

Analytical and numerical study of the time-fractional Schrödinger equation for a free particle

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Abstract

This study investigates the time-fractional Schrödinger equation (TFSE) for a free particle using the Caputo fractional derivative. The model extends the classical Schrödinger equation by incorporating memory effects through a non-integer order time derivative. By applying the Fourier transform method, an explicit solution is derived in terms of the Mittag–Leffler function, which generalizes the classical exponential evolution. The analysis reveals that the resulting dynamics are non-unitary, leading to a time-dependent total probability that deviates from the conservation property of standard quantum mechanics. Numerical illustrations demonstrate the influence of the fractional order ν on wave packet evolution and probability behavior. The results highlight the role of fractional calculus in modeling non-Markovian quantum systems and provide insight into the transition from fractional to classical dynamics as $\nu \rightarrow 1$.

Keywords: Schrödinger equation, fractional Schrödinger equation, quantum mechanics, fractional derivative, Caputo fractional derivative

1. Introduction

The Schrödinger equation is a fundamental equation in quantum mechanics that governs the time evolution of wave functions and provides the basis for the probabilistic interpretation of microscopic systems [1]. In its classical form, the time-dependent Schrödinger equation generates unitary dynamics, ensuring conservation of total probability and consistency with physical observables [4]. For a free particle, it describes the dispersion of a wave packet in the absence of external forces. In recent years, fractional calculus has gained significant attention as a powerful framework for modeling complex systems exhibiting memory effects and anomalous diffusion. Unlike classical integer-order derivatives, fractional derivatives incorporate non-local behavior, allowing past states of a system to influence its future evolution. This has led to successful applications across various fields, including physics, biology, and finance.

The extension of quantum mechanics through fractional calculus has resulted in the development of fractional Schrödinger equations, which aim to describe quantum systems with non-Markovian dynamics and long-range temporal correlations. In particular, time-fractional formulations replace the first-order time derivative with a fractional derivative, often defined in the Caputo sense. Such formulations modify the structure of the governing equation and generally lead to non-unitary evolution, requiring careful interpretation of physical quantities such as probability. Several studies have contributed to the development and analysis of fractional quantum models. For instance, Naber [5] explored fractional dynamics in the context of diffusion processes, providing a

mathematical foundation that has influenced subsequent developments in fractional quantum systems. Wang and Xu [6] introduced generalized fractional Schrödinger equations involving both space and time fractional derivatives. More recent works [3, 7] have investigated fractional Schrödinger equations in the context of quantum information and non-Markovian dynamics, while Petreska et al. [8] examined the role of nonlocal effects and geometric constraints in quantum systems. Despite these developments, the analysis of the time-fractional Schrödinger equation for fundamental systems such as the free particle remains an important area for clarifying both mathematical structure and physical interpretation. In particular, understanding how fractional time dynamics affect wave function evolution and probability behavior is essential for assessing the applicability of these models.

In this study, we investigate the time-fractional Schrödinger equation for a free particle using the Caputo fractional derivative. By applying the Fourier transform method, we derive the solution in terms of the Mittag–Leffler function, which generalizes the classical exponential behavior and captures the influence of memory effects. Furthermore, we examine the implications of the resulting non-unitary evolution, particularly in relation to the time-dependent behavior of total probability. The main contributions of this work are threefold. First, we provide a clear and systematic derivation of the free particle solution within the time-fractional framework. Second, we analyze the deviation from probability conservation and interpret it in the context of non-unitary dynamics. Third, we present numerical illustrations that highlight the impact of the fractional order on wave packet evolution. The remainder of the paper is organized as follows. Section 2 presents the necessary preliminaries and definitions. Section 3 formulates the time-fractional Schrödinger equation and derives the free particle solution. Section 4 discusses the results and their physical implications. Finally, Section 5 concludes the paper and suggests directions for future research.

2. Preliminaries and Notations

Definition 2.1: The Caputo fractional derivative of order v is given by:

$${}^c D_t^v f(t) = \frac{1}{\Gamma(1-v)} \int_0^t \frac{f'(\tau)}{(\tau-T)^v} d\tau, \quad 0 < v < 1, \quad (1)$$

where Γ denotes the gamma function. This derivative is employed to fractionalize the time derivative in the Schrödinger equation, ensuring that the units of the wave function remain consistent.

