy, which is in quantum mechanics, energy levels are discrete, whereas in classical physics, energy can take any value. In the formula of classical physics: $\frac{1}{2}mv^2$, it can have any positive value. Thus, the spectrum is continuous.

For the quantum energy, the boundary conditions impose discrete allowed wavelengths, leading to quantized energies: $En = \frac{n^2h^2}{8mL^2}$, n=1,2,3…

For example: $E1 = \frac{1h^2}{8mL^2}$, $E2 = \frac{4h^2}{8mL^2}$, $E3 = \frac{9^2h^2}{8mL^2}$

Intermediate values such as $En = \frac{1.5h^2}{8mL^2}$are forbidden. This discreteness has no counterpart in classical mechanics and represents one of the defining features of quantum theory. Thus, the particle in a box provides a way to see for the first time and in a very simple setting purely quantum behaviors: (1) non-uniform probability densities, and (2) discrete energy levels. These

are the two central differences from classical mechanics and form the foundation of quantum physics.

The particle in a box idealization is not only a simplified model used in introductory quantum mechanics courses, it also provides an intuitive understanding of the behavior of electrons in atoms. In atomic physics, electrons do not move freely in space. Instead, they are confined to a small region around the atomic nucleus by the Coulomb attraction between positively charged protons and negatively charged electrons. This confinement is analogous to a "box": the electron cannot escape the box without additional energy. Moreover, within the atom, it must satisfy boundary conditions, just like the wave function of a box particle.

In classical physics, one might typically imagine electrons orbiting the atomic nucleus like planets orbiting the sun. However, electrons have discrete energy orbits, just like the particle in a box.

If electrons were classical particles, their energies could assume any value, and atoms would emit a continuous spectrum of light. However, we observe discrete emission and absorption lines, which directly confirms that electrons behave in accordance with quantum mechanics.

The probability density of the particle in a box also reflects the structure of the atomic orbitals. In the ground state ($n = 1$), the probability is highest at the center. Likewise, in the orbits of a hydrogen atom, the electron is most likely to be near the nucleus when $n = 1$, with the probability decreasing outward. For higher energy states ($n = 2, 3, ...$), the box particle forms a node with a probability of exactly zero.

3. Conclusion

The particle-in-a-box model has long been one of the clearest ways to distinguish classical physics from quantum mechanics. In classical physics, a particle inside a box behaves like a bouncing ping-pong ball. It moves at a constant velocity, bounces off the walls, and has equal probability of appearing anywhere in the box. Its energy depends only on its velocity and can therefore take on any positive value. This leads to a simple, flat probability distribution and a continuous energy distribution.

Quantum mechanics tells a very different story. When we solve the Schrödinger equation for an infinitely deep potential well, the particle's wave function appears as standing waves inside the box. These waves must "fit" perfectly within the box, meaning they have only

specific wavelengths and, therefore, only specific energies. The energy is quantized and can only take on values like E1, E2, E3...; no intermediate values are possible. Meanwhile, the square of the wave function, $|| \psi(x) |^2$, gives the probability of finding the particle at each point. This distribution is not uniform: in the ground state (n = 1), the particle is most likely to be at the center; in higher states, the probability splits into several peaks separated by nodes where the particle can never be found. These two features—nonuniform probabilities and discrete energy levels—are the first clear examples of pure quantum behavior Belloni & Doncheski, 2003; Belloni, 2014; Abramson, 2020).

The Python simulations and histograms we created make these ideas very concrete. When the sample size is very small, the histogram is noisy, but as the sample size increases, the shape becomes smoother and closer to the theoretical probability distribution. When the sample size is very large, the histogram matches $|| \psi(x) |^2$ almost exactly. This shows that while a single measurement in quantum mechanics is random, repeated experiments reveal the stable probability pattern predicted by theory (Krijtenburg-Lewerissa, 2020; Wang & Feng, 2024). Comparison with a classical flat line further emphasizes that classical physics cannot explain the structured patterns of quantum mechanics.

The particle in the box model is more than just a classroom example. It is closely related to atomic physics, where electrons are bound to the nucleus by electric forces. Like the particle in the box, electrons can only occupy specific energy states, which explains why atoms emit and absorb light at discrete frequencies (Belloni & Doncheski, 2003; Riggs, 2013). The probability distribution of the box model is also similar to that of atomic orbitals. Without this quantization, atoms would not be stable, and matter as we know it would not exist.

In summary, the particle in the box model helps us understand the main principles and features of quantum mechanics in a very simple setting. It shows that the world of quantum physics does not follow the same rules as everyday objects. Quantum systems are not governed by continuous energy and uniform distribution, but by discrete energy levels and probabilistic patterns. This model lays the foundation for understanding more complex quantum mechanical systems and provides an intuitive understanding for modern applications such as atoms and quantum dots, and nanotechnology.

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