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Research Paper

The Matrix Transformation Technique for the Time- Space Fractional Linear Schrödinger Equation

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Abstract

This paper deals with a time-space fractional Schrödinger equation with homogeneous Dirichlet boundary conditions. A common strategy for discretizing time-fractional operators is finite difference schemes. In these methods, the time-step size should usually be chosen sufficiently small, and subsequently, too many iterations are required which may be time-consuming. To avoid this issue, we utilize the Laplace transform method in the present work to discretize time-fractional operators. By using the Laplace transform, the equation is converted to some time-independent problems. To solve these problems, matrix transformation and improved matrix transformation techniques are used to approximate the spatial derivative terms which are defined by the spectral fractional Laplacian operator. After solving these stationary equations, the numerical inversion of the Laplace transform is used to obtain the solution of the original equation. The combination of finite difference schemes and the Laplace transform creates an efficient and easy-to-implement method for time-space fractional Schrödinger equations. Finally, some numerical experiments are presented and show the applicability and accuracy of this approach.

1 Introduction

By utilizing fractional order derivatives instead of integer derivatives, the concept of integer derivatives can be extended to model complicated phenomena with nonlocality and long-term

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memory effects [1]. Due to their numerous applications in physics [2], chemistry [3], fluid mechanics, mathematical biology [4, 5], and engineering, fractional differential equations have been analyzed by many scientists for decades [6–8].

The Schrödinger equation, is fundamental in the field of quantum mechanics [9, 10]. It is obtained from path integrals over Brownian paths [11]. These equations also occur in many other realms of physics and chemistry, e.g. optics, plasma physics, chemical and biomolecular product design. To predict associated molecular properties in any quantum chemical calculation, the Schrödinger equation must be solved [12]. Nanni in [13] utilized the Schrödinger equation to investigate proton tunneling dynamics. Authors like Laskin [14, 15], Naber [16], and Achar [17] developed generalizations of quantum mechanics. The Riesz space Schrödinger equation was introduced using the Lévy path integral by Laskin [15] and the Caputo time-fractional Schrödinger equation was studied by Naber [16]. Dong and Xu [18] developed a space-time fractional Schrödinger (TS-FS) equation with Caputo fractional and the quantum Riesz fractional operators. Fractional differential equations have numerous applications in the modeling of the anomalous behavior of systems [19]. These applications have attracted many researches [20–24].

Over the past decades, several numerical methods were developed for the standard and fractional Schrödinger equations. Liao et al. [25] and Wang et al. [26] studied and analyzed the fourth-order compact scheme for the solution of standard linear and nonlinear Schrödinger (NS) equations, respectively. Dehghan and Taleei [27] utilized a compact split-step finite difference (FD) method for solving the NS equations with variable coefficients. Mohebbi [28] utilized compact FD scheme for solving the Riesz space fractional diffusion equation. Karamali et al. [29] used particle hydrodynamics method for solving Schrödinger and Schrödinger-Boussinesq equations. Liu et al. [11] proposed finite difference scheme for the TS-FS equation. Fan and Qi [30] introduced the FD and finite element (FE) for temporal and spatial discretization of the Caputo time and the Riesz space fractional Schrödinger equation, respectively. There are several computational methods for time-fractional differential equations that developed by the Laplace transform method (LTM) [31–33].

The LTM has been used in various researches to deal with time derivatives [34, 35]. Here, to recover the numerical solution, at the beginning, we convert the considered equation to some independent and stationary problems by LTM. Then, we will choose a space discretization method to solve each stationary problem. Using the numerical inversion of the Laplace transform (NILT) is the final step to achieve the solution. The LTM and the finite element methods were used for time and space discretization of the parabolic equations, respectively [34, 35]. McLean et al. [36, 37] used this combination for the Volterra type integro-differential equation. Instead of the FEM combined with LTM, RBF method is utilized for the parabolic equation on the sphere [38, 39] by Le Gia and McLean. Jacobs [40] coupled LTM and a fourth-order compact finite difference for time-fractional equations with Dirichlet and Neumann boundary conditions. Uddin et al. [31, 32] worked on time-fractional diffusion and diffusion-wave equations with LTM for temporal term combined with meshless methods. Mohammadi-Firouzjaei et al. [41] combined local discontinuous Galerkin method (LDGM) with LTM to solve distributed-order time-fractional equations. They also compared LDGM and LTM for solving fractional compartmental model that applied in pharmacokinetics in [42]. Kamran et al.[43] proposed a combination of LTM and meshless methods and solved time-fractional telegraph equations.