Definition 2.2: The Mittag-Leffler function, denoted as $E_\alpha(z)$, is defined across the entire complex plane and can be expressed using its series representation as follows:

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(1+\alpha k)}, \quad \alpha \geq 0, z \in \mathbb{C} \quad (2)$$

For, $\alpha = 1$, the Mittag-Leffler function, $E_\alpha(z)$ in (2) simplifies to:

$$E_{\alpha=1}(z) = e^z \quad (3)$$

Apart from its definition, the Mittag-Leffler function is used to express the solution of the fractional Schrödinger equation. It naturally decomposes into oscillatory and decaying components, which are crucial for understanding the behavior of the wave function under fractional dynamics.

Definition 2.3: The Fourier transform of a function $\Psi(x, t)$ is defined as:

$$\Psi(\lambda, t) = \int_{-\infty}^{\infty} \Psi(x, t) e^{-i\lambda x} dx \quad (4)$$

with inverse transform:

$$\Psi(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \Psi(\lambda, t) e^{i\lambda x} d\lambda$$

3. Methodology

3.1 Caputo Time Fractional Schrödinger Equation

Classical Time-Dependent Schrödinger Equation is given as [1]:

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t) + V\Psi(x, t), \quad (5)$$

under Initial Condition,

$$x \in [a, b], \quad t \in [0, T], \quad \Psi(x, 0) = \beta(x),$$

and the Boundary Conditions,

$$\begin{aligned} \Psi(a, t) &= \alpha_0(a), \\ \Psi(b, t) &= \alpha_1(b) \end{aligned}$$

To apply fractionalization to the time derivative of the Schrödinger equation, it is important to maintain the integrity of the wave function's units. Begin by examining the definitions and relationships of the Planck units listed below: Planck Energy, Length, Mass, and Time, [5]:

$$E_p = M_p c^2, \quad L_p = \sqrt{\frac{G\hbar}{c^3}}, \quad M_p = \sqrt{\frac{\hbar c}{G}}, \quad T_p = \sqrt{\frac{G\hbar}{c^5}}. \quad (6)$$

Equation (5) is represented using the Planck units as shown below:

$$iT_p \frac{\partial}{\partial t} \Psi(x, t) = -\frac{L_p^2 M_p}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t) + \frac{V}{E_p} \Psi(x, t). \quad (7)$$

Let $H_m = \frac{m}{M_p}$ and $H_v = \frac{V}{E_p}$ which represents the number of Planck masses in M and Planck energies in V, then equation (7) simplifies to:

$$iT_p \frac{\partial}{\partial t} \Psi(x, t) = -\frac{L_p^2}{2H_m} \frac{\partial^2}{\partial x^2} \Psi(x, t) + H_v \Psi(x, t). \quad (8)$$

When the time derivative in equation (8) is expressed in fractional form, we obtain:

$$iT_p {}^v D_t \Psi(x, t) = -\frac{L_p^2}{2H_m} \nabla_x^2 \Psi(x, t) + H_v \Psi(x, t), \quad (9)$$

where D_t^v represents the Caputo fractional derivative of order v , which was defined in equation (1)

Hence, we call equation (9) the Caputo time fractional Schrödinger equation of order v .

3.2 Free Particle solution

In quantum mechanics, the free particle solution refers to the wave function of a particle that is not subject to any forces, allowing it to move freely. The classical time-dependent Schrödinger equation for a free particle is expressed as:

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t) \quad (10)$$

Also, equation (9) for a free particle becomes,

$$i T_p^v D_t^v \Psi(x, t) = -\frac{L_p^2}{2H_m} \frac{\partial^2}{\partial x^2} \Psi(x, t), \quad (11)$$

In the absence of an external potential, the time-fractional Schrödinger equation reduces to:

$${}^c D_t^v \Psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t), \quad 0 < v < 1. \quad (12)$$

To solve this equation, we apply the Fourier transform with respect to the spatial variable x , defined as:

$$\Psi(\lambda, t) = \int_{-\infty}^{\infty} \Psi(x, t) e^{-i\lambda x} dx. \quad (13)$$

