axioms

MDPI

Article

Numerical Solution of Time-Fractional Schrödinger Equation by Using FDM

Moldir Serik, Rena Eskar * and Pengzhan Huang

College of Mathematics and Systems Science, Xinjiang University, Urumqi 830046, China; moldir114@163.com (M.S.); hpzh@xju.edu.cn (P.H.)
* Correspondence: renaeskar@xju.edu.cn

Abstract: In this paper, we first established a high-accuracy difference scheme for the time-fractional Schrödinger equation (TFSE), where the factional term is described in the Caputo derivative. We used the L1-2-3 formula to approximate the Caputo derivative, and the fourth-order compact finite difference scheme is utilized for discretizing the spatial term. The unconditional stability and convergence of the scheme in the maximum norm are proved. Finally, we verified the theoretical result with a numerical test.

Keywords: time-fractional Schrödinger equation; L1-2-3 formula; compact finite difference method; stability; Caputo derivative

MSC: 65M15; 65Y20

check for updates

Citation: Serik, M.; Eskar, R.; Huang, P. Numerical Solution of Time-Fractional Schrödinger Equation by Using FDM. *Axioms* **2023**, *12*, 816. https://doi.org/10.3390/axioms12090816

Academic Editors: Behzad Djafari-Rouhani and Feliz Manuel Minhós

Received: 16 June 2023
Revised: 16 August 2023
Accepted: 22 August 2023
Published: 25 August 2023

1. Introduction

In 1926, the Schrödinger equation was proposed by Schrödinger, who is a physicist from Austria [1], which combines the concept of matter wave with the wave equation to establish a second-order partial differential equation that describes the motion of microscopic particles, and its general form is as follows:

$$i\hbar\frac{\partial u}{\partial t} = -\frac{\hbar^2}{2m}\Delta u + Vu.$$

where u is the wave function, $\hbar$ is Planck constant, V is the potential function, m denotes the mass of the particle, and Δ represents the Laplace operator. In recent years, there have been many studies on the Schrödinger equation [2–10]. Researchers have found that fractional differential operators are non-local compared to integer differential operators and are very suitable for describing real-world processes of change with memory as well as hereditary properties. It has become one of the most important tools for describing all kinds of complex mechanical and physical behaviors. In 2004, Naber substituted the time term of the classical Schrödinger equation with the Caputo time-fractional derivative to propose the time-fractional Schrödinger equation (TFSE) [11], which describes the dependence of particle motion.

The TFSE is an integral-differential equation, and since it's very difficult to find the analytical solution, it has been a widely discussed hot topic to get a numerical solution of the TFSE with a smaller error and higher order. For example, Wei et al. proposed an LDG finite element method to solve the TFSE, which is implicit and fully discrete [12]. Garrappa R. et al. solved the TFSE based on the Krylov projection methods [13]. Liu et al. obtained the approximation solution of the TFSE based on the reproducing kernel theory and collocation method [14]. Zheng et al. presented a spectral collocation method for solving the TFSE [15].

Some L-type formulas have been exploited to replace the Caputo time-fractional term for discretizing the time derivative term and to reap the approximation solution of the TFSE. For example, Eskar, R. et al. used the L1 and L1-2 formulas to discretize the Caputo derivatives, and the compact difference scheme is exploited for the spatial terms to obtain the finite difference scheme [16]. Fei et al. constructed an implicit scheme by adopting the L2-1_σ formula to approximate the Caputo term; the weighted and shifted Grünwald formula is used for the spatial term [17]. Cen et al. also adopted the L2-1_σ formula on graded meshes for solving the TFKBE with an initial singularity [18]. Ding et al. solved a nonlinear TFSE by using the quintic non-polynomial spline in the spatial term and the L1 formula in the time term [19]. Mokhtari, R. et al. constructed three finite difference schemes by adopting different L-type formulas to approximate the Caputo derivatives in the time direction and the central difference format in the space direction, respectively. The accuracy of the three schemes are $O(\tau^{2-\alpha}+h^2), O(\tau^{3-\alpha}+h^2)$, and $O(\tau^3+h^2)$ [20], where $0 \leqslant \alpha \leqslant 1$, and τ (h) is time (spatial) step size. Hadhoud et al. received the approximation solution of the TFSE by using the L1 formula and proved the conditional stability of the technique [21].

In this paper, we use the L1-2-3 formula to approximate the Caputo derivative, and the fourth-order compact difference scheme is exploited to discretize the spatial derivative term for establishing a high-accuracy difference scheme, where the order in the time direction is 3 and the spatial direction is 4. Furthermore, we will prove the scheme is unconditionally stable and convergent in the maximum norm. At the end of the paper, a numerical test is given to prove the theoretical result.

2. Preliminaries

The following TFSE is considered:

$$i\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), \qquad x \in \Omega = (0,L),\ t \in (0,T], \tag{1}$$

$$u(x,0) = \varphi(x), \qquad x \in \Omega = [0,L], \tag{2}$$

$$u(0,t) = u(L,t) = \phi(t), \qquad t \in [0,T]. \tag{3}$$

where $i = \sqrt{-1}$, $\alpha \in (0,1)$, T and L are positive real numbers, $u_0(x)$ and $f(x,t)$ are given functions, $\frac{\partial^\alpha u(x,t)}{\partial t^\alpha}$ is the Caputo derivative of order $\alpha \in (0,1)$, which is defined as follows [20]:

$$\frac{\partial^\alpha u(\cdot,t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{u_s(\cdot,s)}{(t-s)^\alpha}ds.$$

In order to discretize the continuous problem, we first give a dissected grid of the solution region. Let $h = L/M$ and $\tau = T/N$ be the step sizes in the time and space directions, where M and N are two integers. Then $x_j = jh (j = 0,1,2,\cdots,M)$, $t^n = n\tau(n = 0,1,2,\cdots,N)$. Furthermore, we define a mesh that cover the domain $[0,L]\times[0,T]$. Let $\hat{U} = u_j^n$ is a grid function on the mesh. For any $u, v \in \hat{U}$, we introduce the following notations:

$$\delta_x u_{j+1/2}^n = \frac{u_{j+1}^n - u_j^n}{h}, \quad \delta_x u_{j-1/2}^n = \frac{u_j^n - u_{j-1}^n}{h}, \quad \delta_x^2 u_j^n = \frac{\delta_x u_{j+1/2}^n - \delta_x u_{j-1/2}^n}{h},$$

$$(u,v) = h\sum_{j=1}^{M-1} u_j \bar{v}_j, \quad ||u||^2 = (u,u), \quad ||u||_\infty = \max_{1\leqslant j\leqslant M-1}|u_j|,$$

$$(u,v)_1 = h\sum_{j=0}^{M-1}(\delta_x u_{j+1/2})(\delta_x \bar{v}_{j+1/2}), \quad ||u||_1^2 = (u,u)_1,$$

where the $\bar{v}_j$ and $\bar{v}_{j+1/2}$ denote the complex-conjugate of v_j and $v_{j+1/2}$.