In the present study, we are dealing with space fractional operator. One can follow [44, 45] for the matrix transformation technique (MTT) to deal with fractional spatial term with homogeneous and nonhomogeneous boundary conditions, respectively. Yang et al. [46] developed some numerical methods for solving the Riesz fractional diffusion and advection–dispersion equations utilizing MTT. Ding and Zhang [47] proposed a fourth-order improved matrix transformation technique (IMTT), which was based on a compact FD method for space-fractional diffusion and advection-dispersion equations. Bhatt et al. in [48] considered space-fractional reaction-diffusion equations and used the fourth-order IMTT and compact exponential time differencing methods for space and time variables, respectively. Zhuang et al. used MTT for variable-order space-fractional advection-diffusion equation [49]. For the space-fractional diffusion equation, authors in [50], used a contour integral representation of the fractional power of a matrix and approximated the integral by rational approximation. The MTT is developed for space discretization of a two-dimensional time-space fractional diffusion equation by Yang et al. [51].

The standard Schrödinger equation reads as follows:

$$i\partial_t u(x,t) + \Delta u(x,t) + u(x,t) = f(x,t), \qquad (x,t) \in (a,b) \times (0,T], \tag{1}$$

subject to the initial condition $u(x,0) = u_0(x)$ and

$$u(a,t) = g_1(t), \qquad u(b,t) = g_2(t), \qquad t \in (0,T],$$

in which $i = \sqrt{-1}$, $\partial_t = \frac{\partial}{\partial t}$. Also $-\Delta = -\frac{\partial^2}{\partial x^2}$ is one-dimensional positive self-adjoint elliptic operator and $g_1(t)$ and $g_2(t)$ are some given functions. Decomposing u and f into their real-valued functions as $u = p + iq$ and $f = f_1 + if_2$ converts Equation (1) to following real-valued system of equations

$$\partial_t p(x,t) + \Delta q(x,t) + q(x,t) = f_2(x,t), \tag{2a}$$

$$\partial_t q(x,t) - \Delta p(x,t) - p(x,t) = -f_1(x,t). \tag{2b}$$

In this article, we will focus on the following TS-FS equation

$$i{}_0^C D_t^\alpha u(x,t) - (-\Delta)^{\gamma/2} u(x,t) + u(x,t) = f(x,t), \tag{3}$$

subject to the initial condition $u(x,0) = u_0(x)$ and

$$u(x,t) = 0, \qquad x \in \mathbb{R}\backslash(a,b), \quad t \in (0,T],$$

where ${}_0^C D_t^\alpha$ is the Caputo type fractional derivative of order α, $0 < \alpha \leq 1$ and $1 < \gamma \leq 2$. The corresponding real-valued system of equations, after decomposing the complex function u in Equation (3), is written as:

$${}_0^C D_t^\alpha p(x,t) - (-\Delta)^{\gamma/2} q(x,t) + q = f_2(x,t), \tag{4a}$$

$${}_0^C D_t^\alpha q(x,t) + (-\Delta)^{\gamma/2} p(x,t) - p(x,t) = -f_1(x,t). \tag{4b}$$

There has been some investigation into numerical solutions for linear fractional SE. Zheng et al. [52] utilized the Grünwald–Letnikov formulation and the spectral collocation method for time and space discretization of linear time fractional SE. Ma and Chen [53] utilized L1 formula on graded mesh and central difference scheme for this equation. Authors of [54] studied the numerical solution of linear space fractional SE by using matrix approach. In [55] the Adomian decomposition method is applied for linear space-time fractional SE.

Here, we aim to use a combination of Laplace transform and finite difference methods, along with matrix transformation and improved matrix transformation techniques, to numerically solve linear space-time fractional SE (3).

1.1 Motivations

The main goal of this study is to introduce efficient numerical methods for solving the TS-FS system of Equations (4). We use the LTM based on the FD methods. There are several different approaches to time discretization, such as time-marching methods and Laplace transform approach. Due to the Courant-Friedrichs-Lewy (CFL) condition restriction in the time-marching methods, we employ the LTM via the FD methods to prevent the time-stepping issue. We are also facing the space fractional operator $(-\Delta)^{\gamma/2}$, defined by spectral fractional Laplacian operator. We use the matrix transformation technique (MTT) to deal with the fractional spatial term. One of the advantages of using these techniques with FD method is the simplicity of the development of similar algorithms for high-dimensional problems.

