



Quantum Mechanics Visualization Worksheet: Parameter Exploration

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Abstract

This worksheet is designed to deepen your understanding of quantum mechanics through computational visualization. You are provided with several Python codes that simulate different quantum potentials (e.g., simple harmonic oscillator, infinite and finite wells, anharmonic oscillator, Morse potential, hydrogen orbitals, and quantum tunneling). Your task is to modify parameters in these codes (such as potential heights, widths, grid resolution, initial conditions, etc.) and answer the specific questions below. These explorations will help you study how changes in the model affect the energy eigenvalues, eigenfunctions, and dynamic behaviors.

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1 Simple Harmonic Oscillator (SHO)

Objective: Explore the energy levels and eigenfunctions of the SHO by modifying parameters.

Relevant Equations:

- Potential:

$$V(x) = \frac{1}{2}\omega^2 x^2$$

- Energy eigenvalues (in atomic units, where $\hbar = 1$):

$$E_n = \omega \left(n + \frac{1}{2} \right)$$

- Eigenfunctions: The solutions are given in terms of Hermite polynomials (not shown here).

Instructions:

- Run the provided SHO code.
- Modify the potential to include a frequency parameter (i.e., $V(x) = \frac{1}{2}\omega^2 x^2$) and change ω .
- Change the number of grid points (adjust the variable N).

Answers:

1. Effect of Varying ω on Energy Levels:

The energy levels of the simple harmonic oscillator (SHO) depend linearly on the frequency parameter ω , as described by the theoretical formula:

$$E_n = \hbar\omega \left(n + \frac{1}{2} \right).$$

Since the code uses atomic units where $\hbar = 1$, this simplifies to:

$$E_n = \omega \left(n + \frac{1}{2} \right).$$

Upon modifying the potential in the code to include an adjustable ω , for example:

$$V(x) = \frac{1}{2}\omega^2 x^2,$$

it was observed that increasing ω causes all energy levels to increase proportionally. The spacing between adjacent energy levels also increases linearly with ω , consistent with the theoretical prediction. This validates that the numerically computed eigenvalues match the analytical result.

2. Impact of Increasing Grid Resolution on Accuracy:

The grid resolution, determined by the number of grid points N , significantly affects the numerical accuracy of the computed eigenfunctions and eigenvalues. When N is increased:

- The discretization of the kinetic energy operator becomes finer, yielding a more accurate approximation to the second derivative.
- The shape of the eigenfunctions more closely matches the analytical Hermite-Gaussian forms.
- The computed energy levels converge more closely to their exact values.

Conversely, a low value of N leads to noticeable numerical artifacts, including distortion in the wavefunctions and errors in energy levels, especially for higher excited states.

3. Change in Oscillatory Features of Eigenfunctions with Parameters:

The oscillatory behavior of the eigenfunctions (i.e., the number and position of nodes or extrema) is determined by the quantum number n and the spatial extent of the potential. Key observations include:

- Increasing ω compresses the potential well, localizing the eigenfunctions more tightly around $x = 0$. This results in more rapid oscillations over a smaller spatial region.
- Increasing N improves the resolution of these oscillations, allowing finer features (e.g., sharp peaks or closely spaced nodes) to be captured accurately.
- For higher energy levels (larger n), the number of nodes increases, consistent with quantum mechanical theory. These features are more accurately represented with a larger N and an appropriate spatial domain.

Overall, the combination of increasing ω and N reveals more detailed structure in the eigenfunctions, aligning well with theoretical expectations.

Code Fix:

No major errors were present. However, to enable frequency variation directly from the code, we defined the potential using a frequency parameter `omega`:

$$V = 0.5 \cdot \text{omega}^2 \cdot x^2$$

and allowed `omega` to be adjusted as a variable.

2 Infinite Potential Well

Objective: Investigate the energy spectrum and dynamics in an infinite potential well.

Relevant Equations:

- Potential:

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

- Eigenfunctions:

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

- Energy eigenvalues:

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

(In atomic units, you may set $\hbar = 1$ and $m = 1$.)

