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Numerical analysis for time-fractional Schrödinger equation on two space dimensions

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Abstract

In this paper, we study the numerical methods for solving the time-fractional Schrödinger equation (TFSE) with Caputo or Riemann–Liouville fractional derivative. The numerical schemes are implemented by using the L1 scheme in time direction and Fourier–Galerkin/Legendre–Galerkin spectral methods in spatial variable. We prove that the two schemes are unconditionally stable and numerical solutions converge with the order $\mathcal{O}(\Delta t^{2-\alpha} + N^{-s} + N^{-m})$, where α is the order of the fractional derivative, Δt , N are the step of time and polynomial degree, respectively, m , s are the regularity of u and V . Several numerical results are performed to confirm the theoretical analysis.

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Keywords: Schrödinger equation; Caputo; Riemann–Liouville; Fourier-spectral method; Error estimate

1 Introduction

In this work, we construct numerical methods to solve the following TFSE:

$$\frac{1}{i} \frac{\partial^\alpha u}{\partial t^\alpha} - \Delta u + \beta V(x, y)u = 0 \quad \text{in } \Omega \times [0, T], \quad (1)$$

$$(i) \ u \text{ are periodic; or } (ii) \ u|_{\partial\Omega} = 0, \quad (2)$$

$$u(x, y, 0) = u_0(x, y) \quad \text{on } \partial\Omega \times [0, T], \quad (3)$$

where $i^2 = -1$, $\frac{\partial^\alpha u}{\partial t^\alpha}$ ($0 < \alpha < 1$) denotes the Caputo or Riemann–Liouville fractional derivative, $\Omega \subset \mathbf{R}^2$ is a bound domain, β is a positive constant, and V represents a potential function.

TFSE can be viewed as a generalization of the classical Schrödinger equation. It has emerged as an appropriate model in various applications, such as plasma physics, polymer physics, nonlinear optic, etc. The concept of fractal in quantum mechanics has been developed over the past ten years, since Laskin [1, 2] defined some path integrals and developed the space fractional quantum mechanics on the basis of new fractional path

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integrals method. Naber [3], Wang and Xu [4] constructed a class of TFSE with Caputo fractional derivative and discussed the solutions for a free particle and a potential well. Guo and Xu [5] studied the TSFE with a free particle, and they obtained the fundamental solution of the problem. Cheng [6] proved the existence of ground state for TSFE with unbounded potential by using Lagrange multiplier method. In [7], Felmer and Tan studied the existence, regularity of the ground state for the nonlinear fractional Schrödinger equation. It is remarkable that Wang et al. [8] investigated the existence and uniqueness of optimal controls of TFSE (1)–(3).

It is difficult to find an explicit form of analytical solutions of fractional equation, so some recent contributions have focused on using numerical methods to obtain approximate solutions. Rida et al. [9] proposed an Adomian decomposition method for solving nonlinear TFSE. Li and Xu [10] constructed a time-space spectral method to investigate the solution of fractional partial differential equations. Yildirim [11] introduced a homotopy perturbation method to study analytical solutions for fractional Schrödinger equation. Wei et al. [12, 13] presented a local discontinuous Galerkin (LDG) method to approximate the solution of TFSE. Mohebbi et al. [14] developed a shifted Legendre collocation method to solve TFSE with initial-boundary and nonlocal conditions. Baleanu et al. [15–17] investigated the soliton solutions of the nonlinear Schrödinger equation with Kerr law nonlinearity. They obtained the exact dark optical, dark-singular, and periodic singular soliton solutions of the equation. Garrappa et al. [18] discussed approximating the solution of TFSE by using the Krylov projection methods. Zhu et al. [19] presented a finite element method to solve time-space-fractional Schrödinger equation with Caputo and Riesz derivatives. The other related numerical methods for fractional equation can be found in [20–25] and the references therein.

On the other hand, L1 scheme [26, 27] is an efficient numerical method to approximate Caputo or Riemann–Liouville derivative. Langlands and Henry [28], Sun and Wu [29], Lin and Xu [30] obtained the error estimate of the L1 scheme. Grajales and Vargas [31] constructed a Crank–Nicholson/Fourier–Galerkin method to approximate the solution of the Schrödinger equation. Gong et al. [32] proposed an energy conservative Crank–Nicholson/Fourier pseudo-spectral method to solve the Schrödinger equation. Kumar et al. [33–36] introduced a series of homotopy transform methods to solve some fractional equations.

As a classical high-order method, spectral method has been widely used to solve PDE/ODE equations. In this article, we propose two efficient numerical schemes to approximate the TFSE with Caputo or Riemann–Liouville derivative. The proposed schemes are performed by combining the L1 scheme for fractional derivative and Fourier–Galerkin/Legendre–Galerkin spectral methods for space variable. A detailed analysis of the numerical scheme is provided for both stability and error estimate. Our rigorous analysis results show that numerical methods lead to $2-\alpha$ order accuracy in time direction and spectral accuracy in space direction. At last, some numerical examples are conducted to support the theoretical claims.

The rest of the paper is structured in the following way. Section 2 introduces the L1 scheme for Caputo and Riemann–Liouville derivative. In Sect. 3, we discuss error estimates for the full discrete schemes. In Sect. 4, some numerical experiments are presented to illustrate the validity of the numerical method. The conclusions of this paper are given in Sect. 5.

2 Stability for semi-discretization TFSE

In this part, we present the semi-discrete schemes for the solution of (1)–(3). First, we introduce an L1 scheme to discretize the Caputo and Riemann–Liouville derivatives. Let M be a positive integer, $\Delta t = T/M$ be the time step, and $t_n = n\Delta t, n = 0, 1, \dots, M - 1$ be a mesh point. We introduce the following L1 scheme for Caputo fractional derivative of order α :

$$\frac{1}{\Gamma(2 - \alpha)} \sum_{j=0}^n b_j \frac{u(t_{n+1-j}) - u(t_{n-j})}{\Delta t^\alpha}, \tag{4}$$

and the Riemann–Liouville derivative is approximated by

$$\frac{1}{\Gamma(2 - \alpha)} \sum_{j=0}^n b_j \frac{u(t_{n+1-j}) - u(t_{n-j})}{\Delta t^\alpha} + \frac{u(t_0)(t_{n+1} - t_0)^{-\alpha}}{\Gamma(1 - \alpha)}, \tag{5}$$

where $b_j = (j + 1)^{1-\alpha} - j^{1-\alpha}$.