The rest of this paper is organized as follows: In the next section, we present some important definitions, notations and lemmas which are necessary for future sections. Section 3 provides a brief review of FD methods for spatial discretization of TS-FS Equation (3). Time and space discretizations of the equation are presented in Section 4. Section 5 is devoted to several examples with some discussion about the numerical simulation results. Finally, in Section 6 a conclusion is presented.

2 Preliminaries

Definition 2.1. Let $\alpha > 0$ and $n = \lceil \alpha \rceil$. The Caputo derivative of order α, denoted by ${}_0^C D_t^\alpha$, is defined [1] as:

$$ {}_0^C D_t^\alpha u(t) = \frac{1}{\Gamma(n-\alpha)} \int_0^t (t-\tau)^{n-\alpha-1} \frac{d^n u(\tau)}{d\tau^n}\, d\tau. \tag{5} $$

For example, when $0 < \alpha < 1$ and $n = 1$, Equation (5) gives

$$ {}_0^C D_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-\tau)^{-\alpha} \frac{du(\tau)}{d\tau}\, d\tau, \quad 0 < \alpha < 1. $$

Theorem 2.2. *([1, 31]). If $u(t) \in C^n[0,\infty)$, with $\alpha \in (n-1,n)$, $n \in \mathbb{N}$, the LT formula for the Caputo fractional derivative reads:*

$$ \mathcal{L}\{{}_0^C D_t^\alpha u(t)\} = s^\alpha \mathcal{U}(s) - \sum_{k=0}^{n-1} s^{\alpha-k-1} u^{(k)}(0), \quad n-1 < \alpha < n, \tag{6} $$

in which $\mathcal{U}(s) = \mathcal{L}\{u(t)\}$. Then, for $n = 1$, $0 < \alpha < 1$, we have

$$ \mathcal{L}\{{}_0^C D_t^\alpha u(t)\} = s^\alpha \mathcal{U}(s) - s^{\alpha-1} u(0). $$

We recall the following definitions from [44, 45] for the Laplacian and the homogeneous spectral fractional Laplacian operators when the zero boundary condition is considered.

Definition 2.3. ([44]). Assume that ϕ_j's are the eigenfunctions, corresponding to the eigenvalues of the Laplacian operator $(-\Delta)$, in a bounded domain $\Omega = [0, L_x]$, respectively, i.e.

$$ \begin{aligned} -\Delta \phi_j &= \lambda_j \phi_j, && \textit{in } \Omega, \\ \phi_j &= 0, && \textit{on } \partial\Omega, \end{aligned} \tag{7} $$

where $\lambda_j = \frac{j^2\pi^2}{L^2}$ and $\phi_j = \sin(\frac{j\pi x}{L})$. Now consider

$$\mathcal{G}^1_\eta = \left\{ g : g = \sum_{j=1}^{\infty} g_j\phi_j,\ \ g_j = \langle g, \phi_j \rangle \mid \sum_{j=1}^{\infty} |g_j|^2|\lambda_j|^\eta < \infty,\ \eta = max(\gamma, 0) \right\}. \tag{8}$$

The homogeneous spectral fractional Laplacian operator of a function $g \in \mathcal{G}^1_\eta$ is defined by

$$(-\Delta)^{\frac{\gamma}{2}} g = \sum_{j=1}^{\infty} g_j(\lambda_j)^{\frac{\gamma}{2}}\phi_j. \tag{9}$$

Lemma 2.4. *([56]). Let T be a general tridiagonal Toeplitz matrix of order $n-1$ as:*

$$T = \begin{pmatrix} a & b & & & \\ c & a & b & & \\ & c & \ddots & \ddots & \\ & & \ddots & \ddots & b \\ & & & c & a \end{pmatrix},$$

thus the eigenvalues λ_i and their corresponding eigenvectors of $\boldsymbol{\xi}_i$ are obtained by

$$\lambda_i = a + 2\sqrt{bc}\,cos\left(\frac{i\pi}{n}\right), \qquad \boldsymbol{\xi}_i = \begin{bmatrix} (\frac{c}{b})^{\frac{1}{2}} sin(\frac{1i\pi}{n}) \\ (\frac{c}{b})^{\frac{2}{2}} sin(\frac{2i\pi}{n}) \\ (\frac{c}{b})^{\frac{3}{2}} sin(\frac{3i\pi}{n}) \\ \vdots \\ (\frac{c}{b})^{\frac{n-1}{2}} sin(\frac{(n-1)i\pi}{n}) \end{bmatrix}, \quad i = 1, \ldots, n-1. \tag{10}$$

