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On a conservative Fourier spectral Galerkin method for cubic nonlinear Schrödinger equation with fractional Laplacian

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Abstract

In this paper, a Crank–Nicolson Fourier spectral Galerkin method is proposed for solving the cubic fractional Schrödinger equation. Firstly, we discuss the mass and energy conservation laws for the nonlinear system and its corresponding fully discrete scheme. Secondly, the convergence with the spectral order accuracy in space and the second order of accuracy in time is exhibited. We perform one-dimensional calculation of the fractional derivative differential equation to verify our theoretical findings. Moreover, the proposed scheme is successfully applied to study two- and three-dimensional fractional quantum mechanics. Numerical results clearly exhibit that the fractional order can affect the shapes of soliton and rogue waves. The evolution of ground state solution can be clearly seen to be non-symmetrically configured when the fractional order becomes smaller.

Keywords: Fractional Schrödinger equation; Fourier spectral Galerkin method; Conservative laws; Convergence analysis; Numerical examples

1. Introduction

As is well known, the Schrödinger equation is one of the most important partial differential equations in mathematical physics, which is capable of effectively describing the change of the quantum behavior in some physical systems [3]. During the past few decades, there has been a significant effort dedicated to the numerical analysis and scientific computing for the Schrödinger equation [1,6,11,20,23,24,28].

In a sequence of papers [13–15], Nick Laskin developed the fundamental equation of fractional quantum mechanics as a result of extending the Feynman path integral from the Brownian motion to Lévy-like paths. The consequence is that the linear space-fractional Schrödinger equation has been derived. Hu and Kallianpur [8] investigated the Schrödinger equation with fractional Laplacian and constructed solution in a form of probability. Guo and Xu [7] studied the fundamental solution of fractional Schrödinger equation involving the Green's function. Dong and Xu [4] gave some solutions to the space fractional Schrödinger equation using momentum representation method. Bayln [2] presented a free particle solution in terms of Fox's H-functions for the fractional Schrödinger equation in general coordinates. However, it is hard to compute the special functions in the above referred works.

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Furthermore, derivation of the exact solutions to the fractional Schrödinger equations is very difficult in nonlinear cases. Hence, application of numerical techniques becomes essential to study the behaviors of the fractional quantum systems. Zhao et al. [30] presented a fourth-order compact ADI scheme to solve the two-dimensional nonlinear space-fractional Schrödinger equation. Finite difference methods for the nonlinear space-fractional Schrödinger equation with Riesz space fractional derivative were proposed and analyzed in [19,25–27]. Li et al. [16,17] proposed the finite element model for solving the space-fractional Schrödinger equation. Recently, Kirkpatrick and Zhang [12] applied a split-step Fourier spectral method to study the decoherence of solitons in fractional Schrödinger equation without detailing the numerical properties of this method. Mass-conservation Fourier spectral method for the fractional nonlinear Schrödinger equations was investigated by Duo and Zhang [5]. However, the convergence of this method was not discussed.

The novelty of our paper is to develop a Crank–Nicolson Fourier spectral Galerkin method for cubic nonlinear fractional Schrödinger equation. The superiority of this method is based on the weak formulation and Galerkin approximation so that it can be easily extended to other spatial discretizations, such as the Galerkin finite element method. The fast Fourier transform (FFT) is used to find the Fourier coefficients in our spatial computation. Analysis on the conservation laws and error estimates is performed for the proposed scheme, which is proved to preserve both the mass and energy. Also the proposed method can achieve the desired computational efficiency in the sense that the accuracy order of our method is higher than some recently studied methods.

The rest of this paper is organized as follows. In Section 2, the fractional Schrödinger equations are presented and the existence of the conservation laws for the nonlinear systems is proved. In Section 3, we apply the proposed Crank–Nicolson Fourier spectral Galerkin method to solve the fractional Schrödinger equation. Both of the conservation laws and the error estimates of the proposed scheme are detailed. In Section 4, we perform numerical study to confirm the effectiveness of the proposed method. Finally, some concluding remarks are drawn in Section 5.

2. Mathematic model

In this study, we consider the time-dependent nonlinear Schrödinger equation with fractional Laplacian as follows

$$i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t}=\hbar^{\alpha}(-\Delta)^{\frac{\alpha}{2}}\psi(\mathbf{x},t)+V(\mathbf{x})\psi(\mathbf{x},t)+\beta|\psi(\mathbf{x},t)|^{2}\psi(\mathbf{x},t),\ \ t>0,\tag{2.1}$$

where $i=\sqrt{-1}$. The solution of ψ is sought subject to the initial condition:

$$\psi(\mathbf{x},0)=\psi_{0}(\mathbf{x}).\tag{2.2}$$

In Eq. (2.1), $\hbar$ is the reduced Planck constant, $\psi(\mathbf{x},t)$ is a complex-valued wave function of $\mathbf{x}\in\mathbb{R}^{d}$ (for $d=1,2,$ or 3) and $t\geq 0$, $V(\mathbf{x})$ denotes a potential energy. The parameter β represents the strength of short-range nonlinear interaction. The fractional quantum derivative $(-\Delta)^{\frac{\alpha}{2}}$ in (2.1) is defined by [9,10,18,21]

$$-(-\Delta)^{\frac{\alpha}{2}}u(x,t)=\frac{\partial^{\alpha}}{\partial|x|^{\alpha}}u(x,t)=-\frac{1}{2\cos(\pi\alpha/2)}[\,_{-\infty}D_{x}^{\alpha}u(x,t)+_{x}D_{+\infty}^{\alpha}u(x,t)],$$

where $_{-\infty}D_{x}^{\alpha}$ and $_{x}D_{+\infty}^{\alpha}$ are left and right Riemann–Liouville fractional derivatives, respectively. With periodic boundary conditions, the Riesz fractional derivative $(-\Delta)^{\frac{\alpha}{2}}$ also can be defined by the Fourier transform, which reads

$$\mathcal{F}[-(-\Delta)^{\frac{\alpha}{2}}u(x)](\xi)=-|\xi|^{\alpha}\mathcal{F}[u(x)](\xi),$$

where $\mathcal{F}$ is the Fourier transform.

Note that for $\alpha=2$, the fractional Laplacian in (2.1) is reduced to the standard Laplace operator. For the case of $\alpha\in(1,2)$, the effect of fractional Laplacian operator describing long-range interactions is no longer local. For simplicity, numerical approximation of (2.1) in one dimensional domain will be considered, though the generalization to higher dimension is straightforward. In this study, we will truncate (2.1) into a finite computational domain $\Omega=(a,b)$ with periodic boundary condition.

Let C_{per}^{∞} be the set of all restrictions onto $\mathbb{R}$, and denote by H_{per}^{q} the closure of C_{per}^{∞} with the usual Sobolev norm $\|\cdot\|_q$. We denote the standard inner product and norm as follows

$$(u, v) = \int_{\mathbb{R}} uv dx, \quad \|u\| = (\int_{\mathbb{R}} |u|^2 dx)^{\frac{1}{2}},$$

for any $u, v \in L^2(\mathbb{R})$.

