

Intensive week: Coding in Julia!

An introduction for Master's students

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1 Introduction

The Nonlinear Schrödinger Equation (NLSE) is a fundamental equation in quantum mechanics and nonlinear wave phenomena, describing the time evolution of a complex wave function $\psi(x, t)$. It can be expressed as:

$$i \frac{\partial \psi}{\partial t} = \left[\frac{1}{2} \left(-\frac{\partial^2}{\partial x^2} \right) - |\psi|^2 + V(x) \right] \psi \quad (1)$$

In this equation, the left-hand side represents the time evolution of the wave function, where i is the imaginary unit. The right-hand side comprises several terms that may influence the wave dynamics:

- The kinetic energy operator, $\frac{1}{2} \left(-\frac{\partial^2}{\partial x^2} \right)$
- The nonlinear term, $-|\psi|^2$
- The external potential energy term, $V(x)$

The NLSE encapsulates the interplay between linear dispersion and nonlinear effects, making it a powerful model for various physical systems, such as nonlinear optics, Bose-Einstein condensates, and fluid dynamics. Nonlinearity, indicated by the $-|\psi|^2$ term, leads to phenomena such as solitons and wave breaking, fundamentally altering the behavior of the wave function compared to its linear counterparts. As such, the NLSE serves as a cornerstone for understanding complex wave interactions in both classical and quantum contexts.

The research for the Nonlinear Schrödinger Equation (NLSE) is quite abundant, making it a topic of interest for many researchers. Consequently, there are numerous sources for reference. Rather than simply numerically solving the

NLSE, I chose to pursue a different and more complex approach. For my project, I am implementing the Normalized Nonlinear Fractional Schrödinger Equation (NNFSE) using Julia programming language [1]. This equation represents an advanced extension of the traditional Nonlinear Schrödinger Equation, incorporating fractional derivatives to account for nonlocal and anomalous dispersion effects in wave propagation. In addition to exploring a complex topic, I am employing an advanced technique known as the Split-Step Fourier Method (SSFM). The SSFM is part of the family of pseudo-spectral methods used to solve time-dependent nonlinear partial differential equations. This approach follows the age-old strategy of “divide and conquer,” where the nonlinear PDE is divided into related sub-problems of the original equation.

2 The Normalized Nonlinear Fractional Schrödinger Equation (NNFSE)

The NNFSE can be expressed as [2]:

$$i \frac{\partial \psi}{\partial t} = \left[\frac{1}{2} \left(-\frac{\partial^2}{\partial x^2} \right)^{\alpha/2} - \frac{g|\psi|^2}{1 + s|\psi|^2} + V(x) \right] \psi \quad (2)$$

where $\psi \equiv \psi(x, t)$ denotes the slowly varying complex amplitude of the light field. The parameters g , x , and s signify the nonlinearity activation parameter, the normalized transverse coordinate, and the saturation parameter, respectively. In this formulation, the fractional derivative operator $(-\partial^2/\partial x^2)^{\alpha/2}$ is the fractional Laplacian and α is the Lévy index constrained to the range $(1 < \alpha < 2)$. The inclusion of g and s modifies the nonlinear term, providing a mechanism to regulate the intensity of the wave and mitigate effects like self-focusing.

Notably, when $\alpha = 2$, the equation simplifies to the Normal Schrödinger Equation, illustrating the transition from fractional dynamics to conventional quantum behavior. This characteristic allows for the investigation of various wave phenomena, from solitons to dispersion effects, while maintaining a clear connection to established theories.

3 SSFM Algorithm and Implementation

The Split-Step Fourier Method (SSFM) is an efficient numerical technique used to solve time-dependent nonlinear partial differential equations like the Normalized Nonlinear Fractional Schrödinger Equation (NNFSE)[4]. The algorithm works by dividing the complex evolution of the wave function ψ into two distinct steps: the **nonlinear step** and the **linear step**. In the nonlinear step, the wave function ψ is multiplied by an exponential term that accounts for the nonlinearity and potential, $\exp \left(-i \left(\frac{|\psi|^2}{1 + s|\psi|^2} + V(x) \right) \Delta t \right)$, applied in the spatial

