ARTICLE IN PRESS

Computers and Mathematics with Applications ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Computers and Mathematics with Applications

journal homepage: www.elsevier.com/locate/camwa

An efficient Fourier spectral exponential time differencing method for the space-fractional nonlinear Schrödinger equations

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ARTICLE INFO

Article history:
Received 8 October 2017
Received in revised form 21 February 2018
Accepted 25 March 2018
Available online xxxx

Keywords:
Fractional nonlinear Schrödinger equations
Exponential time differencing
Fourier spectral method
Fractional Laplacian

ABSTRACT

A fourth-order time-discretization scheme based on the exponential time differencing approach with Fourier spectral method in space is proposed for the space-fractional nonlinear Schrödinger equations. The stability and convergence of the numerical scheme are discussed. It is shown that the proposed numerical scheme is fourth-order convergent in time and spectral convergent in space. Numerical experiments are performed on one-, two-, and three-dimensional fractional nonlinear Schrödinger equations and systems of two-, and three-dimensional equations. In addition, a realistic two-dimensional example with the solution of a singularity occurring in finite time is included. The results demonstrate accuracy, efficiency, and reliability of the scheme. Computational results arising from the experiments are compared with relevant known schemes, such as the fourth-order split-step Fourier method, the fourth-order explicit Runge–Kutta method, and a mass-conservative spectral method.

1. Introduction

During the last few decades, the nonlinear Schrödinger equations (NLSEs) have been widely studied and used to model a number of important physical phenomena, including propagations of solitary waves in optical fibers, deep water turbulence, and superfluidity [1,2]. During this time, a great deal of attention has also been directed towards numerical methods for the NLSEs, including finite difference, finite element, pseudo-spectral, and multi-symplectic methods (see, for example, [2,3] and references therein).

Recently, fractional partial differential equations (FPDEs) have been utilized instead of integer-order PDEs in many physical areas [4,5]. For instance, FPDEs are used to model sound wave propagations in rigid porous materials in [6]. In the field of quantum mechanics, the memory and hereditary properties of different substances can be better described by fractional-order derivatives [7], which makes the fractional-order models more adequate than the previously used integer-order models [8,9]. Moreover, space-fractional derivatives are applied to modeling anomalous diffusion or dispersion effects caused by the movement of particles along Lévy-like paths, which is inconsistent with classical Brownian motion [10].

The fractional properties of the space-fractional nonlinear Schrödinger equation (SFNLSE) enable it to describe the evolution of an inviscid perfect fluid with nonlinear dynamics [11]. Modified from the water wave equations, the fractional

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https://doi.org/10.1016/j.camwa.2018.03.042

Laplacian in the SFNLSE represents the dispersion effect of the linearized gravity water wave equation for one- or two-dimensional surfaces [12], while the nonlinear dynamics of water waves are governed by the nonlinear cubic term in the SFNLSE. In the field of biophysics, the SFNLSE can be used as a model for charge transport in large-scale organic polymers such as DNA [13]. In three-dimensional space, a special case of the SFNLSE is named the fractional Gross–Pitaevskii equation, which is used to model the Bose–Einstein condensation in a fractal environment [1,14].

In this paper, we consider the following fractional nonlinear Schrödinger equation with the fractional Laplacian in space:

$$i\frac{\partial u(\mathbf{x},t)}{\partial t} = \gamma(-\Delta)^{\alpha/2}u(\mathbf{x},t) + \beta|u(\mathbf{x},t)|^2u(\mathbf{x},t), \quad 1<\alpha\le 2, \tag{1}$$

with the initial condition $u(\mathbf{x},0)=u_0(\mathbf{x})$, where $i=\sqrt{-1}$, and $u(\mathbf{x},t)$ is a complex-valued wave function of $\mathbf{x}\in\Omega\subset\mathbb{R}^d$ (for $d=1,\ 2$ or 3) and $t\ge 0$, parameters α, γ, and β are real constants. The system is closed with either a homogeneous Dirichlet boundary condition, representing a fixed concentration of u on $\partial\Omega$, or a homogeneous Neumann one, where mass is conserved in Ω [15]. When $\alpha=2$, SFNLSE (1) reduces to the classical cubic nonlinear Schrödinger equation. The fractional Laplacian $-(-\Delta)^{\alpha/2}$ in space can be characterized as [16]:

$$-(-\Delta)^{\alpha/2}u(\mathbf{x},t) := -\mathcal{F}^{-1}\left(|\xi|^\alpha\mathcal{F}\left(u(\mathbf{x},t)\right)\right), \quad \alpha>0, \tag{2}$$

where $\mathcal{F}$ is the Fourier transform, and $\mathcal{F}^{-1}$ denotes its inverse.