Questions:

1. How do the energy eigenvalues scale with the length L of the well?

Answer:

The energy eigenvalues scale inversely with the square of the well length L . That is,

$$E_n \propto \frac{1}{L^2}$$

Therefore, increasing L decreases the energy levels, and decreasing L increases them.

2. How do the eigenfunctions differ when you increase or decrease L ?

Answer:

The eigenfunctions depend on L through their wavelength and normalization. The general form is:

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

As L increases, the sine waves stretch out (longer wavelength), and the functions become wider. As L decreases, the eigenfunctions compress (shorter wavelength), oscillating more rapidly across the smaller domain.

Code Fix:

The original code uses x from 0 to L , which is fine, but we ensured that the spatial domain aligns with boundary conditions by avoiding the endpoints where the wavefunction should be zero. This can be done using:

```
x = np.linspace(dx, L - dx, N)
```

to avoid evaluating at the boundaries exactly.

3 Finite Potential Well

Objective: Explore the eigenvalue spectrum in a finite well.

Relevant Equations:

- Potential:

$$V(x) = \begin{cases} 0, & |x| < a, \\ V_0, & |x| \geq a. \end{cases}$$

- (No simple analytical solution for the eigenfunctions; the problem is solved numerically.)

Instructions:

- Run the finite well code and observe the eigenfunctions and energy levels.
- Change the potential barrier height V_0 and the well half-width a .
- Animate the time evolution of an excited state (e.g., $n = 4$).
- In the eigenfunction plot, overlay the shape of the well (the potential curve).

Answers:

1. **How does increasing V_0 affect the energy eigenvalues and the shape of the eigenfunctions?**

Answer:

Increasing the potential barrier height V_0 makes the finite well more closely resemble an infinite well. This leads to the following effects:

- **Energy eigenvalues increase:** As V_0 increases, the depth of the well effectively increases, allowing for more tightly bound states. However, the eigenvalues still remain below V_0 , and the spacing between levels becomes more like that of an infinite well.
- **Eigenfunctions become more localized:** The wavefunctions are more confined within the region $|x| < a$. The amplitude of the wavefunction in the classically forbidden region (i.e., tunneling outside the well) decreases significantly as V_0 increases.
- **Less tunneling:** For very large V_0 , the wavefunctions approach zero outside the well, mimicking the boundary conditions of an infinite potential well.

2. **How does changing a (the half-width of the well) impact the results?**

Answer:

Changing the width parameter a alters the size of the classically allowed region and has the following effects:

- **Increasing a widens the well, resulting in:**
 - Lower energy eigenvalues (due to a larger spatial confinement region).
 - More energy levels below the barrier V_0 , allowing more bound states.
 - Wavefunctions that are more spread out across the well.

- **Decreasing a** narrows the well, leading to:
 - Higher energy levels and fewer bound states (some may rise above V_0).
 - More rapid oscillations of eigenfunctions within a smaller spatial region.
 - Stronger penetration of the wavefunction into the barrier regions if V_0 is not sufficiently high.

Overall, a controls the spatial extent of the confinement, directly influencing the quantization of energy and the spatial structure of the wavefunctions.

Code Fix:

To make energy levels and wavefunctions easier to distinguish, we individually scaled eigenfunctions so that their maximum absolute amplitude was uniform:

```
scale = 0.5 / np.max(np.abs(eigvecs[:, n]))
```

This was already implemented correctly. Additionally, we verified that the potential plot is correctly overlaid using:

```
plt.plot(x, V, 'k--', label='Potential Well Shape')
```

4 Anharmonic Oscillator and Morse Potential

Objective: Study potentials with real-life applications by varying key parameters.

Relevant Equations:

- **Anharmonic Oscillator:**

$$V(x) = \frac{1}{2}x^2 + \lambda x^4,$$

where λ is the anharmonicity parameter.

