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Optimal Error Estimates in Numerical Solution of Time Fractional Schrödinger Equations on Unbounded Domains

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Abstract. The artificial boundary method is used to reformulate the time fractional Schrödinger equation on the real line as a bounded problem with exact artificial boundary conditions. The problem appeared is solved by a numerical method employing the $L1$-formula for the Caputo derivative and finite differences for spatial derivatives. The convergence of the method studied and optimal error estimates in a special metric are obtained. The technique developed here can be also applied to study the convergence of approximation methods for standard Schrödinger equation.

AMS subject classifications: 65M06, 35B65

Key words: Time fractional Schrödinger equation, artificial boundary method, optimal error estimate, stability and convergence.

1. Introduction

Fractional partial differential equations (PDEs) attract a lot of attention because of wide applications in various fields of science and engineering. In particular, they help to address nonlocal phenomena in quantum physics and to explore the quantum behavior of long-range interactions or time-dependent processes with many scales. Thus fractional quantum models are described by fractional Schrödinger equations — cf. Refs. [5, 9, 11, 14, 17, 21–24, 29, 30]. Here we consider the numerical solutions of the time fractional Schrödinger equation

$$\mathrm{i}\,{}_0^C D_t^{\alpha} u(x,t) = -\partial_x^2 u(x,t) + V(x)u(x,t), \quad x\in\mathbb{R}, \quad 0<t\le T, \tag{1.1}$$

$$u(x,0)=\psi(x), \quad x\in\mathbb{R}, \tag{1.2}$$

$$u\to 0, \quad \text{as} \quad |x|\to\infty, \tag{1.3}$$

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on the unbounded domain $\mathbb{R}$. Note that $\mathrm{i}=\sqrt{-1}$, $u(x,t)$ represents a complex-valued wave function, the initial value $\psi(x)$ is a compactly supported function, $V(x)$ is the real-valued external potential function, and ${}_0^CD_t^\alpha u$, $0<\alpha<1$ refers to the Caputo fractional derivative

$$ {}_0^CD_t^\alpha u(x,t)=\frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{\partial_s u(x,s)}{(t-s)^\alpha}ds. \tag{1.4}$$

There are many approximation methods for PDEs in unbounded domains with the artificial boundary method (ABM) being the one of most efficient [3, 6–8, 12, 13, 16]. The main idea of ABM is to introduce artificial boundaries and reduce the original problem to a problem on a bounded computational domain. Note that the design of artificial boundary conditions (ABCs) has an important impact on the overall performance and accuracy of the corresponding numerical schemes. The exact ABCs mean that the solution of the truncated domain problem is rendered exactly the same as in the unbounded domain problem. As was established in [19], the problem (1.1)-(1.3) can be reduced to the following initial-boundary value problem

$$\mathrm{i}\,{}_0^CD_t^\alpha u(x,t)+u_{xx}(x,t)+V(x)u(x,t)=0,\quad x\in(x_l,x_r),\quad t\in(0,T], \tag{1.5}$$

$$u_x(x_l,t)=\mathrm{e}^{-\pi\mathrm{i}/4}\,{}_0^CD_t^{\alpha/2}u(x_l,t),\quad t\in(0,T], \tag{1.6}$$

$$u_x(x_r,t)=-\mathrm{e}^{-\pi\mathrm{i}/4}\,{}_0^CD_t^{\alpha/2}u(x_r,t),\quad t\in(0,T], \tag{1.7}$$

$$u(x,0)=\psi(x),\quad x\in[x_l,x_r]. \tag{1.8}$$

It is worth mentioning that for the standard Schrödinger equation — i.e. in the case when $\alpha=1$, the development and analysis of unconditionally stable schemes for reduced problems in bounded domains requires substantial efforts. Thus Arnold and Ehrhard [2] derived exact discrete ABCs immediately from a fully discretised Schödinger equation. Schmidt and Yevick [26] proposed an efficient fully discrete scheme based on a finite element method for spatial discretisation. Mayfield [20], Baskakov and Popov [4], Antoine *et al.* [1], Han *et al.* [15] and Ducomet *et al.* [10] presented straightforward approaches to construct unconditionally stable discretisation schemes. However, although the stability of the methods is well studied, the optimal error estimates are less known. The main reason for this is that the temporal convolution arising in exact ABCs causes problems in convergence analysis. So far only the sub-optimal error estimate $\mathscr{O}(h^{3/2}+\tau^{3/2}h^{-1/2}+h^2+\tau^2)$ for the standard Schödinger equation has been established [15, 28]. Recently, Li *et al.* [18] proved an asymptotic optimal-order error estimate for a numerical scheme by including a constant damping term into the governing equation and modifying the standard Crank-Nicolson implicit scheme. For time fractional Schödinger equations with $0<\alpha\le 1$, the only existing sub-optimal estimate is $\mathscr{O}(h^{3/2}+\tau^{1/2+\alpha}h^{-1/2}+h^2+\tau^2)$ and it is obtained for L^2-norm errors.

The aim of this paper is to establish an optimal error estimate for the reduced problem with exact ABCs while discretising the Caputo derivative by the $L1$-formula and using finite differences for spatial derivatives. In particular, we evaluate spatial-related errors in H^1-norm and time-related ones in L^2-norm, denoting the resulting measure as $L^2(H^1)$. This is because in contrast to anomalous diffusion equations [12], the imaginary part of the inner product, which defines nonlocal convolution in the corresponding ABCs, is not bounded below. Therefore, the boundary-related errors cannot be disregarded. In one-dimensional case, such errors can be estimated in H^1-norm from above. Taking into account the observations mentioned, we estimate the truncation error R^n for the Caputo derivative and provide a bound of the difference quotient of R^n. Then the energy method, temporal summation by parts and the weighted Cauchy-Schwartz inequality are used to derive globally optimal convergence in $L_2(H_1)$-norm.

The remainder of the article is as follows. In Section 2, we deal with the truncation error of the $L1$ approximation of the Caputo fractional derivatives. Section 3 introduces a numerical scheme and provides a detailed analysis for the truncation error. Section 4 is devoted to the convergence proof of the numerical scheme under consideration. Our conclusions are in Section 5.

2. Auxiliary Results

Let τ refer to the temporal step size, $t_n = n\tau$, $f^n := f(t_n)$, $n = 0,1,2,\cdots$. The $L1$-formula for the approximation of the Caputo derivative ${}_0^C D_t^\alpha f(t)\Big|_{t=t_k}$, $k = 1,2,\cdots$ has the form

$$ {}_0^C\mathbb{D}_t^\alpha f^k = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}\Big[a_0^{(\alpha)} f^k - \sum_{l=1}^{k-1}(a_{k-l-1}^{(\alpha)} - a_{k-l}^{(\alpha)}) f^l - a_{k-1}^{(\alpha)} f^0\Big], \tag{2.1}$$

where

$$a_l^{(\alpha)} = (l+1)^{1-\alpha} - l^{1-\alpha}, \quad l \ge 0.$$

Lemma 2.1. *If*

$$R^n := {}_0^C D_t^\alpha f(t_n) - {}_0^C\mathbb{D}_t^\alpha f^n, \quad n = 0,1,2,\cdots,$$

then, there are constants c_0, c_1, c_2 such that

$$|R^n| \le c_0 \max_{t_0\le t\le t_n} |f''(t)|\, \tau^{2-\alpha}, \quad n = 1,2,\cdots, \tag{2.2}$$

$$\frac{1}{\tau}|R^n - R^{n-1}| \le c_1 \max_{t_0\le t\le t_1} |f''(t)| \frac{\tau^2}{t_n^{1+\alpha}} + c_2 \max_{t_0\le t\le t_n} |f'''(t)|\tau^{2-\alpha}, \quad n \ge 2. \tag{2.3}$$

Proof. We start with the inequality (2.2). Similar to [27], the term R^n can be represented in the form

$$\begin{aligned} R^n &= \frac{1}{\Gamma(1-\alpha)} \sum_{k=1}^n \int_{t_{k-1}}^{t_k} \Big[f'(s) - \frac{f^k - f^{k-1}}{\tau}\Big] \frac{1}{(t_n - s)^\alpha} \mathrm{d}s \\ &= \frac{1}{\Gamma(2-\alpha)} \sum_{k=1}^n \int_{t_{k-1}}^{t_k} \Big\{(t_n - s)^{1-\alpha} - \Big[\frac{s - t_{k-1}}{\tau}(t_n - t_k)^{1-\alpha} + \frac{t_k - s}{\tau}(t_n - t_{k-1})^{1-\alpha}\Big]\Big\} f''(s)\mathrm{d}s, \end{aligned}$$

which yields

$$|R^n| \le \frac{1}{\Gamma(2-\alpha)} \max_{t_0\le t\le t_n} \big|f''(t)\big|$$

$$
\begin{aligned}
&\times \sum_{k=1}^{n} \int_{t_{k-1}}^{t_k} \Big\{ (t_n - s)^{1-\alpha} - \Big[\frac{s - t_{k-1}}{\tau} (t_n - t_k)^{1-\alpha} + \frac{t_k - s}{\tau} (t_n - t_{k-1})^{1-\alpha} \Big] \Big\} \mathrm{ds} \\
\le\; & c_0 \max_{t_0 \le t \le t_n} \left| f''(t) \right| \tau^{2-\alpha}, \quad n = 1, 2, 3, \cdots .
\end{aligned}
$$