Algorithm 1 SSFM($\psi_0, \alpha, \Delta t, k, g, s, V(x)$)

```

1: Initialize:  $\psi^{(n)} \leftarrow \psi_0$ 
2:  $k \leftarrow \frac{2\pi}{L} \left( -\frac{N}{2} : \frac{N}{2} - 1 \right)$ 
3: for  $n = 1$  to  $M$  do
4:   Nonlinear step:
5:    $\psi^{(n+1/2)} \leftarrow \psi^{(n)} \cdot \exp \left[ -i \left( \frac{g|\psi|^2}{1+s|\psi|^2} + V(x) \right) \Delta t \right]$ 
6:   Linear step:
7:    $\hat{\psi}^{(n+1/2)} \leftarrow \text{FFT}(\psi^{(n+1/2)})$  ▷ Fourier space
8:    $\hat{\psi}^{(n+1/2)} \leftarrow \hat{\psi}^{(n+1/2)} \cdot \exp \left( -i \frac{|k|^\alpha}{2} \Delta t \right)$ 
9:    $\psi^{(n+1)} \leftarrow \text{IFFT}(\hat{\psi}^{(n+1/2)})$ 
10:   $\psi^{(n)} \leftarrow \psi^{(n+1)}$ 
11: end for
12: return  $\psi^{(n)}$ 

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domain. Following this, in the linear step, the wave function is transformed into Fourier space using the Fast Fourier Transform (FFT). Here, the linear dispersive effects are applied via $\exp \left(-i \frac{|k|^\alpha}{2} \Delta t \right)$, where k represents the wavenumbers. The wave function is then transformed back to the spatial domain using the Inverse Fast Fourier Transform (IFFT).

This two-step process is repeated for each time step, updating ψ at every iteration. The discrete Fourier Transform (DFT) and its inverse allow efficient manipulation of the wave function in both domains.

4 Results and Discussion

The following results are distributed in three parts, first to do a sanity check of the code, I solved the NNFSE with $\alpha = 2$ and $s = 0$ to recover the Linear Schrödinger Equation (LSE). The second part is to solve the NLSE to observe the Nonlinear behaviour of the wave function. The third part is to solve the NNFSE with different values of α and s to observe the effect of fractional derivatives and saturation parameter.