From the Taylor expansion, we have:

$$
\begin{aligned}
\delta_x^2 u_j^n &= \frac{1}{h^2}(u_{j-1}^n - 2u_j^n + u_{j+1}^n) \\
&= \frac{2}{h^2}(\frac{h^2 u''(x_j, t_n)}{2!} + \frac{h^4 u^{(4)}(x_j, t_n)}{4!}) + O(h^4) \\
&= (1 + \frac{h^2}{12}\delta_x^2)u''(x_j, t_n) + O(h^4),
\end{aligned}
$$

then, we get:

$$
u''(x_j, t_n) = \frac{\delta_x^2}{(1 + \frac{h^2}{12}\delta_x^2)} u_j^n + O(h^4),
$$

and we define the compact fourth-order difference formula as follow:

$$
Hu_j^n = (I + \frac{h^2}{12}\delta_x^2)u_j^n.
$$

Definition 1 ([22]). *(The L1-2-3 formula). Assuming that $\alpha \in (0,1)$ and $u(x,t) \in C^{6,5}$ $(\Omega \times [0,T])$. We have*

$$
{}_0^C\mathcal{D}_t^\alpha u(\cdot, t^n) = \frac{1}{\tau^\alpha \Gamma(2-\alpha)} \left[d_0 u^n - \sum_{l=1}^{n-1} (d_{n-l-1} - d_{n-l}) u^l - d_{n-1} u^0 \right], \tag{4}
$$

where u^n and u^0 are approximations of $u(\cdot, t^n)$ and $u(\cdot, t^0)$. And for $n = 1$,

$$
d_0 = 1,
$$

for $n = 2$,

$$
d_l = \begin{cases} a_l + b_l, & l = 0 \\ a_l - b_{l-1}, & l = 1 \end{cases}
$$

for $n = 3$,

$$
d_l = \begin{cases} a_l + b_l + g_l, & l = 0 \\ a_l + b_l - b_{l-1} - 2g_{l-1}, & l = 1 \\ a_l - b_{l-1} + g_{l-2}, & l = 2 \end{cases}
$$

and for $n \geqslant 4$,

$$
d_l = \begin{cases} a_l + b_l + g_l, & l = 0 \\ a_l + b_l - b_{l-1} + g_l - 2g_{l-1}, & l = 1 \\ a_l + b_l - b_{l-1} + g_l - 2g_{l-1} + g_{l-2}, & 2 \leqslant l \leqslant n-3 \\ a_l + b_l - b_{l-1} - 2g_{l-1} + g_{l-2}, & l = n-2 \\ a_l - b_{l-1} + g_{l-2}, & l = n-1 \end{cases}
$$

with

$$
a_l = (l+1)^{1-\alpha} - l^{1-\alpha},
$$

$$
b_l = \frac{(l+1)^{2-\alpha} - l^{2-\alpha}}{2-\alpha} - \frac{(l+1)^{1-\alpha} - l^{1-\alpha}}{2},
$$

$$
g_l = \frac{(l+1)^{3-\alpha} - l^{3-\alpha}}{(2-\alpha)(3-\alpha)} - \frac{(l+1)^{1-\alpha} + 2l^{1-\alpha}}{6} - \frac{l^{2-\alpha}}{2-\alpha}.
$$

Lemma 1 ([20]). *If $n \geqslant 4$, then we have:*

$$d_0 > |d_1|,$$

$$d_0 > d_2 \geqslant d_3 \geqslant \cdots \geqslant d_{n-1} > 0.$$

Lemma 2 ([20]). *For $d_j (j = 0, 1, 2)$, we have:*

$$d_0 > 1,$$

$$3d_0 + 2d_1 - 2d_2 > 2,$$

$$d_0 + d_1 - d_2 > 1/3.$$

Theorem 1 ([22]). *Let*

$$\epsilon_3(u(\cdot, t^n)) = \frac{\partial^\alpha u(\cdot, t^n)}{\partial t^\alpha} - {}_0^C\mathcal{D}_t^\alpha u(\cdot, t^n)$$

if $u(x,t) \in C^{6,5}(\Omega \times [0,T])$, then

$$\begin{aligned}
|\epsilon_3(u(\cdot, t^1))| &\leqslant \frac{\alpha}{2\Gamma(3-\alpha)} m_{tt} \tau^{2-\alpha}, \\
|\epsilon_3(u(\cdot, t^2))| &\leqslant \frac{\alpha}{3(1-\alpha)(2-\alpha)\Gamma(1-\alpha)} \left(\frac{1}{2} + \frac{1}{3-\alpha} \right) M_{ttt} \tau^{3-\alpha} \\
&\quad + \frac{\alpha}{12\Gamma(1-\alpha)} (t^2 - t^1)^{-\alpha-1} M_{tt} \tau^3, \\
|\epsilon_3(u(\cdot, t^n))| &\leqslant \frac{12\alpha}{\Gamma(1-\alpha)} (t^n - t^1)^{-\alpha-1} M_{tt} \tau^3 + \frac{\alpha}{8\Gamma(1-\alpha)} (t^n - t^2)^{-\alpha-1} M_{ttt} \tau^4 \\
&\quad + \frac{\alpha}{\Gamma(1-\alpha)} \left(\frac{1}{2} + \frac{1}{12} \frac{27 - 10\alpha + \alpha^2}{\prod_{i=1}^4 (\alpha - i)} \right) M_{tttt} \tau^{4-\alpha}, \quad n \geqslant 3
\end{aligned}$$

where

$$m_{tt} = \max_{0 \leqslant t \leqslant t^1} u_{tt}(\cdot, t), \quad M_{tt} = \max_{0 \leqslant t \leqslant t^1} |u_{tt}(\cdot, t)|, \quad M_{ttt} = \max_{0 \leqslant t \leqslant t^2} |u_{ttt}(\cdot, t)|, \quad M_{tttt} = \max_{0 \leqslant t \leqslant t^n} |u_{tttt}(\cdot, t)|.$$

Lemma 3 ([23]). *For any $u, v \in \hat{U}$, we have $(\delta_x^2 u, v) = -(u, v)_1$.*

Lemma 4 ([23]). *For any $u \in \hat{U}$, we have $||u||_\infty \leqslant h^{-1/2} ||u||$.*

Lemma 5 ([24]). *For any $u \in \hat{U}$, we have $||u||_1^2 \leqslant \frac{4}{h^2} ||u||^2$.*