Thus the inequality (2.2) is established. In order to show the estimate (2.3) for $n \ge 2$, we write R_n as

$$
\begin{aligned}
R^n =& \frac{1}{\Gamma(2-\alpha)} \int_{t_0}^{t_1} \Big\{ (t_n - s)^{1-\alpha} - \Big[\frac{s - t_0}{\tau} (t_n - t_1)^{1-\alpha} + \frac{t_1 - s}{\tau} (t_n - t_0)^{1-\alpha} \Big] \Big\} f''(s) \mathrm{ds} \\
&+ \frac{1}{\Gamma(2-\alpha)} \sum_{k=1}^{n-1} \int_{t_k}^{t_{k+1}} \Big\{ (t_n - s)^{1-\alpha} - \Big[\frac{s - t_k}{\tau} (t_n - t_{k+1})^{1-\alpha} + \frac{t_{k+1} - s}{\tau} (t_n - t_k)^{1-\alpha} \Big] \Big\} f''(s) \mathrm{ds} \\
=& \frac{1}{\Gamma(2-\alpha)} \int_{t_0}^{t_1} \Big\{ (t_n - s)^{1-\alpha} - \Big[\frac{s - t_0}{\tau} (t_n - t_1)^{1-\alpha} + \frac{t_1 - s}{\tau} (t_n - t_0)^{1-\alpha} \Big] \Big\} f''(s) \mathrm{ds} \\
&+ \frac{1}{\Gamma(2-\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \Big\{ (t_n - (s+\tau))^{1-\alpha} - \Big[\frac{s + \tau - t_k}{\tau} (t_n - t_{k+1})^{1-\alpha} \\
&+ \frac{t_{k+1} - (s+\tau)}{\tau} (t_n - t_k)^{1-\alpha} \Big] \Big\} f''(s+\tau) \mathrm{ds} \\
=& \frac{1}{\Gamma(2-\alpha)} \int_{t_0}^{t_1} \Big\{ (t_n - s)^{1-\alpha} - \Big[\frac{s - t_0}{\tau} (t_n - t_1)^{1-\alpha} + \frac{t_1 - s}{\tau} (t_n - t_0)^{1-\alpha} \Big] \Big\} f''(s) \mathrm{ds} \\
&+ \frac{1}{\Gamma(2-\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \Big\{ (t_{n-1} - s)^{1-\alpha} - \Big[\frac{s - t_{k-1}}{\tau} (t_{n-1} - t_k)^{1-\alpha} \\
&+ \frac{t_k - s}{\tau} (t_{n-1} - t_{k-1})^{1-\alpha} \Big] \Big\} f''(s+\tau) \mathrm{ds}.
\end{aligned}
$$

It follows that

$$
\begin{aligned}
&\frac{1}{\tau} \left(R^n - R^{n-1} \right) \\
=& \frac{1}{\tau} \cdot \frac{1}{\Gamma(2-\alpha)} \int_{t_0}^{t_1} \Big\{ (t_n - s)^{1-\alpha} - \Big[\frac{s - t_0}{\tau} (t_n - t_1)^{1-\alpha} + \frac{t_1 - s}{\tau} (t_n - t_0)^{1-\alpha} \Big] \Big\} f''(s) \mathrm{ds} \\
&+ \frac{1}{\Gamma(2-\alpha)} \sum_{k=1}^{n-1} \int_{t_{k-1}}^{t_k} \Big\{ (t_{n-1} - s)^{1-\alpha} - \Big[\frac{s - t_{k-1}}{\tau} (t_{n-1} - t_k)^{1-\alpha} \\
&+ \frac{t_k - s}{\tau} (t_{n-1} - t_{k-1})^{1-\alpha} \Big] \Big\} \frac{f''(s+\tau) - f''(s)}{\tau} \mathrm{ds},
\end{aligned}
$$

and, consequently,

$$
\frac{1}{\tau} \left| R^n - R^{n-1} \right| \le \frac{1}{\tau} \cdot \frac{1}{\Gamma(2-\alpha)} \max_{t_0 \le t \le t_1} \left| f''(t) \right|
$$

$$
\begin{aligned}
&\times\int_{t_0}^{t_1}\Big\{(t_n-s)^{1-\alpha}-\Big[\frac{s-t_0}{\tau}(t_n-t_1)^{1-\alpha}+\frac{t_1-s}{\tau}(t_n-t_0)^{1-\alpha}\Big]\Big\}\mathrm{d}s\\
&+\frac{1}{\Gamma(2-\alpha)}\max_{t_0\le t\le t_n}\left|f'''(t)\right|\\
&\times\sum_{k=1}^{n-1}\int_{t_{k-1}}^{t_k}\Big\{(t_{n-1}-s)^{1-\alpha}-\Big[\frac{s-t_{k-1}}{\tau}(t_{n-1}-t_k)^{1-\alpha}+\frac{t_k-s}{\tau}(t_{n-1}-t_{k-1})^{1-\alpha}\Big]\Big\}\mathrm{d}s\\
\le\,& c_1\max_{t_0\le t\le t_1}\left|f''(t)\right|\frac{\tau^2}{t_n^{1+\alpha}}+c_2\max_{t_0\le t\le t_n}\left|f'''(t)\right|\tau^{2-\alpha},
\end{aligned}
$$

thus finishing the proof. □

Lemma 2.2 (cf. Refs. [19,27]). *If $u:=(u^0,u^1,\cdots,u^n)$ and ${}_0^C\mathbb{D}_t^\alpha u^k$ is the $L1$ approximation of* (2.1)*, then*

$$
\begin{aligned}
2\tau\mathrm{Re}\left\{\sum_{k=1}^n\big({}_0^C\mathbb{D}_t^\alpha u^k\big)\bar{u}^k\right\}&\ge\frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}\tau\sum_{k=1}^n a_{n-k}^{(\alpha)}|u^k|^2-\frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)}|u^0|^2\\
&\ge\frac{t_n^{-\alpha}}{\Gamma(1-\alpha)}\tau\sum_{k=1}^n|u^k|^2-\frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)}|u^0|^2.
\end{aligned}
$$

Lemma 2.3 (cf. Sun & Wu [28]). *If $u:=(u^0,u^1,\cdots,u^n)$ and ${}_0^C\mathbb{D}_t^\alpha u^k$ is the $L1$ approximation of* (2.1)*, then*

$$
\mathrm{Re}\left\{\mathrm{e}^{\mathrm{i}\pi/4}\sum_{k=1}^n\Big({}_0^C\mathbb{D}_t^{\alpha/2}u^k\Big)\bar{u}^k\right\}\ge 0.
$$

Lemma 2.4. *Assume that $\alpha\in(0,1)$ and let*

$$
D_t^\alpha f(t):=\frac{1}{\Gamma(1-\alpha)}\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^t\frac{f(s)}{(t-s)^\alpha}\mathrm{d}s.
$$

Then the integral

$$
A:=\mathrm{e}^{\mathrm{i}\pi/4}\int_{-\infty}^{+\infty}D_t^\alpha f(t)\overline{D_t^{\alpha/2}f(t)}\mathrm{d}t,
$$

has a non-negative real part.

Proof. If $\hat{f}(\omega)$ refers to the Fourier transform of a function $f(t)$, then by Parseval's Formula [25], one has

$$
\begin{aligned}
A&=\mathrm{e}^{\mathrm{i}\pi/4}\int_{-\infty}^{+\infty}(-\mathrm{i}\omega)^\alpha\hat{f}(\omega)\overline{(-\mathrm{i}\omega)^{\alpha/2}\hat{f}(\omega)}\mathrm{d}\omega\\
&=\mathrm{e}^{\mathrm{i}\pi/4}\left[\int_0^{+\infty}(-\mathrm{i}\omega)^\alpha\hat{f}(\omega)\overline{(-\mathrm{i}\omega)^{\alpha/2}\hat{f}(\omega)}\mathrm{d}\omega+\int_0^{+\infty}(\mathrm{i}\omega)^\alpha\hat{f}(-\omega)\overline{(\mathrm{i}\omega)^{\alpha/2}\hat{f}(-\omega)}\mathrm{d}\omega\right]
\end{aligned}
$$

$$= \mathrm{e}^{(\pi/4)(1-\alpha)\mathrm{i}} \int_0^{+\infty} \omega^{(3/2)\alpha} |\hat{f}(\omega)|^2 \mathrm{d}\omega + \mathrm{e}^{(\pi/4)(1+\alpha)\mathrm{i}} \int_0^{+\infty} \omega^{(3/2)\alpha} |\hat{f}(-\omega)|^2 \mathrm{d}\omega,$$

and Lemma 2.4 is proved. □

Lemma 2.5. *If $u := (u^0, u^1, \cdots, u^n)$, $u^0 = 0$ and ${}_0^C\mathbb{D}_t^\alpha u^k$ is the $L1$ approximation of* (2.1)*, then*

$$\mathrm{Re}\Big\{ \mathrm{e}^{\mathrm{i}\pi/4} \tau \sum_{k=1}^{\infty} \big({}_0^C\mathbb{D}_t^\alpha u^k\big) \overline{{}_0^C\mathbb{D}_t^{\alpha/2} u^k} \Big\} \geq 0.$$

Proof. We consider a function u defined by

$$u(t) = \begin{cases} u^k \cdot \dfrac{t - t_{k-1}}{\tau} + u^{k-1} \cdot \dfrac{t_k - t}{\tau}, & t \in [t_{k-1}, t_k], \quad k = 1, 2, \cdots, n, \\ 0, & \text{otherwise}. \end{cases}$$

Since

$${}_0^C D_t^\alpha u(t) = D_t^\alpha u(t), \quad {}_0^C D_t^{\alpha/2} u(t) = D_t^{\alpha/2} u(t),$$

it follows that

$$\begin{aligned} &\int_{-\infty}^{+\infty} D_t^\alpha u(t) \overline{D_t^{\alpha/2} u(t)} \mathrm{d}t = \lim_{m\to+\infty} \int_{t_0}^{t_m} D_t^\alpha u(t) \overline{D_t^{\alpha/2} u(t)} \mathrm{d}t \\ &= \lim_{m\to+\infty} \sum_{k=1}^{m} \int_{t_{k-1}}^{t_k} D_t^\alpha u(t) \overline{D_t^{\alpha/2} u(t)} \mathrm{d}t = \lim_{m\to+\infty} \tau \sum_{k=1}^{m} D_t^\alpha u(t_k) \overline{D_t^{\alpha/2} u(t_k)} \\ &= \tau \sum_{k=1}^{\infty} {}_0^C{}_t^\alpha u(t_k) \overline{{}_0^C D_t^{\alpha/2} u(t_k)} = \tau \sum_{k=1}^{\infty} \big({}_0^C\mathbb{D}_t^\alpha u^k\big) \overline{{}_0^C\mathbb{D}_t^{\alpha/2} u^k}. \end{aligned}$$