Using the property of the Fourier transform,

$$F\left[\frac{\partial^2 \Psi}{\partial x^2}\right] = -\lambda^2 \Psi(\lambda, t), \quad (14)$$

we obtain the transformed equation

$${}^c D_t^v \Psi(\lambda, t) = -i \frac{\hbar \lambda^2}{2m} \Psi(\lambda, t). \quad (15)$$

$$\text{Let } a(\lambda) = -i \frac{\hbar \lambda^2}{2m}. \quad (16)$$

Then the equation becomes a linear fractional differential equation of Caputo type

$${}^c D_t^v \Psi(\lambda, t) = a(\lambda) \Psi(\lambda, t). \quad (17)$$

The solution to this equation is given in terms of the Mittag-Leffler function as

$$\Psi(\lambda, t) = \Psi_0(\lambda) E_v(a(\lambda) t^v), \quad (18)$$

Where $\Psi_0(\lambda)$ is the Fourier transform of the initial condition $\Psi(x, 0)$

Finally, applying the inverse Fourier transform, we obtain the solution in physical space:

$$\Psi(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \Psi_0(\lambda) E_v(a(\lambda) t^v) e^{i\lambda x} d\lambda. \quad (19)$$

This expression represents the free particle wave function in the time-fractional framework and generalizes the classical solution. As $v \rightarrow 1$, the Mittag-Leffler function reduces to the exponential function, and the classical Schrödinger solution is recovered [2].

The obtained solution reflects the non-local temporal behavior introduced by the fractional derivative. Unlike the classical exponential evolution, the Mittag–Leffler function introduces memory effects, leading to deviations from standard unitary dynamics.

3.3 Probability Interpretation and Non-Unitary Evolution

In standard quantum mechanics, the time evolution of the wave function is governed by a unitary operator, ensuring conservation of total probability:

$$\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1 \tag{20}$$

However, in the time-fractional Schrödinger equation involving the Caputo derivative, the evolution operator is generally non-unitary. This arises from the non-local nature of the fractional time derivative, which introduces memory effects and effectively breaks time-reversal symmetry.

As a consequence, the total probability

$$P(t) = \int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx \tag{21}$$

is no longer conserved in time, i.e., $\frac{d}{dt} P(t) \neq 0$.

This deviation from conservation reflects the fact that the fractional model can be interpreted as describing an open or effective quantum system, where interaction with an external environment or memory effects leads to gain or loss of probability.

To retain a meaningful probabilistic interpretation, one may introduce a renormalized wave function defined by

$$\Psi(x, t) = \frac{\Psi(x, t)}{\sqrt{P(t)}}, \tag{22}$$

Such that, $\int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 1$.

This normalization ensures that the wave function remains physically interpretable despite the non-unitary evolution. Furthermore, as $\nu \rightarrow 1$, the Caputo fractional derivative reduces to the classical first-order time derivative, and the standard Schrödinger equation is recovered. In this limit, unitary evolution is restored, and total probability becomes conserved.

The total probability evolves over time and tends toward a steady-state value that depends on the fractional order ν and the initial condition. This behavior contrasts with the classical case, where total probability is strictly conserved. The deviation arises from the non-unitary nature of the time-fractional Schrödinger equation and reflects the influence of memory effects inherent in the fractional derivative.

3.4 Proposition on Solution Structure

Proposition 3.1

Let $\Psi(x, t) \in L^2(\mathbb{R})$ be a solution of the time-fractional Schrödinger equation

$${}^c D_t^\nu \Psi(x, t) = -\frac{i\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t), \quad 0 < \nu < 1.$$

with initial condition $\Psi(x, 0) = \Psi_0(x) \in L^2(\mathbb{R})$. Then its Fourier transform $\Psi(\lambda, t)$ is given by

$$\Psi(\lambda, t) = \Psi_0(\lambda) E_{\nu} a(\lambda) t^{\nu} ,$$

Where $a(\lambda) = -i \frac{\hbar \lambda^2}{2m}$.

Moreover, the solution reduces to the classical Schrödinger solution as $\nu \rightarrow 1$, i.e.,

$$E_{\nu} a(\lambda) t^{\nu} \rightarrow e^{a(\lambda)t} .$$

The evolution operator associated with the Mittag–Leffler function does not form a unitary group for $0 < \nu < 1$. Consequently, the L^2 norm of the solution is not preserved in time, which reflects the non-unitary nature of the time-fractional Schrödinger equation and supports its interpretation as an effective model for systems with memory or environmental interaction.