Here, we focus on a finite (square) barrier potential $V(x) = V_0$ that is restricted to the interval (a, b). The value of V_0 is zero elsewhere. The weak statement of (2.1)–(2.2) in one-dimensional case can be defined as follows.

Definition 2.1. A function $\psi : \Omega \times R^+ \to R$ is called a weak solution of (2.1), if $\psi \in C^2(H_{\text{per}}^{\alpha}(\Omega) \cap H^q(\Omega); [0, T])$ for all $T > 0$, such that for all $\phi \in H_{\text{per}}^2(\Omega)$ the following equation holds

$$(i\hbar \frac{\partial \psi}{\partial t}, \varphi) = (\hbar^{\alpha}(-\Delta)^{\frac{\alpha}{2}} \psi, \varphi) + (V_0 \psi, \varphi) + (\beta|\psi|^2 \psi, \varphi), \tag{2.3}$$

with the initial condition $\psi(0) = \psi_0$.

In the following lemma, we shall give a useful characterization with respect to the fractional Laplacian.

Lemma 2.1. *For any $u, w \in L^2(\mathbb{R})$, then one can have*

$$((-\Delta)^{\frac{\alpha}{2}} u, w) = ((-\Delta)^{\frac{\alpha}{4}} u, (-\Delta)^{\frac{\alpha}{4}} w).$$

Proof. For any $w_1, w_2 \in L^2(\mathbb{R})$, we recall the Parseval identity [29] as

$$\int_{\mathbb{R}} w_1(x)\overline{w_2(x)} dx = \frac{1}{2\pi} \int_{\mathbb{R}} \mathcal{F}[w_1(x)](\xi)\overline{\mathcal{F}[w_2(x)](\xi)} dx.$$

Then, by using the identity $\mathcal{F}[(-\Delta)^{\frac{\alpha}{4}} u(x)](\xi) = |\xi|^{\alpha/2}\mathcal{F}[u(x)](\xi)$, we have

$$\begin{aligned}
\int_{\mathbb{R}} (-\Delta)^{\frac{\alpha}{4}} u(x)(-\Delta)^{\frac{\alpha}{4}} w(x) dx &= \frac{1}{2\pi} \int_{\mathbb{R}} \mathcal{F}[(-\Delta)^{\frac{\alpha}{4}} u(x)](\xi)\overline{\mathcal{F}[(-\Delta)^{\frac{\alpha}{4}} w(x)](\xi)} dx \\
&= \frac{1}{2\pi} \int_{\mathbb{R}} |\xi|^{\alpha} \mathcal{F}[u(x)](\xi)\overline{\mathcal{F}[w(x)](\xi)} dx \\
&= \frac{1}{2\pi} \int_{\mathbb{R}} \mathcal{F}[(-\Delta)^{\frac{\alpha}{2}} u(x)](\xi)\overline{\mathcal{F}[w(x)](\xi)} dx \\
&= \int_{\mathbb{R}} [(-\Delta)^{\frac{\alpha}{2}} u(x)] w(x) dx.
\end{aligned}$$

The proof is completed.

Next, we will give two conservation laws with respect to the fractional Schrödinger equation (2.1) in one dimensional domain.

Theorem 2.1. *The fractional system of Schrödinger equations (2.1)–(2.2) permits the mass and energy conservation laws as follows*

$$Q(t) := \|\psi(x, t)\|^2 = \|\psi_0(x)\|^2 = Q(0), \tag{2.4}$$

and

$$E(t) := \frac{\hbar^{\alpha-1}}{2} \|(-\Delta)^{\frac{\alpha}{4}} \psi(x, t)\|^2 + \frac{V_0}{2\hbar} \|\psi(x, t)\|^2 + \frac{\beta}{4\hbar} \|\psi(x, t)\|_{L^4}^4 = E(0), \tag{2.5}$$

where $\|\cdot\|_{L^4}$ denotes the L^4-norm.

Proof. Taking $\varphi = \psi$ in (2.3), by Lemma 2.1, we get

$$(i \frac{\partial \psi}{\partial t}, \psi) = \hbar^{\alpha-1}((-\Delta)^{\frac{\alpha}{4}} \psi, (-\Delta)^{\frac{\alpha}{4}} \psi) + \frac{V_0}{\hbar}(\psi, \psi) + \frac{\beta}{\hbar}(|\psi|^2 \psi, \psi).$$

Taking the imaginary part of the above equation into account, we arrive at

$$Im\{(i\frac{\partial\psi}{\partial t},\psi)\} = (\frac{\partial\psi}{\partial t},\psi) = 0.$$

Therefore, we deduce that

$$\frac{d}{dt}\|\psi\|^2 = 2(\frac{\partial\psi}{\partial t},\psi) = 0,$$

implying the conservation of mass given in (2.4).

Similarly, setting $\varphi = \frac{\partial\psi}{\partial t}$ in (2.3), we obtain

$$(i\frac{\partial\psi}{\partial t},\frac{\partial\psi}{\partial t}) = \hbar^{\alpha-1}((-\Delta)^{\frac{\alpha}{4}}\psi,(-\Delta)^{\frac{\alpha}{4}}(\frac{\partial\psi}{\partial t})) + \frac{V_0}{\hbar}(\psi,\frac{\partial\psi}{\partial t}) + \frac{\beta}{\hbar}(|\psi|^2\psi,\frac{\partial\psi}{\partial t}).$$

Taking the real part of the above equation, we immediately get

$$\frac{d}{dt}[\frac{\hbar^{\alpha-1}}{2}\|(-\Delta)^{\frac{\alpha}{4}}\psi\|^2 + \frac{V_0}{2\hbar}\|\psi\|^2 + \frac{\beta}{4\hbar}\|\psi\|_{L^4}^4] = 0.$$

If we set $E(t) = \frac{\hbar^{\alpha-1}}{2}\|(-\Delta)^{\frac{\alpha}{4}}\psi\|^2 + \frac{V_0}{2\hbar}\|\psi\|^2 + \frac{\beta}{4\hbar}\|\psi\|_{L^4}^4$, then the conservation of energy given in (2.5) holds.

3. Fourier spectral Galerkin method

In this section, we shall present a Fourier spectral Galerkin method for solving the fractional Schrödinger equation.

For each integer $N \geq 1$, we introduce the following finite dimensional subspace

$$H_N = \text{span}\{e^{i\mu\cdot x}, |\mu| \leq N\}.$$

Denote by $P_N : L^2(\Omega) \to H_N$ the $L^2(\Omega)$-projection onto H_N, which is defined by

$$(P_N\psi - \psi,\varphi) = 0, \ \forall\varphi \in H_N.$$

Let $\psi_N(x,t) \in H_N$ for $t \geq 0$. By performing the Fourier spectral Galerkin approximation on (2.3) we have the following equation for all $\varphi_N \in H_N$

$$(i\hbar\frac{\partial\psi_N}{\partial t},\varphi_N) = (\hbar^{\alpha}(-\Delta)^{\frac{\alpha}{2}}\psi_N,\varphi_N) + (V_0\psi_N,\varphi_N) + (\beta|\psi_N|^2\psi_N,\varphi_N), \ \forall\varphi_N \in H_N, \tag{3.1}$$

with

$$\psi_N(x,0) = P_N\psi_0(x).$$

The Fourier projection P_N is defined as

$$P_N\phi(x) = \sum_{|\xi|\leq N}\widehat{\phi}(\xi)e^{i\xi\cdot x}.$$

In the above equation, the Fourier coefficients are arranged as

$$\widehat{\phi}(\xi) = \frac{1}{2\pi}\int_{\Omega}\phi(x)e^{-i\xi\cdot x}dx.$$

To establish the bound and convergence of the Fourier spectral Galerkin approximation, we shall recall the following lemma and theorems.

