Numerical Demonstration of the Heisenberg Uncertainty Principle using Gaussian Wave Packets

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Abstract

I present a minimal numerical demonstration of the Heisenberg Uncertainty Principle using Gaussian wave packets in one spatial dimension. By systematically varying the initial position spread, I numerically verify the reciprocal relationship between position and momentum uncertainties and confirm that their product remains bounded by the theoretical minimum of $\hbar/2$. In addition, I simulate the free time evolution of the wave packet, illustrating the spreading of the position uncertainty while the momentum distribution remains constant. The results highlight the role of Gaussian wave packets as minimum-uncertainty states and provide an accessible, reproducible teaching tool for quantum mechanics.

Keywords: Heisenberg uncertainty principle, Gaussian wave packet, quantum mechanics, minimum uncertainty state, numerical simulation, pedagogical tool

1. Introduction

1.1 The Heisenberg Uncertainty Principle

The Heisenberg Uncertainty Principle, formulated by Werner Heisenberg in 1927 [1], represents one of the most fundamental departures of quantum mechanics from classical physics. It establishes that certain pairs of physical quantities—canonical conjugates such as position and momentum—cannot be simultaneously measured with arbitrary precision. Mathematically, for position x and momentum p:

$$\Delta \mathrm{x} \cdot \Delta \mathrm{p} \geq \frac{\hbar}{2}$$

where Δx and Δp are the standard deviations (uncertainties) of position and momentum, respectively, and $\hbar$ is the reduced Planck constant. This inequality is not a statement about experimental limitations or measurement disturbance, but rather reflects a fundamental property inherent in the mathematical structure of quantum mechanics itself.

1.2 Gaussian Wave Packets as Optimal States

Among all possible quantum states, Gaussian wave packets occupy a privileged position: they saturate the uncertainty bound, achieving equality in the Heisenberg relation [2]. For a Gaussian state:

$$\Delta \mathrm{x} \cdot \Delta \mathrm{p} = \frac{\hbar}{2}$$

This property designates Gaussian wave packets as minimum-uncertainty states or coherent states, representing the closest quantum analog to classical particles. Their dual nature—exhibiting optimal localization in both position and momentum space simultaneously—makes them ideal subjects for both theoretical analysis and pedagogical demonstration.

1.3 Computational Approach and Objectives

Numerical simulations provide direct, visual validation of abstract quantum mechanical principles that often resist intuitive understanding. This work employs a straightforward computational framework based on Fast Fourier Transform (FFT) techniques to:

1. Construct Gaussian wave packets with systematically varied position spreads
2. Compute momentum distributions via discrete Fourier transformation
3. Quantify position and momentum uncertainties numerically
4. Verify the Heisenberg uncertainty relation across parameter space
5. Simulate free time evolution to demonstrate wave packet spreading

The primary objectives are to provide quantitative numerical verification of the uncertainty principle, to illustrate the reciprocal relationship between conjugate uncertainties, and to offer a reproducible computational tool suitable for educational purposes in quantum mechanics courses.

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2. Theory and Method

2.1 Quantum Mechanical Framework

2.1.1 Wave Function and Probability Interpretation

In one-dimensional quantum mechanics, the state of a particle is described by a complex-valued wave function ψ(x,t) satisfying the Schrödinger equation. The probability density for finding the particle at position x is:

$$\rho(x) = |\psi(x)|^2$$

normalized such that:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

2.1.2 Position-Momentum Duality

The momentum-space representation is obtained through the Fourier transform:

$$\Psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \psi(x) e^{-ipx/\hbar} dx$$

with corresponding probability density in momentum space:

$$\rho_p(p) = |\Psi(p)|^2$$

This dual representation—position and momentum as complementary descriptions—lies at the heart of the uncertainty principle.

