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An improved collocation method for multi-dimensional space–time variable-order fractional Schrödinger equations

A.H. Bhrawy [a,*], M.A. Zaky [b,c]

[a] Department of Mathematics, Faculty of Science, Beni-Suef University, Beni-Suef, Egypt
[b] Department of Applied Mathematics, National Research Centre, Dokki, Giza 12622, Egypt
[c] Zewail City of Science and Technology, University of Science and Technology, Zayed City, Giza 12588, Egypt

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ABSTRACT

Current discretizations of variable-order fractional (V-OF) differential equations lead to numerical solutions of low order of accuracy. This paper explores a high order numerical scheme for multi-dimensional V-OF Schrödinger equations. We derive new operational matrices for the V-OF derivatives of Caputo and Riemann–Liouville type of the shifted Jacobi polynomials (SJPs). These allow us to establish an efficient approximate formula for the Riesz fractional derivative. An operational approach of the Jacobi collocation approach for the approximate solution of the V-OF nonlinear Schrödinger equations. The main characteristic behind this approach is to investigate a space–time spectral approximation for spatial and temporal discretizations. The proposed spectral scheme, both in temporal and spatial discretizations, is successfully developed to handle the two-dimensional V-OF Schrödinger equation. Numerical results indicating the spectral accuracy and effectiveness of this algorithm are presented.

1. Introduction

It is demonstrated that many dynamic processes exhibit fractional order behavior that may vary with time and/or space [26]. This indicates that V-OF calculus is a natural candidate to provide an effective mathematical framework for the description of complex dynamical phenomena, whose behavior otherwise may not be properly understood. Interest in this area started with the studies by Samko, Ross, and collaborators [41–44]. Many authors presented different definitions of V-OF operators to suit desired goals and then studied their properties and applications. Lorenzo and Hartley [34] presented the concept of V-OF operators and investigated several potential V-OF definitions. Coimbra [16] proposed the Laplace transform of Caputo fractional derivative as the starting point to suggest a novel definition for the V-OF differential operator. These pioneering publications focused on mathematical properties of possible candidates for a V-OF operator. The extension from fixed-order to V-OF operators provides an invaluable prospect in modeling diverse physical systems such as linear and nonlinear oscillators with viscoelastic damping [16], modeling of diffusive–convective effects on the oscillatory flows [38], processing of geographical data using V-OF derivatives [17], signature verification through variable/adaptive fractional order differentiators [48], constitutive laws in viscoelastic continuum mechanics [40], anomalous diffusion problems [45], fractional advection–diffusion problem [46], and chloride ions diffusion in concrete structures [13].

* Corresponding author.
E-mail addresses: alibhrawy@yahoo.co.uk (A.H. Bhrawy), mzaky@zewailcity.edu.eg (M.A. Zaky).

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The classical Schrödinger equation is one of the most universal models that describe many physical phenomena and has important applications in nonlinear optics, plasma physics and fluid dynamics [18,19,39]. Feynman and Hibbs [21] reformulated the non relativistic quantum mechanics as a path integral over the Brownian paths, and this background leads to standard (nonfractional) quantum mechanics. Recently, in a series of papers by Laskin (see e.g. [28–30]) and many other papers by different authors [1,4,15,49,52], a space-fractional Schrödinger equation with the quantum Riesz derivative of order β, $1 < \beta \le 2$ (fractional Laplacian) instead of the Laplace operator has been introduced and analyzed on the base of the Feynman path integral. Afterwards, some authors [22,23] discussed the physical applications of fractional Schrödinger equation and obtained the exact solutions with several kinds of potential fields. Amore et al. [2] developed the collocation method for fractional quantum mechanics. Guo et al. [24] proved the existence of the global smooth solution of fractional nonlinear Schrödinger equation with periodic boundary conditions. Zhao et al. [59] proposed a novel compact operator for the approximation of the Riesz fractional derivative which applied to solve the two dimensional nonlinear space fractional Schrödinger equation. Yang [55] proposed a class of linearized energy-conserved finite difference schemes for nonlinear space-fractional Schrödinger equation. Hu et al. [25] studied the existence and uniqueness of the global solution of coupled nonlinear fractional Schrödinger equations. In a series of papers by Wang et al. [51–53], efficient numerical schemes were studied for the coupled nonlinear space-fractional Schrödinger equations with the Riesz fractional derivative. Li et al. [32] used Crank–Nicolson scheme in temporal direction and finite element method in spatial direction to solve a class of nonlinear space-fractional Schrödinger equations.