4.1 Linear Schrödinger Equation (LSE)

In this case, I am solving a time-dependent Schrödinger equation with no nonlinearity, potential, or saturation. Since the parameters - potential (V), and saturation (s) are set to zero, the equation becomes the free particle Schrödinger equation (in the case of $\alpha = 2$, which corresponds to the normal Schrödinger equation).

$$i \frac{\partial \psi}{\partial t} = \left[\frac{1}{2} \left(-\frac{\partial^2}{\partial x^2} \right) + V(x) \right] \psi \quad (3)$$

As seen in the figures 1 and 2, the numerical simulation of

Description	Value
Number of spatial points (N)	1000
Final time (t_{final})	5.0
Time step (Δt)	0.0005
Total number of time steps (M)	10000
Spatial domain length (L)	50.0
Spatial grid range (x_{grid})	[-20.0, 20.0]

Table 1: Parameters used in the numerical simulation.

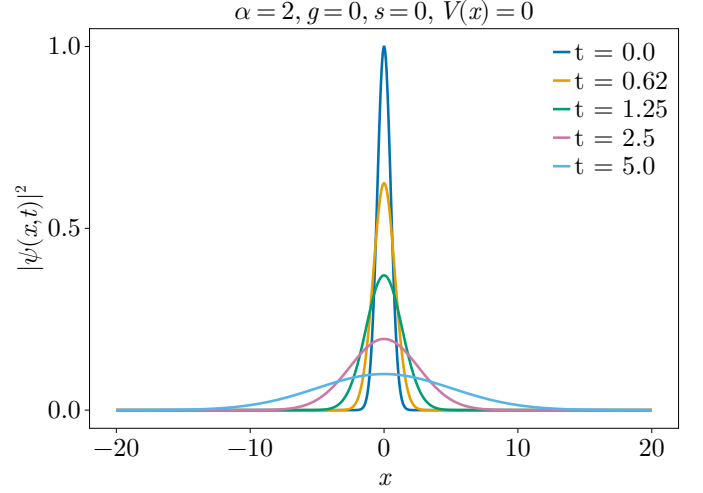


Figure 1: Numerical simulation - Evolution of wave function ψ_0

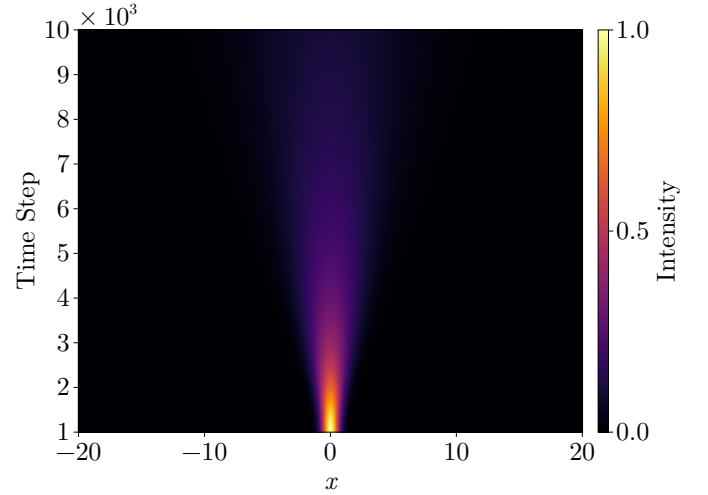


Figure 2: Numerical simulation - Heatmap of the evolution of wave function ψ_0

the Linear Schrödinger Equation (LSE) shows a dispersing Gaussian wave packet. The wave packet spreads out over time, consistent with the analytical solution. Additionally, The heatmap provides a visual representation of the wave packet's evolution, showing the dispersion of the wave function as time progresses.

The exact solution to this problem, when starting with a Gaussian initial condition, $\psi_0(x) = e^{-x^2}$, is known to be a **dispersing Gaussian wave packet**. For the free parti-

cle Schrödinger equation, the time-evolved solution [3] for a Gaussian wave packet is:

$$\psi(x, t) = \frac{1}{\sqrt{1 + 2it}} \exp\left(-\frac{x^2}{1 + 2it}\right) \quad (4)$$

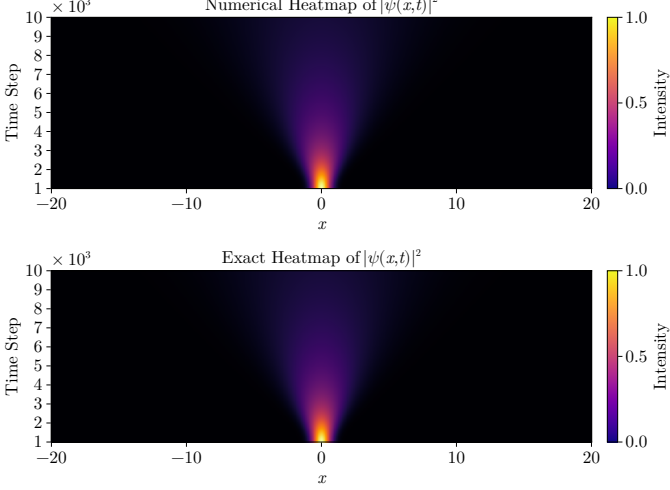


Figure 3: Comparison of Numerical and Analytical solutions of the wave function ψ_0

