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GUI PROJECT

PH311 — Quantum Mechanics and Application

USER MANUAL

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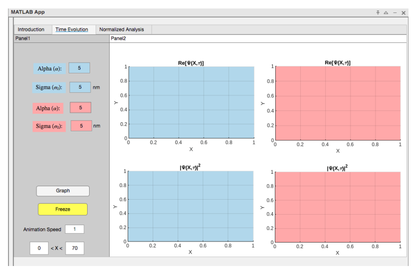
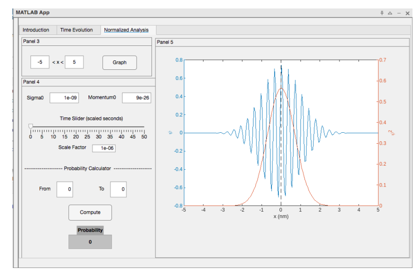
GAUSSIAN WAVE-PACKET

Module 1



Module 2



- Made Using MATLAB App Designer -

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1. Problem and Purpose

Generally solutions to the time independent Schrodinger equation, take bound state problems like rectangular barrier for example, involve planar waves with definite wavelength and indefinite locality. But practically speaking, it cannot be the case considering particles are localised in space, hence its associated matter wave should be localised. What Gaussian wave-packet does is introduce this locality with the expense of there being uncertainty in the particle's momentum; with the superposition of infinite planar waves having different wave numbers and frequencies, waves can constructively and destructively interfere in such a way that they get localised in space.

The aim of this GUI is to aid in analysis of the Gaussian Wave-packet, so that it can be incorporated with main problems in quantum mechanics such that the solution resembles more of reality. The user may grasp the effects of certain Gaussian parameters on the wave-packet itself considering the equation is not intuitive.

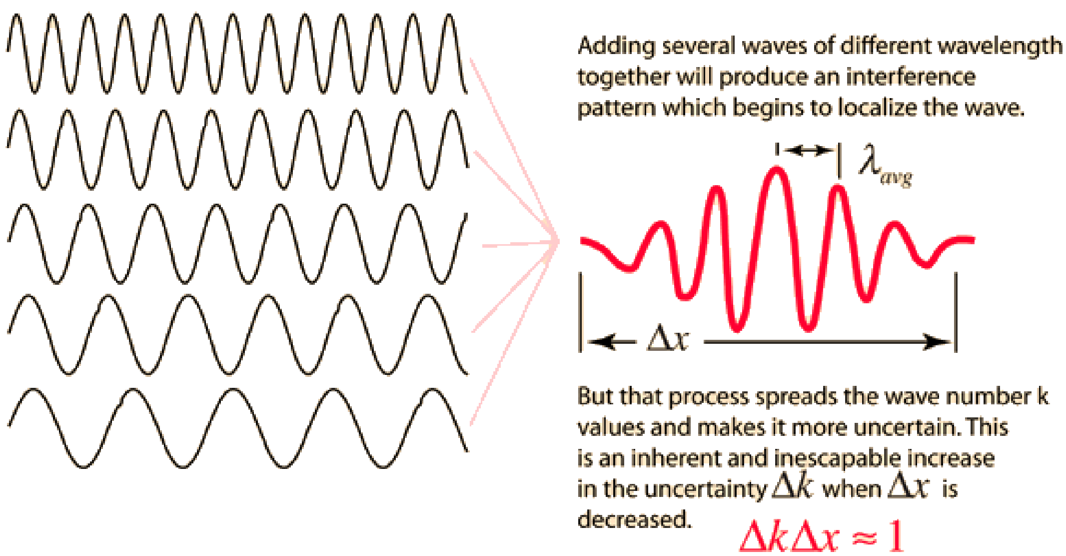
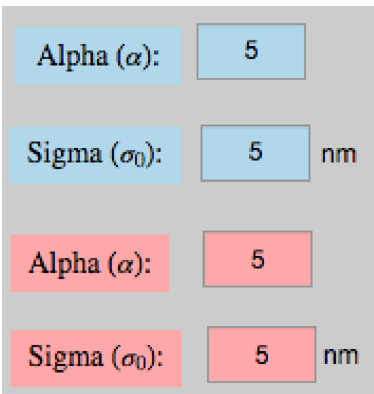


Figure 1: Source: *http://hyperphysics.phy-astr.gsu.edu/hbase/Waves/wpack.html*

2. Module 1: Time Evolution

Overview: This module provides insight on the time evolution of a Gaussian wave-packet, precisely for a free electron. Variation of certain parameters that govern the shape and time evolution of a Gaussian wave-packet, like σ and α, the GUI provides an animation for the evolution of the defined wave-packet across an arbitrary range of time values.