Lemma 3.1 ([22]). *For any $\phi \in H^q_{\text{per}}(\Omega)$, the following estimates hold*

$$\|P_N\phi\|_p \leq \|\phi\|_p, \quad \|\phi - P_N\phi\|_p \leq CN^{p-q}\|\phi\|_q,$$

for all $0 \leq p \leq q$.

Let $\tau = T/K > 0$ be a time step, and denote $t_k = k\tau$ for $k = 0, 1, \ldots, K$. Defining the difference operators as

$$\delta_t\psi_N^k = \frac{\psi_N^{k+1} - \psi_N^k}{\tau}, \quad \psi_N^{k+1/2} = \frac{\psi_N^{k+1} + \psi_N^k}{2}.$$

At each time level k, the time derivative is discretized by the Crank–Nicolson scheme. The fully discrete Fourier spectral Galerkin approximation can then be read as: for all $\varphi_N \in H_N$, find $\psi_N^k \in H_N$ such that

$$(i\hbar\delta_t\psi_N^k, \varphi_N) = (\hbar^\alpha(-\Delta)^{\frac{\alpha}{2}}\psi_N^{k+1/2}, \varphi_N) + (V_0\psi_N^{k+1/2}, \varphi_N) + \frac{\beta}{2}((|\psi_N^{k+1}|^2 + |\psi_N^k|^2)\psi_N^{k+1/2}, \varphi_N), \tag{3.2}$$

with $\psi_N^0 = P_N\psi_0$.

Next, we will prove the existence of conservation laws and establish the error estimation for the Fourier spectral Galerkin approximation.

Theorem 3.1 (*Mass Conservation*). *Assume that ψ_N^k is the numerical solution of (2.1)–(2.2), then we have the discrete mass*

$$Q^k = \|\psi_N^k\|^2 = \|\psi_N^0\|^2 = Q^0. \tag{3.3}$$

Proof. Setting $\varphi_N = \psi_N^{k+1/2}$ in (3.2), then we have

$$(i\delta_t\psi_N^k, \psi_N^{k+1/2}) = \hbar^{\alpha-1}((-\Delta)^{\frac{\alpha}{2}}\psi_N^{k+1/2}, \psi_N^{k+1/2}) + \frac{V_0}{\hbar}(\psi_N^{k+1/2}, \psi_N^{k+1/2}) + \frac{\beta}{2\hbar}((|\psi_N^{k+1}|^2 + |\psi_N^k|^2)\psi_N^{k+1/2}, \psi_N^{k+1/2}). \tag{3.4}$$

Notice that

$$Im\{(\psi_N^{k+1/2}, \psi_N^{k+1/2})\} = 0,$$
$$Im\{((|\psi_N^{k+1}|^2 + |\psi_N^k|^2)\psi_N^{k+1/2}, \psi_N^{k+1/2})\} = 0,$$
$$Im\{((-\Delta)^{\frac{\alpha}{2}}\psi_N^{k+1/2}, \psi_N^{k+1/2})\} = Im\{((-\Delta)^{\frac{\alpha}{4}}\psi_N^{k+1/2}, (-\Delta)^{\frac{\alpha}{4}}\psi_N^{k+1/2})\} = 0.$$

Taking the imaginary part of (3.4) into account, we obtain

$$Re\{(\delta_t\psi_N^k, \psi_N^{k+1/2})\} = \frac{1}{2\tau}(\|\psi_N^{k+1}\|^2 - \|\psi_N^k\|^2) = 0.$$

The above equation implies that $Q^{k+1} = Q^k$ and thus the mass conservation in (3.3) holds for $k \geq 0$.

Theorem 3.2 (*Energy Conservation*). *Assume that ψ_N^k is the numerical solution of (2.1), then the discrete energy given below can be derived*

$$E^k = \frac{\hbar^{\alpha-1}}{2}\|(-\Delta)^{\frac{\alpha}{4}}\psi_N^k\|^2 + \frac{V_0}{2\hbar}\|\psi_N^k\|^2 + \frac{\beta}{4\hbar}\|\psi_N^k\|_{L^4}^4 = E^0. \tag{3.5}$$

Proof. Setting $\varphi_N = \delta_t\psi_N^k$, (3.2) can be rewritten as

$$(i\delta_t\psi_N^k, \delta_t\psi_N^k) = \hbar^{\alpha-1}((-\Delta)^{\frac{\alpha}{2}}\psi_N^{k+1/2}, \delta_t\psi_N^k) + \frac{V_0}{\hbar}(\psi_N^{k+1/2}, \delta_t\psi_N^k) + \frac{\beta}{2\hbar}((|\psi_N^{k+1}|^2 + |\psi_N^k|^2)\psi_N^{k+1/2}, \delta_t\psi_N^k). \tag{3.6}$$

Noticing that $Re\{(i\delta_t\psi_N^k, \delta_t\psi_N^k)\} = 0$ and considering the real part of (3.6), we are led to derive

$$0 = Re\{(\hbar^{\alpha-1}(-\Delta)^{\frac{\alpha}{2}}\psi_N^{k+1/2}, \delta_t\psi_N^k)\} + \frac{V_0}{2\tau\hbar}(\|\psi_N^{k+1}\|^2 - \|\psi_N^k\|^2) + \frac{\beta}{4\tau\hbar}(\|\psi_N^{k+1}\|_{L^4}^4 - \|\psi_N^k\|_{L^4}^4).$$

Owing to

$$Re\{(\hbar^{\alpha-1}(-\Delta)^{\frac{\alpha}{2}}\psi_N^{k+1/2}, \delta_t\psi_N^k)\} = \frac{\hbar^{\alpha-1}}{2\tau}(\|(-\Delta)^{\frac{\alpha}{4}}\psi_N^{k+1}\|^2 - \|(-\Delta)^{\frac{\alpha}{4}}\psi_N^k\|^2),$$

we can conclude that

$$\frac{\hbar^{\alpha-1}}{2}\|(-\Delta)^{\frac{\alpha}{4}}\psi_N^{k+1}\|^2+\frac{V_0}{2\hbar}\|\psi_N^{k+1}\|^2+\frac{\beta}{4\hbar}\|\psi_N^{k+1}\|_{L^4}^4$$
$$=\frac{\hbar^{\alpha-1}}{2}\|(-\Delta)^{\frac{\alpha}{4}}\psi_N^{k}\|^2+\frac{V_0}{2\hbar}\|\psi_N^{k}\|^2+\frac{\beta}{4\hbar}\|\psi_N^{k}\|_{L^4}^4,$$

it is implied that $E^{k+1}=E^k$ for any $k\geq 0$. As a result, the energy conservation law, or (3.5), holds.