- The Gaussian wave packet remains Gaussian at any later time, but it spreads out, meaning the width of the wave packet increases as time progresses.
- The phase of the wave function will evolve over time, as indicated by the imaginary part in the time-evolved solution.

This describes the spreading (dispersing) of the initial Gaussian wave packet over time.

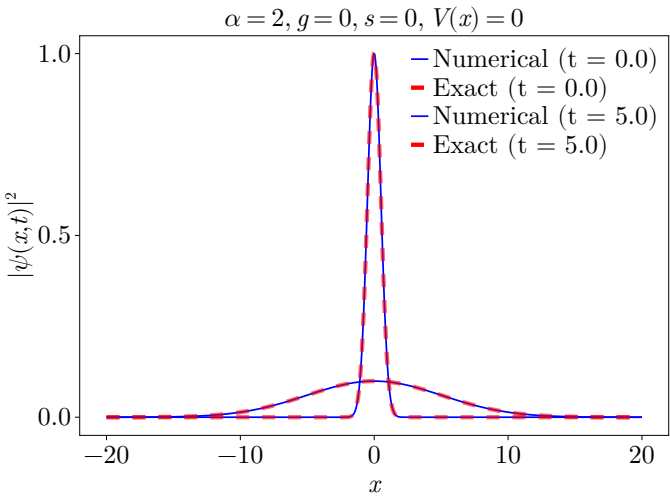


Figure 4: Comparison of Numerical and Analytical solutions of the wave function ψ_0

To further affirm and check the results, I plotted the Numerical and Analytical solutions of the wave function together to compare the results. As one can observe in the figure

3, and the line plot in figure 4, the numerical solution and the exact solution are in excellent agreement, confirming the correctness of the implementation.

4.2 Nonlinear Schrödinger Equation (NLSE)

Description	Value
Number of spatial points (N)	1000
Final time (t_{final})	[5.0, 20.0]
Time step (dt)	0.0005
Total number of time steps (M)	10000
Spatial domain length (L)	50.0
Spatial grid range (x_{grid})	[-20.0, 20.0]
Nonlinearity activation parameter (g)	1.0
Saturation parameter (s)	1.0

Table 2: Parameters used in the numerical simulation.

In this case, I am solving a time-dependent Nonlinear Schrödinger equation with nonlinearity, potential, and saturation all set to one. Additionally, I am setting the $\alpha = 2$ to neglect the fractional derivative term. The equation becomes:

$$i\frac{\partial\psi}{\partial t} = \left[\frac{1}{2}\left(-\frac{\partial^2}{\partial x^2}\right) - |\psi|^2 + V(x)\right]\psi \quad (5)$$

Along with this, the initial wavepacket is a travelling soliton with a Gaussian profile. The soliton is

$$\psi(x, 0) = \exp(x^2 + ix) \quad (6)$$