2.1. Explanation of Input Parameters



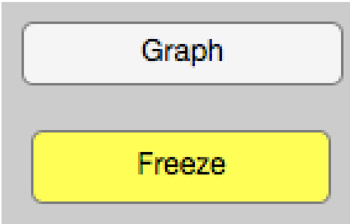
Alpha: A quantitative parameter related to the initial momentum of the Gaussian Wave-packet.

- **Range:** $-\infty < \alpha < \infty$
- Default Value: 5
- Negative Alpha indicates a negative momentum, hence the wave-packet evolves in -X direction with time.
- **Units:** Unit-less

$$\alpha = \frac{p_0 \sigma_0}{\hbar} \tag{1}$$

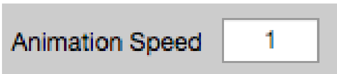
Sigma0: The essential parameter governing the initial spread of the Gaussian wave-packet, i.e the standard deviation from the mean at initial time, and the evolution of amplitude.

- **Range:** $0.1 < \sigma_0 < \infty$
- Default Value: 5
- The greater the value, the more the initial spread and initial amplitude.
- **Units:** Nanometers (nm)



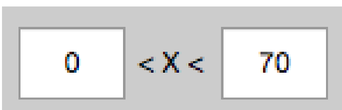
Graph Button: Displays the animation on the four graphs provided.

Freeze Button: Upon pressing, all animations on the four graphs will freeze. It will become slightly darker. In order to display graph again, this button must be clicked again and then the Graph Button must be clicked.



Animation Speed: Controls the speed at which the animation of the time evolution plays out.

- **Range: 0.1 to ∞**
- Default Value: 1
- A number smaller than 1 implies a slow animation and a number greater than 1 indicates animation speed fast relative that amount.

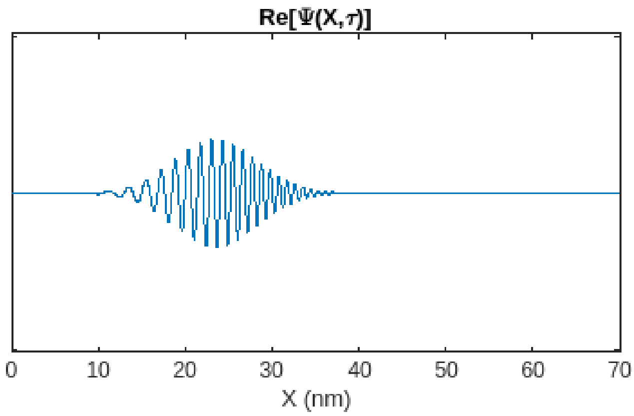


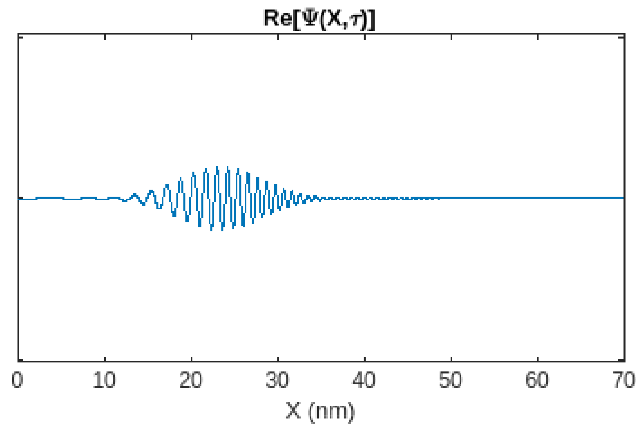
Domain of Graphs: The lower and upper values of the visible domain on graphs are to be put in the left and right box respectively.

- Value on the left must be less than the value on the right. It is possible both are positive or both are negative, or negative and positive; depending on the needs of the user.
- Default Value: $0 < X < 70$