Then, we rewrite the complex function $u(x, y, t)$ into the real part and the imaginary part, that is, $u(x, y, t) = v(x, y, t) + iw(x, y, t)$. Then we get the following coupled system:

$$\begin{cases} \frac{\partial^\alpha v}{\partial t^\alpha} + \Delta w - \beta Vw = 0, \\ \frac{\partial^\alpha w}{\partial t^\alpha} - \Delta v + \beta Vv = 0. \end{cases} \tag{6}$$

Remark 1 It is worth mentioning that there are two different boundary conditions for Caputo and Riemann–Liouville derivatives.

Then we obtain the following semi-discrete schemes for TFSE with Caputo derivative:

$$\begin{cases} (v^{n+1} - \sum_{j=0}^{n-1} (b_j - b_{j+1})v^{n-j} - b_n v^0) + a_0 \Delta w^{n+1} - a_0 \beta Vw^{n+1} = 0, \\ (w^{n+1} - \sum_{j=0}^{n-1} (b_j - b_{j+1})w^{n-j} - b_n w^0) - a_0 \Delta v^{n+1} + a_0 \beta Vv^{n+1} = 0, \end{cases} \tag{7}$$

and Riemann–Liouville derivative:

$$\begin{cases} (v^{n+1} - \sum_{j=0}^{n-1} (b_j - b_{j+1})v^{n-j} - \bar{b}_n v^0) + a_0 \Delta w^{n+1} - a_0 \beta Vw^{n+1} = 0, \\ (w^{n+1} - \sum_{j=0}^{n-1} (b_j - b_{j+1})w^{n-j} - \bar{b}_n w^0) - a_0 \Delta v^{n+1} + a_0 \beta Vv^{n+1} = 0, \end{cases} \tag{8}$$

where $a_0 = \Delta t^\alpha \Gamma(2 - \alpha)$, $\bar{b}_n = b_n - (1 - \alpha)\Delta t^\alpha t_{n+1}^{-\alpha}$.

Lemma 1 For all $\bar{b}_n, n \geq 0$, we have

$$0 < \bar{b}_n \leq \alpha b_n. \tag{9}$$

Proof It is easy to check that

$$\bar{b}_n = (n + 1)^{1-\alpha} - n^{1-\alpha} - (1 - \alpha)(n + 1)^{-\alpha}.$$

Set

$$f(t) = (1 + t)^\alpha - (1 + t\alpha), \quad t \geq 0.$$

Then $f(0) = 0$ and $f'(t) = \alpha((1+t)^{\alpha-1} - 1) < 0, \forall t > 0$, thus $f(t) < f(0) = 0$, then

$$(1+t)^\alpha < (1+t\alpha), \quad \forall t > 0.$$

Let $t = \frac{1}{x}, x > 0$, we have

$$\left(1 + \frac{1}{x}\right)^\alpha < \left(1 + \frac{\alpha}{x}\right).$$

Therefore

$$\left(\frac{1+x}{x}\right)^\alpha < \left(\frac{x+\alpha}{x}\right).$$

That is

$$(1+x)^{-\alpha}(x+\alpha) > x^{1-\alpha}.$$

Hence

$$(1+x)^{-\alpha}(1+x-(1-\alpha)) > x^{1-\alpha}.$$

Namely

$$(1+x)^{1-\alpha} - (1-\alpha)(1+x)^{1-\alpha} - x^{1-\alpha} > 0.$$

On the other hand, there holds

$$\bar{b}_n - \alpha b_n = (1-\alpha)((n+1)^{1-\alpha} - n^{1-\alpha} - (n+1)^{-\alpha}) \leq 0, \quad \forall n \geq 0.$$

The above inequalities can be proved as follows:

$$(n+1)^{1-\alpha} - n^{1-\alpha} - (n+1)^{-\alpha} \leq 0.$$

It follows that

$$(n+1)^{1-\alpha} - (n+1)^{-\alpha} \leq n^{1-\alpha}.$$

Thus, we arrive at

$$(n+1)^{1-\alpha} \left(1 - \frac{1}{n+1}\right) \leq n^{1-\alpha}.$$

That is

$$(n+1)^{-\alpha} \leq n^{-\alpha}.$$

Hence, we finish the proof of (9). \square

We have the following unconditional stability results.

Lemma 2 *The semi-discrete schemes (7) are unconditionally stable such that, for $0 \leq n \leq M - 1$, we have*

$$\|v^{n+1}\|^2 + \|w^{n+1}\|^2 \leq \|v^0\|^2 + \|w^0\|^2. \tag{10}$$

Proof When $n = 0$, computing the L^2 inner product of (7) with $2v^1$ and $2w^1$, we obtain

$$\begin{aligned} (v^1 - v^0, 2v^1) + 2a_0(\Delta w^1, v^1) - 2a_0\beta(Vw^1, v^1) &= 0, \\ (w^1 - w^0, 2w^1) - 2a_0(\Delta v^1, w^1) + 2a_0\beta(Vv^1, w^1) &= 0. \end{aligned}$$

This yields

$$\|v^1\|^2 - \|v^0\|^2 + \|v^1 - v^0\|^2 + \|w^1\|^2 - \|w^0\|^2 + \|w^1 - w^0\|^2 = 0.$$

That is

$$\|v^1\|^2 + \|w^1\|^2 \leq \|v^0\|^2 + \|w^0\|^2.$$

Assume that the following inequality holds:

$$\|v^j\|^2 + \|w^j\|^2 \leq \|v^0\|^2 + \|w^0\|^2, \quad j = 2, 3, \dots, n. \tag{11}$$

Then we need to prove $\|v^{n+1}\|^2 + \|w^{n+1}\|^2 \leq \|v^0\|^2 + \|w^0\|^2$. When $j = n + 1$, computing the L^2 inner product of (7) with $2v^{n+1}$ and $2w^{n+1}$, we derive

$$\begin{aligned} &2\|v^{n+1}\|^2 + 2\|w^{n+1}\|^2 \\ &= 2\left(\sum_{j=0}^{n-1} (b_j - b_{j+1})v^{n-j} + b_n v^0, v^{n+1}\right) + 2\left(\sum_{j=0}^{n-1} (b_j - b_{j+1})w^{n-j} + b_n w^0, w^{n+1}\right) \\ &\leq \sum_{j=0}^{n-1} (b_j - b_{j+1})(\|v^{n-j}\|^2 + \|v^{n+1}\|^2) + b_n(\|v^0\|^2 + \|v^{n+1}\|^2) \\ &\quad + \sum_{j=0}^{n-1} (b_j - b_{j+1})(\|w^{n-j}\|^2 + \|w^{n+1}\|^2) + b_n(\|w^0\|^2 + \|w^{n+1}\|^2). \end{aligned}$$