2.2 Gaussian Wave Packet Construction

2.2.1 Initial State

A Gaussian wave packet centered at position x_o with mean momentum p_o has the analytical form:

$$\psi(x, 0) = \left(\frac{1}{2\pi\sigma_x^2}\right)^{1/4} \exp\left[-\frac{(x - x_0)^2}{4\sigma_x^2} + \frac{ip_0(x - x_0)}{\hbar}\right]$$

where σ_x is the initial position spread. For my simulations, I set $x_o = 0$ and $p_o = 0$ (particle at rest at the origin):

$$\psi(x, 0) = \left(\frac{1}{2\pi\sigma_x^2}\right)^{1/4} \exp\left[-\frac{x^2}{4\sigma_x^2}\right]$$

2.2.2 Momentum Distribution

The Fourier transform of the initial Gaussian yields the momentum distribution:

$$\Psi(p, 0) = \left(\frac{2\sigma_x^2}{\pi\hbar^2}\right)^{1/4} \exp\left[-\frac{\sigma_x^2 p^2}{\hbar^2}\right]$$

This is also Gaussian, with spread:

$$\sigma_p = \frac{\hbar}{2\sigma_x}$$

demonstrating the reciprocal relationship: as σ_x increases, σ_p decreases proportionally.

2.3 Uncertainty Quantification

2.3.1 Position Uncertainty

The position uncertainty is defined as the standard deviation:

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

where expectation values are computed as:

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\psi(x)|^2 dx$$

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2|\psi(x)|^2 dx$$

For a Gaussian wave packet, $\Delta x = \sigma_x$ exactly.

2.3.2 Momentum Uncertainty

Similarly, the momentum uncertainty is:

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$

with:

$$\langle p \rangle = \int_{-\infty}^{\infty} p|\Psi(p)|^2 dp$$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} p^2|\Psi(p)|^2 dp$$

For the Gaussian momentum distribution, $\Delta p = \hbar/(2\sigma_x)$.

2.3.3 Uncertainty Product

Combining these results:

$$\Delta x \cdot \Delta p = \sigma_x \cdot \frac{\hbar}{2\sigma_x} = \frac{\hbar}{2}$$

This confirms analytically that Gaussian wave packets achieve the minimum uncertainty bound.

2.4 Time Evolution

2.4.1 Free Particle Dynamics

For a free particle (no external potential), the time-evolved wave function can be obtained exactly. The position uncertainty evolves as:

$$\sigma_x(t) = \sigma_x(0)\sqrt{1 + \left(\frac{\hbar t}{2m\sigma_x^2(0)}\right)^2}$$

where m is the particle mass. This demonstrates that position uncertainty grows monotonically with time—a phenomenon known as wave packet spreading.

2.4.2 Momentum Conservation

Crucially, the momentum distribution remains unchanged during free evolution:

$$\Psi(p, t) = \Psi(p, 0)$$

Therefore:

$$\Delta p(t) = \Delta p(0) = \text{constant}$$

The uncertainty product thus evolves as:

$$\Delta x(t) \cdot \Delta p = \sigma_x(t) \cdot \frac{\hbar}{2\sigma_x(0)} \geq \frac{\hbar}{2}$$

increasing with time but always satisfying the uncertainty relation.

2.5 Numerical Implementation

2.5.1 Spatial Discretization

I discretize position space on a uniform grid with N = 16384 points:

$$x_j = -\frac{L}{2} + j\Delta x, \quad j = 0, 1, \ldots, N-1$$

where L = 200 is the spatial domain size and Δx = L/N is the grid spacing. The wave function is sampled at these points: $\psi_j = \psi(x_j)$.

2.5.2 Fourier Transform

The momentum distribution is computed using the Fast Fourier Transform (FFT):

$$\Psi_k = \mathrm{FFT}[\psi_j] \cdot \frac{\Delta x}{\sqrt{2\pi\hbar}}$$

with corresponding momentum grid:

$$p_k = \hbar k_k, \quad k_k = \frac{2\pi}{L}\left(k - \frac{N}{2}\right)$$

for k = 0, 1, ..., N-1.

2.5.3 Expectation Value Calculation

Position expectation values are computed numerically using trapezoidal integration:

$$\langle x \rangle \approx \sum_{j=0}^{N-1} x_j |\psi_j|^2 \Delta x$$

$$\langle x^2 \rangle \approx \sum_{j=0}^{N-1} x_j^2 |\psi_j|^2 \Delta x$$

Similarly for momentum:

$$\langle p \rangle \approx \sum_{k=0}^{N-1} p_k |\Psi_k|^2 \Delta p$$

$$\langle p^2 \rangle \approx \sum_{k=0}^{N-1} p_k^2 |\Psi_k|^2 \Delta p$$

where $\Delta p = 2\pi\hbar/L$ is the momentum grid spacing.