Similar to the classical cubic NLSE, the SFNLSE (1) conserves two quantities [17–19]: the mass of the wave function:

$$\mathrm{M}(t) := \|u(\cdot,t)\|_{L^2}^2 = \int_{\mathbb{R}^d}|u(\mathbf{x},t)|^2d\mathbf{x} \equiv \mathrm{M}(0), \tag{3}$$

and the total energy (or Hamiltonian):

$$\mathrm{E}(t) := \int_{\mathbb{R}^d}[\gamma\,\mathrm{Re}(u^*(\mathbf{x},t)(-\Delta)^{\alpha/2}u(\mathbf{x},t)) + \frac{\beta}{2}|u(\mathbf{x},t)|^4]d\mathbf{x} \equiv \mathrm{E}(0), \tag{4}$$

where $\mathrm{Re}(\phi)$ and ϕ^* represent the real part and the complex conjugate of a function ϕ, respectively.

Numerical simulations play an important role in the study of the SFNLSE. To solve a space-fractional PDE numerically, we could combine a spatial discretization scheme with a time integrator. For spatial discretization, numerical methods can be found in [20–22], where one-dimensional space-fractional equations are solved. A fast finite difference method was developed by Wang and Du [23] for the three-dimensional time-dependent space-fractional diffusion equations with a linear source term. Yu et al. [24] utilized a fourth-order compact scheme for the two-dimensional nonlinear fractional reaction–subdiffusion equation in which the trapezoid formula is used to approximate the integration of the nonlinear source term. Zhao et al. [25] developed a fourth-order compact ADI scheme for the two-dimensional SFNLSE. A spectral approach is used in [26] to solve the space–time fractional diffusion equation. In this paper, a Fourier spectral method will be used for the spatial discretization of the SFNLSE, because it deals with different kinds of boundary conditions and solves multiple space-dimensional problems fast and accurately.

The exponential time differencing (ETD) method is one of the many time integrators developed to solve stiff semi-linear problems. In this paper, we propose a modified exponential time differencing Runge–Kutta (ETDRK4) scheme with Padé approximation to the exponential function (ETDRK4-P). The ETDRK4 method uses the same techniques as the Krylov subspace methods and Chebyshev approximations of the matrix exponential operator used in [27]. A similar method, which is named the implicit–explicit multi-step time-discretization scheme is also used for time-dependent partial differential equations (PDEs), such as PDEs of convection–diffusion type [28]. This paper utilizes the ETDRK4-P scheme that treats the linear terms in the SFNLSEs implicitly and the nonlinear terms explicitly.

This paper is organized as follows. In Section 2, we briefly introduce the Fourier spectral method, utilized as the spatial discretization scheme for the SFNLSE. In Section 3, we provide descriptions of the fourth-order split-step scheme and the ETDRK4-P scheme as time integrators for the SFNLSE. We perform the analytical discussion of the stability and truncation errors of the ETDRK4-P scheme in Section 4. In Section 5, extensive numerical results of the SFNLSE are given, demonstrating the convergence rate and efficiency of the proposed scheme. Mass and energy conservation properties of the proposed scheme are also numerically discussed. Finally, we present conclusions and possible future extensions for this research in Section 6.

2. The Fourier spectral method for the fractional Laplacian in space

Spectral decomposition is critical in interpreting the fractional Laplacian. Suppose the Laplacian $(-\Delta)$ has a complete set of orthonormal eigenfunctions φ_j satisfying standard boundary conditions on a bounded region $\Omega\subset\mathbb{R}^d$, with corresponding eigenvalues λ_j, i.e.,$(-\Delta)\varphi_j=\lambda_j\varphi_j$ on Ω, then the fractional Laplacian can be interpreted as [29]:

$$(-\Delta)^{\alpha/2}u = \sum_{j=0}^{\infty}\hat{u}_j\lambda_j^{\alpha/2}\varphi_j,$$

Please cite this article in press as: X. Liang, A.Q.M. Khaliq, An efficient Fourier spectral exponential time differencing method for the space-fractional nonlinear Schrödinger equations, Computers and Mathematics with Applications (2018), https://doi.org/10.1016/j.camwa.2018.03.042.