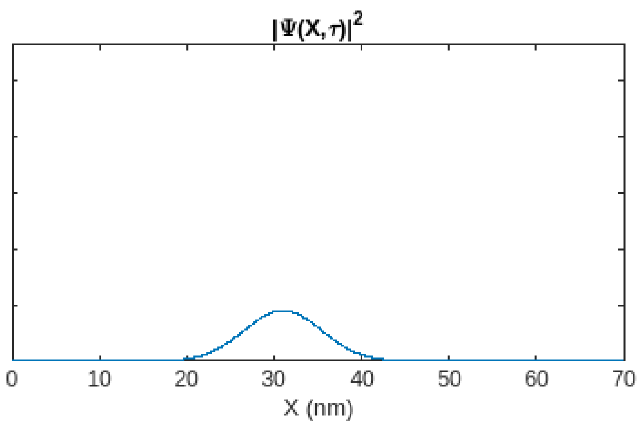
2.2. Outputs

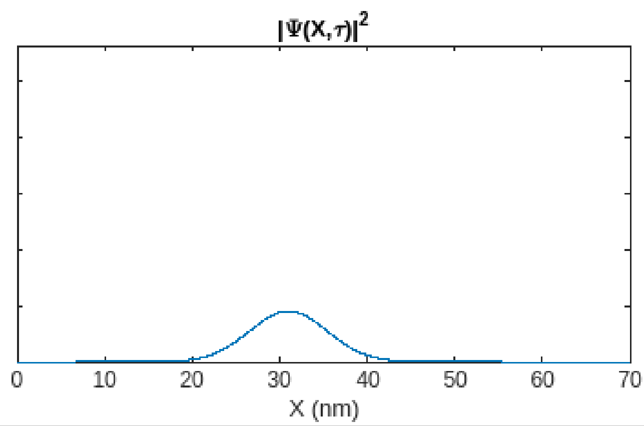
Real Component of the time evolution of wave-packet: It is on an arbitrary scale due to the denormalised parameters that define it. Across time, it is visible that the travelling wave-packet has a dispersion overtime and its amplitude decreases.





Probability Distribution of the time evolution of wave-packet: It is also on an arbitrary scale due to the denormalised parameters that define it. Across time, it is visible that probability distribution spreads and its amplitude decreases; ensuring that the total area under the graph remains constant due to necessity of particle existence.

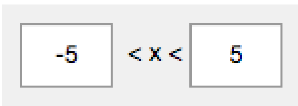




3. Module 2: Study of the Normalised Wave

Overview: This module fills the hole the previous module leaves, which is quantitatively analysing the variation of wave function and probability density. At precise time values, the user can compute the probability of finding the electron within a certain range they may define.

3.1. Explanation of Input Parameters

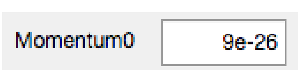


x: Position of the wave-packet in space, the parameters tell the lower and upper values of the visible domain on graphs are to be put in the left and right box respectively.
Value on the left must be less than the value on the right. It is possible both are positive or both are negative, or negative and positive; depending on the needs of the user.

- Default Value: -5 < x < 5

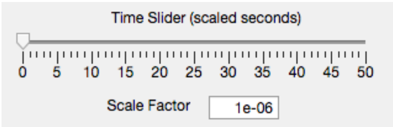
Sigma0 (σ_0): The normalised parameter governing the initial spread of the Gaussian wave-packet, i.e the standard deviation from the mean at initial time, and the evolution of amplitude.

- **Range:** 0.1e-09 $< \sigma_0 < \infty$
- Default Value: 1e-09
- The #e-09 syntax is used to denote "times ten to the power -9"
- The greater the value, the more the initial spread and initial amplitude.
- **Units:** Meters (m)



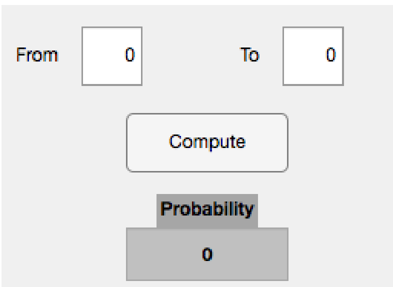
Momentum0 (p_0): Instead of Alpha in previous module, the user directly plays with the momentum of the local particle.

- **Range:** $-\infty < p_0 < \infty$
- Default Value: 9e-26
- A positive value implies particle moving in the positive x-direction. A negative value hence implies in the negative x-direction.
- **Units:** Standard, $Kg \cdot ms^{-1}$



Time Slider: To selectively choose the point in time the wave-packet and probability is to be studied. There is a scale factor that essentially changes the unit of the time value on the slider. For example, if slider is at '15' and scale factor is 1, then t=15s. Then if scale factor is 1e-06, then t=15 microseconds.