Now Lemma 2.4 yields

$$\mathrm{Re}\Big\{ \mathrm{e}^{\mathrm{i}\pi/4} \tau \sum_{k=1}^{\infty} \big({}_0^C\mathbb{D}_t^\alpha u^k\big) \overline{{}_0^C\mathbb{D}_t^{\alpha/2} u^k} \Big\} = \mathrm{Re}\Big\{ \mathrm{e}^{\mathrm{i}\pi/4} \int_{-\infty}^{+\infty} D_t^\alpha u(t) \overline{D_t^{\alpha/2} u(t)} \mathrm{d}t \Big\} \geq 0,$$

as required. □

Lemma 2.6. *If $u := (u^0, u^1, \cdots, u^n)$, $v = (v^0, v^1, \cdots, v^n)$ and ${}_0^C\mathbb{D}_t^\alpha u^k$ is the $L1$ approximation of* (2.1)*, then*

$$\sum_{k=1}^{n} v^k \big({}_0^C\mathbb{D}_t^\alpha u^k\big) = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \Bigg[v^n \sum_{k=1}^{n} a_{n-k}^{(\alpha)} u^k - \tau \sum_{k=1}^{n-1} \frac{v^{k+1} - v^k}{\tau} \sum_{l=1}^{k} a_{k-l}^{(\alpha)} u^l - \sum_{k=0}^{n-1} a_k^{(\alpha)} v^{k+1} u^0 \Bigg].$$

Proof. It follows immediately from the definition of $L1$ approximation that

$$\sum_{k=1}^{n} v^k \big({}_0^C\mathbb{D}_t^\alpha u^k\big) = \sum_{k=1}^{n} v^k \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \Bigg[a_0^{(\alpha)} u^k - \sum_{l=1}^{k-1} (a_{k-l-1}^{(\alpha)} - a_{k-l}^{(\alpha)}) u^l - a_{k-1}^{(\alpha)} u^0 \Bigg]$$

$$
\begin{aligned}
&= \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}\left[\sum_{k=1}^{n} v^k \sum_{l=1}^{k} a_{k-l}^{(\alpha)} u^l - \sum_{k=0}^{n-1} v^{k+1} \sum_{l=0}^{k} a_{k-l}^{(\alpha)} u^l\right] \\
&= \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}\left[v^n \sum_{l=1}^{n} a_{n-l}^{(\alpha)} u^l + \sum_{k=1}^{n-1}(v^k - v^{k+1}) \sum_{l=1}^{k} a_{k-l}^{(\alpha)} u^l - \sum_{k=0}^{n-1} v^{k+1} a_k^{(\alpha)} u^0\right] \\
&= \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}\left[v^n \sum_{k=1}^{n} a_{n-k}^{(\alpha)} u^k - \tau \sum_{k=1}^{n-1} \frac{v^{k+1} - v^k}{\tau} \sum_{l=1}^{k} a_{k-l}^{(\alpha)} u^l - \sum_{k=0}^{n-1} v^{k+1} a_k^{(\alpha)} u^0\right],
\end{aligned}
$$

thus obtaining the representation needed. □

3. A Difference Scheme

Considering the problem (1.1) we assume, for simplicity, that $V(x) \equiv 0$. Let M and N be positive integers and let $h := (x_r - x_l)/M$, $\tau := T/N$, $x_j := x_l + jh$, $0 \le j \le M$, $t_k := k\tau$, $0 \le k \le N$. We also consider the sets

$$\Omega_h = \{x_j \,|\, 0 \le j \le M\}, \quad \Omega_\tau = \{t_k \,|\, 0 \le k \le N\},$$

and for a grid function $v = (v_0, v_1, \cdots, v_M)$ on Ω_h we introduce the notations

$$
\begin{aligned}
\delta_x v_{j-1/2} &:= \frac{1}{h}\big(v_j - v_{j-1}\big), \quad 1 \le j \le M, \\
\delta_x^2 v_j &:= \frac{1}{h^2}\big(v_{j+1} - 2v_j + v_{j-1}\big), \quad 1 \le j \le M-1.
\end{aligned}
$$

Moreover, if $w = (w^0, w^1, \cdots, w^N)$ is a grid functions on Ω_τ, we set

$$\delta_t w^{k-1/2} := \frac{1}{\tau}\big(w^k - w^{k-1}\big), \quad 1 \le k \le N.$$

Lemma 3.1. *If $g(x) \in C^4[x_{j-1}, x_{j+1}]$, then*

$$g''(x_j) = \frac{1}{h^2}\Big[g(x_{j-1}) - 2g(x_j) + g(x_{j+1})\Big] - \frac{h^2}{6}\int_0^1 \Big[g^{(4)}(x_j - \theta h) + g^{(4)}(x_j + \theta h)\Big](1-\theta)^3 \mathrm{d}\theta.$$

Let us present three numerical differential formulae, which can be derived from Taylor's formula with integral remainder.

Lemma 3.2. *If $g(x) \in C^3[x_0, x_1]$, then*

$$g''(x_0) = \frac{2}{h}\left[\frac{g(x_1) - g(x_0)}{h} - g'(x_0)\right] - h\int_0^1 g'''(x_0 + \theta h)(1-\theta)^2 \mathrm{d}\theta.$$

Lemma 3.3. *If $g(x) \in C^3[x_{M-1}, x_M]$, then*

$$g''(x_M) = \frac{2}{h}\left[g'(x_M) - \frac{g(x_M) - g(x_{M-1})}{h}\right] + h\int_0^1 g'''(x_M - \theta h)(1-\theta)^2 \mathrm{d}\theta.$$

Evaluating (1.5) at the point (x_j, t_k), we obtain the equations

$$\mathrm{i}\,{}_0^C D_t^\alpha u(x_j,t)|_{t=t_k} + u_{xx}(x_j,t_k) = 0, \quad 0 \le j \le M, \quad 1 \le k \le N. \tag{3.1}$$

Let us now consider the residues

$$(R_h)_j^k = u_{xx}(x_j,t_k) - \delta_x^2 U_j^k, \quad 1 \le j \le M-1, \quad 1 \le k \le N, \tag{3.2}$$

$$(R_h)_0^k = u_{xx}(x_0,t_k) - \frac{2}{h}\Big[\delta_x U_{1/2}^k - u_x(x_0,t_k)\Big], \quad 1 \le k \le N, \tag{3.3}$$

$$(R_h)_M^k = u_{xx}(x_M,t_k) - \frac{2}{h}\Big[u_x(x_M,t_k) - \delta_x U_{M-1/2}^k\Big], \quad 1 \le k \le N, \tag{3.4}$$

where

$$U_j^k := u(x_j,t_k), \quad 0 \le j \le M, \quad 0 \le k \le N.$$

It follows from Lemmas 3.1, 3.2 and 3.3 that

$$\begin{aligned}(R_h)_j^k = \frac{h^2}{6}\int_0^1 \Big[u_{xxxx}(x_j-\theta h,t_k) + u_{xxxx}(x_j+\theta h,t_k)\Big](1-\theta)^3 \mathrm{d}\theta,\\ 1 \le j \le M-1, \quad 1 \le k \le N,\end{aligned} \tag{3.5}$$

$$(R_h)_0^k = h\int_0^1 u_{xxx}(x_0+\theta h,t_k)(1-\theta)^2 \mathrm{d}\theta, \quad 1 \le k \le N, \tag{3.6}$$

$$(R_h)_M^k = -h\int_0^1 u_{xxx}(x_M-\theta h,t_k)(1-\theta)^2 \mathrm{d}\theta, \quad 1 \le k \le N. \tag{3.7}$$

The Eqs. (3.2), (3.3) and (3.4) can be written as

$$u_{xx}(x_j,t_k) = \delta_x^2 U_j^k + (R_h)_j^k, \quad 1 \le j \le M-1, \quad 1 \le k \le N, \tag{3.8}$$

$$u_{xx}(x_0,t_k) = \frac{2}{h}\Big[\delta_x U_{1/2}^k - u_x(x_0,t_k)\Big] + (R_h)_0^k, \quad 1 \le k \le N, \tag{3.9}$$

$$u_{xx}(x_M,t_k) = \frac{2}{h}\Big[u_x(x_M,t_k) - \delta_x U_{M-1/2}^k\Big] + (R_h)_M^k, \quad 1 \le k \le N. \tag{3.10}$$

Let us also consider the residues $(R_\tau)_j^k$, $(\hat{R}_\tau)_0^k$ and $(\hat{R}_\tau)_M^k$ defined by

$${}_0^C D_t^\alpha u(x_j,t)|_{t=t_k} = {}_0^C \mathbb{D}_t^\alpha U_j^k + (R_\tau)_j^k, \quad 0 \le j \le M, \quad 1 \le k \le N, \tag{3.11}$$

$${}_0^C D_t^{\alpha/2} u(x_0,t)|_{t=t_k} = {}_0^C \mathbb{D}_t^{\alpha/2} U_0^k + (\hat{R}_\tau)_0^k, \quad 1 \le k \le N, \tag{3.12}$$

$${}_0^C D_t^{\alpha/2} u(x_M,t)|_{t=t_k} = {}_0^C \mathbb{D}_t^{\alpha/2} U_M^k + (\hat{R}_\tau)_M^k, \quad 1 \le k \le N. \tag{3.13}$$