Additionally, T is diagonalizable and P diagonalizes T, i.e., $T = P\Lambda P^{-1}$ where

$$P = (\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \boldsymbol{\xi}_3, \ldots, \boldsymbol{\xi}_{n-1}) \ \ \text{and} \ \ \Lambda = diag(\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_{n-1}).$$

Consider a positive definite matrix, T, such that $T = P\Lambda P^{-1}$, in which P is an orthogonal matrix. A fractional power of T is defined as [49] :

$$T^\gamma = P\Lambda^\gamma P^{-1} = P\, diag(\lambda_1^\gamma, \lambda_2^\gamma, \lambda_3^\gamma, \ldots, \lambda_{n-1}^\gamma)\, P^{-1}. \tag{11}$$

3 A brief review of the spatial discretization schemes

In this section, at first, the FD methods are presented for the following TF-SE

$${}^C_0D^\alpha_t p + \Delta q + q = f_2, \tag{12a}$$

$${}^C_0D^\alpha_t q - \Delta p - p = -f_1. \tag{12b}$$

Then, we use the concluded semi-discrete scheme and also the matrix transform technique to provide a semi-discrete scheme for Equation (4).

3.1 Time fractional equation

This part is devoted to a brief review of the second-order central and the fourth-order compact FD methods to approximate the solution of Equation (12).

Let n_x be a positive integer and $h_x = \frac{L_x}{n_x}$ denotes the step size of spatial variable, i.e. $x_i = ih_x$, $i = 0, \ldots, n_x$. The second-order central FD scheme is denoted as:

$$p_{xx} \approx \frac{1}{h_x^2}\delta_x^2 p_i + \tau_i = \frac{p_{i+1} - 2p_i + p_{i-1}}{h_x^2} + \tau_i, \tag{13}$$

with the following truncation error

$$\tau_i = \frac{h_x^2}{12}\left(\frac{d^4 p(x)}{dx^4}\right) + O(h_x^4). \tag{14}$$

The central difference scheme gives a bounded matrix operator, $\mathcal{A}_{cn}^{1d}$, for approximation of the Laplacian operator $(-\Delta)$. The matrix representation of the semi-discretization of Equation (12) is

$$ {}_0^C D_t^\alpha \boldsymbol{p} - \mathcal{A}_{cn}^{1d}\boldsymbol{q} + \boldsymbol{q} = \boldsymbol{F}_2, \tag{15a}$$

$$ {}_0^C D_t^\alpha \boldsymbol{q} + \mathcal{A}_{cn}^{1d}\boldsymbol{p} - \boldsymbol{p} = -\boldsymbol{F}_1, \tag{15b}$$

in which $\mathcal{A}_{cn}^{1d} = \frac{1}{h_x^2}\tilde{\mathcal{A}}$ and

$$\tilde{\mathcal{A}} = \begin{bmatrix} 2 & -1 & & & 0 \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & \ddots & -1 \\ 0 & & & -1 & 2 \end{bmatrix}, \quad \boldsymbol{p} = \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ \vdots \\ p_{n_x-1} \end{bmatrix}, \quad \boldsymbol{q} = \begin{bmatrix} q_1 \\ q_2 \\ q_3 \\ \vdots \\ q_{n_x-1} \end{bmatrix}, \quad \boldsymbol{F}_i = \begin{bmatrix} f_{i,1} \\ f_{i,2} \\ f_{i,3} \\ \vdots \\ f_{i,n_x-1} \end{bmatrix}, \quad i = 1, 2. \tag{16}$$

Note that $\mathcal{A}_{cn}^{1d}$ is a symmetric positive definite matrix. Also we can approximate the second-order derivative by the high-order compact FD scheme [57, 58] as follows:

$$u_{xx} \approx \frac{1}{h_x^2}\frac{\delta_x^2}{1 + \frac{1}{12}\delta_x^2}u_i + O(h_x^4). \tag{17}$$