Now, we will give the convergence analysis of the semi-discrete form.

Theorem 3.3. *Let* $1<\alpha\leq 2$ *and* $q\geq 1$*, assume that* $\psi\in C^2(H^{\alpha}_{\text{per}}(\Omega)\cap H^q(\Omega);[0,T])$ *is the exact solution to* (2.1) *and* ψ_N *is the solution of* (3.1)*, respectively. Then, there exists a constant* $C>0$ *such that*

$$\|\psi-\psi_N\|\leq CN^{-q}\|\psi\|_q.$$

Proof. Let $e=\psi-\psi_N=(\psi-P_N\psi)+(P_N\psi-\psi_N):=\rho+\theta$. Setting $\varphi=\varphi_N\in H_N$ in (2.3) and subtracting (3.1) from (2.3), one can arrive at

$$i(\frac{\partial e}{\partial t},\varphi_N)=\hbar^{\alpha-1}((-\Delta)^{\frac{\alpha}{2}}e,\varphi_N)+\frac{V_0}{\hbar}(e,\varphi_N)$$
$$+\frac{\beta}{\hbar}(|\psi|^2\psi-|\psi_N|^2\psi_N,\varphi_N). \tag{3.7}$$

By exploiting the orthogonal property in the operator P_N, we have

$$(e,\varphi_N)=(\rho,\varphi_N)+(\theta,\varphi_N)=(\theta,\varphi_N),$$
$$((-\Delta)^{\frac{\alpha}{2}}e,\varphi_N)=((-\Delta)^{\frac{\alpha}{4}}\rho,(-\Delta)^{\frac{\alpha}{4}}\varphi_N)+((-\Delta)^{\frac{\alpha}{4}}\theta,(-\Delta)^{\frac{\alpha}{4}}\varphi_N)=((-\Delta)^{\frac{\alpha}{4}}\theta,(-\Delta)^{\frac{\alpha}{4}}\varphi_N).$$

Let $\varphi_N=\theta$ in (3.7). Owing to $Im\{((-\Delta)^{\frac{\alpha}{4}}\theta,(-\Delta)^{\frac{\alpha}{4}}\theta)\}=0$, by taking the imaginary part of (3.7), we can derive the following equation

$$(\frac{\partial\theta}{\partial t},\theta)=Im\{\frac{\beta}{\hbar}(|\psi|^2\psi-|\psi_N|^2\psi_N,\theta)\}.$$

Making use of the Cauchy–Schwarz inequality, we have

$$\frac{1}{2}\frac{d}{dt}\|\theta\|^2\leq\frac{\beta\Psi_{\max}}{\hbar}(\|\rho\|+\|\theta\|)\|\theta\|, \tag{3.8}$$

where $\Psi_{\max}=\max\{|\psi|^2,|\psi_N|^2\}$.

By means of Lemma 3.1, we get

$$\|\rho\|\leq CN^{-q}\|\psi\|_q.$$

Therefore, application of inequality (3.8) yields

$$\frac{d}{dt}\|\theta\|\leq C(\|\theta\|+N^{-q}\|\psi\|_q). \tag{3.9}$$

By integrating (3.9) from 0 to t, the following inequality equation holds

$$\|\theta\|\leq C\|\theta(0)\|+CN^{-q}\|\psi\|_q+C\int_0^t\|\theta\|d\sigma.$$

Owing to $\theta(0)=0$ and by virtue of the Gronwall's lemma, we get

$$\|\theta\|\leq CN^{-q}\|\psi\|_q.$$

By Lemma 3.1 and the triangle inequality, finally we obtain

$$\|e\|\leq\|\rho\|+\|\theta\|\leq CN^{-q}\|\psi\|_q.$$

This completes the proof.

Theorem 3.4. *Let $1 < \alpha \leq 2$ and $q \geq 1$, assume that $\psi \in C^2(H^\alpha_{per}(\Omega) \cap H^q(\Omega); [0,T])$ is the exact solution of Eq. (2.1) and ψ_N^k is the solution of (3.2), respectively. Then, there exists a constant $C > 0$ such that*

$$\|\psi^k - \psi_N^k\| \leq C(\tau^2 + N^{-q}).$$

Proof. The employed Crank–Nicolson scheme for (2.1) is given by

$$i\hbar\delta_t\psi^k = \hbar^\alpha(-\Delta)^{\frac{\alpha}{2}}\psi^{k+1/2} + V_0\psi^{k+1/2} + \frac{\beta}{2}(|\psi^{k+1}|^2 + |\psi^k|^2)\psi^{k+1/2} + T^k, \tag{3.10}$$

where $T^k = O(\tau^2)$ is the truncation error.

Let $e^k = \psi^k - \psi_N^k = (\psi^k - P_N\psi^k) + (P_N\psi^k - \psi_N^k) := \rho^k + \theta^k$. Taking the inner product of (3.10) with φ_N and subtracting it from (3.2), we have

$$\begin{aligned} i(\frac{e^{k+1}-e^k}{\tau}, \varphi_N) &= \frac{\hbar^{\alpha-1}}{2}((-\Delta)^{\frac{\alpha}{2}}(e^{k+1}+e^k), \varphi_N) + \frac{V_0}{2\hbar}(e^{k+1}+e^k, \varphi_N) \\ &+ \frac{\beta}{2\hbar}(|\psi^{k+1}|^2\psi^{k+1/2} - |\psi_N^{k+1}|^2\psi_N^{k+1/2}, \varphi_N) \\ &+ \frac{\beta}{2\hbar}(|\psi^k|^2\psi^{k+1/2} - |\psi_N^k|^2\psi_N^{k+1/2}, \varphi_N) + (T^k, \varphi_N). \end{aligned} \tag{3.11}$$

Similarly, by virtue of the orthogonality of the operator P_N, we have

$$(e^{k+1} \pm e^k, \varphi_N) = (\theta^{k+1} \pm \theta^k, \varphi_N),$$

$$Im\{((-\Delta)^{\frac{\alpha}{2}}(e^{k+1}+e^k), \theta^{k+1}+\theta^k)\} = Im\{((-\Delta)^{\frac{\alpha}{4}}(\theta^{k+1}+\theta^k), (-\Delta)^{\frac{\alpha}{4}}(\theta^{k+1}+\theta^k))\} = 0.$$

Setting $\varphi_N = \theta^{k+1} + \theta^k$. By taking into account the imaginary part of (3.11) the following equation can be derived

$$\begin{aligned} \frac{\|\theta^{k+1}\|^2 - \|\theta^k\|^2}{\tau} &= Im\{\frac{\beta}{2\hbar}(|\psi^{k+1}|^2\psi^{k+1/2} - |\psi_N^{k+1}|^2\psi_N^{k+1/2}, \theta^{k+1}+\theta^k)\} \\ &+ Im\{\frac{\beta}{2\hbar}(|\psi^k|^2\psi^{k+1/2} - |\psi_N^k|^2\psi_N^{k+1/2}, \theta^{k+1}+\theta^k)\} \\ &+ Im\{(T^k, \theta^{k+1}+\theta^k)\}. \end{aligned}$$

By virtue of the Hölder inequality and Theorem 3.3, we have

$$\|\theta^{k+1}\|^2 - \|\theta^k\|^2 \leq C(N^{-2q}\|\psi\|_q^2 + \tau^4 + \|\theta^{k+1}\|^2 + \|\theta^k\|^2), \tag{3.12}$$

where C depends on $\Psi_{\max} = \max\{|\psi^k|^2, |\psi^{k+1}|^2, |\psi_N^k|^2, |\psi_N^{k+1}|^2\}$.