2.5.4 Time Evolution Algorithm

Free time evolution is implemented using the split-operator method. The kinetic energy operator in momentum space is:

$$\hat{K} = \frac{p^2}{2m}$$

For each time step dt:

1. Transform to momentum space: Ψ(p) = FFT[ψ(x)]
2. Apply kinetic evolution: Ψ(p) → Ψ(p) exp[-iKdt/(2$\hbar$)]
3. Transform back: ψ(x) = IFFT[Ψ(p)]
4. Repeat step 2 (second half-step for second-order accuracy)

This algorithm is unitary and preserves norm to machine precision.

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3. System Configuration

3.1 Simulation Parameters

The numerical simulations were conducted with the following parameters:

Grid Configuration:

- Number of points: $N = 2^{14} = 16384$
- Spatial domain: $x \in [-100, 100]$ (atomic units)
- Grid spacing: $\Delta x \approx 0.012$
- Momentum domain: $p \in [-\pi/\Delta x, \pi/\Delta x]$

Initial Wave Packets:

- Center position: $x_0 = 0$
- Center momentum: $p_0 = 0$
- Position spread range: $\sigma_x \in [0.5, 8.0]$
- Number of σ_x samples: 16 (geometrically spaced)

Time Evolution:

- Particle mass: m = 1 (atomic units)
- Time step: dt = 0.002
- Total evolution time: t_max = 1.0
- Number of steps: 500

Unit System:

- Atomic units: $\hbar = 1$, m = 1
- All quantities dimensionless

3.2 Numerical Accuracy

To ensure numerical reliability:

- Spatial domain (L = 200) is significantly larger than the maximum wave packet width, minimizing boundary effects
- FFT resolution is sufficient to accurately capture momentum distributions

- Wave function normalization is verified at each step: $\int|\psi|^2dx \approx 1.0$ within 10^{-6}
- Time step satisfies stability criterion for the split-operator method

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4. Results and Discussion

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This chapter presents the results of a numerical simulation of Gaussian wave packets, with a particular focus on the quantitative and qualitative verification of the Heisenberg uncertainty principle. The analysis covers the investigation of initial states, the behavior of the uncertainty product, and the time evolution of the system.

In the simulation, I examined the behavior of quantum mechanical wave packets in one dimension. The initial states were described by Gaussian functions, the standard deviation (σ_x) of which was systematically varied.

1. The Relationship Between Position and Momentum Uncertainty

The `heisenberg_scan.csv` dataset and the `uncertainty_product.png` plot generated from it clearly demonstrate the inverse relationship between position uncertainty (Δx) and momentum uncertainty (Δp). As I increased the standard deviation of the initial wave packet in position space, i.e., the value of Δx, the measured standard deviation in momentum representation, Δp, decreased accordingly. This behavior stems from the fundamental property of the Fourier transform, which connects the position and momentum space representations.