As seen in the figures 5 and 6, the numerical simulation of the Nonlinear Schrödinger Equation (NLSE) shows no interesting behavior. The wave packet travels but the spreading is more faster than the linear case. Now, let's make things interesting by manipulating the parameters g and s and add some nice potentials.

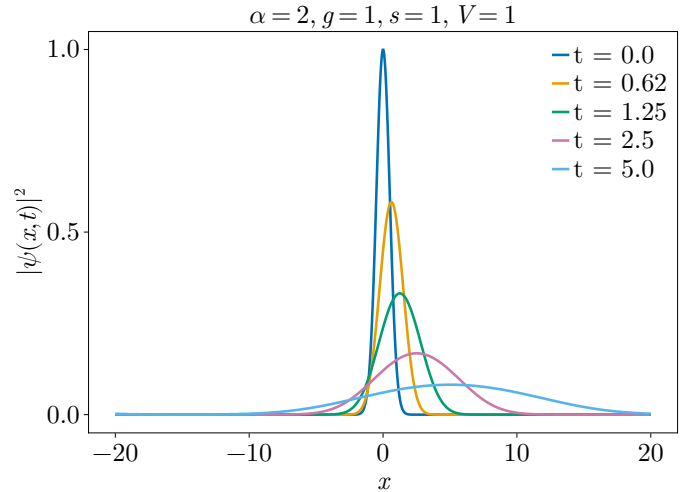


Figure 5: Numerical simulation - Evolution of wave function ψ_0

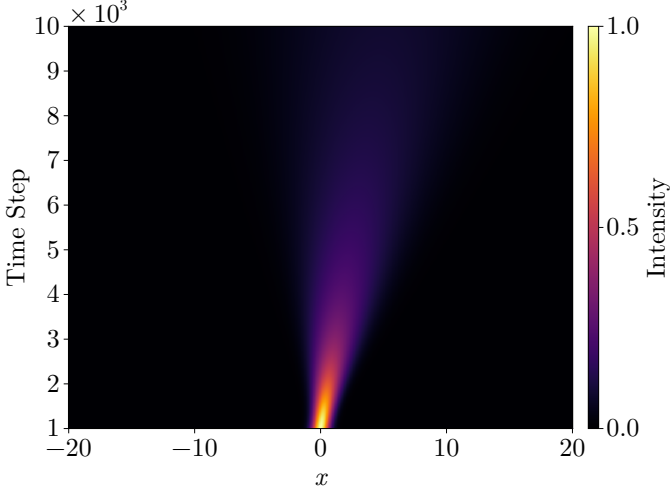


Figure 6: Numerical simulation - Heatmap of the evolution of wave function ψ_0

4.2.1 Effect of Step Potential

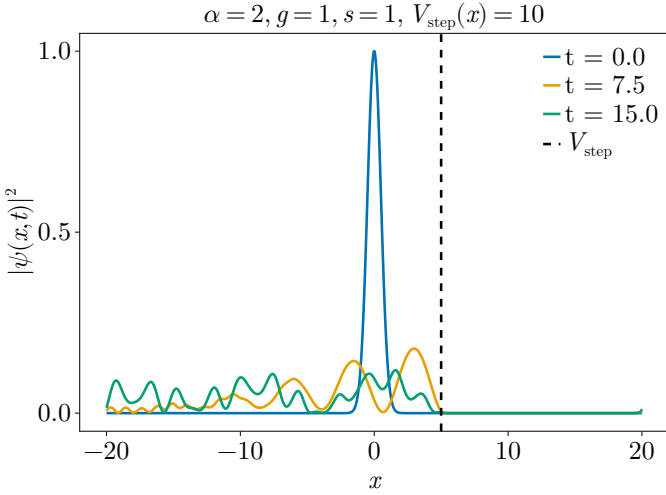


Figure 7: Numerical simulation - Evolution of wave function ψ_0 with step potential

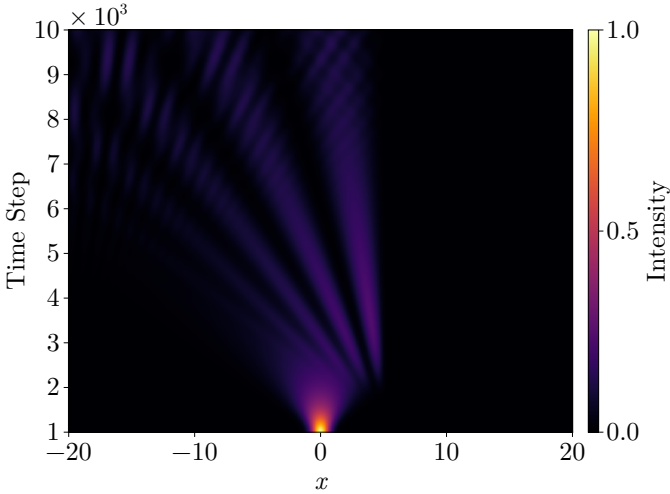


Figure 8: Numerical simulation - Heatmap of the evolution of wave function ψ_0 with step potential

$$V(x) = \begin{cases} 0, & \text{if } x < 5 \\ 10, & \text{if } x \geq 5 \end{cases} \quad (7)$$

I implemented a step potential in the simulation to observe the effect of the potential on the wave which can be seen in the figures 7 and 8. Since $V(x) = 10$ is significantly higher than the wave packet's energy, most of the wave packet gets reflected back, forming an interference pattern between the incoming and reflected waves. This results in sharp oscillations, where the amplitude oscillates rapidly due to constructive and destructive interference.

4.2.2 Effect of Harmonic Potential

$$V(x) = x^2 \quad (8)$$

I implemented a harmonic potential in the simulation to observe the effect of the potential on the wave which can be seen in the figures 9 and 10.

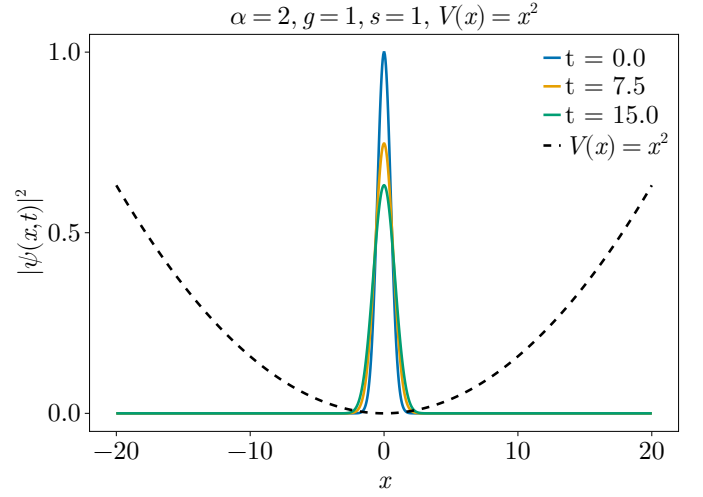


Figure 9: Numerical simulation - Evolution of wave function ψ_0 with harmonic potential

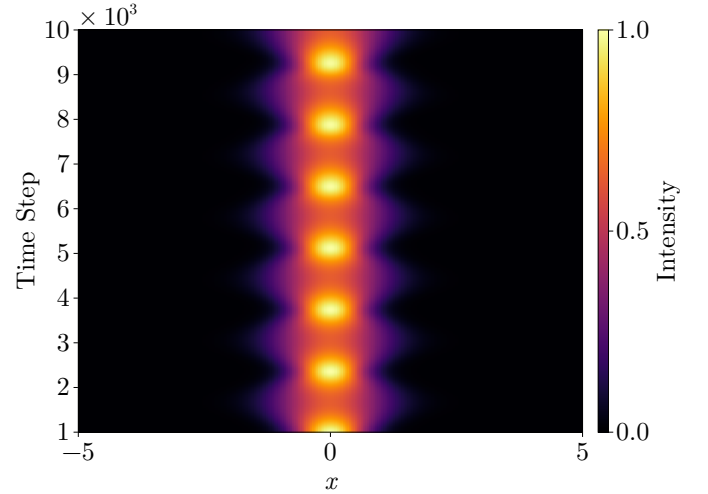


Figure 10: Numerical simulation - Heatmap of the evolution of wave function ψ_0 with harmonic potential