- **Morse Potential:**

$$V(x) = D_e \left(1 - e^{-a(x-x_e)}\right)^2,$$

where D_e is the dissociation energy, a controls the width of the potential, and x_e is the equilibrium bond length.

Answers:

1. **How does increasing λ affect the energy levels compared to the harmonic oscillator case?**

Answer:

In the harmonic oscillator ($\lambda = 0$), the energy levels are equally spaced and given by:

$$E_n = \left(n + \frac{1}{2}\right), \quad \text{with } \hbar = \omega = 1.$$

In your code, the potential is modified to:

$$V(x) = \frac{1}{2}x^2 + \lambda x^4,$$

where $\lambda > 0$ adds an anharmonic term. As λ increases:

- The potential becomes steeper at larger $|x|$, making the well deeper at the edges.
- The energy levels become *non-uniformly spaced*.
- Higher energy levels increase more rapidly than lower ones.
- The spacing between adjacent levels increases with energy level n .

This leads to more realistic behavior for vibrational systems compared to the ideal harmonic oscillator.

2. **In the Morse potential, how do changes in D_e and a alter the depth and width of the potential well?**

Answer:

The Morse potential is defined in the code as:

$$V(x) = D_e \left(1 - e^{-a(x-x_e)}\right)^2,$$

where:

- D_e : Controls the **depth** of the potential well.
 - Increasing D_e : Deepens the well, allowing more bound vibrational states and lowering their energies.
 - Decreasing D_e : Shallower well, fewer bound states.
- a : Controls the **width** of the potential.
 - Increasing a : Narrows the well, resulting in stiffer potential walls and larger energy spacing.
 - Decreasing a : Widens the well, leading to looser confinement and more closely spaced levels.

These parameter changes visibly affect the potential shape and the computed eigenstates in your simulation.

3. What are the applications of the Morse and Anharmonic potentials?

Answer:

- **Morse Potential:**
 - Models vibrational energy levels of diatomic molecules.
 - Accurately represents bond dissociation (unlike the harmonic oscillator).
 - Useful in infrared spectroscopy, molecular dynamics, and chemical bonding analysis.
- **Anharmonic Oscillator:**
 - Used in quantum field theory (e.g., ϕ^4 theory) and perturbation theory.
 - Describes nonlinear interatomic forces and vibrational modes in solids and molecules.
 - Relevant in thermal expansion, crystal lattice modeling, and nonlinear optics.

Both potentials go beyond the harmonic approximation, making them essential tools for more realistic quantum mechanical modeling.

Code Fix:

The code currently only includes the anharmonic oscillator. To address the full assignment, we added a separate block to simulate the Morse potential:

```
# Morse potential:  $V(x) = D_e (1 - \exp(-a(x - x_e)))^2$ 
D_e = 10
a = 1.0
x_e = 0.0
V_morse = D_e * (1 - np.exp(-a * (x - x_e)))**2
H_morse = T + np.diag(V_morse)
eigvals_morse, eigvecs_morse = eigh(H_morse)
```

This block mirrors the structure used in other sections, with the Hamiltonian and eigenvalue problem solved numerically.

5 Hydrogen Atom Orbitals

Objective: Visualize and compare the electron density distributions for the Hydrogen 1s and 2p_z orbitals.

Relevant Equations:

- **Hydrogen 1s Orbital:**

$$\psi_{1s}(r) = \frac{1}{\sqrt{\pi}} e^{-r}, \quad |\psi_{1s}(r)|^2 = \frac{1}{\pi} e^{-2r},$$

where $r = \sqrt{x^2 + y^2 + z^2}$ (for a 2D slice, set one coordinate to 0).

- **Hydrogen 2p_z Orbital:**

$$\psi_{2p_z}(x, y, z) = \frac{1}{4\sqrt{2\pi}} z e^{-r/2},$$

with probability density $|\psi_{2p_z}(x, y, z)|^2$. (For a 2D slice, set $y = 0$.)

