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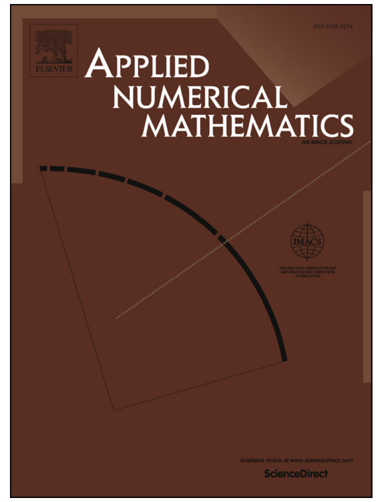

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Structure-preserving numerical methods for the fractional Schrödinger equation

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Abstract

This paper considers the long-time integration of the nonlinear fractional Schrödinger equation involving the fractional Laplacian from the point of view of symplectic geometry. By virtue of a variational principle with the fractional Laplacian, the equation is first reformulated as a Hamiltonian system with a symplectic structure. Then, by introducing a pair of intermediate variables with a fractional operator, the equation is reformulated in another form for which more conservation laws are found. When reducing to the case of integer order, they correspond to multi-symplectic conservation law and local energy conservation law for the the classic Schrödinger equation. After that, structure-preserving algorithms with the Fourier pseudospectral approximation to the spatial fractional operator are constructed. It is proved that the semi-discrete and fully discrete systems satisfy the corresponding symplectic or other conservation laws in the discrete sense. Numerical tests are performed to validate the efficiency of the methods by showing their remarkable conservation properties in the long-time simulation.

Key words: Fractional Schrödinger equation; Fractional Laplacian; Hamiltonian system; Symplectic method; Generalized multi-symplectic method; Conservation law

1. Introduction

Fractional quantum mechanics is a natural extension of quantum mechanics that has been attracting great interest since its introduction by Laskin via replacing Brownian trajectories in Feynman path integrals by the Lévy ones [1, 2]. It leads to the fractional Schrödinger equation (FSE) − a generalization of the classical Schrödinger equation, which involves the fractional Laplacian with the Lévy index $1 < \alpha \leqslant 2$ instead of the usual one. The FSE also arises in the continuum limit of a family of discrete models for charge transport in biopolymers like the DNA [3]. In the special case of $\alpha = 2$, the equation reduces to the classical Schrödinger equation which describes a

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