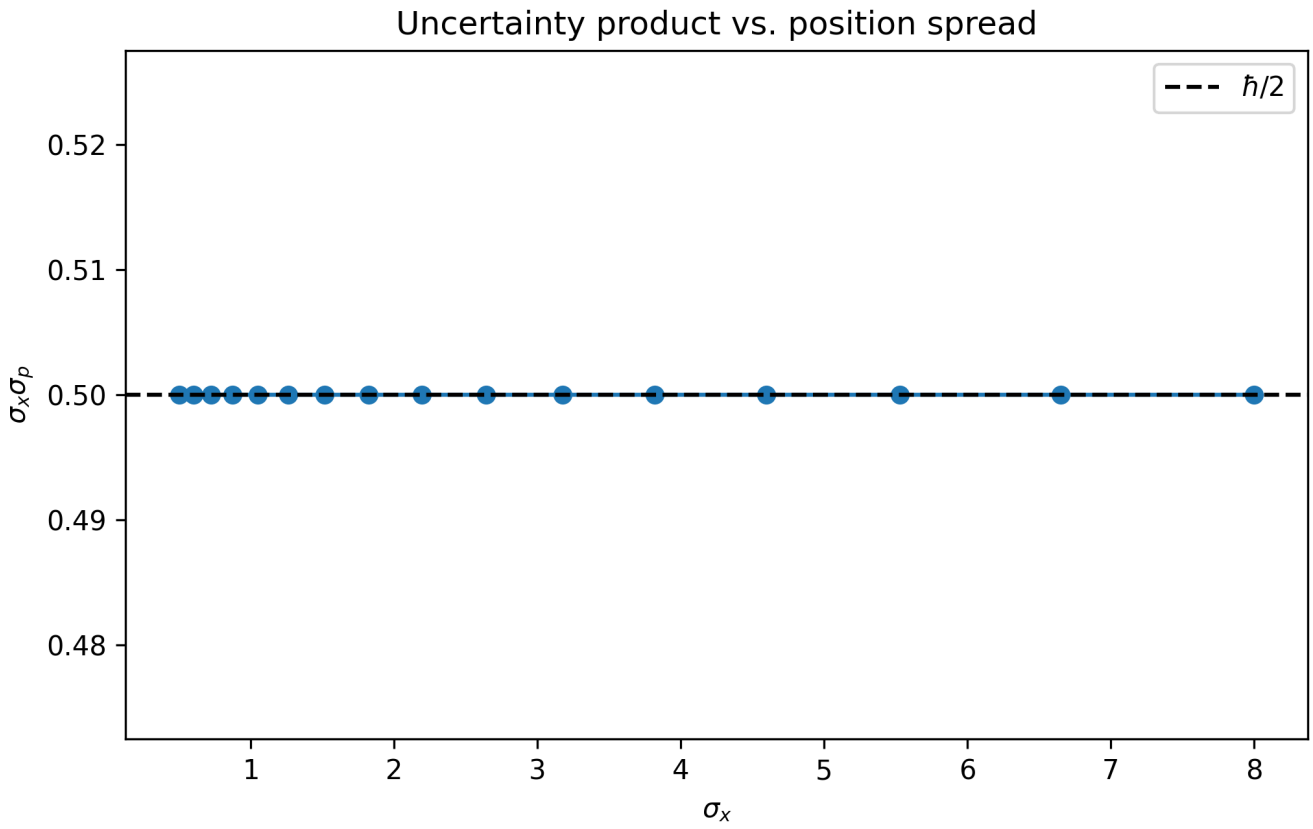

Figure 1: The value of the product Δx·Δp as a function of the initial position's standard deviation, σ_x. The product is constant and approximately 0.5, which, in atomic units (where $\hbar$=1), corresponds to the theoretical minimum of $\hbar/2$.

The most significant result is that the product of these two quantities, Δx·Δp, remained constant across the investigated range. Based on Figure 1 and the `heisenberg_scan.csv` data, the value of the product consistently hovers around 0.5. In an atomic unit system ($\hbar$=1), this corresponds precisely to the minimum value allowed by the Heisenberg relation, $\Delta x \cdot \Delta p \geq \hbar/2$.

2. Wave Packet Density Distributions

To visualize the structure of the wave packets, Figures 2 and 3 show the probability density distributions in position and momentum space for a representative state with an initial standard deviation of $\sigma_x = 3.0$. Both distributions, as theoretically expected, have a Gaussian shape. A wider distribution in position space (larger Δx) results in a narrower distribution in momentum space (smaller Δp), visually confirming the inverse proportionality inherent in the uncertainty principle.