Summing up the above inequality, or (3.12), for $k = 0, 1, \ldots, n$, we find

$$\|\theta^{n+1}\|^2 \leq \|\theta^0\|^2 + C(N^{-2q}\|\psi^k\|_q^2 + \tau^4) + C\sum_{k=0}^{n}(\|\theta^{k+1}\|^2 + \|\theta^k\|^2).$$

Based on $\theta^0 = 0$, by virtue of the discrete version of the Gronwall's lemma, we have

$$\|\theta^{n+1}\|^2 \leq C(N^{-2q}\|\psi\|_q^2 + \tau^4).$$

Using Theorem 3.3 and the triangle inequality we are led to get

$$\|e^n\| \leq \|\rho^n\| + \|\theta^n\| \leq C(\tau^2 + N^{-q}\|\psi\|_q).$$

The proof is completed.

4. Numerical examples

For a positive integer J, define the spatial grid points $x_j = 2\pi j/J$ with $j = 0, 1, \ldots, J-1$. The discrete Fourier coefficients of function $\psi(x)$ with respect to the points x_j are defined as

$$\hat{\psi}_l = \frac{1}{J}\sum_{j=0}^{J-1}\psi(x_j)e^{i\xi_l x_j}, \ l = -J/2, \ldots, J/2-1.$$

Table 1
The errors and convergence orders obtained under different values of α when $N = 128$ for example 1.

τ	$\alpha = 1.2$		$\alpha = 1.6$		$\alpha = 2.0$	
	Error	Order	Error	Order	Error	Order
0.1	7.3864e−02	–	7.1036e−02	–	7.0035e−02	–
0.05	1.8592e−02	1.9903	1.7820e−02	1.9952	1.7509e−03	2.0001
0.025	4.6085e−03	2.0010	4.4370e−03	2.0004	4.3772e−03	1.9997
0.0125	1.1531e−03	2.0005	1.1073e−03	2.0012	1.0919e−03	2.0011
0.00625	2.8870e−04	1.9998	2.7679e−04	2.0009	2.7335e−04	2.0003

The inversion formula is expressed as

$$\psi(x_j) = \sum_{l=J/2}^{J/2-1} \hat{\psi}_l e^{i\xi_l x_j}, \quad j = 0, 1, \ldots, J-1.$$

Based on the above notations, the fully discrete Fourier spectral Galerkin equation, or (3.2), can be rewritten as

$$\begin{aligned}&(1 + \frac{i\tau\hbar^{\alpha-1}}{2}(-\Delta)^{\frac{\alpha}{2}} + \frac{i\tau V_0}{2\hbar})\psi_N^{k+1}(x_j)\\ &\quad = (1 - \frac{i\tau\hbar^{\alpha-1}}{2}(-\Delta)^{\frac{\alpha}{2}} - \frac{i\tau V_0}{2\hbar})\psi_N^k(x_j) - \frac{i\tau\beta}{2\hbar} Q_N^k(x_j),\end{aligned} \tag{4.1}$$

where $Q_N^k(x_j) = (|\psi_N^{k+1}(x_j)|^2 + |\psi_N^k(x_j)|^2)\psi_N^{k+1/2}(x_j)$ with $\psi_N^0(x_j) = P_N\psi_0(x_j)$.

Applying the Fourier transformation on both hand sides of (4.1) yields

$$(1 + \frac{i\tau\hbar^{\alpha-1}|\xi_l|^\alpha}{2} + \frac{i\tau V_0}{2\hbar})\widehat{\psi}_N^{k+1} = (1 - \frac{i\tau\hbar^{\alpha-1}|\xi_l|^\alpha}{2} - \frac{i\tau V_0}{2\hbar})\widehat{\psi}_N^k - \frac{i\tau\beta}{2\hbar}\widehat{Q}_N^k, \tag{4.2}$$

with $\widehat{\psi}_N^0 = P_N\widehat{\psi}_0$. It should be noted that the fast Fourier transform (FFT) is used to find the Fourier coefficients in our computation. The following three numerical examples are presented to demonstrate the effectiveness of our proposed method.

4.1. Example 1

In the first example, we consider the following one-dimensional fractional Schrödinger equation

$$i\frac{\partial\psi(x,t)}{\partial t} = (-\Delta)^{\frac{\alpha}{2}}\psi(x,t) + \psi(x,t) - |\psi(x,t)|^2\psi(x,t), \quad x \in [-\pi,\pi], t \in [0,T],$$

subject to the initial condition

$$\psi(x,0) = \operatorname{sech}(x)\cdot\exp(-x^2).$$

Firstly, we need to check the spatial and temporal convergence orders of the Fourier spectral Galerkin scheme (3.2). Since the exact solution of this problem is not known explicitly, in order to quantify the approximation error, we obtain the "true" solution ψ by performing computation in a sufficiently small time step and a very fine mesh size. To examine the spatial and temporal convergence orders separately, the orders of convergence in time and space shall be determined from the computed L^2-error norms defined as:

$$\text{Order} = \begin{cases} \frac{\ln(\|e(\tau_1,N)\|/\|e(\tau_2,N)\|)}{\ln(\tau_1/\tau_2)}, & \text{in time,}\\ \frac{\ln(\|e(\tau,N_1)\|/\|e(\tau,N_2)\|)}{\ln(N_2/N_1)}, & \text{in space,}\end{cases}$$

where $\tau_2 \neq \tau_1$ and $N_2 \neq N_1$. The errors are measured by $e(\tau,N) := \|\psi - \psi_N^k\|$.

Tables 1 and 2 give the numerical results about the temporal and spatial convergence orders, from which we know that the temporal order is $\mathcal{O}(\tau^2)$, which is the theoretical order, and the spatial order is spectral accuracy. All the convergence results are in agreement with the theoretical ones. Fig. 1 displays the time evolution of mass Q^n and energy E^n. It is clearly shown that the two conserved quantities are well preserved with respect to time.

Table 2
The errors and convergence orders obtained under different values of α when $\tau = 0.0125$ for example 1.