Noting that

$$\sum_{j=0}^{n-1} (b_j - b_{j+1}) + b_n = 1.$$

Thus, we get

$$\begin{aligned} \|v^{n+1}\|^2 + \|w^{n+1}\|^2 &\leq \sum_{j=0}^{n-1} (b_j - b_{j+1})(\|v^{n-j}\|^2 + \|w^{n-j}\|^2) + b_n(\|v^0\|^2 + \|w^0\|^2) \\ &\leq \left(\sum_{j=0}^{n-1} (b_j - b_{j+1}) + b_n\right)(\|v^0\|^2 + \|w^0\|^2) \end{aligned}$$

$$= \|v^0\|^2 + \|w^0\|^2.$$

The proof is completed. □

Lemma 3 *Semi-discrete equations (8) are unconditionally stable, and v^{n+1}, w^{n+1} satisfy*

$$\|v^{n+1}\|^2 + \|w^{n+1}\|^2 \leq \alpha \|v^0\|^2 + \alpha \|w^0\|^2, \quad 0 \leq n \leq M - 1. \tag{12}$$

Proof For $n = 0$, taking the L^2 inner product of (8) with $2v^1, 2w^1$, we get

$$\begin{aligned} (v^1 - \alpha v^0, 2v^1) + 2a_0(\Delta w^1, v^1) - 2a_0\beta(Vw^1, v^1) &= 0, \\ (w^1 - \alpha w^0, 2w^1) - 2a_0(\Delta v^1, w^1) + 2a_0\beta(Vv^1, w^1) &= 0. \end{aligned}$$

Consequently,

$$\|v^1\|^2 - \alpha^2 \|v^0\|^2 + \|v^1 - \alpha v^0\|^2 + \|w^1\|^2 - \alpha^2 \|w^0\|^2 + \|w^1 - \alpha w^0\|^2 = 0.$$

We arrive at

$$\|v^1\|^2 + \|w^1\|^2 \leq \alpha \|v^0\|^2 + \alpha \|w^0\|^2.$$

Suppose

$$\|v^j\|^2 + \|w^j\|^2 \leq \alpha \|v^0\|^2 + \alpha \|w^0\|^2, \quad j = 2, 3, \dots, n. \tag{13}$$

For $k = n + 1$, taking the L^2 inner product of (7) with $2v^{n+1}$ and $2w^{n+1}$, we find that

$$\begin{aligned} &2\|v^{n+1}\|^2 + 2\|w^{n+1}\|^2 \\ &= 2\left(\sum_{j=0}^{n-1} (b_j - b_{j+1})v^{n-j} + \bar{b}_n v^0, v^{n+1}\right) + 2\left(\sum_{j=0}^{n-1} (b_j - b_{j+1})w^{n-j} + \bar{b}_n w^0, w^{n+1}\right) \\ &\leq \sum_{j=0}^{n-1} (b_j - b_{j+1})(\|v^{n-j}\|^2 + \|v^{n+1}\|^2) + \bar{b}_n(\|v^0\|^2 + \|v^{n+1}\|^2) \\ &\quad + \sum_{j=0}^{n-1} (b_j - b_{j+1})(\|w^{n-j}\|^2 + \|w^{n+1}\|^2) + \bar{b}_n(\|w^0\|^2 + \|w^{n+1}\|^2). \end{aligned}$$

By using (9), we have

$$\begin{aligned} \|v^{n+1}\|^2 + \|w^{n+1}\|^2 &\leq \sum_{j=0}^{n-1} (b_j - b_{j+1})(\|v^{n-j}\|^2 + \|w^{n-j}\|^2) + \bar{b}_n(\|v^0\|^2 + \|w^0\|^2) \\ &\leq \left(\sum_{j=0}^{n-1} (b_j - b_{j+1})\right)(\alpha \|v^0\|^2 + \alpha \|w^0\|^2) + \alpha b_n(\|v^0\|^2 + \|w^0\|^2) \\ &= \alpha \|v^0\|^2 + \alpha \|w^0\|^2. \end{aligned}$$

This concludes the proof. □

3 Error estimates for full discretization

In this section, we discuss fully discrete schemes. Considering different boundary conditions, we choose a Fourier–Galerkin spectral method to discretize semi-discrete scheme (7) and a Legendre–Galerkin method to discretize semi-discrete scheme (8). We present some error estimates for full-discretization schemes in L^2 norm. First, we define S_N to be the Fourier or Legendre polynomial space. Denote $\pi_N : L^2(\Omega) \rightarrow S_N$ to be the L^2 -projection operator which satisfies

$$(\pi_N \phi - \phi, \psi) = 0, \quad \forall \psi \in S_N.$$

We also define the H^1 -projection operator $\pi_N^1 : H^1(\Omega) \rightarrow S_N$ by

$$(\nabla(\pi_N^1 \phi - \phi), \nabla \psi) = 0, \quad \forall \psi \in S_N.$$

We have the following estimate [37]:

$$\|\phi - \pi_N \phi\|_0 \leq CN^{-m} \|\phi\|_m, \quad \forall \phi \in H^m(\Omega), m \geq 0. \tag{14}$$

Consider the full-discretization Fourier–Galerkin/Legendre–Galerkin spectral method to equations (7) and (8) as follows: find $v_N^{n+1}, w_N^{n+1} \in S_N$ such that, for all $\phi_N, \psi_N \in S_N$, they satisfy

$$\begin{cases} (v_N^{n+1} - \sum_{j=0}^{n-1} (b_j - b_{j+1})v_N^{n-j} - b_n v_N^0, \phi_N) + a_0(\Delta w^{n+1}, \phi_N) - a_0\beta(I_N V w^{n+1}, \phi_N) = 0, \\ (w_N^{n+1} - \sum_{j=0}^{n-1} (b_j - b_{j+1})w_N^{n-j} - b_n w_N^0, \psi_N) - a_0(\Delta v_N^{n+1}, \psi_N) + a_0\beta(I_N V v_N^{n+1}, \psi_N) = 0, \end{cases} \tag{15}$$

and

$$\begin{cases} (v_N^{n+1} - \sum_{j=0}^{n-1} (b_j - b_{j+1})v_N^{n-j} - \bar{b}_n v_N^0, \phi_N) + a_0(\Delta w^{n+1}, \phi_N) - a_0\beta(I_N V w^{n+1}, \phi_N) = 0, \\ (w_N^{n+1} - \sum_{j=0}^{n-1} (b_j - b_{j+1})w_N^{n-j} - \bar{b}_n w_N^0, \psi_N) - a_0(\Delta v_N^{n+1}, \psi_N) + a_0\beta(I_N V v_N^{n+1}, \psi_N) = 0, \end{cases} \tag{16}$$

where $I_N V$ is the interpolation function of V .

We now state the stability results for equations (15) and (16).