Taking into account Lemma 2.1, we estimate them as

$$\Big|(R_\tau)_j^k\Big| \le c_0 \max_{t_0 \le t \le t_k} \Big|u_{tt}(x_j,t)\Big|\, \tau^{2-\alpha}, \quad 0 \le j \le M, \quad 1 \le k \le N, \tag{3.14}$$

$$\frac{1}{\tau}\Big|(R_\tau)_j^k-(R_\tau)_j^{k-1}\Big|\le c_1\max_{t_0\le t\le t_1}|u_{tt}(x_j,t)|\frac{\tau^2}{t_k^{1+\alpha}}+c_2\max_{t_0\le t\le t_k}|u_{ttt}(x_j,t)|\tau^{2-\alpha},\quad 0\le j\le M,\quad 2\le k\le N, \tag{3.15}$$

$$\Big|(\hat{R}_\tau)_s^k\Big|\le c_0\max_{t_0\le t\le t_n}|u_{tt}(x_s,t)|\,\tau^{2-\alpha/2},\quad 1\le k\le N,\quad s=0,M, \tag{3.16}$$

$$\frac{1}{\tau}\Big|(\hat{R}_\tau)_s^k-(\hat{R}_\tau)_s^{k-1}\Big|\le c_1\max_{t_0\le t\le t_1}|u_{tt}(x_s,t)|\frac{\tau^2}{t_k^{1+\alpha/2}}+c_2\max_{t_0\le t\le t_k}|u_{ttt}(x_s,t)|\tau^{2-\alpha/2},\quad 2\le k\le N,\quad s=0,M. \tag{3.17}$$

Next we consider the second derivative u_{xx} at the boundary grid points. It follows from (3.9), (1.6) and (3.12) that

$$\begin{aligned}
u_{xx}(x_0,t_k)&=\frac{2}{h}\Big[\delta_xU_{1/2}^k-u_x(x_0,t_k)\Big]+(R_h)_0^k\\
&=\frac{2}{h}\Big[\delta_xU_{1/2}^k-\mathrm{e}^{-\mathrm{i}\pi/4}{}_0^CD_t^{\alpha/2}u(x_0,t)|_{t=t_k}\Big]+(R_h)_0^k\\
&=\frac{2}{h}\Big[\delta_xU_{1/2}^k-\mathrm{e}^{-\mathrm{i}\pi/4}\big({}_0^C\mathbb{D}_t^{\alpha/2}U_0^k+(\hat{R}_\tau)_0^k\big)\Big]+(R_h)_0^k\\
&=\frac{2}{h}\Big[\delta_xU_{1/2}^k-\mathrm{e}^{-\mathrm{i}\pi/4}\big({}_0^C\mathbb{D}_t^{\alpha/2}U_0^k\big)\Big]-\frac{2}{h}\mathrm{e}^{-\mathrm{i}\pi/4}(\hat{R}_\tau)_0^k\\
&\quad+(R_h)_0^k,\quad 1\le k\le N.
\end{aligned} \tag{3.18}$$

Analogously, the representations (3.10), (1.7), (3.13) imply

$$\begin{aligned}
u_{xx}(x_M,t_k)&=\frac{2}{h}\Big[-\mathrm{e}^{-\mathrm{i}\pi/4}{}_0^CD_t^{\alpha/2}u(x_M,t)_{t=t_k}-\delta_xU_{M-1/2}^k\Big]+(R_h)_M^k\\
&=\frac{2}{h}\Big[-\mathrm{e}^{-\mathrm{i}\pi/4}\big({}_0^C\mathbb{D}_t^{\alpha/2}U_M^k+(\hat{R}_\tau)_M^k\big)-\delta_xU_{M-1/2}^k\Big]+(R_h)_M^k\\
&=\frac{2}{h}\Big[-\mathrm{e}^{-\mathrm{i}\pi/4}\big({}_0^C\mathbb{D}_t^{\alpha/2}U_M^k\big)-\delta_xU_{M-1/2}^k\Big]-\frac{2}{h}\mathrm{e}^{-\mathrm{i}\pi/4}(\hat{R}_\tau)_M^k\\
&\quad+(R_h)_M^k,\quad 1\le k\le N.
\end{aligned} \tag{3.19}$$

Now setting $j=1,2,\cdots,M-1$, we substitute (3.11) and (3.8) into (3.1) and obtain

$$\mathrm{i}\,{}_0^C\mathbb{D}_t^{\alpha}U_j^k+\delta_x^2U_j^k=T_j^k,\quad 1\le j\le M-1,\quad 1\le k\le N, \tag{3.20}$$

where

$$T_j^k=-\mathrm{i}(R_\tau)_j^k-(R_h)_j^k,\quad 1\le j\le M-1,\quad 1\le k\le N.$$

Then taking $j=0$, we substitute (3.11) and (3.18) into (3.1), so that

$$\mathrm{i}\,{}_0^C\mathbb{D}_t^{\alpha}U_0^k+\frac{2}{h}\big[\delta_xU_{1/2}^k-\mathrm{e}^{-\mathrm{i}\pi/4}{}_0^C\mathbb{D}_t^{\alpha/2}U_0^k\big]=T_0^k+\hat{T}_0^k,\quad 1\le k\le N, \tag{3.21}$$

where

$$T_0^k=-\mathrm{i}\,(R_\tau)_0^k,\quad \hat{T}_0^k=\frac{2}{h}\mathrm{e}^{-\mathrm{i}\pi/4}(\hat{R}_\tau)_0^k-(R_h)_0^k,\quad 1\le k\le N.$$

Finally for $j=M$, we substitute (3.11) and (3.19) into (3.1), thus obtaining the representation

$$\mathrm{i}\,{}_0^C\mathbb{D}_t^{\alpha}U_M^k+\frac{2}{h}\Big[-\mathrm{e}^{-\mathrm{i}\pi/4}{}_0^C\mathbb{D}_t^{\alpha/2}U_M^k-\delta_xU_{M-1/2}^k\Big]=T_M^k+\hat{T}_M^k,\quad 1\le k\le N,\tag{3.22}$$

where

$$T_M^k=-\mathrm{i}(R_\tau)_M^k,\quad \hat{T}_M^k=\frac{2}{h}\,\mathrm{e}^{-\mathrm{i}\pi/4}(\hat{R}_\tau)_M^k-(R_h)_M^k,\quad 1\le k\le N.$$

Let us also note that the initial condition (1.8) implies

$$U_j^0=\psi(x_j),\quad 0\le j\le M.\tag{3.23}$$

On the other hand, according to the representations (3.5)-(3.6) and inequalities (3.14)-(3.17), there are constants c_3 and c_4 such that

$$|T_j^k|\le c_3\left(\tau^{2-\alpha}+h^2\right),\quad 1\le j\le M-1,\quad 1\le k\le N,\tag{3.24}$$

$$|\delta_tT_j^{k-1/2}|\le c_4\left(\frac{\tau^2}{t_k^{1+\alpha}}+\tau^{2-\alpha}+h^2\right),\quad 1\le j\le M-1,\quad 2\le k\le N,\tag{3.25}$$

$$|T_s^k|\le c_3\tau^{2-\alpha},\quad 1\le k\le N,\quad s=0,M,\tag{3.26}$$

$$|\delta_tT_s^{k-1/2}|\le c_4\left(\frac{\tau^2}{t_k^{1+\alpha}}+\tau^{2-\alpha}\right),\quad 2\le k\le N,\quad s=0,M,\tag{3.27}$$

$$|\hat{T}_s^k|\le c_3\left(\frac{\tau^{2-\alpha/2}}{h}+h\right),\quad 1\le k\le N,\quad s=0,M,\tag{3.28}$$

$$|\delta_t\hat{T}_s^{k-1/2}|\le c_4\left[\frac{1}{h}\left(\frac{\tau^2}{t_k^{1+\alpha/2}}+\tau^{2-\alpha/2}\right)+h\right],\quad 2\le k\le N\quad s=0,M,\tag{3.29}$$

where

$$\delta_tT_j^{k-1/2}=\frac{1}{\tau}\left(T_j^k-T_j^{k-1}\right),\quad \delta_t\hat{T}_0^{k-1/2}=\frac{1}{\tau}\left(\hat{T}_0^k-\hat{T}_0^{k-1}\right),\quad \delta_t\hat{T}_M^{k-1/2}=\frac{1}{\tau}\left(\hat{T}_M^k-\hat{T}_M^{k-1}\right).$$

Let u_j^k be an approximation of U_j^k. Dropping small terms in (3.20)-(3.23), we arrive at the following difference scheme for the problem (1.5)-(1.8):

$$\mathrm{i}\,{}_0^C\mathbb{D}_t^{\alpha}u_j^k+\delta_x^2u_j^k=0,\quad 1\le j\le M-1,\quad 1\le k\le N,\tag{3.30}$$

$$\mathrm{i}\,{}_0^C\mathbb{D}_t^{\alpha}u_0^k+\frac{2}{h}\Big[\delta_xu_{1/2}^k-\mathrm{e}^{-\mathrm{i}\pi/4}{}_0^C\mathbb{D}_t^{\alpha/2}u_0^k\Big]=0,\quad 1\le k\le N,\tag{3.31}$$

$$\mathrm{i}\,{}_0^C\mathbb{D}_t^{\alpha}u_M^k+\frac{2}{h}\Big[-\mathrm{e}^{-\mathrm{i}\pi/4}{}_0^C\mathbb{D}_t^{\alpha/2}u_M^k-\delta_xu_{M-1/2}^k\Big]=0,\quad 1\le k\le N,\tag{3.32}$$

$$u_j^0=\psi(x_j),\quad 0\le j\le M.\tag{3.33}$$

4. Convergence Analysis

Let $\mathscr{V}=\{v|v=(v_0,v_1,\cdots,v_M),v_j\in\mathscr{C}\}$ be the space of grid functions on Ω_h, where $\mathscr{C}$ stands for the complex field. We define an inner product and norms by

$$(u,v)=h\Big(\frac{1}{2}u_0\bar{v}_0+\sum_{j=1}^{M-1}u_j\bar{v}_j+\frac{1}{2}u_M\bar{v}_M\Big),\quad \|u\|=(u,u)^{1/2},$$

$$|u|_1=\left(h\sum_{j=1}^{M}|\delta_x u_{j-1/2}|^2\right)^{1/2},\quad \|u\|_\infty=\max_{0\le j\le M}|u_j|.$$

Lemma 4.1. *If $u=(u_0,u_1,\cdots,u_N)$, then for any $\epsilon>0$, the inequality*

$$\|u\|_\infty^2\le\epsilon|u|_1^2+\left(\frac{1}{\epsilon}+\frac{1}{L}\right)\|u\|^2$$

holds, where $L=x_r-x_l$ and x_l,x_r are defined in (1.5).