N	$\alpha = 1.2$		$\alpha = 1.6$		$\alpha = 2.0$	
	Error	Order	Error	Order	Error	Order
16	9.8257e−01	–	9.5603e−01	–	9.4320e−01	–
32	4.8685e−01	1.0132	4.4558e−01	1.1015	4.5449e−01	1.0534
64	4.7927e−02	2.1788	4.5472e−02	2.1970	4.3418e−02	2.2206
128	2.3391e−04	4.0122	1.9829e−04	4.0785	1.9489e−04	4.0803
256	2.4089e−08	6.3204	2.7871e−08	6.2579	1.8493e−08	6.4010

Table 3
Comparison of CPU-time with those using the Crank–Nicolson finite difference method (CN-FDM), Crank–Nicolson finite element method (CN-FEM) and Crank–Nicolson Fourier spectral Galerkin method (CN-FSGM) for $\alpha = 1.6$.

L^2-norm	CN-FDM			CN-FEM			CN-FSGM		
	τ	h	CPU-time	τ	h_K	CPU-time	τ	N	CPU-time
$\mathcal{O}(10^{-1})$	0.050	0.100	1.8319 s	0.050	0.200	1.8765 s	0.050	32	0.0955 s
$\mathcal{O}(10^{-2})$	0.025	0.050	20.3285 s	0.025	0.100	25.6679 s	0.020	64	0.1673 s
$\mathcal{O}(10^{-3})$	0.001	0.005	877.1152 s	0.010	0.050	160.4458 s	0.010	100	0.2887 s
$\mathcal{O}(10^{-4})$	–	–	–	0.005	0.010	725.7064 s	0.005	128	0.7564 s
$\mathcal{O}(10^{-5})$	–	–	–	–	–	–	0.002	128	1.1225 s
$\mathcal{O}(10^{-6})$	–	–	–	–	–	–	0.001	200	1.7899 s

Table 4
Comparison of CPU-time with those using the Crank–Nicolson finite difference method (CN-FDM), Crank–Nicolson finite element method (CN-FEM) and Crank–Nicolson Fourier spectral Galerkin method (CN-FSGM) for $\alpha = 2.0$.

L^2-norm	CN-FDM			CN-FEM			CN-FSGM		
	τ	h	CPU-time	τ	h_K	CPU-time	τ	N	CPU-time
$\mathcal{O}(10^{-1})$	0.050	0.100	1.5465 s	0.050	0.200	1.2711 s	0.050	32	0.0104 s
$\mathcal{O}(10^{-2})$	0.025	0.050	12.6249 s	0.025	0.100	20.5576 s	0.025	64	0.0822 s
$\mathcal{O}(10^{-3})$	0.010	0.010	30.1255 s	0.010	0.050	116.5846 s	0.015	80	0.1051 s
$\mathcal{O}(10^{-4})$	0.001	0.005	240.5897 s	0.005	0.010	408.2305 s	0.010	128	0.4876 s
$\mathcal{O}(10^{-5})$	–	–	–	–	–	–	0.005	128	0.8024 s
$\mathcal{O}(10^{-6})$	–	–	–	–	–	–	0.002	168	1.2435 s

Fig. 2 presents the numerical solutions with different values of α. It is easy to see that the order α can affect the shape of the soliton in the sense that when α becomes smaller, the shape of the soliton changes more quickly. Moreover, the symmetry-breaking ground state solution occurs for the fractional Schrödinger equation investigated under $\alpha \in (1, 2)$.

Now, we compare our proposed Crank–Nicolson Fourier spectral Galerkin method (CN-FSGM) with some existing methods, e.g. the Crank–Nicolson finite difference method (CN-FDM) [27] and Crank–Nicolson finite element method (CN-FEM) [17]. The numerical solutions are carried out on the same hardware platform. The comparison results for the three methods are described in Tables 3 and 4, where h is the space step-size of CN-FDM and h_K is the spatial mesh size of CN-FEM. The accuracy of the solutions with L^2-norm is obtained at time $t = 1.0$ and the requisite CPU-time for the three schemes is also listed. It can be seen that the CN-FDM cannot achieve the error level $\mathcal{O}(10^{-4})$ for $\alpha = 1.6$ and $\mathcal{O}(10^{-5})$ for $\alpha = 2.0$, and the CN-FEM cannot achieve the error level $\mathcal{O}(10^{-5})$. Moreover, the CN-FSGM takes less computing time than the other two methods. The efficiency of CN-FSGM can be seen, in addition to the high order accuracy. In short, the CN-FSGM has a high convergence order in space and demands less CPU-time for solving the cubic space-fractional Schrödinger equations.

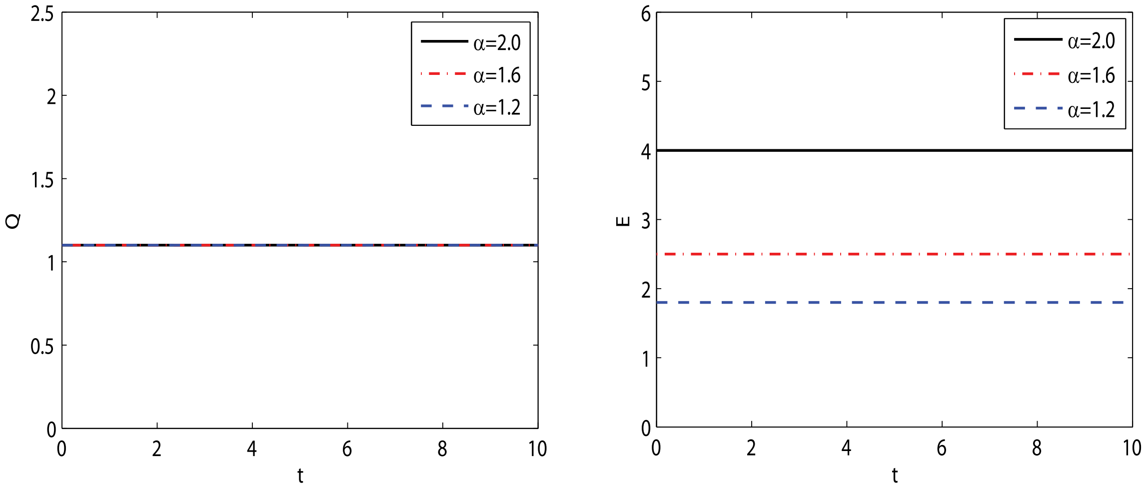

Fig. 1. The time evolution of the computed mass Q^n (left) and energy E^n (right) with $\alpha = 1.2, 1.6, 2.0$ in the example 1.

