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Efficient Numerical Computation of Time-Fractional Nonlinear Schrödinger Equations in Unbounded Domain

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Abstract. The aim of this paper is to derive a stable and efficient scheme for solving the one-dimensional time-fractional nonlinear Schrödinger equation set in an unbounded domain. We first derive absorbing boundary conditions for the fractional system by using the unified approach introduced in [47,48] and a linearization procedure. Then, the initial boundary-value problem for the fractional system with ABCs is discretized, a stability analysis is developed and the error estimate $\mathcal{O}(h^2+\tau)$ is stated. To accelerate the L1-scheme in time, a sum-of-exponentials approximation is introduced to speed-up the evaluation of the Caputo fractional derivative. The resulting algorithm is highly efficient for long time simulations. Finally, we end the paper by reporting some numerical simulations to validate the properties (accuracy and efficiency) of the derived scheme.

AMS subject classifications: 35R11, 35Q41, 65L20

Key words: Time-fractional nonlinear Schrödinger equation, absorbing boundary condition, stability analysis, convergence analysis, sum-of-exponentials approximation.

1 Introduction

The classical Schrödinger equation serves as the Feynman propagator for nonrelativistic quantum mechanics by using a Gaussian probability distribution in the space of all possible paths. This provides a useful mechanism that accounts naturally for the non-Gaussian distributions corresponding to fractional structures. By extending the Feynman

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path integral from Gaussian distribution to Lévy-like quantum mechanical paths, Laskin [28, 29] proposed a space fractional Schrödinger equation. Naber [39] built the Time Fractional Schrödinger Equation (TFSE) in analogy with the fractional Fokker-Planck equation as well as with the application of the time Wich rotation. Related works have next been developed [10, 15, 32, 35, 40, 45], including e.g. the generalization of the TFSE to a full space and some new results on the correct continuity equation for the probability density. The fractional nonlinear Schrödinger equation is used to describe the nonlocal quantum phenomena in quantum physics and explore the quantum behaviors of either long-range interactions or multi-scale time-dependent processes. Many possible applications explain why this new direction in quantum physics is rapidly emerging [26, 28, 29, 35, 39, 40, 46]. Some analytical and approximate solutions have first been considered for the TFSE [23, 41]. Nevertheless, the complexity of the mathematical structure of the TFSE with different potentials and nonlinearities leads to extremely difficult detailed analytical studies of its non standard properties, which are sometimes impossible to derive. Therefore, efficient and accurate numerical simulations [3, 6, 11, 17, 19] are urgently needed to understand them.

In this paper, we develop and analyze some original accurate and efficient numerical methods for computing the solution to the general 1D Time-Fractional Nonlinear Schrödinger Equation (TFNSE)

$$\begin{cases} \mathrm{i}\,{}_0^C\mathcal{D}_t^\alpha \psi(x,t) = -\psi_{xx} + V(x)\psi + f(|\psi|^2)\psi, & (x,t)\in\mathbb{R}\times(0,T], \\ \psi(x,0) = \psi_0(x), & x\in\mathbb{R}, \\ \psi(x,t)\to 0 \quad \text{when} \quad |x|\to+\infty, \quad t\in(0,T], \end{cases} \tag{1.1}$$

where $\mathrm{i}=\sqrt{-1}$ and $V(x)$ is the external potential. The function f models general nonlinear effects with respect to ψ, e.g. for the case of the cubic nonlinearity $f(|\psi|^2)\psi = g|\psi|^2\psi$ that arises in nonlinear optics. If $g=+1$, one gets the well-known *defocusing* nonlinearity while $g=-1$ corresponds to the *focusing* situation. The operator ${}_0^C\mathcal{D}_t^\alpha$ denotes the Caputo fractional derivative of order α $(0<\alpha<1)$ with respect to t [49] and given by

$${}_0^C\mathcal{D}_t^\alpha \psi(x,t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{1}{(t-s)^\alpha}\frac{\partial\psi(x,s)}{\partial s}ds, \quad 0<\alpha<1, \tag{1.2}$$

where $\Gamma(\cdot)$ is the Gamma special function. Three crucial and fundamental difficulties appear when numerically solving problem (1.1)

(i) the spatial domain is unbounded,

(ii) the TFNSE is a nonlinear equation,

(iii) the (nonlocal) Caputo derivative *a priori* needs a huge storage and a high computational cost when discretized.

Over the past few decades, many contributions were made to overcome the numerical difficulties arising from solving PDEs in unbounded domains. For example, the method