Theorem 1 *Let $(\{v_N^n\}_{n=1}^{M-1}, \{w_N^n\}_{n=1}^{M-1})$ be the numerical solutions of (15), then we derive*

$$\|v_N^{n+1}\|^2 + \|w_N^{n+1}\|^2 \leq \|v_N^0\|^2 + \|w_N^0\|^2. \tag{17}$$

Theorem 2 *Let $(\{v_N^n\}_{n=1}^{M-1}, \{w_N^n\}_{n=1}^{M-1})$ be the numerical solutions of (16), then we have*

$$\|v_N^{n+1}\|^2 + \|w_N^{n+1}\|^2 \leq \alpha \|v_N^0\|^2 + \alpha \|w_N^0\|^2. \tag{18}$$

Next, we begin to analyze the error estimates of the full-discretization schemes (15) and (16). We denote the truncation error as follows:

$$r_1^{n+1} = \frac{1}{\Gamma(2-\alpha)} \sum_{j=0}^n b_j \frac{v(t_{n+1-j}) - v(t_{n-j})}{\Delta t^\alpha} - \frac{1}{\Gamma(1-\alpha)} \int_0^{t_{n+1}} \frac{\partial v(s)}{\partial s} \frac{ds}{(t_{n+1}-s)^\alpha},$$

$$r_2^{n+1} = \frac{1}{\Gamma(2-\alpha)} \sum_{j=0}^n b_j \frac{w(t_{n+1-j}) - w(t_{n-j})}{\Delta t^\alpha} - \frac{1}{\Gamma(1-\alpha)} \int_0^{t_{n+1}} \frac{\partial w(s)}{\partial s} \frac{ds}{(t_{n+1}-s)^\alpha}.$$

From [29, 30], we have

$$\|r_1^{n+1}\| \leq C\Delta t^{2-\alpha}, \quad \|r_2^{n+1}\| \leq C\Delta t^{2-\alpha}. \tag{19}$$

We also define the following error functions:

$$\tilde{e}_v^n = \pi_N v(t_n) - u_N^n, \quad \hat{e}_v^n = v(t_n) - \pi_N v(t_n), \quad e_v^n = \hat{e}_v^n + \tilde{e}_v^n = v(t_n) - v_N^n, \tag{20}$$

$$\tilde{e}_w^n = \pi_N w(t_n) - w_N^n, \quad \hat{e}_w^n = w(t_n) - \pi_N w(t_n), \quad e_w^n = \hat{e}_w^n + \tilde{e}_w^n = w(t_n) - w_N^n. \tag{21}$$

The following lemma can help us to analyze the error estimates.

Lemma 4 For $a_0, b_n, n \geq 0$, we have the following result:

$$\frac{a_0}{b_n} \leq 2\Gamma(1-\alpha)T^\alpha. \tag{22}$$

Proof

$$\begin{aligned} b_n &= ((n+1)^{1-\alpha} - n^{1-\alpha}) = n^{1-\alpha} \left(\left(1 + \frac{1}{n}\right)^{1-\alpha} - 1 \right) \\ &= n^{1-\alpha} \left(\frac{(1-a)}{n} + \frac{(1-\alpha)(-\alpha)}{2!} \frac{1}{n^2} + \dots \right) \\ &\geq n^{1-\alpha} \left(\frac{(1-a)}{n} + \frac{(1-\alpha)(-\alpha)}{2!} \frac{1}{n^2} \right) \\ &= n^{1-\alpha} \left(\frac{(1-a)}{2n} + \frac{(1-a)}{2n} + \frac{(1-\alpha)(-\alpha)}{2!} \frac{1}{n^2} \right). \end{aligned}$$

Note that

$$\frac{(1-a)}{2n} + \frac{(1-\alpha)(-\alpha)}{2!} \frac{1}{n^2} \geq 0.$$

Therefore, we obtain

$$\frac{a_0}{b_n} \leq \frac{2n^\alpha \Delta t^\alpha \Gamma(2-\alpha)}{(1-\alpha)} \leq 2\Gamma(1-\alpha)T^\alpha. \quad \square$$

We show the error estimate of full-discretization problem (15) in the following theorem.

Theorem 3 Suppose that $u = v + iw$ is the exact solution of (1)–(3), (v, w) and $(\{v_N^n\}_{n=1}^{M-1}, \{w_N^n\}_{n=1}^{M-1})$ are the solutions of (6) and (15), respectively, then we have

$$\|v(\cdot, t_n) - v_N^n\| + \|w(\cdot, t_n) - w_N^n\| \leq C(\Delta t^{2-\alpha} + N^{-s} + N^{-m}), \tag{23}$$

where C depends only on u, V, T, α, β .

Proof We will utilize mathematical induction to prove the above conclusion. For $n = 0$, equation (15) can be written as

$$\begin{cases} \frac{1}{a_0}(v_N^1 - v_N^0, \phi_N) + (\Delta w_N^1, \phi_N) - \beta(I_N V w_N^1, \phi_N) = 0, \\ \frac{1}{a_0}(w_N^1 - w_N^0, \psi_N) - (\Delta v_N^1, \psi_N) + \beta(I_N V v_N^1, \psi_N) = 0. \end{cases} \tag{24}$$

Subtracting (24) from a reformulation of (6) at t_1 , we obtain

$$\begin{aligned} & (\tilde{e}_v^1 - \tilde{e}_v^0, \phi_N) + a_0(\Delta \tilde{e}_w^1, \phi_N) - a_0\beta(Vw(t_1) - I_N V w_N^1, \phi_N) \\ & = a_0(r_1^1, \phi_N) + ((\pi_N - I)(v(t_1) - v(t_0)), \phi_N) - a_0(\nabla(\pi_N^1 - I)w(t_1), \nabla\phi_N), \\ & (\tilde{e}_w^1 - \tilde{e}_w^0, \psi_N) - a_0(\Delta \tilde{e}_v^1, \psi_N) + a_0\beta(Vv(t_1) - I_N V v_N^1, \psi_N) \\ & = a_0(r_2^1, \psi_N) + ((\pi_N - I)(w(t_1) - w(t_0)), \psi_N) + a_0(\nabla(\pi_N^1 - I)v(t_1), \nabla\psi_N). \end{aligned}$$

Let $\phi_N = 2\tilde{e}_v^1, \psi_N = 2\tilde{e}_w^1$, we have

$$\begin{aligned} 2\|\tilde{e}_v^1\|^2 + 2\|\tilde{e}_w^1\|^2 & \leq 2a_0(r_1^1, \tilde{e}_v^1) + 2a_0(r_2^1, \tilde{e}_w^1) \\ & \quad + 2((\pi_N - I)(v(t_1) - v(t_0)), \tilde{e}_v^1) + 2((\pi_N - I)(w(t_1) - w(t_0)), \tilde{e}_w^1) \\ & \quad + 2a_0\beta(w(t_1)(V - I_N V) + I_N V(w(t_1) - w_N^1), \tilde{e}_v^1) \\ & \quad - 2a_0\beta(v(t_1)(V - I_N V) + I_N V(v(t_1) - v_N^1), \tilde{e}_w^1). \end{aligned}$$