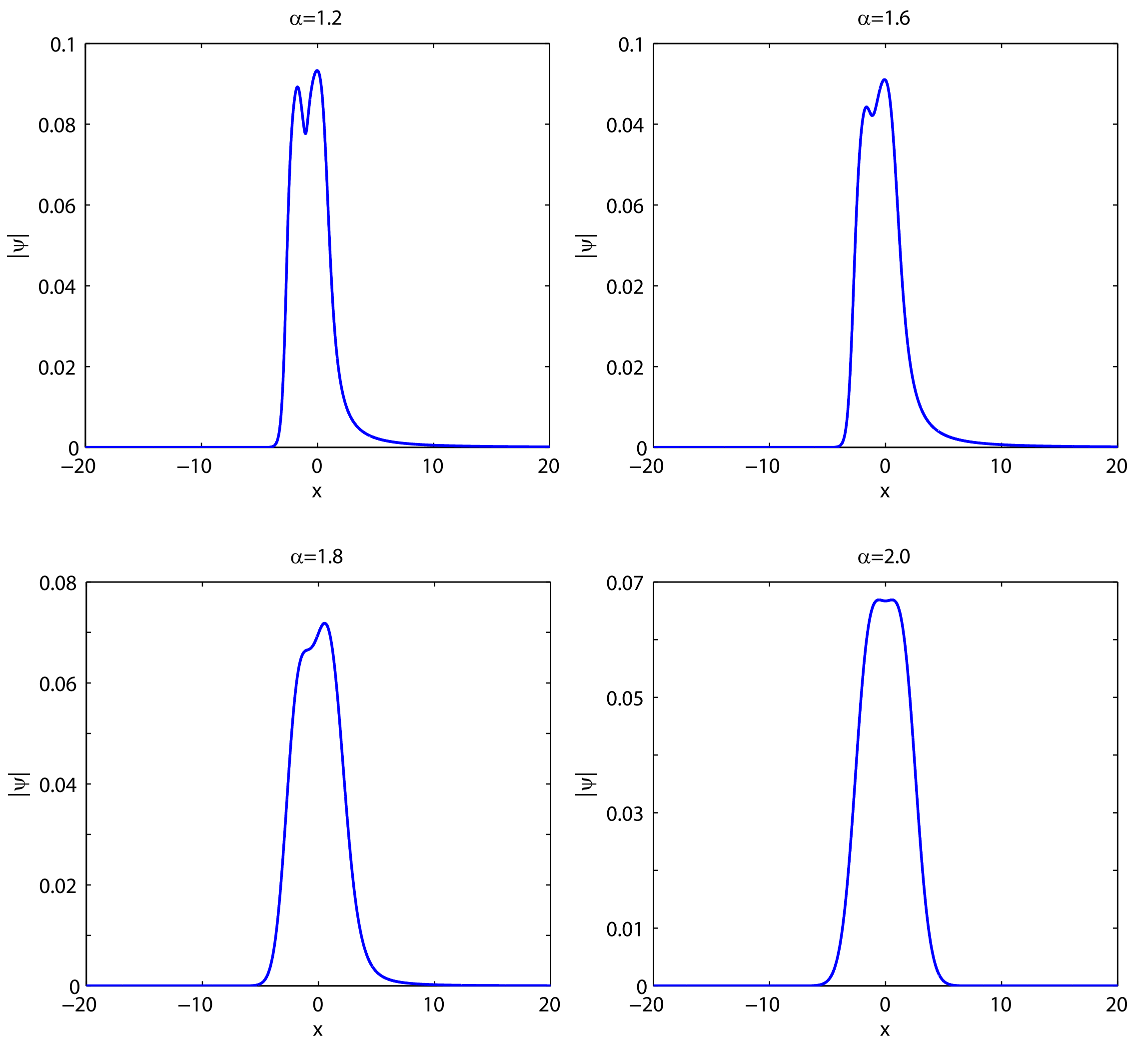

Fig. 2. Numerical solutions obtained at $\alpha = 1.4, 1.6, 1.8, 2.0$ for example 1 at $t = 2.0$ when $\tau = 0.0125$ and $N = 128$.

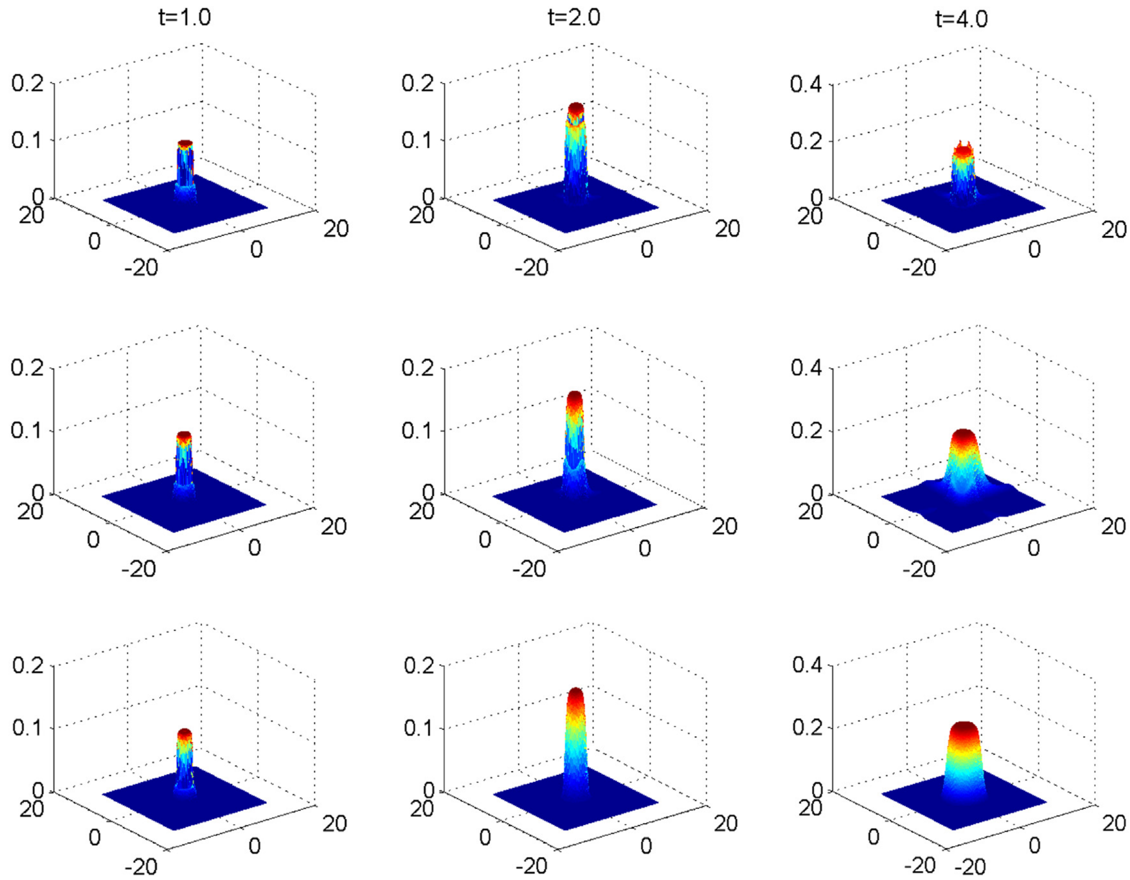

Fig. 3. Numerical solutions, for example 2, predicted at time $t = 1.0, 2.0, 4.0$ when $\tau = 0.01$ and $N = 128$ with (1) $\alpha = 1.2$ (Top line) (2) $\alpha = 1.6$ (Middle line) (3) $\alpha = 2.0$ (Bottom line).