Answers:

1. **How does changing the grid resolution affect the visualization of the orbital shapes?**

Answer:

Grid resolution determines how finely the space is sampled when calculating and plotting the wavefunctions. Increasing the resolution (i.e., using more grid points):

- Produces smoother and more detailed contour plots.
- Reveals finer structures in the probability distributions, especially near nodal surfaces.
- Improves the accuracy of radial symmetry in the 1s orbital and the angular nodal plane in the 2p_z orbital.

Conversely, lower resolution can lead to pixelation, loss of detail, and incorrect representation of orbital symmetry.

2. **Compare the probability distributions of the 1s and 2p_z orbitals. What are the key differences, and how do they relate to the underlying quantum numbers?**

Answer:

The 1s and 2p_z orbitals differ significantly in shape and symmetry due to their quantum numbers:

- **1s Orbital** ($n = 1, \ell = 0, m = 0$):
 - Spherically symmetric (isotropic in all directions).
 - Probability density is highest at the nucleus and decreases monotonically outward.
 - No nodes (excluding the boundary at infinity).

- **$2p_z$ Orbital** ($n = 2, \ell = 1, m = 0$):
 - Has directional character aligned along the z -axis.
 - Contains a nodal plane at $z = 0$ where the probability density is zero.
 - Electron density is distributed in two lobes above and below the nucleus.

These differences arise from the angular momentum quantum number ℓ , which controls the presence of angular nodes and directional behavior in the orbital shape.

3. How can these visualizations help you understand electron density distributions in atoms?

Answer:

Visualizations of orbital probability densities make abstract quantum concepts tangible. They help in:

- Understanding where electrons are most likely to be found around the nucleus.
- Identifying nodal structures (regions of zero probability) associated with specific quantum numbers.
- Building intuition about chemical bonding, molecular orbital shapes, and electron cloud overlap.
- Relating theoretical wavefunctions to experimental observations like scanning tunneling microscopy and spectroscopy data.

These graphical insights are especially valuable when transitioning from single-electron atoms to more complex, multi-electron systems.

Code Fix:

We ensured the plotted ranges are symmetric and large enough to capture the full spatial structure of both $1s$ and $2p_z$ orbitals. To enhance clarity, we increased the number of contour levels:

```
contourf(..., levels=200, ...)
```

6 Quantum Tunneling Through a Potential Barrier

Objective: Explore the dynamic tunneling process by modifying barrier and wave packet parameters.

Relevant Equations:

- **Potential Barrier:**

$$V(x) = \begin{cases} V_0, & |x| < a, \\ 0, & |x| \geq a. \end{cases}$$

- **Transmission Coefficient (approximate for a rectangular barrier):**

$$T \approx e^{-2\kappa a}, \quad \kappa = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}},$$

where E is the energy of the incident particle.

Answers:

1. **How does increasing V_0 affect the transmission and reflection coefficients? Explain your observations.**

Answer:

Increasing the barrier height V_0 increases the potential energy difference between the wave packet and the barrier. When the particle energy $E < V_0$, the transmission coefficient T decreases exponentially according to the approximation:

$$T \approx e^{-2\kappa a}, \quad \kappa = \sqrt{2m(V_0 - E)}.$$

As a result, higher V_0 values cause:

- Lower transmission probability (less of the wave packet passes through).
- Higher reflection coefficient (more of the wave packet is reflected).

In the simulation, this is observed as a greater portion of the wave packet bouncing back from the barrier and a diminished transmitted wave on the far side.

2. **What is the effect of increasing the barrier width on the tunneling probability?**

Answer:

Increasing the width a of the potential barrier decreases the tunneling probability. This is because the wave function must decay exponentially within a wider classically forbidden region. From the same transmission approximation:

$$T \approx e^{-2\kappa a},$$

it is evident that T decreases exponentially with increasing a . Physically, a wider barrier provides more space for the wavefunction to decay, resulting in:

- Reduced amplitude of the transmitted wave.

- Longer interaction time with the barrier.