On the other hand, the time-fractional Schrödinger equation with Caputo fractional derivative was derived and studied on the basis of fractional Brownian motion [37]. In addition, Naber [37] showed that the time-fractional Schrödinger equation is equivalent to the classical Schrödinger equation but with a time dependent Hamiltonian. More recently, Wang and Xu [50] investigated a Schrödinger equation with both space- and time-fractional derivatives and solved the generalized Schrödinger equation for free particle and an infinite rectangular potential well. Several global numerical methods were proposed and developed, in the last few years, for solving space- and time-fractional Schrödinger equations [20], like Galerkin method [54], collocation method with radial basis functions [36] and Legendre collocation method [6].

As a natural generalization of the fractional Schrödinger equation, the V-OF Schrödinger equation has been exploited to study fractional quantum phenomena. Atangana and Cloot [3] studied the stability and convergence of the Crank–Nicolson difference scheme for the space V-OF Schrödinger equation with V-OF Caputo derivative. Since the kernel of the V-OF operators has a variable exponent, analytical solutions to the resulting equations are hard to obtain compared with its counterpart constant-order one. Therefore, numerical approaches are needed for solving V-OF differential equations. Several numerical methods have been developed for solving numerically the fractional partial differential equations [5,7,9,10,57]. From the numerical point of view for V-OF partial differential equations, Lin et al. [33] studied the stability and convergence of an explicit finite-difference approximation for the space V-OF nonlinear diffusion equation. Zhuang et al. [60] discussed the stability and convergence of Euler approximation for the space V-OF advection-diffusion equation with a nonlinear source term. A new two-dimensional space V-OF percolation equation is considered by Chen et al. [14], who gave an implicit numerical scheme by an alternating direct method. Zhang et al. [58] provided a novel numerical method for the time V-OF mobile–immobile advection–dispersion model. Recently, we proposed an accurate collocation scheme for solving V-OF cable equation [8].

The main objective of the present work is to investigate new Jacobi operational matrices for left-side and right-side Riemann–Liouville and Caputo V-OF derivatives, which in turn allow us to establish an efficient approximate formula for the V-OF Riesz derivative. Therefore, we propose a high order numerical scheme for solving the one-dimensional space–time V-OF Schrödinger equation. This method is based on Jacobi collocation technique in conjunction with the new operational matrices of V-OF derivatives of SJPs. The highly accurate scheme, both in temporal and spatial discretizations, is successfully extended to solve the two-dimensional V-OF Schrödinger equation. Illustrative test problems are carried out to demonstrate the spectral accuracy and efficiency of the proposed algorithms. Indeed, there are no high order methods in the literatures for the numerical solution of multi-dimensional V-OF Schrödinger equations, and this motivated our interest to propose such new method.

The article is structured as follows. Section 2 introduces fractional calculus and some characteristics of SJPs. In Section 3, we derive new operational matrices of SJPs. In Section 4, V-OF Schrödinger equation in one and two dimensions are solved by Jacobi collocation technique in conjunction with the operational matrices of V-OF Caputo and Riemann–Liouville derivatives. Numerical examples and comparisons are reported in Section 5. A conclusion is highlighted in Section 6.

2. Preliminaries

In this section, we make necessary preparations for subsequent discussions. We divide this section into two main parts. In the first part, we recollect some definitions and mathematical preliminaries of the V-OF derivatives. In the second part, we collect some important properties of SJPs.

2.1. Variable-order fractional Laplacian

The V-OF operator definitions that have been proposed are either direct extensions of the fractional calculus definitions or generalizations that arise from Laplace or Fourier transformations. In the direct extension approach, the constant exponent in the fractional operator is replaced with a function [43,56,60].