Lemma 6. *For any $u \in \hat{U}$, we have $\frac{2}{3} ||u||^2 \leqslant (Hu, u)$..*

Proof. Using Lemma 3 and Lemma 5,we have:

$$\begin{aligned}
(Hu, u) &= ((I + \frac{h^2}{12} \delta_x^2) u, u) = (u, u) + (\frac{h^2}{12} \delta_x^2 u, u) \\
&= ||u||^2 - \frac{h^2}{12} (u, u)_1 = ||u||^2 - \frac{h^2}{12} ||u||_1^2 \\
&\geqslant ||u||^2 - \frac{1}{3} ||u||^2 = \frac{2}{3} ||u||^2.
\end{aligned}$$

□

Lemma 7 ([25])**.** *Let $\{u^n\}$ and $\{v^n\}$ be nonnegative sequences, and c is a nonnegative constant, for all $n \geqslant 1$, if*

$$u^n \leqslant c + \sum_{l=0}^{n-1} u^l v^l,$$

then,

$$u^n \leqslant c \prod_{l=0}^{n-1}(1+v^n) \leqslant cexp(\sum_{l=0}^{n-1} v^l).$$

Lemma 8 ([26])**.** *For any $u \in \hat{U}$, we have $||u|| \leqslant \frac{L}{\sqrt{6}}||u||_1$.*

Lemma 9 ([27])**.** *For any $u \in \hat{U}$, we have $(Hu, v) = (u, Hv)$.*

Lemma 10. *For any $u \in \hat{U}$, we have $||Hu|| \leqslant \frac{4}{3}||u||$.*

Proof. Applying the inverse estimate $||\delta_x^2 u|| \leqslant \frac{4}{h^2}||u||$, we have:

$$||Hu|| = ||u + \frac{h^2}{12}\delta_x^2 u|| \leqslant ||u|| + \frac{h^2}{12}||\delta_x^2 u|| \leqslant ||u|| + \frac{1}{3}||u|| = \frac{4}{3}||u||.$$

□

3. Analysis of the Method

3.1. Construction of the Difference Scheme

To solve Equation (1), we discretize the time term by using the L1-2-3 formula, and the compact difference scheme is exploited for the spatial term, then we obtain the finite difference scheme as follows:

$$i{}_0^C\mathcal{D}_t^\alpha u_j^n = H^{-1}\delta_x^2 u_j^n + f_j^n, \quad 1 \leqslant j \leqslant M-1, \ \ 1 \leqslant n \leqslant N \tag{5}$$

$$u_j^0 = \varphi_j, \qquad 0 \leqslant j \leqslant M \tag{6}$$

$$u_0^n = u_M^n = \phi^n, \qquad 0 \leqslant n \leqslant N \tag{7}$$

where u_j^n is an approximation to $u(x_j, t^n)$, and $\varphi_j = \varphi(x_j)$, $\phi^n = \phi(t^n)$, $f_j^n = f(x_j, t^n)$. Since f_j^n has no effect on the discussion of the study that follows, for convenience, we assume $f_j^n = 0$.

3.2. Analysis of Stability

In this section, we will analyze the unconditional stability of the scheme (5) that was established in the previous subsection.

Theorem 2. *Difference scheme (5) is unconditionally stable.*

Proof. For $n = 1$, the inner product of Equation (5) and Hu^1 gives:

$$(i{}_0^C D_t^\alpha u^1, Hu^1) = (H^{-1}\delta_x^2 u^1, Hu^1) = (\delta_x^2 u^1, u^1).$$

From the Lemma 3, we have:

$$id_0(Hu^1, u^1) - id_0(Hu^1, u^0) = -\mu(u^1, u^1)_1 = -\mu||u^1||_1^2,$$

where $\mu = \tau^\alpha \Gamma(2-\alpha)$.

According to the Lemma 6 and Cauchy-Schwarz inequality, we can obtain:

$$\frac{2}{3}||u^1||^2 \leqslant \frac{1}{4}||Hu^1||^2 + ||u^0||^2.$$

From Lemma 10, here is:

$$\frac{2}{3}||u^1||^2 \leqslant \frac{1}{3}||u^1||^2 + ||u^0||^2.$$

Eventually, we can get $||u^1|| \leqslant \sqrt{3}||u^0||$.

For $n = 2$, we can obtain the following equation by inner product of Equation (5) and Hu^2:

$$(i_0^C D_t^\alpha u^2, Hu^2) = (H^{-1}\delta_x^2 u^2, Hu^2) = (\delta_x^2 u^2, u^2).$$

From Lemma 3, we have:

$$id_0(Hu^2, u^2) - i(d_0 - d_1)(Hu^2, u^1) - id_1(Hu^2, u^0) = -\mu||u^2||_1^2.$$

Further, we have:

$$d_0(Hu^2, u^2) \leqslant (d_0 - d_1)(Hu^2, u^1) + d_1(Hu^2, u^0).$$

Using the Lemma 6 and Cauchy-Schwarz inequality, we can obtain:

$$\frac{2}{3}d_0||u^2||^2 \leqslant (d_0 - d_1)(\frac{1}{4}||Hu^2||^2 + ||u^1||^2) + d_1(\frac{1}{4}||Hu^2||^2 + ||u^0||^2).$$

From Lemma 10, we can eventually obtain:

$$||u^2||^2 \leqslant \frac{3(d_0 - d_1)}{d_0}||u^1||^2 + \frac{3d_1}{d_0}||u^0||^2.$$

Then, for $\eta \geqslant 0$, we now have:

$$||u^2||^2 \leqslant \eta||u^0||^2 + \sum_{l=0}^{1} v^l||u^l||^2,$$

in which $v^0 = \frac{3d_1}{d_0}$, and $v^1 = \frac{3(d_0-d_1)}{d_0}$.

According to Lemma 1, $v^l > 0$, then using Lemma 7 ,we can obtain:

$$||u^2||^2 \leqslant \eta exp(\sum_{l=0}^{1} v^l)||u^0||^2 = \eta exp(3)||u^0||^2,$$

choosing $\eta \leqslant 3/exp(3)$ gives $||u^2|| \leqslant \sqrt{3}||u^0||$.