Thus, the matrix representation of the semi-discretization of Equation (12) is

$$ {}_0^C D_t^\alpha P - \mathcal{A}_{cp}^{1d}Q + Q = F_2, \tag{18a}$$

$$ {}_0^C D_t^\alpha Q + \mathcal{A}_{cp}^{1d}P - P = -F_1, \tag{18b}$$

where $\mathcal{A}_{cp}^{1d} = \mathcal{B}^{-1}\mathcal{A}_{cn}^{1d}$ and

$$\mathcal{B} = \begin{bmatrix} \frac{5}{6} & \frac{1}{12} & & & 0 \\ \frac{1}{12} & \frac{5}{6} & \frac{1}{12} & & \\ & \frac{1}{12} & \frac{5}{6} & \ddots & \\ & & \ddots & \ddots & \frac{1}{12} \\ 0 & & & \frac{1}{12} & \frac{5}{6} \end{bmatrix}. \tag{19}$$

Now the goal is to get the power of the fractional order operator. To do this, one can use Lemma 2.4. To accomplish this, we decompose $\mathcal{A}_{cn}^{1d}$ and $\mathcal{B}$ as:

$$\mathcal{A}_{cn}^{1d} = \frac{1}{h_x^2}\tilde{\boldsymbol{p}}\Lambda_{cn}\tilde{\boldsymbol{p}}^{-1}, \quad \mathcal{B} = \boldsymbol{p}\Lambda\boldsymbol{p}^{-1}, \tag{20}$$

where

$$\begin{aligned} \tilde{\boldsymbol{p}} &= (\tilde{\xi}_1, \tilde{\xi}_2, \tilde{\xi}_3, \dots, \tilde{\xi}_{n_x-1}), \quad \Lambda_{cn} = diag(\tilde{\lambda}_1, \tilde{\lambda}_2, \tilde{\lambda}_3, \dots, \tilde{\lambda}_{n_x-1}), \\ \boldsymbol{p} &= (\xi_1, \xi_2, \xi_3, \dots, \xi_{n_x-1}), \quad \Lambda_B = diag(\lambda_1, \lambda_2, \lambda_3, \dots, \lambda_{n_x-1}), \end{aligned} \tag{21}$$

such that

$$\tilde{\xi}_i = \xi_i = \begin{bmatrix} sin(\frac{1i\pi}{n_x}) \\ sin(\frac{2i\pi}{n_x}) \\ sin(\frac{3i\pi}{n_x}) \\ \vdots \\ sin(\frac{(n_x-1)i\pi}{n_x}) \end{bmatrix}, \quad \tilde{\lambda}_i = 4sin^2(\frac{i\pi}{2n_x}), \quad \lambda_i = 1 - \frac{1}{3}sin^2(\frac{i\pi}{2n_x}), \quad i = 1 : n_x - 1. \tag{22}$$

Now, according to the Lemma 2.4, we have $\mathcal{A}_{cp}^{1d} = \frac{1}{h_x^2}\boldsymbol{p}\Lambda_{cp}\boldsymbol{p}^{-1}$, subject to

$$\boldsymbol{p} = (\xi_1, \xi_2, \xi_3, \dots, \xi_{n_x-1}), \quad \Lambda_{cp} = diag\left(\frac{\tilde{\lambda}_1}{\lambda_1}, \frac{\tilde{\lambda}_2}{\lambda_2}, \frac{\tilde{\lambda}_3}{\lambda_3}, \dots, \frac{\tilde{\lambda}_{n_x-1}}{\lambda_{n_x-1}}\right). \tag{23}$$

3.2 Time-space fractional equation

Let us consider the TS-FS equation

$${}_0^C D_t^\alpha p - (-\Delta)^{\gamma/2} q + q = f_2, \tag{24a}$$

$${}_0^C D_t^\alpha q + (-\Delta)^{\gamma/2} p - p = -f_1. \tag{24b}$$

The space fractional order γ will be integer when $\gamma = 2$ and non-integer, when $1 < \gamma < 2$.

If $\gamma = 2$, one can use the FD schemes mentioned above. Now consider $1 < \gamma \leq 2$. When $\mathcal{A}$ is the approximation of the the fractional Laplacian operator, using Definition 2.3, then $(-\Delta)^{\frac{\gamma}{2}}$ is approximated as $(-\Delta)^{\frac{\gamma}{2}} \approx \mathcal{A}^{\frac{\gamma}{2}}$ by means of the matrix transformation technique. If so, utilizing the central FD or compact FD, the semi-discrete scheme for Equation (24) is

$${}_0^C D_t^\alpha \boldsymbol{p} - \mathcal{A}_\varrho^{\frac{\gamma}{2}} \boldsymbol{q} + \boldsymbol{q} = \boldsymbol{F}_2, \tag{25a}$$