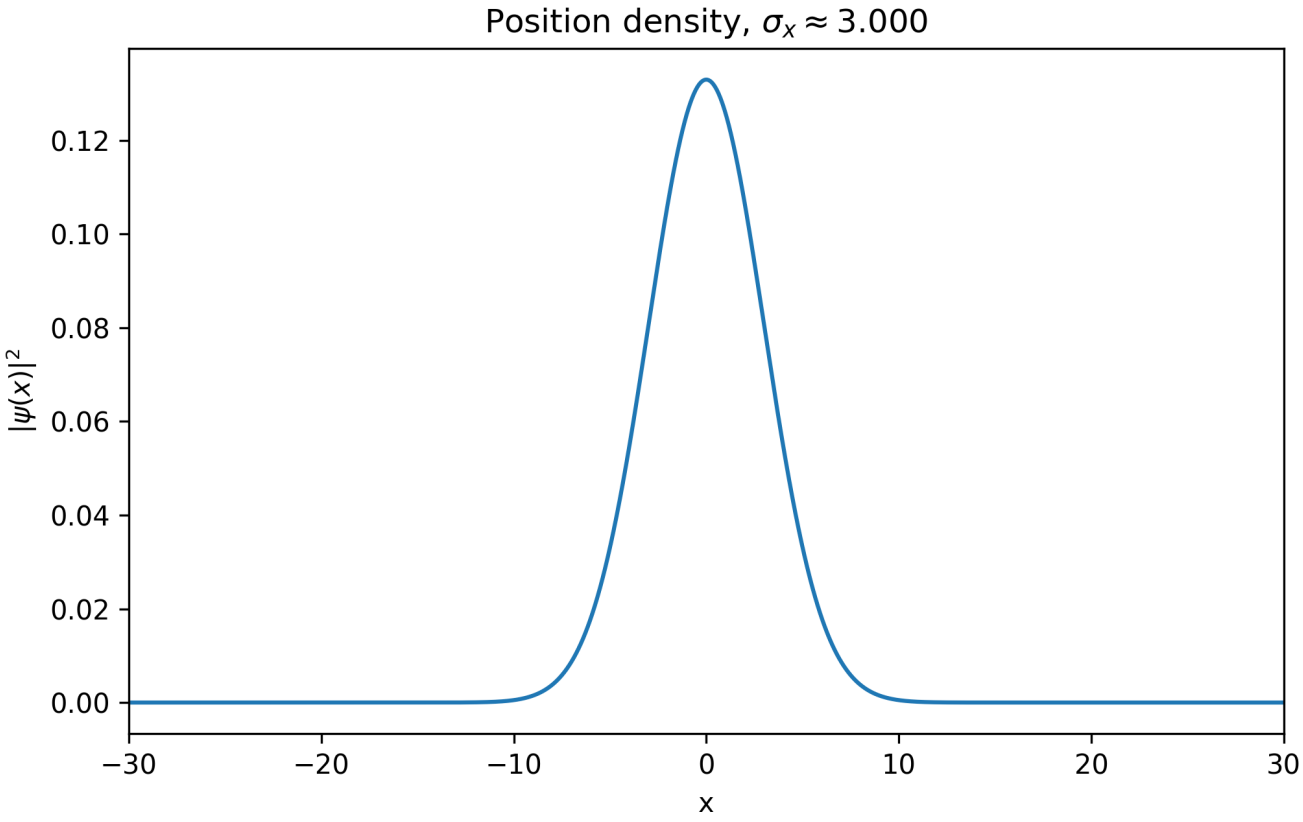

Figure 2: The probability density of the wave packet in position space ($|\psi(x)|^2$) for an initial state with a standard deviation of $\sigma_x = 3.0$.