The harmonic potential $V(x) = x^2$ acts as a restoring force, confining the wave packet to the center of the potential well. The wave packet oscillates back and forth within the potential well, exhibiting a harmonic motion. The potential well acts as a trap, preventing the wave packet from dispersing and maintaining its shape over time.

4.3 Normalized Nonlinear Fractional Schrödinger Equation (NNFSE)

Finally, I implemented the evolution of Normalized Nonlinear Fractional Schrödinger Equation (NNFSE) with different values of α observe the effect of fractional derivatives on the wave function.

Description	Value
Number of spatial points (N)	1000
Final time (t_{final})	[5.0, 15, 20.0]
Time step (dt)	0.0005
Total number of time steps (M)	10000
Spatial domain length (L)	50.0
Spatial grid range (x_{grid})	[-20.0, 20.0]
Nonlinearity activation parameter (g)	[1.0, 2]
Saturation parameter (s)	[1.0, 1.5]

Table 3: Parameters used in the numerical simulation.

The initial wavepacket is the same 6, a travelling soliton with a Gaussian profile.

4.3.1 Effect of Fractional Derivative ($\alpha = 1.2$)

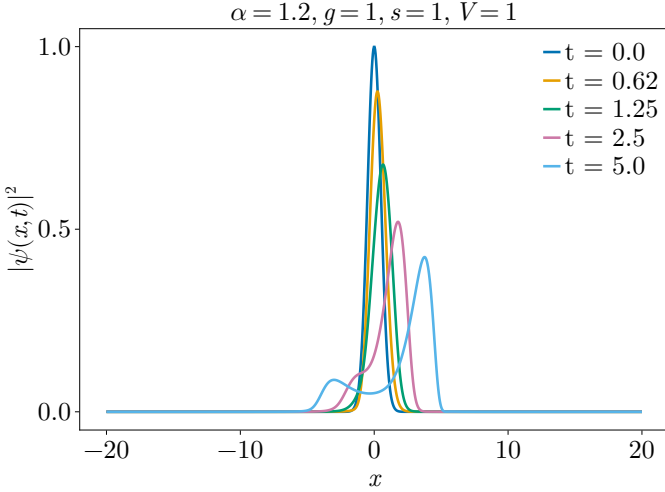


Figure 11: Numerical simulation - Evolution of wave function ψ_0

As seen in the figures 11 and 12, The wave packet is sharp and does not disperse as much as the linear case.

4.3.2 Effect of Fractional Derivative ($\alpha = 1.5$)

As seen in the figures 13 and 14, The wave packet starts dispersing faster now as it should because as the value of alpha increases it starts behaving more like the normal Schrödinger equation.

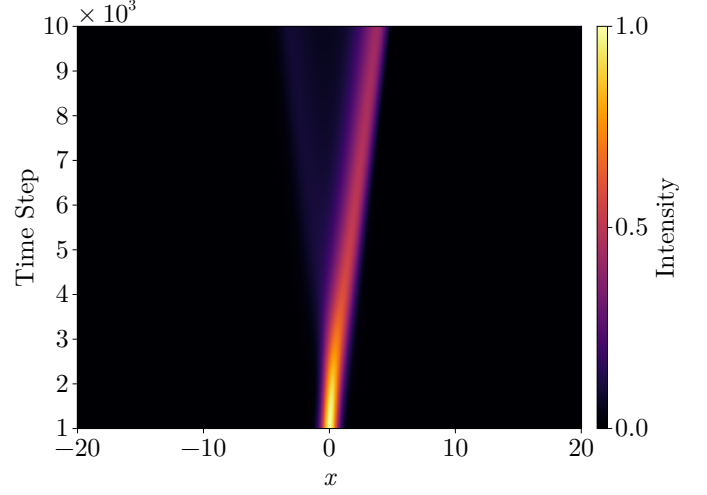


Figure 12: Numerical simulation - Heatmap of the evolution of wave function ψ_0

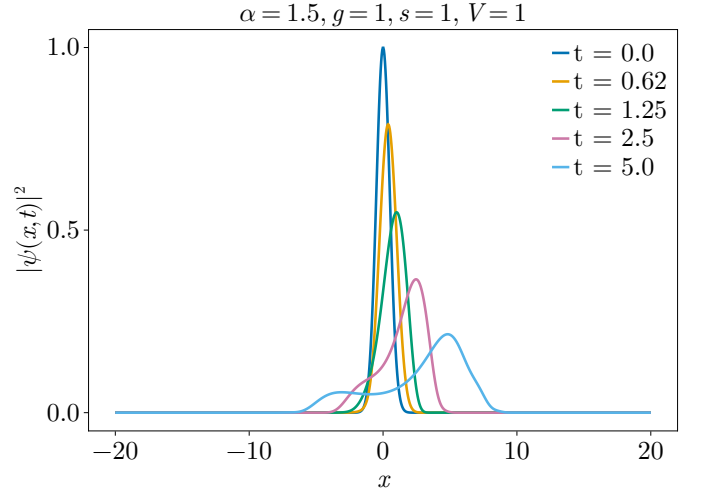


Figure 13: Numerical simulation - Evolution of wave function ψ_0

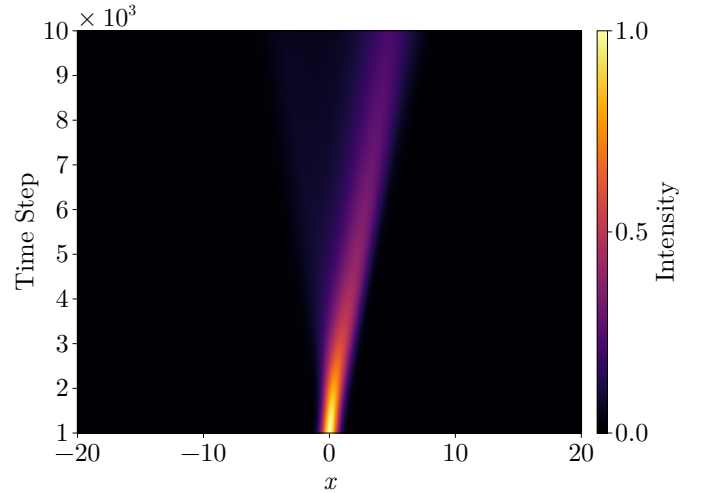


Figure 14: Numerical simulation - Heatmap of the evolution of wave function ψ_0