Note that

$$\begin{aligned} & 2a_0(w(t_1)(V - I_N V) + I_N V(w(t_1) - w_N^1), \tilde{e}_v^1) \\ & \quad - 2a_0(v(t_1)(V - I_N V) + I_N V(v(t_1) - v_N^1), \tilde{e}_w^1) \\ & = 2a_0(w(t_1)(V - I_N V) + I_N V(\tilde{e}_w^1 + \hat{e}_w^1), \tilde{e}_v^1) - 2a_0(v(t_1)(V - I_N V) + I_N V(\tilde{e}_v^1 + \hat{e}_v^1), \tilde{e}_w^1) \\ & = 2a_0(w(t_1)(V - I_N V) + I_N V\tilde{e}_w^1, \tilde{e}_v^1) - 2a_0(v(t_1)(V - I_N V) + I_N V\tilde{e}_v^1, \tilde{e}_w^1). \end{aligned}$$

Using Young's inequality, we get

$$\begin{aligned} & 2\|\tilde{e}_v^1\|^2 + 2\|\tilde{e}_w^1\|^2 \\ & \leq a_0\left(4a_0\|r_1^1\|^2 + \frac{1}{4a_0}\|\tilde{e}_v^1\|^2\right) + a_0\left(4a_0\|r_2^1\|^2 + \frac{1}{4a_0}\|\tilde{e}_w^1\|^2\right) \\ & \quad + 4\|(\pi_N - I)(v(t_1) - v(t_0))\|^2 + \frac{1}{4}\|\tilde{e}_v^1\|^2 + 4\|(\pi_N - I)(w(t_1) - w(t_0))\|^2 + \frac{1}{4}\|\tilde{e}_w^1\|^2 \\ & \quad + a_0\beta\left(4a_0\beta\|I_N V\tilde{e}_w^1\|^2 + \frac{1}{4a_0\beta}\|\tilde{e}_v^1\|^2\right) \\ & \quad + a_0\beta\left(4a_0\beta\|w(t_1)(V - I_N V)\|^2 + \frac{1}{4a_0\beta}\|\tilde{e}_v^1\|^2\right) \\ & \quad + a_0\beta\left(4a_0\beta\|I_N V\tilde{e}_v^1\|^2 + \frac{1}{4a_0\beta}\|\tilde{e}_w^1\|^2\right) \\ & \quad + a_0\beta\left(4a_0\beta\|v(t_1)(V - I_N V)\|^2 + \frac{1}{4a_0\beta}\|\tilde{e}_w^1\|^2\right) \end{aligned}$$

$$\begin{aligned} &\leq 4a_0^2(\|r_1\|^2 + \|r_2\|^2) + 4\|(\pi_N - I)(v(t_1) - v(t_0))\|^2 + 4\|(\pi_N - I)(w(t_1) - w(t_0))\|^2 \\ &\quad + 4a_0^2\beta^2\|I_N V\|_\infty\|\tilde{e}_w^1\|^2 + 4a_0^2\beta^2\|w(t_1)\|_\infty\|V - I_N V\|^2 + \|\tilde{e}_w^1\|^2 + \|\tilde{e}_v^1\|^2 \\ &\quad + 4a_0^2\beta^2\|I_N V\|_\infty\|\tilde{e}_v^1\|^2 + 4a_0^2\beta^2\|v(t_1)\|_\infty\|V - I_N V\|^2. \end{aligned}$$

That is

$$\|\tilde{e}_v^1\|^2 + \|\tilde{e}_w^1\|^2 \leq C_1 a_0^2 \Delta t^{4-2\alpha} + C_2 a_0^2 N^{-s} + C_3 a_0^2 N^{-m}.$$

Assume

$$\|\tilde{e}_v^j\|^2 + \|\tilde{e}_w^j\|^2 \leq \frac{C_1 a_0^2 \Delta t^{4-2\alpha}}{b_{j-1}^2} + \frac{C_2 a_0^2 N^{-s}}{b_{j-1}^2} + \frac{C_3 a_0^2 N^{-m}}{b_{j-1}^2}, \quad j = 2, 3, \dots, n. \tag{25}$$

Next, we need to prove that it also holds for $j = n + 1$. Setting $\phi_N = 2\tilde{e}_v^{n+1}$ and $\psi_N = 2\tilde{e}_w^{n+1}$ in (15), we have

$$\begin{aligned} &2\|\tilde{e}_v^{n+1}\|^2 + 2\|\tilde{e}_w^{n+1}\|^2 \\ &\leq 2a_0(r_1^{n+1}, \tilde{e}_v^{n+1}) + 2a_0(r_2^{n+1}, \tilde{e}_w^{n+1}) \\ &\quad + 2\left(\sum_{j=0}^{n-1} (b_j - b_{j+1})\tilde{e}_v^{n-j} + b_n \tilde{e}_v^0, \tilde{e}_v^{n+1}\right) + 2\left(\sum_{j=0}^{n-1} (b_j - b_{j+1})\tilde{e}_w^{n-j} + b_n \tilde{e}_w^0, \tilde{e}_w^{n+1}\right) \\ &\quad + 2\left((\pi_N - I)\left(v(t_{n+1}) - \sum_{j=0}^n (b_j - b_{j+1})v(t_{n-j}) - b_n v(t_0)\right), \tilde{e}_v^{n+1}\right) \\ &\quad + 2\left((\pi_N - I)\left(w(t_{n+1}) - \sum_{j=0}^n (b_j - b_{j+1})w(t_{n-j}) - b_n w(t_0)\right), \tilde{e}_w^{n+1}\right) \\ &\quad + 2a_0\beta(w(t_{n+1})(V - I_N V) + I_N V(w(t_{n+1}) - w_N^{n+1}), \tilde{e}_v^{n+1}) \\ &\quad - 2a_0\beta(v(t_{n+1})(V - I_N V) + I_N V(v(t_{n+1}) - v_N^{n+1}), \tilde{e}_w^{n+1}) \\ &\leq a_0\left(\frac{4a_0}{b_n}\|r_1^{n+1}\|^2 + \frac{b_n}{4a_0}\|\tilde{e}_v^{n+1}\|^2\right) + a_0\left(\frac{4a_0}{b_n}\|r_2^{n+1}\|^2 + \frac{b_n}{4a_0}\|\tilde{e}_w^{n+1}\|^2\right) \\ &\quad + \sum_{j=0}^{n-1} (b_j - b_{j+1})(\|\tilde{e}_v^{n-j}\|^2 + \|\tilde{e}_v^{n+1}\|^2) + \sum_{j=0}^{n-1} (b_j - b_{j+1})(\|\tilde{e}_w^{n-j}\|^2 + \|\tilde{e}_w^{n+1}\|^2) \\ &\quad + \frac{4}{b_n}\left\|\left(\pi_N - I\right)\left(v(t_{n+1}) - \sum_{j=0}^n (b_j - b_{j+1})v(t_{n-j}) - b_n v(t_0)\right)\right\|^2 + \frac{b_n}{4}\|\tilde{e}_v^{n+1}\|^2 \\ &\quad + \frac{4}{b_n}\left\|\left(\pi_N - I\right)\left(w(t_{n+1}) - \sum_{j=0}^n (b_j - b_{j+1})w(t_{n-j}) - b_n w(t_0)\right)\right\|^2 + \frac{b_n}{4}\|\tilde{e}_w^{n+1}\|^2 \\ &\quad + a_0\beta\left(\frac{4a_0\beta}{b_n}\|I_N V\tilde{e}_w^{n+1}\|^2 + \frac{b_n}{4a_0\beta}\|\tilde{e}_v^{n+1}\|^2\right) \\ &\quad + a_0\beta\left(\frac{4a_0\beta}{b_n}\|w(t_{n+1})(V - I_N V)\|^2 + \frac{b_n}{4a_0\beta}\|\tilde{e}_v^{n+1}\|^2\right) \\ &\quad + a_0\beta\left(\frac{4a_0\beta}{b_n}\|I_N V\tilde{e}_v^{n+1}\|^2 + \frac{b_n}{4a_0\beta}\|\tilde{e}_w^{n+1}\|^2\right) \end{aligned}$$