$${}_0^C D_t^\alpha \boldsymbol{q} + \mathcal{A}_\varrho^{\frac{\gamma}{2}} \boldsymbol{p} - \boldsymbol{p} = -\boldsymbol{F}_1. \tag{25b}$$

in which $\varrho = cn, cp$. Now, when $\mathcal{A}_\varrho^{\frac{\gamma}{2}} = \mathcal{P}\Lambda^{\frac{\gamma}{2}}\mathcal{P}^{-1}$, close inspection of (11) reveals

$${}_0^C D_t^\alpha \boldsymbol{p} - \mathcal{P}\Lambda^{\frac{\gamma}{2}}\mathcal{P}^{-1}\boldsymbol{q} + \boldsymbol{q} = \boldsymbol{F}_2, \tag{26a}$$

$${}_0^C D_t^\alpha \boldsymbol{q} + \mathcal{P}\Lambda^{\frac{\gamma}{2}}\mathcal{P}^{-1}\boldsymbol{p} - \boldsymbol{p} = -\boldsymbol{F}_1. \tag{26b}$$

The compact form of Equation (26) is

$$ {}_0^C D_t^{\alpha} \chi + \Xi \chi = \boldsymbol{F}, \tag{27}$$

where

$$ \chi = \begin{bmatrix} P \\ Q \end{bmatrix}, \qquad \Xi = \begin{bmatrix} \boldsymbol{O} & -\mathcal{P}\Lambda^{\frac{\gamma}{2}}\mathcal{P}^{-1} + \boldsymbol{I} \\ \mathcal{P}\Lambda^{\frac{\gamma}{2}}\mathcal{P}^{-1} - \boldsymbol{I} & \boldsymbol{O} \end{bmatrix}, \qquad \boldsymbol{F} = \begin{bmatrix} F_2 \\ -F_1 \end{bmatrix}. \tag{28}$$

4 Numerical description

In this section, the Laplace transform-finite difference (LT-FD) method is used for time and space discretizations of the TS-FS Equations (3). To do this, we implement FD method, use MTT and obtain Equation (27) and finally, the LTM will be utilized for time discretization of Equation (27). In the following subsection, a time discretization by the LTM and also a NILT are presented.

4.1 The Laplace transform method

Taking Laplace transform from Equation (27) yields

$$ s^{\alpha}\widehat{\chi}(s) - s^{\alpha-1}\chi(0) + \Xi\widehat{\chi}(s) = \mathcal{F}(s). \tag{29}$$

Rearranging gives

$$ \widehat{\chi}(s) = [s^{\alpha} I + \Xi]^{-1}\left(s^{\alpha-1}\chi(0) + \mathcal{F}(s)\right). \tag{30}$$

Invertibility of above operators analyzed by McLean et al. [36, 37, 59, 60]. By using the ILT, the solution is:

$$ \chi(t) = \frac{1}{2\pi i}\int_B e^{st}\widehat{\chi}(s)\,ds, \tag{31}$$

in which B, the Bromwich line, is the line $Re(s) = \sigma > \sigma_0$ [33]. The constant σ_0 is considered large enough such that all singularities of $\widehat{\chi}(s)$ lie in the left side of B. We follow the approach presented in [34] and use notations therein. The key idea of this method is deformation of the Bromwich line into a curve Γ, such that begins and ends in the left half-plane and $Re(s) \to -\infty$ at the contour ends [33], in such a way the exponential term in the ILT decays rapidly. Then the following contour is considered

$$ \Gamma := \{s : \; s(\theta) = \varphi(\theta) + i\sigma\theta, \quad -\infty < \theta < \infty\}, \tag{32}$$

where $\sigma \in \mathbb{R}^+$ and φ is a smooth function such that

$$ \varphi(\theta) \approx -|\theta|, \;\; \text{for large } |y|, \qquad \text{and} \;\; \varphi(\theta) \le \varsigma - |\theta|. $$

Sheen et al. in [34] suggest that

$$ \varphi(\theta) = \varsigma - \sqrt{\theta^2 + \nu^2}, \quad \theta \in \mathbb{R}, \tag{33}$$

where ς and ν are real and strictly positive parameters, respectively. Also, $s^{'}(\theta) = \varphi^{'}(\theta) + i\sigma$. If so, integral (31) is converted to the integral with an unbounded domain as follows

$$\chi(t) = \frac{1}{2\pi i}\int_{B} e^{st}\widehat{\chi}(s)\,ds = \frac{1}{2\pi i}\int_{-\infty}^{\infty} e^{s(\theta)t}\widehat{\chi}(s(\theta))s^{'}(\theta)\,d\theta. \tag{34}$$