4.2. Example 2

Two-dimensional fractional Schrödinger equation given below is also studied here

$$i\frac{\partial\psi(x, y, t)}{\partial t} = (-\Delta)^{\frac{\alpha}{2}}\psi(x, y, t) + \psi(x, y, t) - |\psi(x, y, t)|^2\psi(x, y, t),\ (x, y) \in \Omega, t \in [0, T],$$

where $\Omega = [-\pi, \pi] \times [-\pi, \pi]$. The solution of ψ is sought subject to the following initial condition

$$\psi(x, y, 0) = \sin(x^2 + y^2) \cdot \exp(-x^2 - y^2).$$

In this example for modeling rouge wave propagation, we set $\tau = 0.01$ and $N = 128$. Fig. 3 displays the numerical solutions obtained under different values of α. We can see that the order α indeed affects the shape of rogue wave. When α becomes smaller, the height and the width of the rogue wave solution are changed, which are not observed in the case of $\alpha = 2.0$.

4.3. Example 3

In this example, we extend our method and solve the following three-dimensional fractional Schrödinger equation in $\Omega = [-\pi, \pi] \times [-\pi, \pi] \times [-\pi, \pi]$:

$$i\frac{\partial\psi(x, y, z, t)}{\partial t} = (-\Delta)^{\frac{\alpha}{2}}\psi(x, y, z, t) + \psi(x, y, z, t) - |\psi(x, y, z, t)|^2\psi(x, y, z, t),\ (x, y, z) \in \Omega.$$

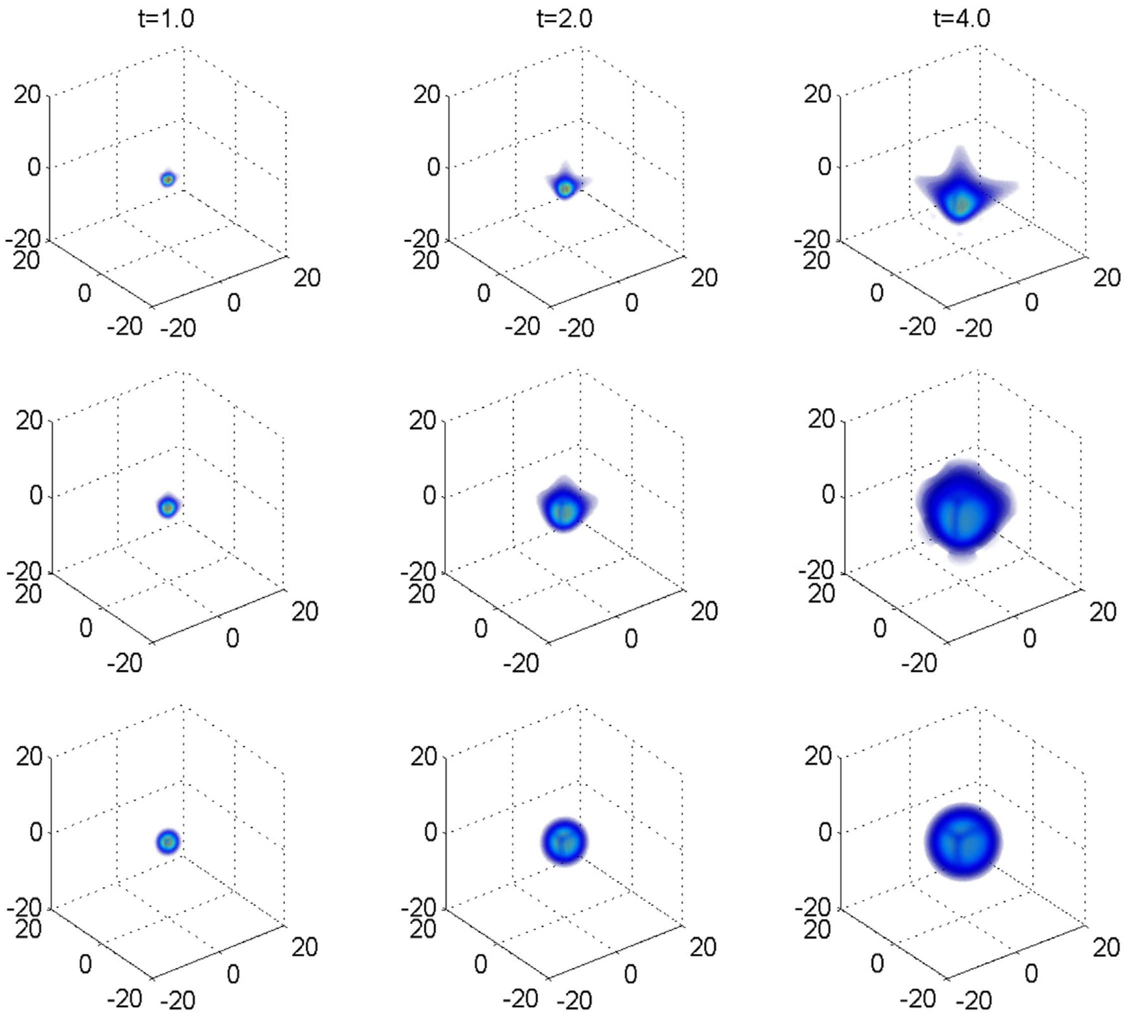

Fig. 4. Numerical solutions, for example 3, predicted at time $t = 1.0, 2.0, 4.0$ when $\tau = 0.01$ and $N = 128$ with (1) $\alpha = 1.2$ (Top line) (2) $\alpha = 1.6$ (Middle line) (3) $\alpha = 2.0$ (Bottom line).

The initial condition is taken as

$$\psi(x, y, z, 0) = \sin(x^2 + y^2 + z^2) \cdot \exp(-x^2 - 2y^2 - z^2).$$

We take $\tau = 0.01$ and $N = 128$. Fig. 4 plots the numerical solutions at $t = 1.0, 2.0, 4.0$ with $\alpha = 1.2$ (Top line), $\alpha = 1.6$ (Middle line) and $\alpha = 2.0$ (Bottom line). It can be found that the results are symmetric with respect to the x, y, z axis for $\alpha = 2.0$. However, when the value of α becomes smaller, the ground state solution, under our expectation, will be evolved to exhibit non-symmetric solution.

5. Concluding remarks

In this study, we have developed a Fourier spectral Galerkin method for solving the space-fractional nonlinear Schrödinger equation. The proposed numerical scheme is proved to be able to preserve both the mass and energy conservations. The convergence of the discrete scheme is also rigorously analyzed to show the second order accuracy in time and the convergence with the spectral order accuracy in space. The superiority of the proposed schemes is rooted in the weak formulation so that it can be easily extended to other spatial discretizations. Numerical examples are provided to demonstrate the effectiveness of our method, which is also applicable to solve the two- and three-dimensional fractional Schrödinger equations. Numerical results show that the fractional quantum mechanics has some interesting properties which are not observed in the classical Schrödinger where α is equal to 2. One can also clearly see that the fractional order α can affect the shapes of the soliton and rogue wave, in the sense that symmetry breaking indeed occurs in the solutions. Our future work will discuss the physical mechanism leading to the currently observed bifurcation in the nonlinear fractional quantum mechanics.

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