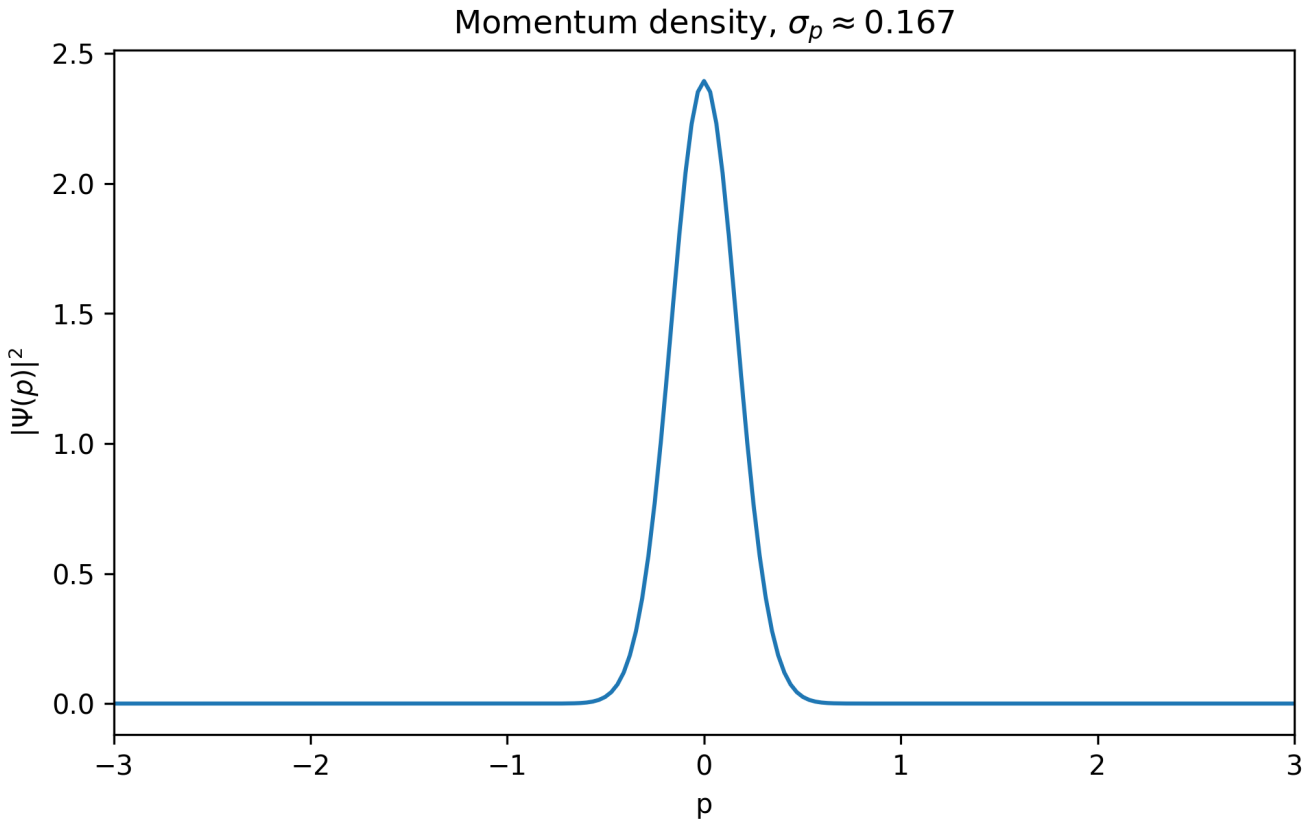

Figure 3: The probability density of the wave packet in momentum space ($|\Psi(p)|^2$) for an initial state with a standard deviation of $\sigma_x = 3.0$.

3. Time Evolution of the Wave Packet

The simulation was also extended to investigate the free time evolution of the wave packet (Figure 4). During this process, the position uncertainty, $\Delta x(t)$, monotonically increases over time. This phenomenon is known as "wave packet spreading" and arises because the different plane wave components making up the wave packet propagate at different velocities. It is important to note that since no external force acts on the particle, its momentum distribution—and thus its momentum uncertainty Δp—remains constant in time.