Now, define $\mathcal{W}(\theta) := \frac{1}{2\pi i}e^{s(\theta)t}\widehat{\chi}(s(\theta))s^{'}(\theta)$, so that

$$\chi(t) = \int_{-\infty}^{\infty}\mathcal{W}(\theta)\,d\theta = \int_{-1}^{1}\mathcal{W}(\theta(\eta))\theta^{'}(\eta)\,d\eta, \tag{35}$$

where

$$\theta(\eta) = \frac{\varphi(\eta)}{\tau}, \quad \varphi(\eta) = log(\frac{1+\eta}{1-\eta}).$$

As for the numerical integration, the trapezoidal rule with $2M+1$ points, $\eta_m = \frac{m}{M}, \ -M \leq m \leq M$ is simple to carry out. We now write the approximation of the above integral as:

$$\chi_M(t) = \frac{1}{M}\left[\frac{\mathcal{W}(\theta_{-M})\theta^{'}_{-M} + \mathcal{W}(\theta_M)\theta^{'}_{M}}{2} + \sum_{m=-M+1}^{M-1}\mathcal{W}(\theta_m)\theta^{'}_{m}\right]. \tag{36}$$

As a final result, one obtains the fully discretization solution as:

$$\chi_{M,h}(t) = \frac{1}{M}\left[\frac{\mathcal{W}_h(\theta_{-M})\theta^{'}_{-M} + \mathcal{W}_h(\theta_M)\theta^{'}_{M}}{2} + \sum_{n=-M+1}^{M-1}\mathcal{W}_h(\theta_m)\theta^{'}_{m}\right]. \tag{37}$$

Here $\mathcal{W}_h(\theta_m) = \frac{1}{2\pi i}e^{s(\theta_m)t}\widehat{\chi}(s(\theta_m))s^{'}(\theta_m)$ and each $\widehat{\chi}(s(\theta_m))$ can be evaluated by (30) using provided methods. Note that, McLean and Thomée [59] proposed an approach based on Duhamel's formula such that the scheme does not use the Laplace transform of the source term.

Remark 1. As demonstrated by [36] and [61], when $t > 0$, the quadrature error of (37) is $O(e^{-\varrho\frac{N^s}{logN^s}})$. On the other hand, the expected convergence rate of errors obtained by the FD and compact FD is $O(h_x^2)$ and $O(h_x^4)$, respectively. As a result, the Laplace transform combined with FD and compact FD are expected to have convergent rates $O(h^2 + e^{-\varrho\frac{N^s}{logN^s}})$ and $O(h^4 + e^{-\varrho\frac{N^s}{logN^s}})$, respectively.

5 Numerical results

Here, we present the definition of error and the integration contour to illustrate more for what we use in examples. We denote T, $\tilde{u}$, and u as the final time, numerical approximation and exact solution of the equations, respectively. The maximum norm of errors, $\|E_n\|_{L_\infty}$, and the convergence rate are given as:

$$\|E_n\|_{L_\infty} = \max_{0\leq i\leq n}|\tilde{u}_i - u(x_i,T)|, \qquad Rate = (\ln(\frac{n_2}{n_1}))^{-1}\ln\left(\frac{\|E_{n_1}\|_{L_\infty}}{\|E_{n_2}\|_{L_\infty}}\right).$$

For solving the following examples, the we consider the integration contour (32) such that $\varsigma = 2, \ \nu = 0.5, \ \sigma = 1$

For the ease of notation, we consider $u(x,t) = p(x,t) + iq(x,t)$ as the exact solution of the first three cases below, where $p(x,t) = t^{\beta}\psi_0(x)$, $q(x,t) = t^{\beta}\phi_0(x)$, such that

$$\psi_r(x) = \sum_{j=1}^{\infty} \frac{8(-1)^{j+1}-4}{j^6}(\frac{j}{2})^r \sin(\frac{jx}{2}), \qquad \phi_r(x) = \sum_{j=1}^{\infty} \frac{16(-1)^{j+1}-8}{j^6}(\frac{j}{4})^r \sin(\frac{jx}{4}).$$