For $n \geqslant 3$, we can obtain the following equation by inner product of Equation (5) and Hu^n:

$$(i_0^C D_t^\alpha u^n, Hu^n) = (H^{-1}\delta_x^2 u^n, Hu^n) = (\delta_x^2 u^n, u^n).$$

From Lemma 3, we get:

$$id_0(Hu^n, u^n) - i\sum_{l=1}^{n-1}(d_{n-l-1} - d_{n-l})(Hu^n, u^l) - id_{n-1}(Hu^n, u^0) = -\mu||u^n||_1^2.$$

Furthermore, we can obtain:

$$d_0(Hu^n, u^n) \leqslant \sum_{l=1}^{n-1}(d_{n-l-1} - d_{n-l})(Hu^n, u^l) + d_{n-1}(Hu^n, u^0).$$

Since only $d_1 - d_2$ is unknown positive or negative in $d_{n-l-1} - d_{n-l}$, for $l = 1, 2, \cdots$, $n - 1$, so we discuss it in two cases.

Case1. If $d_2 < d_1$, from Lemma 6 and Cauchy-Schwarz inequality:

$$\frac{2}{3}d_0||u^n||^2 \leqslant \sum_{l=1}^{n-1}(d_{n-l-1}-d_{n-l})(\frac{1}{4}||Hu^n||^2+||u^l||^2)+d_{n-1}(\frac{1}{4}||Hu^n||^2+||u^0||^2).$$

From Lemma 10, we can obtain:

$$||u^n||^2 \leqslant \frac{3\sum_{l=1}^{n-1}(d_{n-l-1}-d_{n-l})}{d_0}||u^l||^2+\frac{3d_{n-1}}{d_0}||u^0||^2.$$

Then, for $\eta \geqslant 0$, we now have:

$$||u^n||^2 \leqslant \eta||u^0||^2+\sum_{l=0}^{n-1}v^l||u^l||^2,$$

in which $v^0=\frac{3d_{n-1}}{d_0}$, and $v^l=\frac{3(d_{n-l-1}-d_{n-l})}{d_0}$ for $l=1,2,\cdots,n-1$. According to Lemma 1, $v^l>0$, then using Lemma 7:

$$||u^n||^2 \leqslant \eta exp(\sum_{l=0}^{n-1}v^l)||u^0||^2=\eta exp(3)||u^0||^2,$$

choosing $\eta \leqslant 3/exp(3)$ gives $||u^n|| \leqslant \sqrt{3}||u^0||$.

Eventually, for $n \geqslant 1$, using Lemma 4, we have:

$$||u^n||_\infty \leqslant \sqrt{h}||u^n|| \leqslant \sqrt{3h}||u^0||.$$

Case2. If $d_2 > d_1$, then we have:

$$\frac{2}{3}d_0||u^n||^2 \leqslant \sum_{l=1,l\neq n-2}^{n-1}(d_{n-l-1}-d_{n-l})(Hu^n,u^l)+(d_2-d_1)(Hu^n,u^{n-2})+d_{n-1}(Hu^n,u^0).$$

From Lemma 6 and Cauchy-Schwarz inequality we can obtain:

$$\begin{aligned}\frac{2}{3}d_0||u^n||^2 \leqslant &\sum_{l=1,l\neq n-2}^{n-1}(d_{n-l-1}-d_{n-l})(\frac{1}{8}||Hu^n||^2+2||u^l||^2)+(d_2-d_1)(\frac{1}{8}||Hu^n||^2+2||u^{n-2}||^2)\\ &+d_{n-1}(\frac{1}{8}||Hu^n||^2+2||u^0||^2).\end{aligned}$$

Furthermore, using Lemma 10 and Lemma 2, we have:

$$\begin{aligned}||u^n||^2 \leqslant &\frac{12}{3d_0-2d_2+2d_1}\times(\sum_{l=1,l\neq n-2}^{n-1}(d_{n-l-1}-d_{n-l})||u^l||^2+(d_2-d_1)||u^{n-2}||^2+d_{n-1}||u^0||^2)\\ \leqslant &6\sum_{l=1,l\neq n-2}^{n-1}(d_{n-l-1}-d_{n-l})||u^l||^2+6(d_2-d_1)||u^{n-2}||^2+6d_{n-1}||u^0||^2.\end{aligned}$$

Then, for $\eta \geqslant 0$, we now have:

$$||u^n||^2 \leqslant \eta||u^0||^2+\sum_{l=0}^{n-1}v^l||u^l||^2,$$

in which $v^0=6d_{n-1}$, $v^{n-2}=6(d_2-d_1)$, and $v^l=6(d_{n-l-1}-d_{n-l})$ for $l=1,2,\cdots,n-3,n-1$.

According to Lemma 1, $v^l > 0$, then using Lemma 7, we can obtain:

$$||u^n||^2 \leqslant \eta exp(\sum_{l=0}^{n-1} v^l)||u^0||^2 = \eta exp(C)||u^0||^2,$$

where $C = 6(d_0 - 2d_1 + 2d_2)$, based on Lemma 1, $C > 0$. Choosing $\eta \leqslant 3/exp(C)$ gives $||u^n|| \leqslant \sqrt{3}||u^0||$.

Eventually, for $n \geqslant 1$, using Lemma 4, we have:

$$||u^n||_\infty \leqslant \sqrt{h}||u^n|| \leqslant \sqrt{3h}||u^0||.$$

In conclusion, scheme (5) is unconditionally stable. □

3.3. Analysis of Convergence

In the following, we consider the convergence of the difference scheme (5). The error equation holds:

$$e_j^n = u(x_j, t^n) - u_j^n, \tag{8}$$

where $u(x_j, t^n)$ denotes the exact solution of Equation (1), while u_j^n denotes the numerical solution.

Theorem 3. *Finite difference scheme (5) is always consistent with 3 order accuracy for $n > 2$, where $u \in C^{6,5}(\Omega \times [0, T])$.*

Proof. The local truncation error of the scheme (5) is:

$$T(x_j, t^n) = i{}_0^C D_t^\alpha u(x_j, t^n) - H^{-1}\delta_x^2 u(x_j, t^n) - f(x_j, t^n), \tag{9}$$

using Taylor expansion and Theorem 1, we have:

$$\begin{aligned} T(x_j, t^n) &= i\frac{\partial^\alpha u(x_j, t^n)}{\partial t^\alpha} - \frac{\partial^2 u(x_j, t^n)}{\partial x^2} - i\epsilon_3(u(x_j, t^n)) + O\left(h^4\right) \\ &= -i\epsilon_3(u(x_j, t^n)) + O\left(h^4\right). \end{aligned}$$

Let $T_m = \max_{(x,t)\in\Omega\times I} |T(x, t)|$, then:

$$T_m \leqslant \begin{cases} \frac{M_{tt}}{2}\tau^{2-\alpha} + O(h^4), & t \in \left[0, t^1\right], \\ \frac{M_{tt}}{40}\tau^{2-\alpha} + \frac{M_{tt}}{3}\tau^{3-\alpha} + O(h^4), & t \in \left(t^1, t^2\right], \\ \frac{7M_{tt}}{2}\tau^3 + \frac{M_{tt}}{25}\tau^4 + \frac{M_{ttt}}{4}\tau^{4-\alpha} + O(h^4), & t \in \left(t^2, t^n\right]. \end{cases}$$