$$+ a_0\beta \left(\frac{4a_0\beta}{b_n} \|v(t_{n+1})(V - I_N V)\|^2 + \frac{b_n}{4a_0\beta} \|\tilde{e}_w^{n+1}\|^2 \right).$$

That is

$$\begin{aligned} \|\tilde{e}_v^{n+1}\|^2 + \|\tilde{e}_w^{n+1}\|^2 &\leq \frac{4a_0^2}{b_n} (\|r_1^{n+1}\|^2 + \|r_2^{n+1}\|^2) + \sum_{j=0}^{n-1} (b_j - b_{j+1}) (\|\tilde{e}_v^{n-j}\|^2 + \|\tilde{e}_w^{n-j}\|^2) \\ &\quad + \frac{4}{b_n} \left\| (\pi_N - I) \left(v(t_{n+1}) - \sum_{j=0}^n (b_j - b_{j+1})v(t_{n-j}) - b_n v(t_0) \right) \right\|^2 \\ &\quad + \frac{4}{b_n} \left\| (\pi_N - I) \left(w(t_{n+1}) - \sum_{j=0}^n (b_j - b_{j+1})w(t_{n-j}) - b_n w(t_0) \right) \right\|^2 \\ &\quad + \frac{4a_0^2\beta^2}{b_n} \|I_N V\|_\infty \|\tilde{e}_w^{n+1}\|^2 + \frac{4a_0^2\beta^2}{b_n} \|w(t_{n+1})\|_\infty \|V - I_N V\|^2 \\ &\quad + \frac{4a_0^2\beta^2}{b_n} \|I_N V\|_\infty \|\tilde{e}_v^{n+1}\|^2 + \frac{4a_0^2\beta^2}{b_n} \|v(t_{n+1})\|_\infty \|V - I_N V\|^2. \end{aligned}$$

Using assumption (25) and the fact that $b_{n-1-j} > b_n$, we obtain

$$\begin{aligned} \|\tilde{e}_v^{n+1}\|^2 + \|\tilde{e}_w^{n+1}\|^2 &\leq \left(\frac{C_1 a_0^2 \Delta t^{4-2\alpha}}{b_n} + \frac{C_2 a_0^2 N^{-s}}{b_n} + \frac{C_3 a_0^2 N^{-m}}{b_n} \right) \\ &\quad + \sum_{j=0}^{n-1} (b_j - b_{j+1}) \left(\frac{C_1 a_0^2 \Delta t^{4-2\alpha}}{b_{n-j-1}^2} + \frac{C_2 a_0^2 N^{-s}}{b_{n-j-1}^2} + \frac{C_3 a_0^2 N^{-m}}{b_{n-j-1}^2} \right) \\ &\leq \left(\frac{C_1 a_0^2 \Delta t^{4-2\alpha}}{b_n} + \frac{C_2 a_0^2 N^{-s}}{b_n} + \frac{C_3 a_0^2 N^{-m}}{b_n} \right) \\ &\quad + \sum_{j=0}^{n-1} (b_j - b_{j+1}) \left(\frac{C_1 a_0^2 \Delta t^{4-2\alpha}}{b_n^2} + \frac{C_2 a_0^2 N^{-s}}{b_n^2} + \frac{C_3 a_0^2 N^{-m}}{b_n^2} \right) \\ &= \left(\frac{C_1 a_0^2 \Delta t^{4-2\alpha}}{b_n^2} + \frac{C_2 a_0^2 N^{-s}}{b_n^2} + \frac{C_3 a_0^2 N^{-m}}{b_n^2} \right) \left(b_n + \sum_{j=0}^{n-1} (b_j - b_{j+1}) \right) \\ &= \left(\frac{C_1 a_0^2 \Delta t^{4-2\alpha}}{b_n^2} + \frac{C_2 a_0^2 N^{-s}}{b_n^2} + \frac{C_3 a_0^2 N^{-m}}{b_n^2} \right). \end{aligned}$$

Combining with (14) and (22), estimate (23) is proved. □

Theorem 4 Suppose that $u = v + iw$ is the exact solution of (1)–(3), (v, w) and $(\{v_N^n\}_{n=1}^{M-1}, \{w_N^n\}_{n=1}^{M-1})$ are the solutions to (6) and (16), respectively, then we obtain

$$\|v(\cdot, t_n) - v_N^n\| + \|w(\cdot, t_n) - w_N^n\| \leq C(\Delta t^{2-\alpha} + N^{-s} + N^{-m}). \tag{26}$$

Proof The proof process is similar to the above theorem, and we omit it here. □

4 Numerical results

This section presents several numerical examples to confirm the accuracy and applicability of schemes (15)–(16) for solving Caputo/Riemann–Liouville Schrödinger equations. First, we need an exact solution to evaluate the accuracy of the numerical solution.