- Scale Factor Default Value: 1e-06

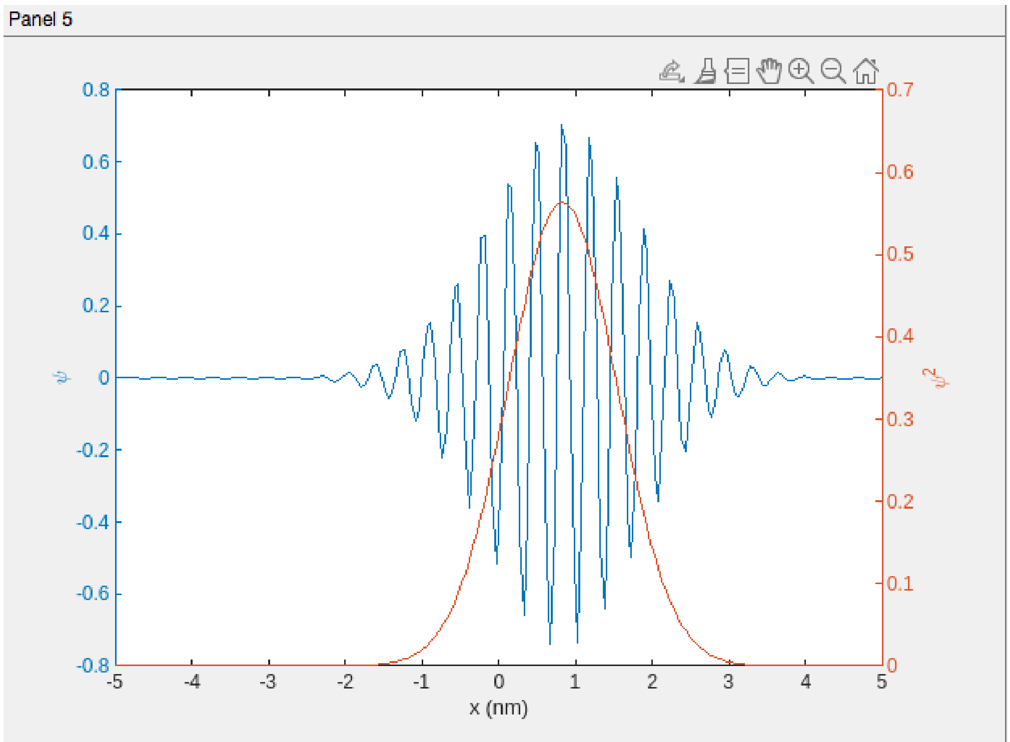


Probability Calculator: The user can calculate the total probability (area under graph of probability density function) of the Gaussian wave-packet. Left and right boxes correspond to From __ and To __ respectively. After pressing Compute, the numerical answer is given in the dark grey box labelled Probability.

- **Range:** Any as long as left value is smaller than right value.
- Infinity may be input as inf. Negative infinity may be input as -inf
- Press Graph on the top to reset the interval region shown on main graph after computing probability.

3.2. Outputs

Normalised Wave function and probability density: Both of the graphs are combined into one for more efficient analysis; with wave function scale on the left in blue and probability density scale on the right in red. There also appears the interval region when the user tries to compute the numerical probability, given that the parameters fall within the current graph domain.



4. Research Applications

The GUI with time evolution visualisation has many applications in quantum mechanics. The key application is demonstrating the dispersion of a free particle wave-packet. Users can observe how the wave-packet spreads over time, illustrating the fundamental quantum principle that a localised particle in space has an uncertain momentum. Additionally, the GUI can be implemented in other projects to simulate the interaction of the wave-packet with potential barriers, enabling exploration of quantum tunneling, reflection, and transmission phenomena, which are central to quantum devices.

5. Important Equations

$$\Psi(X,\tau) = \frac{1}{\pi^{\frac{1}{4}}[\sigma_0(1+i\tau)]^{\frac{1}{2}}} \exp\left[-\frac{(X-\alpha\tau)^2}{2(1+\tau^2)} + \frac{i}{2(1+\tau^2)}\left[2\alpha X + \tau(X^2-\alpha^2)\right]\right] \tag{2}$$

$$|\Psi(X,\tau)|^2 = \frac{1}{\sqrt{\pi}\,\sigma(\tau)} \exp\left[-\frac{(X-\alpha\tau)^2}{1+\tau^2}\right] \tag{3}$$

$$\Re[\Psi(X,\tau)] = \frac{\cos\left(\frac{\tan^{-1}(\tau)}{2}\right)}{\pi^{1/4}\sqrt{\sigma_0(1+\tau^2)}} \exp\left(-\frac{(X-\alpha\tau)^2}{2(1+\tau^2)}\right)\cos\left(\frac{2\alpha X + \tau(X^2-\alpha^2)}{2(1+\tau^2)}\right) \tag{4}$$

$$\Im[\Psi(X,\tau)] = \frac{\sin\left(\frac{\tan^{-1}(\tau)}{2}\right)}{\pi^{1/4}\sqrt{\sigma_0(1+\tau^2)}} \exp\left(-\frac{(X-\alpha\tau)^2}{2(1+\tau^2)}\right)\sin\left(\frac{2\alpha X + \tau(X^2-\alpha^2)}{2(1+\tau^2)}\right) \tag{5}$$