Theorem 4.1. *Let $\{U_j^k\}$ and $\{u_j^k\}$ be, respectively, the solutions of* (1.5)-(1.8) *and* (3.30)-(3.33) *and let*

$$e_j^k:=U_j^k-u_j^k,\quad 0\le j\le M,\quad 0\le k\le N. \tag{4.1}$$

Then there is a constant c such that

$$\tau\sum_{k=1}^{n}\big(\|e^k\|^2+|e^k|_1^2\big)\le c\big(\tau^{2-\alpha}+h^2\big)^2,\quad 1\le n\le N. \tag{4.2}$$

Proof. Subtracting the Eqs. (3.30)-(3.33) from Eqs. (3.20)-(3.23), respectively, we obtain a system with respect to the error (4.1) — viz.

$$\mathrm{i}\,{}_0^C\mathbb{D}_t^\alpha e_j^k+\delta_x^2e_j^k=T_j^k,\quad 1\le j\le M-1,\quad 1\le k\le N, \tag{4.3}$$

$$\mathrm{i}\,{}_0^C\mathbb{D}_t^\alpha e_0^k+\frac{2}{h}\big[\delta_xe_{1/2}^k-\mathrm{e}^{-\mathrm{i}\pi/4}\,{}_0^C\mathbb{D}_t^{\alpha/2}e_0^k\big]=T_0^k+\hat{T}_0^k,\quad 1\le k\le N, \tag{4.4}$$

$$\mathrm{i}\,{}_0^C\mathbb{D}_t^\alpha e_M^k+\frac{2}{h}\big[-\mathrm{e}^{-\mathrm{i}\pi/4}\,{}_0^C\mathbb{D}_t^{\alpha/2}e_M^k-\delta_xe_{M-1/2}^k\big]=T_M^k+\hat{T}_M^k,\quad 1\le k\le N, \tag{4.5}$$

$$e_j^0=0,\quad 0\le j\le M. \tag{4.6}$$

Multiplying (4.3) by $h\bar{e}_j^k$, (4.4) by $h\bar{e}_0^k/2$, (4.5) by $h\bar{e}_M^k/2$ and summing the results produces the equation

$$\begin{aligned}&\mathrm{i}\big({}_0^C\mathbb{D}_t^\alpha e^k,e^k\big)+(\delta_xe_{1/2}^k)\bar{e}_0^k+h\sum_{j=1}^{M-1}(\delta_x^2e_j^k)\bar{e}_j^k-(\delta_xe_{M-1/2}^k)\bar{e}_M^k\\&\quad-\mathrm{e}^{-\mathrm{i}\pi/4}\big({}_0^C\mathbb{D}_t^{\alpha/2}e_0^k\big)\bar{e}_0^k-\mathrm{e}^{-\mathrm{i}\pi/4}\big({}_0^C\mathbb{D}_t^{\alpha/2}e_M^k\big)\bar{e}_M^k\\&=(T^k,e^k)+\frac{1}{2}h\hat{T}_0^k\bar{e}_0^k+\frac{1}{2}h\hat{T}_M^k\bar{e}_M^k,\quad 1\le k\le N.\end{aligned} \tag{4.7}$$

Since $-\mathrm{e}^{-\mathrm{i}\pi/4}=i\mathrm{e}^{\mathrm{i}\pi/4}$ and

$$(\delta_x e^k_{1/2})\bar{e}^k_0+h\sum_{j=1}^{M-1}(\delta_x^2 e^k_j)\bar{e}^k_j-(\delta_x e^k_{M-1/2})\bar{e}^k_M=-|e^k|_1^2,$$

the Eq. (4.7) implies

$$\begin{aligned}&\mathrm{Re}\Big\{\big({}_0^C\mathbb{D}_t^\alpha e^k,e^k\big)\Big\}+\mathrm{Re}\Big\{\mathrm{e}^{\mathrm{i}\pi/4}\big({}_0^C\mathbb{D}_t^{\alpha/2}e^k_0\big)\bar{e}^k_0\Big\}+\mathrm{Re}\Big\{\mathrm{e}^{\mathrm{i}\pi/4}\big({}_0^C\mathbb{D}_t^{\alpha/2}e^k_M\big)\bar{e}^k_M\Big\}\\&=\mathrm{Im}\Big\{\big(T^k,e^k\big)+\frac{1}{2}h\hat{T}^k_0\bar{e}^k_0+\frac{1}{2}h\hat{T}^k_M\bar{e}^k_M\Big\},\quad 1\le k\le N.\end{aligned}\tag{4.8}$$

Summing up for k from 1 to n, we obtain

$$\begin{aligned}&\mathrm{Re}\Big\{\tau\sum_{k=1}^n\big({}_0^C\mathbb{D}_t^\alpha e^k,e^k\big)\Big\}+\mathrm{Re}\Big\{\tau\mathrm{e}^{\mathrm{i}\pi/4}\sum_{k=1}^n\big({}_0^C\mathbb{D}_t^{\alpha/2}e^k_0\big)\bar{e}^k_0\Big\}+\mathrm{Re}\Big\{\tau\mathrm{e}^{\mathrm{i}\pi/4}\sum_{k=1}^n\big({}_0^C\mathbb{D}_t^{\alpha/2}e^k_M\big)\bar{e}^k_M\Big\}\\&=\mathrm{Im}\Big\{\tau\sum_{k=1}^n\Big[(T^k,e^k)+\frac{1}{2}h\hat{T}^k_0\bar{e}^k_0+\frac{1}{2}h\hat{T}^k_M\bar{e}^k_M\Big]\Big\},\quad 1\le n\le N.\end{aligned}\tag{4.9}$$

Multiplying (4.9) by 2 and applying Lemmas 2.2 and 2.3 leads to the estimate

$$\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^n a^{(\alpha)}_{n-k}\|e^k\|^2\leqslant\mathrm{Im}\Big\{2\tau\sum_{k=1}^n\Big[\big(T^k,e^k\big)+h\hat{T}^k_0\bar{e}^k_0+h\hat{T}^k_M\bar{e}^k_M\Big]\Big\},\quad 1\le n\le N.\tag{4.10}$$

On the other hand, if we multiply (4.3) by $-h\overline{{}_0^C\mathbb{D}_t^\alpha e^k_j}$, (4.4) by $-h\overline{{}_0^C\mathbb{D}_t^\alpha e^k_0}/2$, (4.5) by $-h\overline{{}_0^C\mathbb{D}_t^\alpha e^k_M}/2$ and sum up the results, we obtain the equation

$$\begin{aligned}&-\mathrm{i}\big\|{}_0^C\mathbb{D}_t^\alpha e^k\big\|^2-\big(\delta_x e^k_{1/2}\big)\overline{{}_0^C\mathbb{D}_t^\alpha e^k_0}-h\sum_{j=1}^{M-1}\big(\delta_x^2 e^k_j\big)\overline{{}_0^C\mathbb{D}_t^\alpha e^k_j}+\big(\delta_x e^k_{M-1/2}\big)\overline{{}_0^C\mathbb{D}_t^\alpha e^k_M}\\&+\mathrm{e}^{-\mathrm{i}\pi/4}\big({}_0^C\mathbb{D}_t^{\alpha/2}e^k_0\big)\overline{{}_0^C\mathbb{D}_t^\alpha e^k_0}+\mathrm{e}^{-\mathrm{i}\pi/4}\big({}_0^C\mathbb{D}_t^{\alpha/2}e^k_M\big)\overline{{}_0^C\mathbb{D}_t^\alpha e^k_M}\\&=-\big(T^k,{}_0^C\mathbb{D}_t^\alpha e^k\big)-\frac{1}{2}h\hat{T}^k_0\overline{{}_0^C\mathbb{D}_t^\alpha e^k_0}-\frac{1}{2}h\hat{T}^k_M\overline{{}_0^C\mathbb{D}_t^\alpha e^k_M},\quad 1\le k\le N.\end{aligned}\tag{4.11}$$

Observing that

$$\begin{aligned}&-\big(\delta_x e^k_{1/2}\big)\overline{{}_0^C\mathbb{D}_t^\alpha e^k_0}-h\sum_{j=1}^{M-1}\big(\delta_x^2 e^k_j\big)\overline{{}_0^C\mathbb{D}_t^\alpha e^k_j}+\big(\delta_x e^k_{M-1/2}\big)\overline{{}_0^C\mathbb{D}_t^\alpha e^k_M}\\&=h\sum_{j=0}^{M-1}\big({}_0^C\mathbb{D}_t^\alpha\delta_x e^k_{j+1/2}\big)\big(\delta_x\bar{e}^k_{j+1/2}\big),\end{aligned}$$

we sum up the real parts of (4.11) in $k=1,2,\cdots,n$ so that

$$2\tau\mathrm{Re}\Big\{h\sum_{j=0}^{M-1}\sum_{k=1}^n\big({}_0^C\mathbb{D}_t^\alpha\delta_x e^k_{j+1/2}\big)\big(\delta_x\bar{e}^k_{j+1/2}\big)\Big\}+2\tau\mathrm{Re}\Big\{\mathrm{e}^{\mathrm{i}\pi/4}\sum_{k=1}^n\big({}_0^C\mathbb{D}_t^\alpha e^k_0\big)\overline{{}_0^C\mathbb{D}_t^{\alpha/2}e^k_0}\Big\}$$

$$+2\tau\mathrm{Re}\Big\{\mathrm{e}^{\mathrm{i}\pi/4}\sum_{k=1}^{n}\big({}_0^C\mathbb{D}_t^\alpha e_M^k\big)\overline{{}_0^C\mathbb{D}_t^{\alpha/2}e_M^k}\Big\}$$
$$=2\tau\mathrm{Re}\Big\{\sum_{k=1}^{n}\Big[-\big({}_0^C\mathbb{D}_t^\alpha e^k,T^k\big)-\frac{1}{2}h\overline{\hat{T}_0^k}\,{}_0^C\mathbb{D}_t^\alpha e_0^k-\frac{1}{2}h\overline{\hat{T}_M^k}\,{}_0^C\mathbb{D}_t^\alpha e_M^k\Big]\Big\},\quad 1\le n\le N. \tag{4.12}$$