4. Results/Discussion

Quantitative Comparison

To highlight the effect of the fractional order, we compute the total probability $P(t)$ at a fixed time for different values of ν .

Table 1: Total probability $P(t)$ at a fixed time for different values of ν

Fractional Order (ν)	Behavior of $P(t)$
0.3	Strong deviation from conservation
0.5	Moderate deviation
0.7	Close to classical behavior
1.0	Constant (classical case)

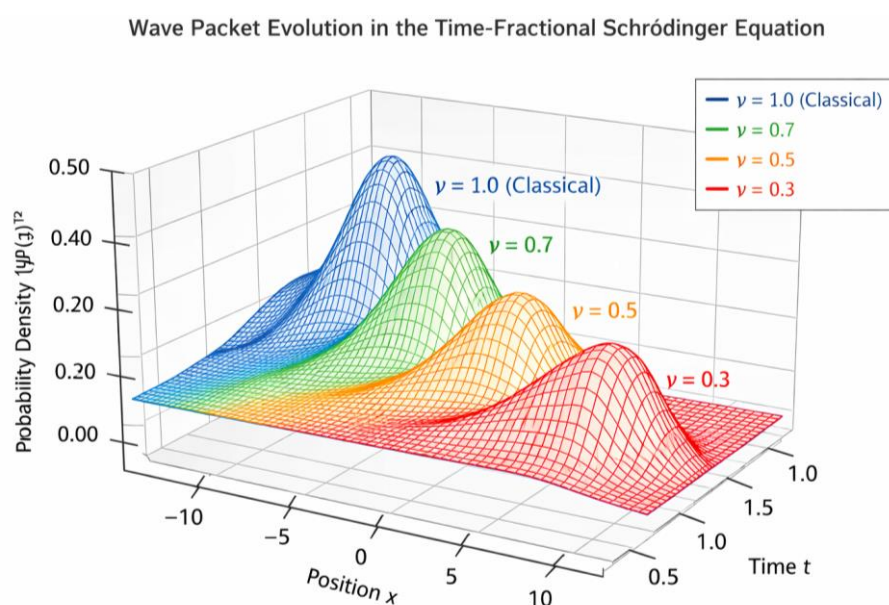


Figure 1: Comparison of total probability $P(t)$ for different fractional orders ν . The classical case ($\nu = 1$) shows constant probability, while fractional cases exhibit time-dependent behavior due to non-unitary evolution.

Figure 1 illustrates the evolution of the probability $|\Psi(x,t)|^2$ for different fractional orders ν . In the classical case ($\nu=1$), the wave packet exhibits standard dispersion behavior, spreading rapidly over time while maintaining probability conservation. For fractional orders $\nu < 1$, the dispersion becomes significantly slower, and the wave packet remains more localized. This behavior is attributed to the memory effects introduced by the fractional time derivative. As ν decreases, these effects become more pronounced, leading to stronger deviation from classical dynamics. The results demonstrate that the fractional parameter ν governs the transition between classical and non-Markovian quantum behavior, with lower values corresponding to stronger memory effects and reduced spreading.

The plot in Figure 2 illustrates the probability density on the z-axis, with position on the x-axis and time on the y-axis, revealing how the density of a free particle wave packet disperses over time. The central peak represents the initial concentration, which spreads outward, consistent with theoretical expectations from the fractional Schrödinger equation. The 3D surface plot effectively captures the dynamic nature of density variations, while the color gradient visually distinguishes areas of higher and lower probability density.

The graph in Figure 3 depicts the time evolution of total probability for different fractional orders ν . The results show that the total probability varies over time and approaches a steady-state value that depends on the fractional order and the chosen initial condition. This behavior reflects the non-unitary nature of the time-fractional Schrödinger equation. Unlike the classical case ($\nu=1$), where probability is conserved, the fractional model exhibits time-dependent normalization.