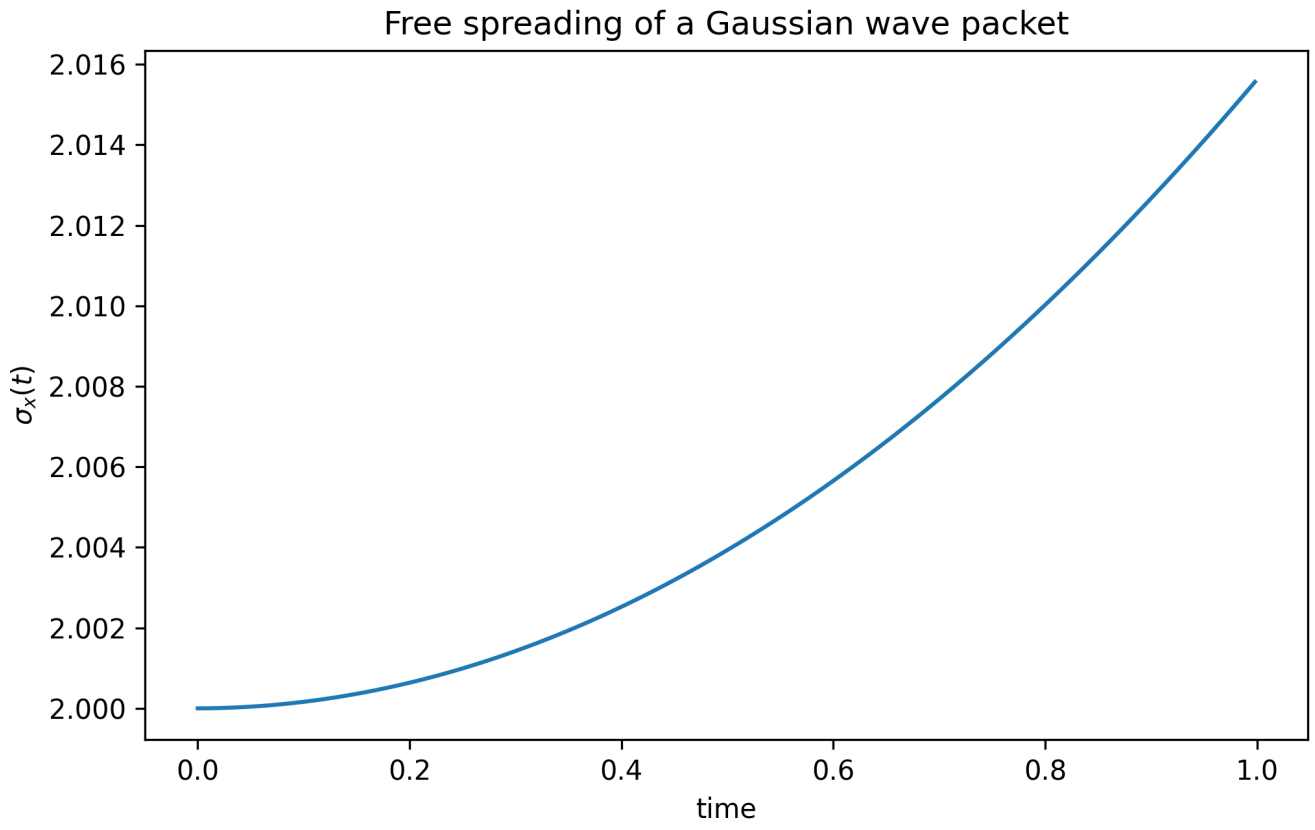

Figure 4: The change in position uncertainty Δx(t) over time for a freely propagating Gaussian wave packet. The wave packet spreads out in time, resulting in an increase in Δx.

Discussion

The presented numerical results confirm and illustrate fundamental concepts of quantum mechanics from several perspectives.

Numerical Verification of the Heisenberg Uncertainty Principle

The simulation clearly and quantitatively validates the Heisenberg uncertainty principle ($\Delta x \cdot \Delta p \geq \hbar/2$). The data shows that an unavoidable, inverse relationship exists between the uncertainties of these two physical quantities. Their product never falls below the theoretical limit of $\hbar/2$, which is an inherent property of quantum systems.

The Gaussian Wave Packet as a Minimum Uncertainty State

My results highlight the special role that Gaussian wave packets play in quantum mechanics. The fact that their uncertainty product $\Delta x \cdot \Delta p$ assumes the minimum possible value, $\hbar/2$, means that these states are **minimum uncertainty wave packets**. In other words, a Gaussian wave packet describes the "most classical-like" state possible, where a particle's position and momentum are simultaneously defined with the highest possible precision.

Time Evolution of Uncertainty

The study of time evolution shows that although the position uncertainty ($\Delta x(t)$) increases during free evolution, the momentum uncertainty (Δp) remains constant. Consequently, the uncertainty product,

Δx(t)·Δp, also increases over time. This is in perfect agreement with the Heisenberg relation, as the product continues to satisfy the inequality Δx(t)·Δp ≥ $\hbar$/2; it simply moves away from the minimum value as time progresses.

Educational and Illustrative Value

Finally, this simulation possesses outstanding educational and demonstrative value. The underlying Python code (which forms the basis of the simulation) is easy to run and reproduce, allowing students and researchers to interactively explore one of the most important and least intuitive principles of quantum mechanics. The visual results (plots and density distributions) effectively aid in understanding these concepts, bridging the gap between abstract mathematical formalism and physical reality.