3. **How does changing the initial momentum k_0 of the wave packet alter the tunneling dynamics?**

Answer:

The initial momentum k_0 sets the kinetic energy of the wave packet via $E = \frac{k_0^2}{2}$. Increasing k_0 increases the particle's energy, which leads to:

- Greater likelihood of $E > V_0$, in which case the particle can classically pass over the barrier, resulting in near-complete transmission.
- A narrower wave packet in real space (due to the uncertainty principle), causing more precise and directed interaction with the barrier.
- Faster movement of the wave packet, reducing interaction time with the barrier.

Lowering k_0 , on the other hand, results in higher reflection and more pronounced tunneling behavior when $E < V_0$.

4. **Under which parameter regimes do you observe nearly complete transmission or reflection? Explain your reasoning.**

Answer:

- **Nearly complete transmission** is observed when the wave packet's energy exceeds the barrier height, i.e., $E = \frac{k_0^2}{2} > V_0$. In this case, the particle can pass over the barrier with minimal reflection. This can be achieved by increasing k_0 or lowering V_0 .
- **Nearly complete reflection** occurs when $E \ll V_0$ or the barrier is both tall and wide. In such regimes, the wavefunction decays significantly inside the barrier, leading to negligible tunneling probability.

These behaviors are consistent with the analytical tunneling probability expression and are visually apparent in the simulation through the dominance of either the reflected or transmitted components of the wave packet.

Code Fixes:

- Defined the wave packet energy explicitly as:

```
E_packet = 0.5 * k0**2
```

and printed it to validate against barrier height.

- To prevent unphysical reflections at the domain boundaries, we optionally implemented absorbing boundaries by multiplying `psi` with a decaying window (e.g., using a cosine mask).

7 General Discussion Questions

- **How do the numerical methods (e.g., finite differences, split-operator method) influence the accuracy of the simulation?**

Answer:

The accuracy of quantum simulations is closely tied to the choice and implementation of numerical methods:

- **Finite difference methods** approximate derivatives by discrete differences. They are simple to implement and effective for eigenvalue problems (e.g., in potential wells), but their accuracy depends on grid resolution. Too coarse a grid leads to poor approximation of the kinetic energy operator and eigenfunctions.
- **Split-operator methods** (used in time evolution problems like tunneling) leverage the separability of the Hamiltonian into kinetic and potential components. They are both stable and efficient for propagating wavefunctions in time, especially when combined with fast Fourier transforms (FFT). Their accuracy hinges on small time steps and well-resolved spatial grids.

Both methods strike a balance between computational cost and precision. However, care must be taken with boundary conditions and numerical stability, especially during long-time simulations.

- **What limitations did you encounter when changing parameters? Discuss possible reasons and solutions.**

Answer:

Several limitations were observed when exploring parameter space:

- **Grid resolution issues:** Increasing spatial or temporal resolution improves accuracy but significantly increases computational time and memory usage.
- **Unphysical artifacts:** For low grid resolution or large time steps, simulations may show spurious reflections or distorted wavefunctions. This is due to poor derivative approximations or numerical dispersion.
- **Normalization errors:** Extreme values of parameters (e.g., very narrow Gaussian wave packets or large barrier heights) may lead to normalization loss due to underflow or overflow in numerical computations.

Solutions: Use adaptive step sizes, verify convergence with finer grids, apply absorbing boundary conditions, and test edge cases to ensure robustness.

- **Reflect on how these computational explorations enhance your understanding of quantum mechanical phenomena.**

Answer:

These simulations bridge abstract theory with visual intuition. They allow:

- Dynamic observation of wave packet evolution, tunneling, and stationary states — phenomena that are otherwise difficult to visualize.
- Hands-on experimentation with parameters like potential shapes, barrier widths, and initial momentum, deepening insight into their physical significance.
- Better conceptual grasp of foundational ideas such as quantization, uncertainty, eigenstates, probability distributions, and superposition.

Overall, computational quantum mechanics serves as a powerful supplement to analytical methods, fostering a deeper and more interactive understanding of the quantum world.