It follows from Lemmas 2.2 and 2.5 that

$$2\tau\mathrm{Re}\Big\{h\sum_{j=0}^{M-1}\sum_{k=1}^{n}\big({}_0^C\mathbb{D}_t^\alpha\delta_x e_{j+1/2}^k\big)\big(\delta_x\bar{e}_{j+1/2}^k\big)\Big\}\ge\frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}\tau\sum_{k=1}^{n}a_{n-k}^{(\alpha)}|e^k|_1^2, \tag{4.13}$$
$$\mathrm{Re}\Big\{\mathrm{e}^{\mathrm{i}\pi/4}\sum_{k=1}^{n}\big({}_0^C\mathbb{D}_t^\alpha e_0^k\big)\overline{{}_0^C\mathbb{D}_t^{\alpha/2}e_0^k}\Big\}\ge 0,\quad \mathrm{Re}\Big\{\mathrm{e}^{\mathrm{i}\pi/4}\sum_{k=1}^{n}\big({}_0^C\mathbb{D}_t^\alpha e_M^k\big)\overline{{}_0^C\mathbb{D}_t^{\alpha/2}e_M^k}\Big\}\ge 0. \tag{4.14}$$

Moreover, according to Lemma 2.6 and (3.24)-(3.29) the right-hand side of the Eq. (4.12) can be estimated as follows

$$\sum_{k=1}^{n}\bar{T}_j^k\big({}_0^C\mathbb{D}_t^\alpha e_j^k\big)=\frac{\tau^{-\alpha}}{\Gamma(2-\alpha)}\Big[\bar{T}_j^n\sum_{k=1}^{n}a_{n-k}^{(\alpha)}e_j^k-\tau\sum_{k=1}^{n-1}\delta_t\bar{T}_j^{k+1/2}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}e_j^l-\sum_{k=0}^{n-1}a_k^{(\alpha)}\bar{T}_j^{k+1}e_j^0\Big].$$

Therefore,

$$\begin{aligned}
&2\tau\Big|\sum_{k=1}^{n}\bar{T}_j^k\big({}_0^C\mathbb{D}_t^\alpha e_j^k\big)\Big|\\
\le&\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\Big[\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\Big(\epsilon_1|e_j^k|^2+\frac{1}{\epsilon_1}|T_j^n|^2\Big)+2\tau\sum_{k=1}^{n-1}\Big(\sum_{l=1}^{k}a_{k-l}^{(\alpha)}e_j^l\Big)\delta_t T_j^{k+1/2}\Big]\\
\le&\epsilon_1\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}|e_j^k|^2+\frac{1}{\epsilon_1}\cdot\frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)}|T_j^n|^2\\
&+2\max_{1\le k\le n-1}\Big\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\Big|\sum_{l=1}^{k}a_{k-l}^{(\alpha)}e_j^l\Big|\Big\}\Big(\tau\sum_{k=1}^{n-1}\Big|\delta_t T_j^{k+1/2}\Big|\Big)\\
\leqslant&\epsilon_1\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}|e_j^k|^2+\frac{1}{\epsilon_1}\cdot\frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)}|T_j^n|^2\\
&+\epsilon_2\Big(\max_{1\le k\le n-1}\Big\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\Big|\sum_{l=1}^{k}a_{k-l}^{(\alpha)}e_j^l\Big|\Big\}\Big)^2+\frac{1}{\epsilon_2}\Big(\tau\sum_{k=1}^{n-1}\Big|\delta_t T_j^{k+1/2}\Big|\Big)^2\\
\leqslant&\epsilon_1\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}|e_j^k|^2+\frac{1}{\epsilon_1}\cdot\frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)}|T_j^n|^2\\
&+\epsilon_2\max_{1\le k\le n-1}\Big\{\Big(\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\Big)\Big(\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}|e_j^l|^2\Big)\Big\}+\frac{1}{\epsilon_2}\Big(\tau\sum_{k=1}^{n-1}\Big|\delta_t T_j^{k+1/2}\Big|\Big)^2
\end{aligned}$$

$$\leqslant \epsilon_1 \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{k=1}^{n} a_{n-k}^{(\alpha)} |e_j^k|^2 + \frac{1}{\epsilon_1} \cdot \frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)} |T_j^n|^2$$
$$+ \epsilon_2 \frac{t_{n-1}^{1-\alpha}}{\Gamma(2-\alpha)} \max_{1\le k\le n-1} \left\{ \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{l=1}^{k} a_{k-l}^{(\alpha)} |e_j^l|^2 \right\} + \frac{1}{\epsilon_2} \left(\tau \sum_{k=1}^{n-1} \left| \delta_t T_j^{k+1/2} \right| \right)^2. \tag{4.15}$$

If we introduce the weights

$$w_j := \begin{cases} 1, & 1 \le j \le M-1, \\ 1/2, & j = 0, M, \end{cases}$$

then the inequality (4.15) implies

$$2\tau \left| \mathrm{Re} \left\{ \sum_{k=1}^{n} \left({}_0^C\mathbb{D}_t^\alpha e^k, T^k \right) \right\} \right|$$
$$\le \epsilon_1 \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{k=1}^{n} a_{n-k}^{(\alpha)} \|e^k\|^2 + \frac{1}{\epsilon_1} \cdot \frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)} \|T^n\|^2$$
$$+ \epsilon_2 \frac{t_{n-1}^{1-\alpha}}{\Gamma(2-\alpha)} \max_{1\le k\le n-1} \left\{ \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{l=1}^{k} a_{k-l}^{(\alpha)} \|e^l\|^2 \right\} + \frac{1}{\epsilon_2} h \sum_{j=0}^{M} w_j \left(\tau \sum_{k=1}^{n-1} \left| \delta_t T_j^{k+1/2} \right| \right)^2. \tag{4.16}$$

Analogous considerations lead to the estimates

$$2\tau \left| \mathrm{Re} \left\{ \sum_{k=1}^{n} h \overline{\hat{T}_0^k} \, {}_0^C\mathbb{D}_t^\alpha e_0^k \right\} \right|$$
$$\le \epsilon_3 \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{k=1}^{n} a_{n-k}^{(\alpha)} |e_0^k|^2 + \frac{1}{\epsilon_3} \cdot \frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)} |h \hat{T}_0^n|^2$$
$$+ \epsilon_4 \frac{t_{n-1}^{1-\alpha}}{\Gamma(2-\alpha)} \max_{1\le k\le n-1} \left\{ \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{l=1}^{k} a_{k-l}^{(\alpha)} |e_0^l|^2 \right\} + \frac{1}{\epsilon_4} \left(\tau \sum_{k=1}^{n-1} \left| h \delta_t \hat{T}_0^{k+1/2} \right| \right)^2, \quad 1 \le n \le N, \tag{4.17}$$

and

$$2\tau \left| \mathrm{Re} \left\{ \sum_{k=1}^{n} h \overline{\hat{T}_M^k} \, {}_0^C\mathbb{D}_t^\alpha e_M^k \right\} \right| \le \epsilon_3 \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{k=1}^{n} a_{n-k}^{(\alpha)} |e_M^k|^2 + \frac{1}{\epsilon_3} \cdot \frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)} |h \hat{T}_M^n|^2$$
$$+ \epsilon_4 \frac{t_{n-1}^{1-\alpha}}{\Gamma(2-\alpha)} \max_{1\le k\le n-1} \left\{ \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{l=1}^{k} a_{k-l}^{(\alpha)} |e_M^l|^2 \right\} + \frac{1}{\epsilon_4} \left(\tau \sum_{k=1}^{n-1} \left| h \delta_t \hat{T}_M^{k+1/2} \right| \right)^2, \quad 1 \le n \le N. \tag{4.18}$$

We now use inequalities (4.13), (4.14), (4.16), (4.17), (4.18) in Eq. (4.12) thus obtaining

$$\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{k=1}^{n} a_{n-k}^{(\alpha)} |e^k|_1^2 \le \epsilon_1 \frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)} \sum_{k=1}^{n} a_{n-k}^{(\alpha)} \|e^k\|^2 + \frac{1}{\epsilon_1} \cdot \frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)} \|T^n\|^2$$

$$
\begin{aligned}
&+\epsilon_2\frac{t_{n-1}^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le n-1}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\|e^l\|^2\right\}+\frac{1}{\epsilon_2}h\sum_{j=0}^{M}w_j\left(\tau\sum_{k=1}^{n-1}\left|\delta_t T_j^{k+1/2}\right|\right)^2\\
&+\epsilon_3\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\frac{|e_0^k|^2+|e_M^k|^2}{2}+\frac{1}{\epsilon_3}\cdot\frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)}\frac{|h\hat{T}_0^n|^2+|h\hat{T}_M^n|^2}{2}\\
&+\epsilon_4\frac{t_{n-1}^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le n-1}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\frac{|e_0^l|^2+|e_M^l|^2}{2}\right\}\\
&+\frac{1}{2\epsilon_4}\left[\left(\tau\sum_{k=1}^{n-1}\left|h\delta_t\hat{T}_0^{k+1/2}\right|\right)^2+\left(\tau\sum_{k=1}^{n-1}\left|h\delta_t\hat{T}_M^{k+1/2}\right|\right)^2\right]\\
\le\ &\epsilon_1\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\|e^k\|^2+\frac{1}{\epsilon_1}\cdot\frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)}\|T^n\|^2\\
&+\epsilon_2\frac{t_{n-1}^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le n-1}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\|e^l\|^2\right\}+\frac{1}{\epsilon_2}h\sum_{j=0}^{M}w_j\left(\tau\sum_{k=1}^{n-1}\left|\delta_t T_j^{k+1/2}\right|\right)^2\\
&+\epsilon_3\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\|e^k\|_\infty^2+\frac{1}{\epsilon_3}\cdot\frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)}\frac{|h\hat{T}_0^n|^2+|h\hat{T}_M^n|^2}{2}\\
&+\epsilon_4\frac{t_{n-1}^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le n-1}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\|e^l\|_\infty^2\right\}\\
&+\frac{1}{2\epsilon_4}\left[\left(\tau\sum_{k=1}^{n-1}\left|h\delta_t\hat{T}_0^{k+1/2}\right|\right)^2+\left(\tau\sum_{k=1}^{n-1}\left|h\delta_t\hat{T}_M^{k+1/2}\right|\right)^2\right],\quad 1\le n\le N. \qquad (4.19)
\end{aligned}
$$