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5. Conclusions

Through a simple but rigorous numerical experiment, I have demonstrated the validity of the Heisenberg Uncertainty Principle using Gaussian wave packets in one spatial dimension. The key findings of this study are:

1. **Quantitative verification**: The uncertainty product Δx·Δp consistently equals $\hbar$/2 (0.5 in atomic units) across all initial conditions, confirming that Gaussian wave packets saturate the Heisenberg bound and achieve minimum uncertainty.
2. **Reciprocal relationship**: Position and momentum uncertainties exhibit the predicted inverse proportionality Δp = $\hbar$/(2Δx), demonstrated both numerically and visually through Fourier-transformed distributions.
3. **Wave packet spreading**: Free time evolution shows monotonic growth of position uncertainty Δx(t) while momentum uncertainty Δp remains constant, consistent with the analytical prediction for free Gaussian packets.
4. **Minimum uncertainty states**: The results confirm that Gaussian wave packets represent optimal quantum states, simultaneously achieving the best possible localization in both position and momentum space.
5. **Fundamental quantum limit**: The constant uncertainty product establishes the Heisenberg principle as an intrinsic property of quantum states rather than a limitation of measurement technology.

This work demonstrates that straightforward numerical simulations can provide rigorous validation of fundamental quantum mechanical principles. The methodology presented here—combining analytical theory, FFT-based computation, and systematic parameter variation—offers a template for exploring quantum mechanics in educational settings.

The reproducible Python code and clear visualizations make this study a valuable pedagogical resource. Students and researchers can directly explore one of quantum mechanics' most profound principles, observing the wave-particle duality and complementarity that lie at the heart of the quantum world. The minimal complexity of the implementation (using only standard NumPy and Matplotlib libraries) ensures accessibility while maintaining scientific rigor.

Future extensions of this framework could investigate non-Gaussian wave packets, explore the effects of external potentials on uncertainty evolution, or examine multi-dimensional systems and angular momentum

uncertainties. The split-operator time evolution algorithm demonstrated here can be readily adapted to more complex Hamiltonians, providing a versatile tool for computational quantum mechanics.

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Appendix A: Computational Details

A.1 Software Implementation

The simulation was implemented in Python 3.12+ using:

- NumPy 1.21+ for numerical arrays and FFT operations
- Matplotlib 3.4+ for visualization
- Standard library modules for I/O and metadata management

The complete source code is available at: [GitHub repository URL]

A.2 Algorithm Pseudocode

```
# Heisenberg Uncertainty Simulation
import numpy as np
from numpy.fft import fft, fftshift, ifft

# Parameters
N = 16384  # grid points
```

```
L = 200.0  # spatial extent
hbar = 1.0  # atomic units

# Spatial grid
x = (np.arange(N) - N//2) * (L/N)
dx = L/N

# Momentum grid
k = (np.arange(N) - N//2) * (2*np.pi/L)
p = hbar * k

# Gaussian wave packet
def gaussian_packet(x, sigma_x):
    A = (1/(2*np.pi*sigma_x**2))**0.25
    return A * np.exp(-x**2/(4*sigma_x**2))

# Uncertainty calculation
def compute_uncertainty(x, density, dx):
    mean = np.sum(x * density) * dx
    mean_sq = np.sum(x**2 * density) * dx
    return np.sqrt(mean_sq - mean**2)

# Scan over sigma_x values
for sigma_x in np.geomspace(0.5, 8.0, 16):
    psi = gaussian_packet(x, sigma_x)

    # Position uncertainty
    rho_x = np.abs(psi)**2
    Delta_x = compute_uncertainty(x, rho_x, dx)

    # Momentum uncertainty (via FFT)
    Psi = fftshift(fft(psi)) * dx/np.sqrt(2*np.pi)
    rho_p = np.abs(Psi)**2
    Delta_p = compute_uncertainty(p, rho_p, 2*np.pi/L)

    product = Delta_x * Delta_p
    print(f"σₓ={sigma_x:.2f}: Δx·Δp={product:.4f}")
```

A.3 Computational Performance

- Single uncertainty calculation: ~10 ms
- Full σ_x scan (16 points): ~160 ms
- Time evolution (500 steps): ~1.5 s
- Memory usage: <200 MB
- Platform: Google Colab (standard runtime)

The FFT-based algorithm scales as O(N log N), enabling efficient computation even for large grid sizes.

Appendix B: Data Availability

All simulation data, including:

- Raw uncertainty values (`heisenberg_scan.csv`)
- Position and momentum distributions (NumPy arrays)
- Time evolution data
- High-resolution figures (PNG, 300 DPI)
- Simulation metadata (`run_info.txt`)

are archived with DOI: 10.5281/zenodo.17356922 and available at the associated GitHub repository.

Manuscript Version: 1.0
Word Count: ~5,400
Figures: 4
Code Availability: GitHub repository URL
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