Obviously, for $n > 2, T_m = O(\tau^3 + h^4)$. Eventually, we have the following result:

$$\|T_j^n\| \leqslant C_1(\tau^3 + h^4),$$

where C_1 is a positive integer. □

Theorem 4. *Finite difference scheme (5) is convergent if $u \in C^{4,4}(\Omega \times I)$.*

Proof. Subtracting Equation (5) from Equation (9) leads to :

$$T_j^n = i{}_0^C D_t^\alpha e_j^n - H^{-1}\delta_x^2 e_j^n. \tag{10}$$

Multiplying H on both sides of Equation (10), we have:

$$HT_j^n = i_0^C D_t^\alpha He_j^n - \delta_x^2 e_j^n.$$

Taking the inner product with respect to e_j^n and fetching the real part, then the following equation holds:

$$-(\delta_x^2 e^n, e^n) = \mathrm{Re}(HT^n, e^n).$$

By Lemma 3 and Lemma 8, we get :

$$6\|e^n\|^2 \leqslant L^2\|e^n\|_1^2 = L^2\,\mathrm{Re}(HT^n, e^n) \leqslant L^2|(HT^n, e^n)|.$$

Using Lemma 9, Cauchy-Schwarz inequality and Lemma 10, we can obtain:

$$6\|e^n\|^2 \leqslant L^2|\frac{3}{4L^2}\|T^n\|^2 + \frac{L^2}{3}\|He^n\|^2| \leqslant \frac{L^4}{3}\|T^n\|^2 + \|e^n\|^2.$$

Further, we can get :

$$\|e^n\| \leqslant \frac{L^2}{\sqrt{15}}\|T^n\| \leqslant \frac{L^2}{\sqrt{15}}C_1(\tau^3 + h^4),$$

where Theorem 3 used. Eventually, we have :

$$\|e^n\| \leqslant C\left(\tau^3 + h^4\right),$$

where C is a positive integer. Therefore, for $n \geqslant 1$, finite difference scheme (5) is convergent when $u \in C^{6,5}(\Omega \times [0,T])$. □

4. Numerical Experiment

Furthermore, two numerical examples are given to demonstrate the theoretical analyses of the scheme (5). The following notations will be used when presenting the result,

$$L^\infty - error = \max_{0\leqslant j\leqslant M, 0\leqslant n\leqslant N} |e_j^n|.$$

$$Order = log_2\left[\frac{L^\infty - error(2h,\tau)}{L^\infty - error(h,\tau)}\right].$$

Example 1. *The one-dimensional TFSE is considered as follows:*

$$\begin{aligned}
i\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} &= \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), && x \in \Omega = (0,2),\ t \in (0,1],\\
u(x,0) &= 0, && x \in [0,2],\\
u(0,t) &= u(2,t) = 0, && t \in [0,1]
\end{aligned}$$

where $f(x,t) = \frac{2t^{2-\alpha}}{\Gamma(3-\alpha)}(i-1)sin\pi x + (1+i)t^2\pi^2 sin\pi x$, *and the exact solution is given by*

$$u(x,t) = (1+i)t^2 sin\pi x.$$

Tables 1 and 2 indicate the maximum norm errors and the convergence orders in spatial direction. When taking different values of $\alpha(0.1, 0.5, 0.9)$ for $N = 2000$; we can know that the order of convergence in spatial direction is 4.

In Figure 1, we show the errors in the maximum norm for time direction attaining the third order of accuracy for $M = 2000$ for $\alpha = 0.1$ and $\alpha = 0.5$.

Table 1. Numerical error and convergence order in spatial direction for Example 1.

α	h	L^{∞}-Error	Order
	$1/2$	0.0395	-
	$1/4$	2.2777×10^{-3}	4.1107
0.1	$1/8$	1.4014×10^{-4}	4.0268
	$1/16$	8.7188×10^{-6}	4.0066
	$1/32$	5.4430×10^{-7}	4.0017
	$1/2$	0.0393	-
	$1/4$	2.2777×10^{-3}	4.1104
0.5	$1/8$	1.3974×10^{-4}	4.0258
	$1/16$	8.6938×10^{-6}	4.0066
	$1/32$	5.4273×10^{-7}	4.0017
	$1/2$	0.0396	-
	$1/4$	2.2935×10^{-3}	4.1108
0.9	$1/8$	1.4073×10^{-4}	4.0265
	$1/16$	8.7792×10^{-6}	4.0027
	$1/32$	5.7222×10^{-7}	3.9395

Table 2. Numerical error and convergence order in spatial direction for Example 2.

α	h	L^{∞}-Error	Order
	$\pi/2$	0.0240	-
	$\pi/4$	1.4026×10^{-3}	4.0953
0.1	$\pi/8$	8.6104×10^{-5}	4.0260
	$\pi/16$	5.3570×10^{-6}	4.0066
	$\pi/32$	3.3509×10^{-7}	3.9990
	$\pi/2$	0.0181	-
	$\pi/4$	1.0620×10^{-3}	4.0891
0.5	$\pi/8$	6.6241×10^{-5}	4.0028
	$\pi/16$	4.1390×10^{-6}	4.0004
	$\pi/32$	2.5174×10^{-7}	4.0393
	$\pi/2$	0.0117	-
	$\pi/4$	6.9124×10^{-4}	4.0856
0.9	$\pi/8$	4.4740×10^{-5}	3.9500
	$\pi/16$	2.7902×10^{-6}	4.0031
	$\pi/32$	1.7359×10^{-7}	4.0066

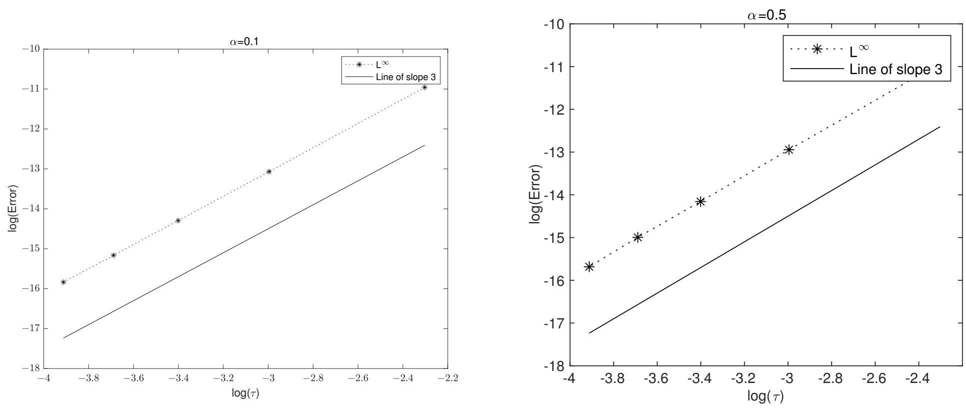

Figure 1. Convergence rates of numerical solutions at $M = 2000$ with different α for Example 1.