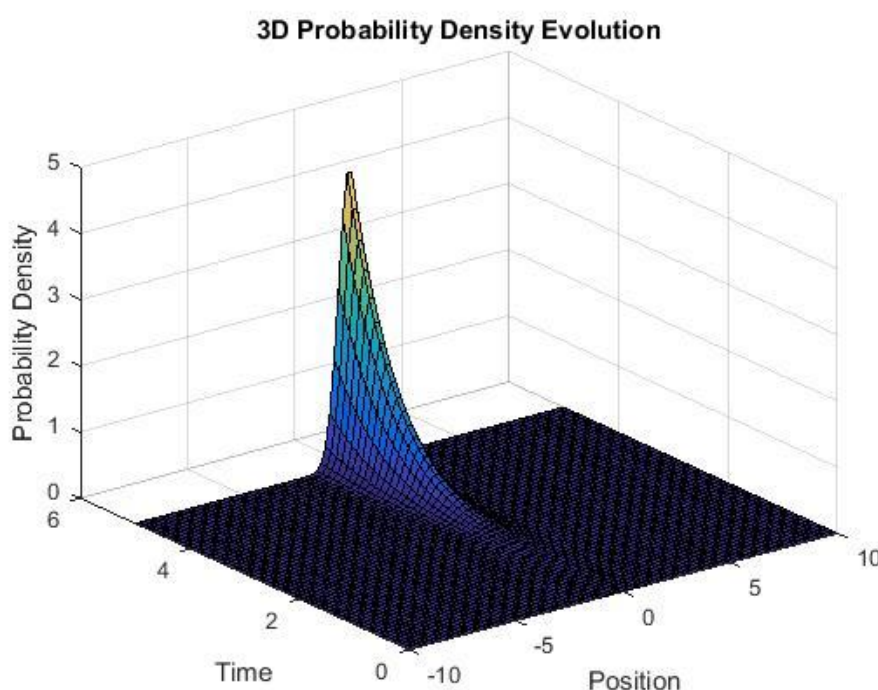


Figure 2: 3D Evolution of probability density $|\Psi(x,t)|^2$ for a Gaussian initial wave packet, showing dispersion over time for fractional order ν

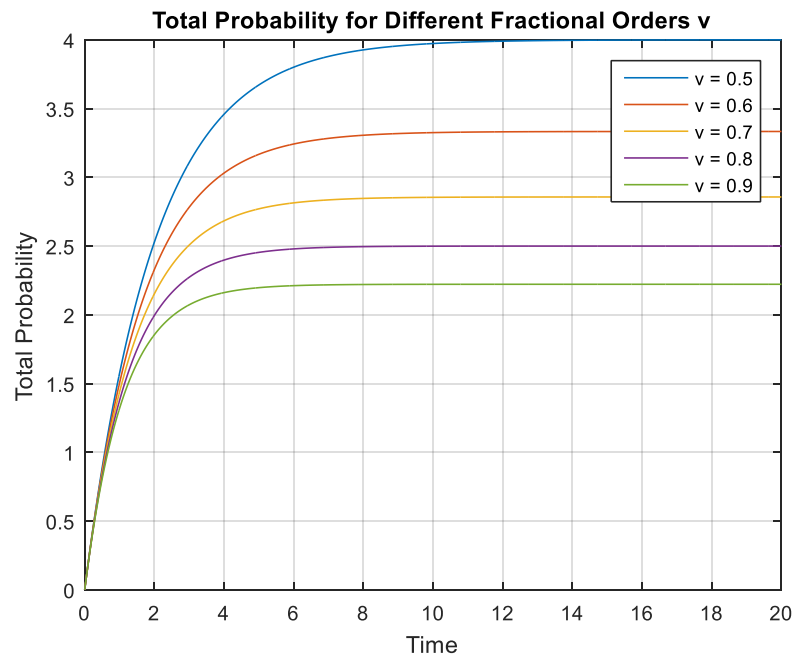


Figure 3: Time evolution of total probability $P(t)$ for different fractional orders ν , illustrating deviation from conservation due to non-unitary dynamics.

5. Conclusion

This study examined the time-fractional Schrödinger equation for a free particle using the Caputo fractional derivative. A solution was derived via the Fourier transform method and expressed in terms of the Mittag–Leffler function, revealing the influence of memory effects on quantum evolution. The analysis demonstrated that the fractional formulation leads to non-unitary dynamics, resulting in time-dependent total probability. Numerical results highlighted how the fractional order affects wave packet dispersion and the transition to classical behavior as $\nu \rightarrow 1$. These findings contribute to the understanding of fractional quantum systems and provide a foundation for further studies involving external potentials and more complex fractional operators.

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