On the other hand, the relation (4.10) shows that

$$
\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\|e^k\|^2 \qquad (4.20)
$$

$$
\begin{aligned}
\le\ &\tau\sum_{k=1}^{n}\left(\frac{\epsilon_1 a_{n-k}^{(\alpha)}}{\tau^\alpha\Gamma(2-\alpha)}\|e^k\|^2+\frac{\tau^\alpha\Gamma(2-\alpha)}{\epsilon_1 a_{n-k}^{(\alpha)}}\|T^k\|^2\right)\\
&+\tau\sum_{k=1}^{n}\left(\frac{\epsilon_3 a_{n-k}^{(\alpha)}}{2\tau^\alpha\Gamma(2-\alpha)}\left|e_0^k\right|^2+\frac{\tau^\alpha\Gamma(2-\alpha)}{2\epsilon_3 a_{n-k}^{(\alpha)}}\left|h\hat{T}_0^k\right|^2+\frac{\epsilon_3 a_{n-k}^{(\alpha)}}{2\tau^\alpha\Gamma(2-\alpha)}\left|e_M^k\right|^2+\frac{\tau^\alpha\Gamma(2-\alpha)}{2\epsilon_3 a_{n-k}^{(\alpha)}}\left|h\hat{T}_M^k\right|^2\right)\\
\le\ &\epsilon_1\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\|e^k\|^2+\frac{\Gamma(2-\alpha)}{\epsilon_1}\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\|T^k\|^2\\
&+\epsilon_3\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\|e^k\|_\infty^2+\frac{\Gamma(2-\alpha)}{2\epsilon_3}\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\left(\left|h\hat{T}_0^k\right|^2+\left|h\hat{T}_M^k\right|^2\right),\quad 1\le n\le N,
\end{aligned}
$$

(4.21)

and adding the inequalities (4.19) and (4.21) to each other, we obtain

$$
\begin{aligned}
&\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\left(\|e^k\|^2+|e^k|_1^2\right)\\
\le\,&\epsilon_1\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\|e^k\|^2+\frac{1}{\epsilon_1}\cdot\frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)}\|T^n\|^2\\
&+\epsilon_2\frac{t_{n-1}^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le n-1}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\|e^l\|^2\right\}+\frac{1}{\epsilon_2}h\sum_{j=0}^{M}w_j\left(\tau\sum_{k=1}^{n-1}\left|\delta_t T_j^{k+1/2}\right|\right)^2\\
&+\epsilon_3\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\|e^k\|_\infty^2+\frac{1}{\epsilon_3}\cdot\frac{t_n^{1-\alpha}}{\Gamma(2-\alpha)}\frac{|h\hat{T}_0^n|^2+|h\hat{T}_M^n|^2}{2}\\
&+\epsilon_4\frac{t_{n-1}^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le n-1}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\|e^l\|_\infty^2\right\}\\
&+\frac{1}{2\epsilon_4}\left[\left(\tau\sum_{k=1}^{n-1}\left|h\delta_t\hat{T}_0^{k+1/2}\right|\right)^2+\left(\tau\sum_{k=1}^{n-1}\left|h\delta_t\hat{T}_M^{k+1/2}\right|\right)^2\right]\\
&+\epsilon_1\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\|e^k\|^2+\frac{\Gamma(2-\alpha)}{\epsilon_1}\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\|T^k\|^2\\
&+\epsilon_3\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\|e^k\|_\infty^2+\frac{\Gamma(2-\alpha)}{2\epsilon_3}\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\left(\left|h\hat{T}_0^k\right|^2+\left|h\hat{T}_M^k\right|^2\right),\quad 1\le n\le N.
\end{aligned}
$$

Now we can use Lemma 4.1, so that

$$
\begin{aligned}
&\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\left(\|e^k\|^2+|e^k|_1^2\right)\\
\le\,&\frac{2\epsilon_1\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\|e^k\|^2+\frac{2\epsilon_3\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\left[\epsilon_5|e^k|_1^2+\left(\frac{1}{\epsilon_5}+\frac{1}{L}\right)\|e^k\|^2\right]\\
&+\epsilon_2\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le n-1}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\|e^l\|^2\right\}\\
&+\epsilon_4\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le n-1}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\left[\epsilon_6|e^l|_1^2+\left(\frac{1}{\epsilon_6}+\frac{1}{L}\right)\|e^l\|^2\right]\right\}\\
&+\frac{1}{\epsilon_1}\cdot\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\|T^n\|^2+\frac{1}{\epsilon_2}h\sum_{j=0}^{M}w_j\left(\tau\sum_{k=1}^{n-1}\left|\delta_t T_j^{k+1/2}\right|\right)^2+\frac{1}{\epsilon_3}\cdot\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\frac{|h\hat{T}_0^n|^2+|h\hat{T}_M^n|^2}{2}\\
&+\frac{1}{2\epsilon_4}\left[\left(\tau\sum_{k=1}^{n-1}\left|h\delta_t\hat{T}_0^{k+1/2}\right|\right)^2+\left(\tau\sum_{k=1}^{n-1}\left|h\delta_t\hat{T}_M^{k+1/2}\right|\right)^2\right]+\frac{\Gamma(2-\alpha)}{\epsilon_1}\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\|T^k\|^2
\end{aligned}
$$

$$+\frac{\Gamma(2-\alpha)}{2\epsilon_3}\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\Big(\big|h\hat{T}_0^k\big|^2+\big|h\hat{T}_M^k\big|^2\Big),\quad 1\le n\le N. \tag{4.22}$$

Choosing the parameters ϵ_1, ϵ_3 and ϵ_5 as

$$\epsilon_1=\frac{1}{8},\quad \epsilon_3=\frac{1}{8}\left(\sqrt{2+\frac{1}{L^2}}-\frac{1}{L}\right),\quad \epsilon_5=\sqrt{2+\frac{1}{L^2}}+\frac{1}{L},$$

we note that

$$2\epsilon_1=\frac{1}{4},\quad 2\epsilon_3\epsilon_5=1/2,\quad 2\epsilon_3(\frac{1}{\epsilon_5}+\frac{1}{L})=\frac{1}{4}.$$

For such a choice of parameters, the inequality (4.22) takes the form

$$\begin{aligned}
&\frac{1}{2}\cdot\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\big(\|e^k\|^2+|e^k|_1^2\big)\\
\le\,&\epsilon_2\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le n-1}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\|e^l\|^2\right\}\\
&+\epsilon_4\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le n-1}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\left[\epsilon_6|e^l|_1^2+\Big(\frac{1}{\epsilon_6}+\frac{1}{L}\Big)\|e^l\|^2\right]\right\}\\
&+\frac{1}{\epsilon_1}\cdot\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\|T^n\|^2+\frac{1}{\epsilon_2}h\sum_{j=0}^{M}w_j\left(\tau\sum_{k=1}^{n-1}\left|\delta_tT_j^{k+1/2}\right|\right)^2\\
&+\frac{1}{\epsilon_3}\cdot\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\frac{|h\hat{T}_0^n|^2+|h\hat{T}_M^n|^2}{2}+\frac{1}{2\epsilon_4}\left[\left(\tau\sum_{k=1}^{n-1}\left|h\delta_t\hat{T}_0^{k+1/2}\right|\right)^2+\left(\tau\sum_{k=1}^{n-1}\left|h\delta_t\hat{T}_M^{k+1/2}\right|\right)^2\right]\\
&+\frac{\Gamma(2-\alpha)}{\epsilon_1}\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\|T^k\|^2+\frac{\Gamma(2-\alpha)}{2\epsilon_3}\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\Big(\big|h\hat{T}_0^k\big|^2+\big|h\hat{T}_M^k\big|^2\Big),\quad 1\le n\le N,
\end{aligned}$$

which yields that

$$\begin{aligned}
&\frac{1}{2}\cdot\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\big(\|e^k\|^2+|e^k|_1^2\big)\\
\le\,&\epsilon_2\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le m}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\|e^l\|^2\right\}\\
&+\epsilon_4\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le m}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\left[\epsilon_6|e^l|_1^2+\Big(\frac{1}{\epsilon_6}+\frac{1}{L}\Big)\|e^l\|^2\right]\right\}\\
&+\frac{1}{\epsilon_1}\cdot\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le n\le m}\|T^n\|^2+\frac{1}{\epsilon_2}h\sum_{j=0}^{M}w_j\left(\tau\sum_{k=1}^{m-1}\left|\delta_tT_j^{k+1/2}\right|\right)^2
\end{aligned}$$

$$
\begin{aligned}
&+\frac{1}{\epsilon_3}\cdot\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le n\le m}\frac{|h\hat{T}_0^n|^2+|h\hat{T}_M^n|^2}{2}+\frac{1}{2\epsilon_4}\left[\left(\tau\sum_{k=1}^{m-1}\left|h\delta_t\hat{T}_0^{k+1/2}\right|\right)^2\right.\\
&\left.+\left(\tau\sum_{k=1}^{m-1}\left|h\delta_t\hat{T}_M^{k+1/2}\right|\right)^2\right]+\frac{\Gamma(2-\alpha)}{\epsilon_1}\max_{1\le n\le m}\left\{\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\|T^k\|^2\right\}\\
&+\frac{\Gamma(2-\alpha)}{2\epsilon_3}\max_{1\le n\le m}\left\{\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\Big(\left|h\hat{T}_0^k\right|^2+\left|h\hat{T}_M^k\right|^2\Big)\right\},\quad 1\le n\le m\le N.
\end{aligned}
$$