Example 4.1 Let $\beta = 1$ and $V = 1$, we consider numerical results for the following Caputo time-fractional Schrödinger equation:

$$\frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x, y, \mu)}{\partial \mu} \frac{d\mu}{(t-\mu)^\alpha} - i\Delta u + iu = f(x, y, t),$$

where

$$f(x, y, t) = \frac{2t^{2-\alpha}}{\Gamma(3-\alpha)} (\cos 8x + i \sin 8y) + t^2(-65 \sin 8y + i65 \cos 8x).$$

Then the exact solution is $u = t^2(\cos 8x + i \sin 8y)$.

Full-discrete scheme (15) is solved in $\Omega = (0, 2\pi)^2$ with $T = 1$. Tables 1–2 display the temporal convergence orders at $N = 20$ for v, w , respectively. It shows that for $\alpha = 0.1, 0.3, 0.5, 0.6, 0.7, 0.9$, the convergence orders of v and w are approximately 1.9, 1.7, 1.5, 1.4, 1.3, 1.1, respectively, which indicates that numerical scheme (15) can achieve $2 - \alpha$ order accuracy in time, which confirms the result in Theorem 3. Table 3 shows the L^2 error and the L^∞ error in space with $\alpha = 0.1, 0.3, 0.5, 0.7$. It confirms that the numerical solutions are in good agreement with the exact solutions and the error is influenced by the time direction error. It ascertains that, if the error in the time direction is negligible, our numerical method can theoretically achieve exponential order accuracy in space.

Table 1 Temporal convergence orders of v for Example 4.1

$\alpha \setminus \Delta t$	$\Delta t = 1.00E-2$	$\Delta t = 5.00E-3$	$\Delta t = 1.00E-3$	$\Delta t = 5.00E-4$
$\alpha = 0.1$	1.8015	1.8138	1.8349	1.8418
$\alpha = 0.3$	1.6588	1.6674	1.6807	1.6845
$\alpha = 0.5$	1.4857	1.4900	1.4956	1.4969
$\alpha = 0.6$	1.3923	1.3949	1.3981	1.3987
$\alpha = 0.7$	1.2962	1.2976	1.2992	1.2995
$\alpha = 0.9$	1.0995	1.0997	1.0999	1.1000

Table 2 Temporal convergence orders of w for Example 4.1

$\alpha \setminus \Delta t$	$\Delta t = 1.00E-2$	$\Delta t = 5.00E-3$	$\Delta t = 1.00E-3$	$\Delta t = 5.00E-4$
$\alpha = 0.1$	1.8015	1.8138	1.8349	1.8418
$\alpha = 0.3$	1.6588	1.6674	1.6807	1.6845
$\alpha = 0.5$	1.4857	1.4900	1.4956	1.4969
$\alpha = 0.6$	1.3923	1.3949	1.3981	1.3987
$\alpha = 0.7$	1.2961	1.2976	1.2992	1.2995
$\alpha = 0.9$	1.0994	1.0997	1.0999	1.1000

Table 3 L^2, L^∞ errors of v and w at $\Delta t = 10^{-4}$ for Example 4.1

$\alpha \setminus error$	N	$\ v(T) - v_N^M\ $	$\ v(T) - v_N^M\ _\infty$	$\ w(T) - w_N^M\ $	$\ w(T) - w_N^M\ _\infty$
$\alpha = 0.1$	18	1.7195E-10	5.6609E-10	1.7196E-10	5.7301E-10
	20	1.8126E-10	5.4817E-11	1.8125E-10	5.7301E-11
$\alpha = 0.3$	18	2.2952E-09	7.5500E-10	2.2952E-09	7.6500E-10
	20	2.4193E-09	7.3044E-10	1.8125E-10	5.7301E-11
$\alpha = 0.5$	18	2.1610E-08	7.1047E-10	2.1610E-08	7.2032E-09
	20	2.2779E-08	6.8701E-09	2.2779E-08	7.2032E-09
$\alpha = 0.7$	18	1.9066E-07	6.2644E-08	1.9066E-07	6.3553E-08
	20	2.0098E-07	6.0544E-08	2.0098E-07	6.3553E-08

Example 4.2 Let $\beta = 1$ and $V = 1$, we consider the following Riemann–Liouville time-fractional Schrödinger equation:

$$\frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t (t-\mu)^{-\alpha} u(x, y, \mu) d\mu - i\Delta u + iu = f(x, y, t),$$

where

$$f(x, y, t) = \left(\frac{t^{-\alpha}}{\Gamma(1-\alpha)} + \frac{2t^{2-\alpha}}{\Gamma(3-\alpha)} \right) (\sin 8x + i \cos 8y) + (t^2 + 1)(-65 \cos 8y + i65 \sin 8x).$$

Then the exact solution is $u = (t^2 + 1)(\sin 8x + i \cos 8y)$.

Full-discrete scheme (16) is solved at $\Omega = (0, 2\pi)^2$ with $T = 1$. The convergence orders in time direction are listed in Tables 4–5, and the L^2 and L^∞ errors in spatial direction are also listed in Table 6. It is obvious that numerical scheme (16) achieves $2 - \alpha$ order accuracy in time direction. Table 6 shows that numerical schemes (15)–(16) have good convergence behavior.

We fix $u(x, y, 0) = \cos 6x + i \sin y$, $\Delta t = 0.001$, $N = 20$, we also use numerical method (15) to simulate the dynamic behavior of the solution for different α . The results are summarized in Figs. 1–3. The results show that the wavelength becomes larger when the fractional diffusion coefficient α increases due to the long tail mechanism of the fractional operator.