Figure 2 (Figure 3) represents the real (imaginary) part of the numerical solution and the exact solution for $\alpha = 0.7$, $h = 1/100$ and $\tau = 1/200$; it can be seen that our resulting numerical solution is very close to the exact solution.

Figure 4 gives the absolute modulus error between the numerical and exact solution when $M = 20$ and $N = 400$ for different $\alpha(0.2, 0.8)$, and we can observe that the error is very small.

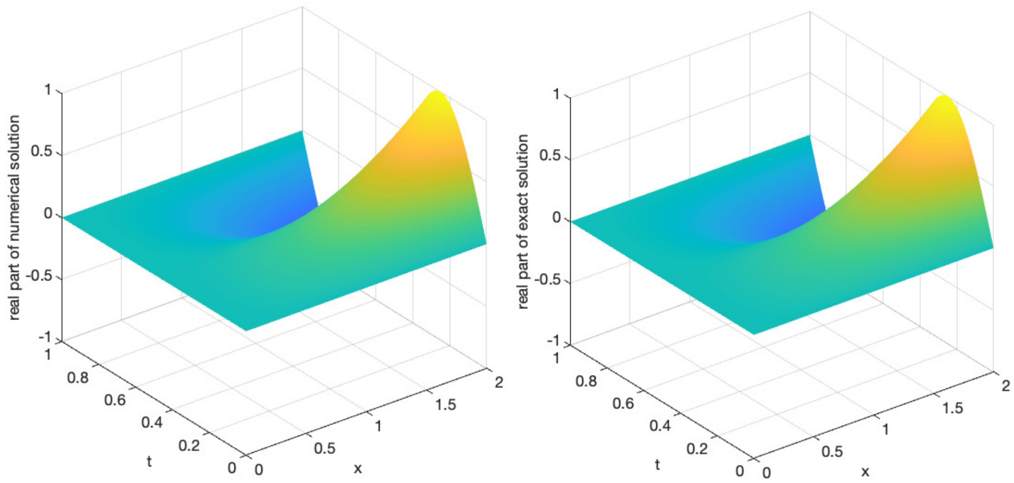

Figure 2. Real part of numerical solution and exact solution of Example 1.

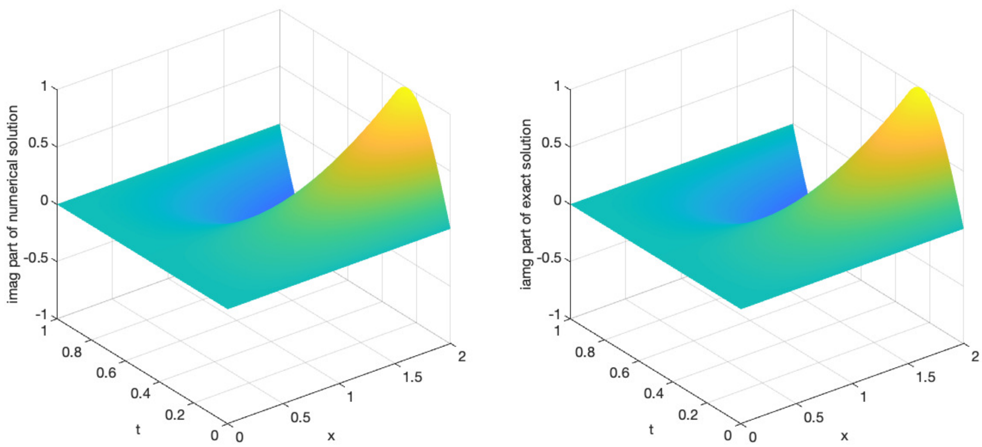

Figure 3. Imaginary part of numerical solution and exact solution of Example 1.

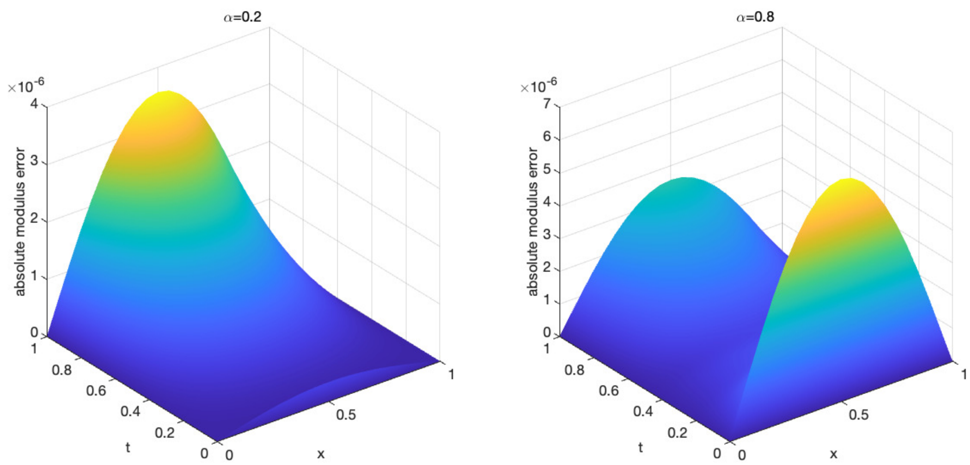

Figure 4. Absolute modulus error of Example1 for different α.

Example 2. *The one-dimensional TFSE is considered as follows:*

$$
\begin{aligned}
i\frac{\partial^{\alpha} u(x,t)}{\partial t^{\alpha}} &= \frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), && x \in \Omega = (0,2\pi),\ t \in (0,1],\\
u(x,0) &= 0, && x \in [0,2\pi],\\
u(0,t) = u(2,t) &= t^2, && t \in [0,1]
\end{aligned}
$$

where $f(x,t) = -\frac{2t^{2-\alpha}}{\Gamma(3-\alpha)}\sin x + t^2\cos x + i(\frac{2t^{2-\alpha}}{\Gamma(3-\alpha)}\cos x + t^2 \sin x)$, *and the exact solution is given by*

$$u(x,t) = t^2(\cos x + i \sin x).$$

In Figure 5, we show the errors in the maximum norm for time direction attaining the third order of accuracy for $M = 2000$ for $\alpha = 0.1$ and $\alpha = 0.5$.