4.3.3 Effect of Fractional Derivative ($\alpha = 1.8$)

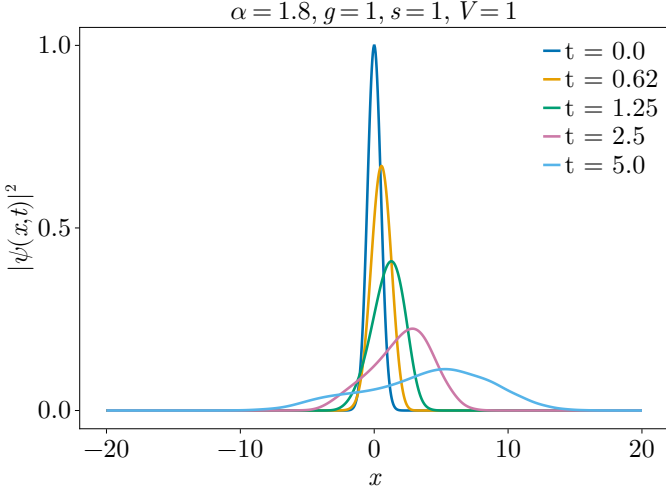


Figure 15: Numerical simulation - Evolution of wave function ψ_0

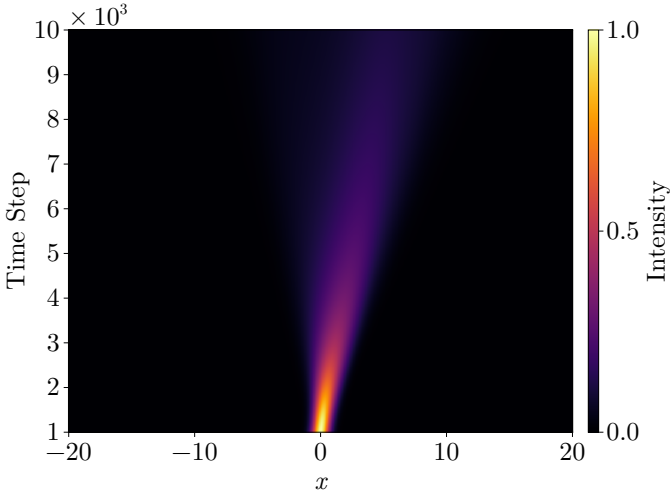


Figure 16: Numerical simulation - Heatmap of the evolution of wave function ψ_0

The wave packet is dispersing faster now as the value of α is closer to 2. This once again confirms the correctness of the implementation. This can be observed in the figures 15 and 16.

4.3.4 Effect of Harmonic Potential

The harmonic potential $V(x) = x^2$ acts as a restoring force, confining the wave packet to the center of the potential well. The wave packet oscillates back and forth within the potential well, exhibiting a harmonic motion. The potential well acts as a trap, preventing the wave packet from dispersing and maintaining its shape over time. This can be clearly seen in the figures 17 and 18. Also, I changed $\alpha = 1.1$ to observe the effect of fractional derivatives on the wave function. This makes it more fractional than other cases. The effect of this can be observed as the oscillations are more erratic and spread out than the Nonlinear Schrödinger Equation (NLSE).

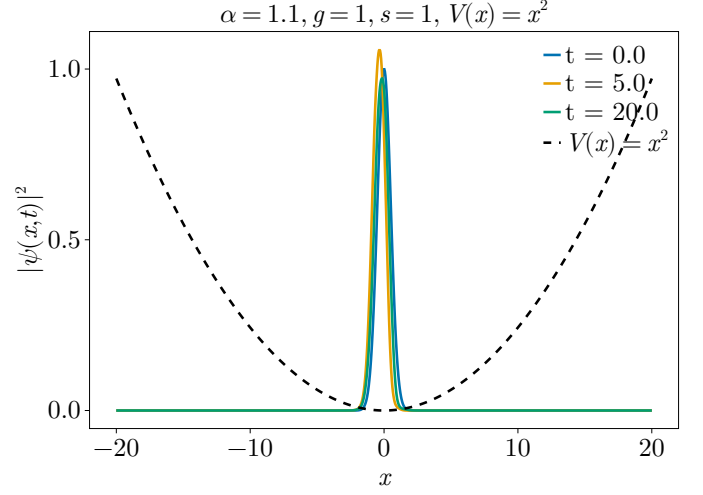


Figure 17: Numerical simulation - Evolution of wave function ψ_0 with harmonic potential

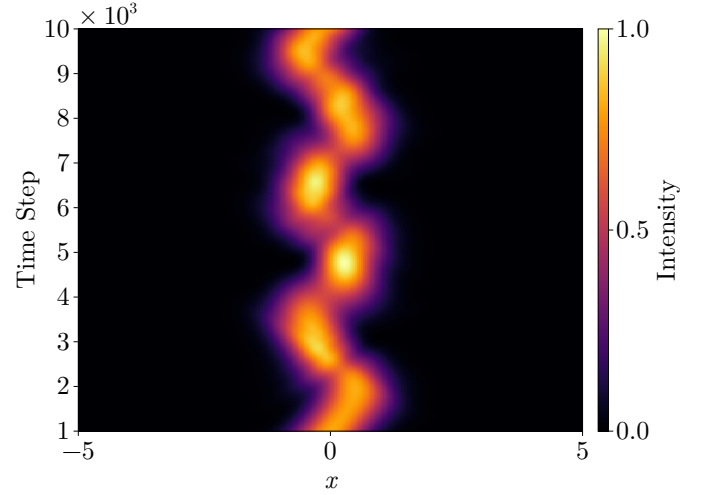


Figure 18: Numerical simulation - Heatmap of the evolution of wave function ψ_0 with harmonic potential

4.3.5 Effect of Quartic Potential

$$V(x) = x^4 \quad (9)$$

I implemented a quartic potential in the simulation with $\alpha = 1.1$ and a stronger value of nonlinearity $g = 1$, and saturation $s = 1.5$ to observe the effect of the potential on the wave which can be seen in the figures 19 and 20.