Table 4 Temporal convergence orders of v for Example 4.2

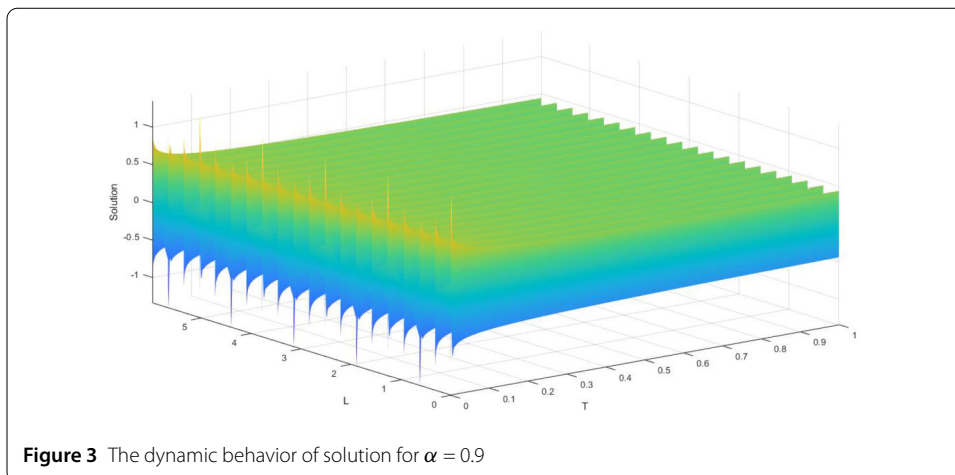
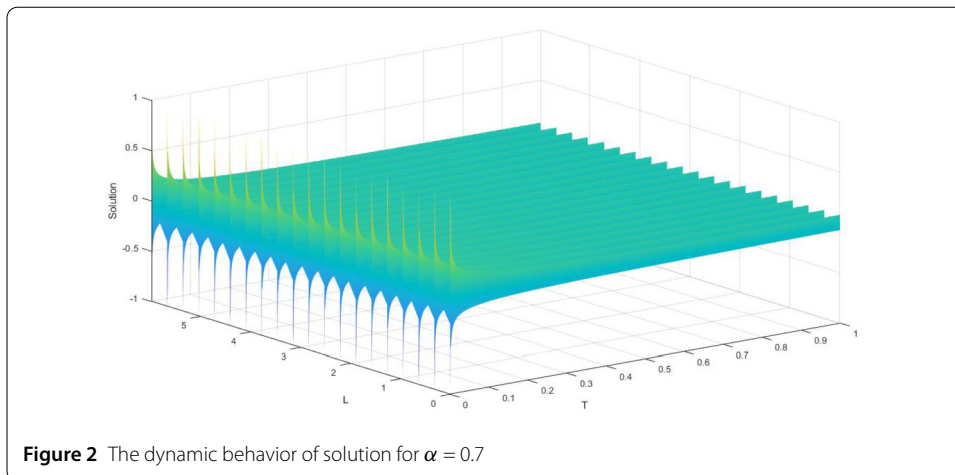
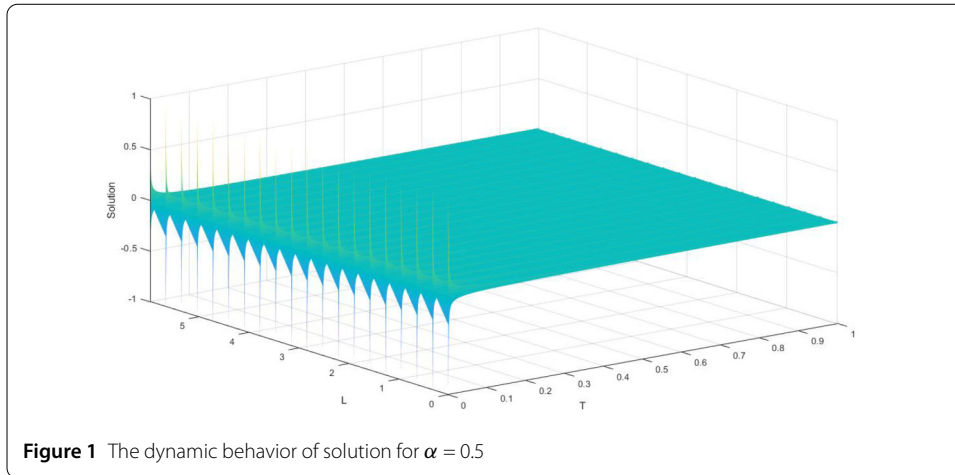
$\alpha \setminus \Delta t$	$\Delta t = 1.00E-2$	$\Delta t = 5.00E-3$	$\Delta t = 1.00E-3$	$\Delta t = 5.00E-4$
$\alpha = 0.1$	1.8015	1.8138	1.8349	1.8418
$\alpha = 0.3$	1.6588	1.6674	1.6807	1.6845
$\alpha = 0.5$	1.4857	1.4900	1.4956	1.4969
$\alpha = 0.6$	1.3923	1.3949	1.3981	1.3987
$\alpha = 0.7$	1.2961	1.2976	1.2992	1.2995
$\alpha = 0.9$	1.0994	1.0997	1.0999	1.1000

Table 5 Temporal convergence orders of w for Example 4.2

$\alpha \setminus \Delta t$	$\Delta t = 1.00E-2$	$\Delta t = 5.00E-3$	$\Delta t = 1.00E-3$	$\Delta t = 5.00E-4$
$\alpha = 0.1$	1.8015	1.8138	1.8349	1.8418
$\alpha = 0.3$	1.6588	1.6674	1.6807	1.6845
$\alpha = 0.5$	1.4857	1.4900	1.4956	1.4969
$\alpha = 0.6$	1.3923	1.3949	1.3981	1.3987
$\alpha = 0.7$	1.2961	1.2976	1.2992	1.2995
$\alpha = 0.9$	1.0994	1.0997	1.0999	1.1000

Table 6 L^2, L^∞ errors of v and w at $\Delta t = 10^{-4}$ for Example 4.2

$\alpha \setminus \Delta t$	N	$\ v(T) - v_N^M\ $	$\ v(T) - v_N^M\ _\infty$	$\ w(T) - w_N^M\ $	$\ w(T) - w_N^M\ _\infty$
$\alpha = 0.1$	18	1.7193E-10	5.7337E-11	1.7195E-10	5.6706E-11
	20	1.8124E-10	5.7430E-11	1.8124E-10	5.4762E-11
$\alpha = 0.3$	18	2.2951E-09	7.6502E-10	2.2952E-09	7.5509E-10
	20	2.4193E-09	7.6511E-10	2.4193E-09	7.3037E-10
$\alpha = 0.5$	18	2.1610E-08	7.2032E-09	2.1610E-08	7.1048E-09
	20	2.2779E-08	7.2033E-09	2.2779E-08	6.8700E-09
$\alpha = 0.7$	18	1.9066E-07	6.3553E-08	1.9066E-07	6.2645E-08
	20	2.0098E-07	6.3553E-08	2.0098E-07	6.0544E-08



5 Conclusion

We have constructed two efficient numerical schemes to solve time-fractional Schrödinger equation with Caputo/Riemann–Liouville derivative. These two numerical methods have been proved to be unconditionally stable. In addition, we have also discussed the conver-

gence of the numerical methods, and numerical convergence results show that the two schemes converge with the order $\mathcal{O}(\Delta t^{2-\alpha} + N^{-s} + N^{-m})$. Numerical examples are consistent with the theoretical prediction.

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Availability of data and materials

Data sharing not applicable to this article as no datasets were generated or analyzed during the current study.

Ethics approval and consent to participate

Not applicable.

Competing interests

The authors declare that they have no competing interests.

Consent for publication

We agree.

Authors' contributions

JZ carried out an efficient numerical approach to solve time-fractional Schrödinger. JRW helped to draft the manuscript. YZ helped to correct some typos and grammar errors. All authors read and approved the final manuscript.

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