In Figure 6 (Figure 7), we plot the real (imaginary) part of the numerical solution and the exact solution for $\alpha = 0.3$, $h = \pi/100$ and $\tau = 1/200$, it can be seen that our resulting numerical solution gives a great approximation of the exact solution.

Figure 8 gives the absolute modulus error between the numerical and exact solution when $M = 20$ and $N = 400$ for different $\alpha(0.2, 0.8)$, and we can observe that the error is very small.

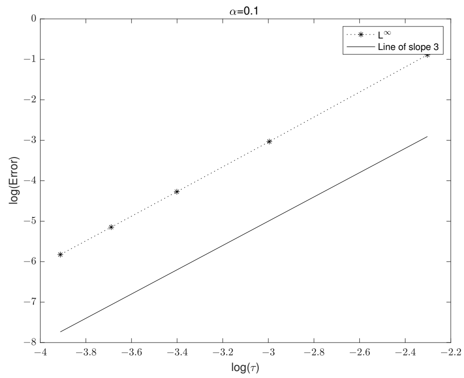

Figure 5. Convergence rates of numerical solutions at $M = 2000$ with different α for Example 2.

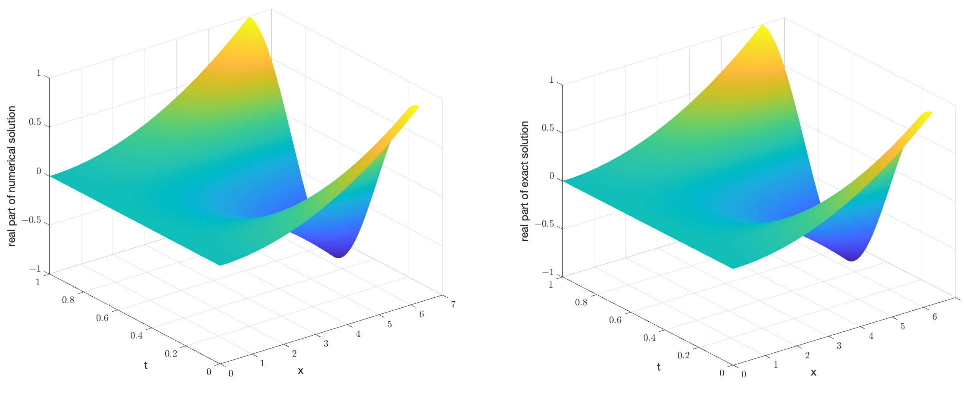

Figure 6. Real part of numerical solution and exact solution of Example 2.

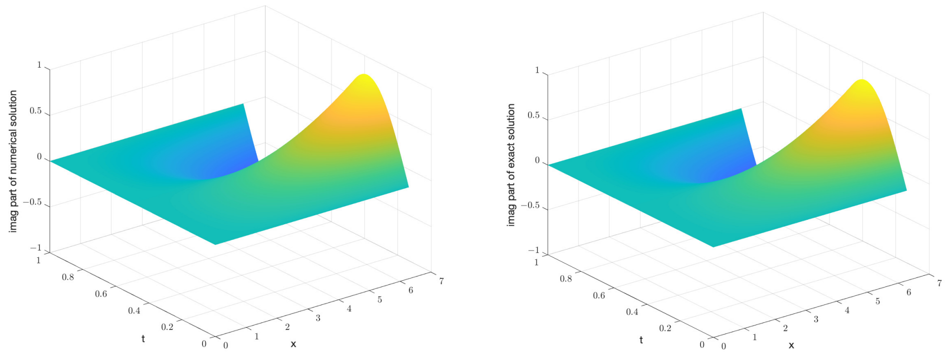

Figure 7. Imaginary part of numerical solution and exact solution of Example 2.

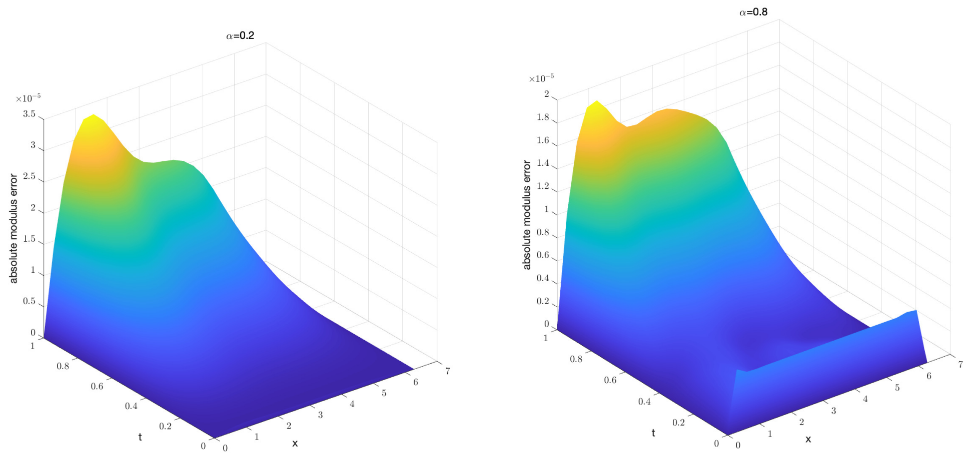

Figure 8. Absolute modulus error of Example 2 for different α.

Ref. [16] has used two L-type formulas to approximate the time fractional derivatives to establish two finite difference schemes, and the convergence orders are fourth order accuracy in the spatial direction and $2-\alpha$ and $3-\alpha$ in the temporal direction, respectively. The convergence order in the time direction for two schemes is shown in the Table 3:

Table 3. The convergence order in time direction [16].

α	τ	Example 1		Example 2	
		Order(L1)	**Order(L1-2)**	**Order(L1)**	**Order(L1-2)**
0.1	1/10	-	-	-	-
	1/20	1.768	3.042	1.764	3.010
	1/40	1.787	3.021	1.784	2.981
	1/80	1.802	3.010	1.800	2.965
0.5	1/10	-	-	-	-
	1/20	1.472	2.872	1.448	2.553
	1/40	1.480	2.699	1.468	2.524
	1/80	1.486	2.547	1.478	2.511
0.9	1/10	-	-	-	-
	1/20	1.089	1.397	1.051	2.086
	1/40	1.136	1.995	1.074	2.124
	1/80	1.157	2.162	1.087	2.100

By following Figures 1 and 5, we can know that with our method, we can achieve third order accuracy in the time direction, which is higher than [16].