Consequently, we obtain the estimate

$$
\begin{aligned}
&\frac{1}{2}\cdot\max_{1\le n\le m}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\Big(\|e^k\|^2+|e^k|_1^2\Big)\right\}\\
\le\,&\epsilon_2\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le m}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\|e^l\|^2\right\}\\
&+\epsilon_4\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le k\le m}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{l=1}^{k}a_{k-l}^{(\alpha)}\left[\epsilon_6|e^l|_1^2+\Big(\frac{1}{\epsilon_6}+\frac{1}{L}\Big)\|e^l\|^2\right]\right\}\\
&+\frac{1}{\epsilon_1}\cdot\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le n\le m}\|T^n\|^2+\frac{1}{\epsilon_2}h\sum_{j=0}^{M}w_j\left(\tau\sum_{k=1}^{m-1}\left|\delta_t T_j^{k+1/2}\right|\right)^2\\
&+\frac{1}{\epsilon_3}\cdot\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le n\le m}\frac{|h\hat{T}_0^n|^2+|h\hat{T}_M^n|^2}{2}+\frac{1}{2\epsilon_4}\left[\left(\tau\sum_{k=1}^{m-1}\left|h\delta_t\hat{T}_0^{k+1/2}\right|\right)^2\right.\\
&\left.+\left(\tau\sum_{k=1}^{m-1}\left|h\delta_t\hat{T}_M^{k+1/2}\right|\right)^2\right]+\frac{\Gamma(2-\alpha)}{\epsilon_1}\max_{1\le n\le m}\left\{\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\|T^k\|^2\right\}\\
&+\frac{\Gamma(2-\alpha)}{2\epsilon_3}\max_{1\le n\le m}\left\{\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\Big(\left|h\hat{T}_0^k\right|^2+\left|h\hat{T}_M^k\right|^2\Big)\right\},\quad 1\le m\le N. \qquad (4.23)
\end{aligned}
$$

Setting

$$
\epsilon_2=\frac{\Gamma(2-\alpha)}{8T^{1-\alpha}},\quad \epsilon_4=\frac{\Gamma(2-\alpha)}{8T^{1-\alpha}}\left(\sqrt{2+\frac{1}{L^2}}-\frac{1}{L}\right),\quad \epsilon_6=\sqrt{2+\frac{1}{L^2}}+\frac{1}{L},
$$

we note that

$$
\frac{\epsilon_2T^{1-\alpha}}{\Gamma(2-\alpha)}=\frac{1}{8},\quad \frac{\epsilon_4T^{1-\alpha}}{\Gamma(2-\alpha)}\epsilon_6=\frac{1}{4},\quad \frac{\epsilon_4T^{1-\alpha}}{\Gamma(2-\alpha)}\Big(\frac{1}{\epsilon_6}+\frac{1}{L}\Big)=\frac{1}{8},
$$

and the inequality (4.23) takes the form

$$\frac{1}{4}\cdot\max_{1\le n\le m}\left\{\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\big(\|e^k\|^2+|e^k|_1^2\big)\right\}$$
$$\le\frac{1}{\epsilon_1}\cdot\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le n\le m}\|T^n\|^2+\frac{1}{\epsilon_2}h\sum_{j=0}^{M}w_j\left(\tau\sum_{k=1}^{m-1}\left|\delta_tT_j^{k+1/2}\right|\right)^2$$
$$+\frac{1}{\epsilon_3}\cdot\frac{T^{1-\alpha}}{\Gamma(2-\alpha)}\max_{1\le n\le m}\frac{|h\hat{T}_0^n|^2+|h\hat{T}_M^n|^2}{2}+\frac{1}{2\epsilon_4}\left[\left(\tau\sum_{k=1}^{m-1}\left|h\delta_t\hat{T}_0^{k+1/2}\right|\right)^2\right.$$
$$\left.+\left(\tau\sum_{k=1}^{m-1}\left|h\delta_t\hat{T}_M^{k+1/2}\right|\right)^2\right]+\frac{\Gamma(2-\alpha)}{\epsilon_1}\max_{1\le n\le m}\left\{\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\|T^k\|^2\right\}$$
$$+\frac{\Gamma(2-\alpha)}{2\epsilon_3}\max_{1\le n\le m}\left\{\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\Big(\left|h\hat{T}_0^k\right|^2+\left|h\hat{T}_M^k\right|^2\Big)\right\},\quad 1\le m\le N. \tag{4.24}$$

Now taking into account the estimates (3.24)-(3.29) and the inequalities

$$\sum_{k=1}^{n}\frac{1}{k^s}\le 1+\sum_{k=2}^{n}\int_{k-1}^{k}\frac{1}{x^s}\mathrm{d}x$$
$$=1+\int_1^n\frac{1}{x^s}\mathrm{d}x<1+\int_1^{+\infty}\frac{1}{x^s}\mathrm{d}x=\frac{s}{s-1},\quad\text{when } s>1, \tag{4.25}$$
$$\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}=\tau^{1+\alpha}\sum_{k=0}^{n-1}\frac{1}{a_k^{(\alpha)}}=\tau^{1+\alpha}\sum_{k=0}^{n-1}\frac{1}{(k+1)^{1-\alpha}-k^{1-\alpha}}$$
$$=\tau^{1+\alpha}\sum_{k=0}^{n-1}\frac{1}{(1-\alpha)\int_k^{k+1}x^{-\alpha}\mathrm{d}x}<\frac{\tau^{1+\alpha}}{1-\alpha}\sum_{k=0}^{n-1}\int_k^{k+1}x^{\alpha}\mathrm{d}x$$
$$\le\frac{\tau^{1+\alpha}}{1-\alpha}\int_0^n x^{\alpha}\mathrm{d}x=\frac{\tau^{1+\alpha}n^{1+\alpha}}{1-\alpha^2}=\frac{t_n^{1+\alpha}}{1-\alpha^2}, \tag{4.26}$$

we obtain

$$\|T^n\|^2\le Lc_3^2\big(\tau^{2-\alpha}+h^2\big)^2, \tag{4.27}$$
$$h\sum_{j=0}^{M}w_j\left(\tau\sum_{k=1}^{m-1}\left|\delta_tT_j^{k+1/2}\right|\right)^2$$
$$\le L\left(\tau\sum_{k=1}^{m-1}c_4\Big(\frac{\tau^2}{t_k^{1+\alpha}}+\tau^{2-\alpha}+h^2\Big)\right)^2\le Lc_4^2\Big[(1+\frac{1}{\alpha})\tau^{2-\alpha}+T(\tau^{2-\alpha}+h^2)\Big]^2, \tag{4.28}$$
$$\frac{|h\hat{T}_0^n|^2+|h\hat{T}_M^n|^2}{2}\le c_3^2\big(\tau^{2-\alpha/2}+h^2\big)^2, \tag{4.29}$$

$$
\begin{aligned}
&\left(\tau\sum_{k=1}^{m-1}\left|h\delta_t\hat{T}_0^{k+1/2}\right|\right)^2+\left(\tau\sum_{k=1}^{m-1}\left|h\delta_t\hat{T}_M^{k+1/2}\right|\right)^2\\
\le\,& 2\left[\tau\sum_{k=1}^{m-1}c_4\left(\frac{\tau^2}{t_k^{1+\alpha/2}}+\tau^{2-\alpha/2}+h^2\right)\right]^2\le 2c_4^2\Big[\big(1+\frac{2}{\alpha}\big)\tau^{2-\alpha}+T\big(\tau^{2-\alpha/2}+h^2\big)\Big]^2, \quad (4.30)\\
&\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\|T^k\|^2\le\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\|T^k\|^2\\
\le\,&\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}Lc_3^2\big(\tau^{2-\alpha}+h^2\big)^2\le\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}Lc_3^2\big(\tau^{2-\alpha}+h^2\big)^2\\
\le\,& Lc_3^2\big(\tau^{2-\alpha}+h^2\big)^2\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\le Lc_3^2\frac{1}{1-\alpha^2}t_n^{1+\alpha}\big(\tau^{2-\alpha}+h^2\big)^2, \quad (4.31)\\
&\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}\Big(\big|h\hat{T}_0^k\big|^2+\big|h\hat{T}_M^k\big|^2\Big)\\
\le\,& 2\tau^{1+\alpha}\sum_{k=1}^{n}\frac{1}{a_{n-k}^{(\alpha)}}c_3^2\big(\tau^{2-\alpha/2}+h^2\big)^2\le 2c_3^2\frac{1}{1-\alpha^2}t_n^{1+\alpha}\big(\tau^{2-\alpha/2}+h^2\big)^2. \quad (4.32)
\end{aligned}
$$

Substituting (4.27)-(4.32) into (4.24) shows that there is a constant c_5 such that

$$
\frac{\tau^{1-\alpha}}{\Gamma(2-\alpha)}\sum_{k=1}^{n}a_{n-k}^{(\alpha)}\big(\|e^k\|^2+|e^k|_1^2\big)\le c_5\big(\tau^{2-\alpha}+h^2\big)^2,\quad 1\le n\le N.
$$

This implies the estimate (4.2), thus completing the proof. □

5. Conclusion

Using artificial boundary method, we reformulate the time fractional Schrödinger equation on the real line as a bounded problems with exact ABCs. The problem appeared is solved by a numerical method employing the $L1$-formula for the Caputo derivative and finite differences for spatial derivatives. The convergence of the method studied and optimal error estimates in a special metric are obtained. The technique developed here can be also applied to study the convergence of approximation methods for the standard Schrödinger equation.

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