This is more interesting to observe as I increase the value of nonlinearity and saturation, the wave packet becomes more sharp and the oscillations are more erratic and spread out. The quartic potential acts as a stronger restoring force, confining the wave packet to the center of the potential well. Also the combat between the confining potential and strong nonlinearity and saturation can be clearly observed as there are constructive and destructive interference patterns forming in the wave packet in the heatmap.

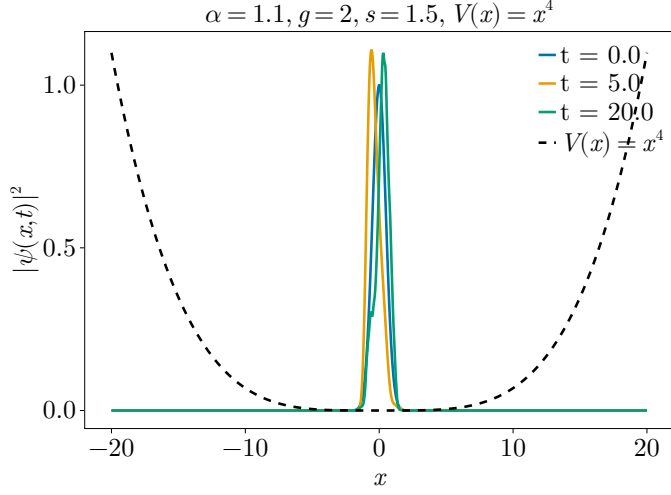


Figure 19: Numerical simulation - Evolution of wave function ψ_0 with quartic potential

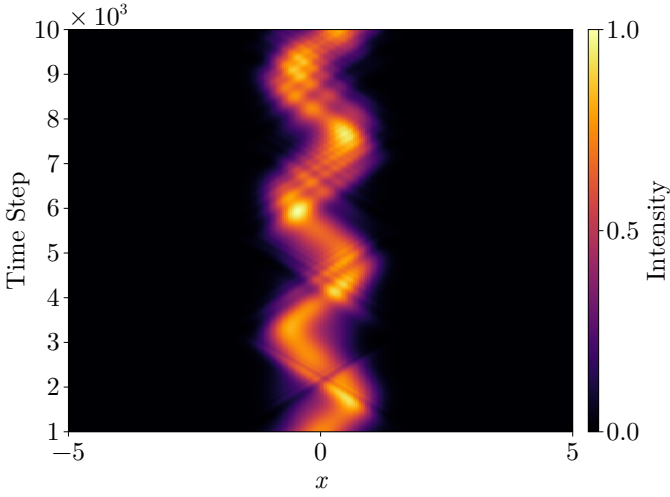


Figure 20: Numerical simulation - Heatmap of the evolution of wave function ψ_0 with quartic potential

5 Conclusion

In this project, I implemented the Split-Step Fourier Method (SSFM) to solve the Normalized Nonlinear Fractional Schrödinger Equation (NNFSE). I started by solving the Linear Schrödinger Equation (LSE) to do a sanity check of the code. Then I solved the Nonlinear Schrödinger Equation (NLSE) to observe the nonlinear behavior of the wave function. Finally, I solved the NNFSE with different values of α , s and g , to observe the effect of fractional derivatives and saturation parameter. The results show that the implementation is promising and the wave packet behaves as anticipated. The SSFM is an efficient numerical technique for solving time-dependent nonlinear partial differential equations, providing insights into the complex dynamics of wave phenomena. The project demonstrates the power of computational methods in exploring nonlinear wave interactions and the impact of fractional derivatives on wave propagation. Future work could involve extending the simulation to higher dimensions, exploring additional potential

profiles, and investigating the interplay between nonlinearity and dispersion in wave dynamics.

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