5. Conclusions

In this paper, we first proposed a time-fractional Schrödinger equation with the Caputo time-fractional derivative of order $\alpha \in (0,1)$ for constructing the finite difference scheme to obtain the approximation solution of the equation; we approximated the Caputo derivative using the L1-2-3 formula to discretize the time term, and the spatial term is discretized by the fourth-order compact difference scheme; we then analyzed the unconditional stability of the scheme and also proved that the scheme is convergent in the maximum norm with an accuracy of $O(\tau^3 + h^4)$. At the end of this article, we give a numerical example to verify the theoretical result.

Author Contributions: Formal analysis, M.S. and R.E.; methodology, R.E. and P.H. All authors have read and agreed to the published version of the manuscript.

Funding: This research work was funded by Natural Science Foundation of Xinjiang Uygur Autonomous Region, 2021D01C068.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: Not applicable.

Conflicts of Interest: The authors declare no conflict of interest.

Abbreviations

TFSE	Time-fractional Schrödinger equation
LDG	Local discontinuous Galerkin
TFKBE	Time-fractional KdV Burgres' equation

References

1. Schrödinger, E. An undulatory theory of the mechanics of atoms and molecules. *Phys. Rev.* **1926**, *28*, 1049–1070. [CrossRef]
2. Chang, Q.; Jia, E.; Sun, W. Difference schemes for solving the generalized nonlinear Schrödinger equation. *J. Comput. Phys.* **1999**, *148*, 397–415. [CrossRef]
3. Dai, W. An unconditionally stable three-level explicit difference scheme for the Schrödinger equation with a variable coefficient. *SIAM J. Numer. Anal.* **1992**, *29*, 174–181. [CrossRef]
4. Ivanauskas, F.; Radziunas, M. On convergence and stability of the explicit difference method for solution of nonlinear Schrödinger equations. *SIAM J. Numer. Anal.* **1999**, *36*, 1466–1481. [CrossRef]
5. Nash, P.L.; Chen, L. Efficient finite difference solutions to the time-dependent Schrödinger equation. *J. Comput. Phys.* **1997**, *130*, 266–268. [CrossRef]
6. Sun, Z.; Wu, X. The stability and convergence of a difference scheme for the Schrödinger equation on an infinite domain by using artificial boundary conditions. *J. Comput. Phys.* **2006**, *214*, 209–223. [CrossRef]
7. Karakashian, O.A.; Akrivis, G.D.; Dougalis, V.A. On optimal order error estimates for the nonlinear Schrödinger equation. *SIAM J. Numer. Anal.* **1993**, *30*, 377–400. [CrossRef]
8. Bao, W.; Jaksch, D. An explicit unconditionally stable numerical method for solving damped nonlinear Schrödinger equations with a focusing nonlinearity. *SIAM J. Numer. Anal.* **2003**, *41*, 1406–1426. [CrossRef]
9. Li, B.; Fairweather, G.; Bialecki, B. Discrete-time orthogonal spline collocation methods for Schrödinger equations in two space variables. *SIAM J. Numer. Anal.* **1998**, *35*, 453–477. [CrossRef]
10. Robinson, M.P.; Fairweather, G. Orthogonal spline collocation methods for Schrödinger-type equations in one space variable. *Numer. Math.* **1994**, *68*, 355–376. [CrossRef]
11. Naber, M. Time fractional Schrödinger equation. *J. Math. Phys.* **2004**, *45*, 3339–3352. [CrossRef]
12. Wei, L.; He, Y.; Zhang, X.; Wang, S. Analysis of an implicit fully discrete local discontinuous Galerkin method for the time-fractional Schrödinger equation. *Finite Elem. Anal. Des.* **2012**, *59*, 28–34. [CrossRef]
13. Garrappa, R.; Moret, I.; Popolizio, M. Solving the time-fractional Schrödinger equation by Krylov projection methods. *J. Comput. Phys.* **2015**, *293*, 115–134. [CrossRef]
14. Liu, N.; Jiang, W. A numerical method for solving the time fractional Schrödinger equation. *Adv. Comput. Math.* **2018**, *44*, 1235–1248. [CrossRef]

15. Zheng, M.; Liu, F.; Jin, Z. The global analysis on the spectral collocation method for time fractional Schrödinger equation. *Appl. Math. Comput.* **2020**, *365*, 124689. [CrossRef]
16. Eskar, R.; Feng, X.; Kasim, E. On high-order compact schemes for the multidimensional time-fractional Schrödinger equation. *Adv. Differ. Equ.* **2020**, *1*, 1–18. [CrossRef]
17. Fei, M.; Wang, N.; Huang, C. A second-order implicit difference scheme for the nonlinear time-space fractional Schrödinger equation. *Appl. Numer. Math.* **2020**, *153*, 399–411. [CrossRef]
18. Cen, D.; Wang, Z.; Mo, Y. Second order difference schemes for time-fractional KdV–Burgers' equation with initial singularity. *Appl. Math. Lett.* **2021**, *112*, 106829. [CrossRef]
19. Ding, Q.; Wong, P.J.Y. Quintic non-polynomial spline for time-fractional nonlinear Schrödinger equation. *Adv. Differ. Equ.* **2020**, *46*, 1–27. [CrossRef]
20. Mokhtari, R.; Ramezani, M.; Haase, G. Stability and convergence analyses of the FDM based on some L-type formulae for solving the subdiffusion equation. *Numer. Math. Theor. Meth. Appl.* **2021**, *14*, 945–971.
21. Hadhoud, A.R.; Rageh, A.A.M.; Radwan, T. Computational solution of the time-fractional Schrödinger equation by using trigonometric B- Spline collocation method. *Fractal Fract.* **2022**, *6*, 127. [CrossRef]
22. Mokhtari, R.; Mostajeran, F. A high order formula to approximate the Caputo fractional derivative. *Commun. Appl. Math. Comput.* **2020**, *2*, 1–29. [CrossRef]
23. Xie, S.; Li, G.; Yi, S. Compact finite difference schemes with high accuracy for one-dimensional nonlinear Schrödinger equation. *Comput. Methods Appl. Mech. Eng.* **2009**, *198*, 1052–1060. [CrossRef]
24. Gao, Z.; Xie, S. Fourth-order alternating direction implicit compact finite difference schemes for two-dimensional Schrödinger equations. *Appl. Numer. Math.* **2011**, *61*, 593–614. [CrossRef]
25. Holte, J.M. Discrete Gronwall lemma and applications. *MAA-NCS Meet. Univ. North Dakota.* **2009**, *24*, 1–7.
26. Sun, Z. *The Numerical Methods for Partial Equations*; Science Press: Beijing, China, 2005; pp. 2–3. (In Chinese)
27. Wang, B.; Liang, D.; Sun, T. The conservative splitting high-order compact finite difference scheme for two-dimensional Schrödinger equations. *Int. J. Comput. Methods* **2017**, *14*, 1750079. [CrossRef]