Example 5.1. Consider the Schrödinger equation

$$i\partial_t u(x,t) + \Delta u(x,t) + u(x,t) = f(x,t), \quad x \in (0,4\pi), \tag{38}$$

where, the right-hand side (RHS) of the Equation (38) is

$$f(x,t) = i\beta t^{\beta-1}\left(\psi_0(x) + i\phi_0(x)\right) - t^{\beta}\left(\psi_2(x) + i\phi_2(x)\right) + t^{\beta}\left(\psi_0(x) + i\phi_0(x)\right),$$

that means

$$f_1(x,t) = -\beta t^{\beta-1}\phi_0(x) - t^{\beta}\psi_2(x) + t^{\beta}\psi_0(x), \tag{39a}$$

$$f_2(x,t) = \beta t^{\beta-1}\psi_0(x) - t^{\beta}\phi_2(x) + t^{\beta}\phi_0(x). \tag{39b}$$

Then

$$\mathcal{F}_1(x,s) = -\beta\frac{\Gamma(\beta)}{s^{\beta}}\phi_0(x) - \frac{\Gamma(1+\beta)}{s^{1+\beta}}\psi_2(x) + \frac{\Gamma(1+\beta)}{s^{1+\beta}}\psi_0(x), \tag{40a}$$

$$\mathcal{F}_2(x,s) = \beta\frac{\Gamma(\beta)}{s^{\beta}}\psi_0(x) - \frac{\Gamma(1+\beta)}{s^{1+\beta}}\phi_2(x) + \frac{\Gamma(1+\beta)}{s^{1+\beta}}\phi_0(x). \tag{40b}$$

Table 1: Errors in maximum norm and computational order obtained for the first problem with $M = 150$ and $\beta = 3$.

	Central FD				Compact FD			
	p		q		p		q	
n_x	error	*Rate*	error	*Rate*	error	*Rate*	error	*Rate*
10	1.7097e-03	–	1.1470e-02	–	7.7038e-05	–	6.6452e-04	–
20	4.1180e-04	2.540	3.1111e-03	1.882	2.6661e-05	1.531	5.6250e-05	3.562
40	1.2242e-04	1.750	7.8223e-04	1.992	2.4723e-06	3.431	4.0652e-06	3.790
80	3.2620e-05	1.908	1.9744e-04	1.986	1.6962e-07	3.865	2.7034e-07	3.910
160	8.2290e-06	1.987	4.9377e-05	1.999	1.1141e-08	3.928	1.7319e-08	3.964
320	2.0646e-06	1.995	1.2345e-05	2.000	7.1484e-10	3.962	1.0977e-09	3.980

Example 5.2. Consider the time fractional Schrödinger equation

$$i\,{}_0^C D_t^{\alpha} u(x,t) + \Delta u(x,t) + u(x,t) = f(x,t), \quad x \in (0,4\pi), \tag{41}$$

with a RHS as:

$$f(x,t) = i\frac{\Gamma(1+\beta)}{\Gamma(1+\beta-\alpha)}t^{\beta-\alpha}\left(\psi_0(x) + i\phi_0(x)\right) - t^{\beta}\left(\psi_2(x) + i\phi_2(x)\right) + t^{\beta}\left(\psi_0(x) + i\phi_0(x)\right), \tag{42}$$

that means

$$f_1(x,t) = -\frac{\Gamma(1+\beta)}{\Gamma(\beta-\alpha+1)} t^{\beta-\alpha}\phi_0(x) - t^{\beta}\psi_2(x) + t^{\beta}\psi_0(x), \tag{43a}$$

$$f_2(x,t) = \frac{\Gamma(1+\beta)}{\Gamma(1+\beta-\alpha)} t^{\beta-\alpha}\psi_0(x) - t^{\beta}\phi_2(x) + t^{\beta}\phi_0(x). \tag{43b}$$

Then

$$\mathcal{F}_1(x,s) = \Gamma(1+\beta)\left[-\frac{\phi_0(x)}{s^{1+\beta-\alpha}} - \frac{\psi_2(x)}{s^{1+\beta}} + \frac{\psi_0(x)}{s^{1+\beta}}\right], \tag{44a}$$

$$\mathcal{F}_2(x,s) = \Gamma(1+\beta)\left[\frac{\psi_0(x)}{s^{1+\beta-\alpha}} - \frac{\phi_2(x)}{s^{1+\beta}} + \frac{\phi_0(x)}{s^{1+\beta}}\right]. \tag{44b}$$

Table 2: Errors in maximum norm and computational order obtained for the second problem with $M = 150$, $\beta = 4 - \frac{\alpha}{2}$ and $\alpha = 0.5$.

	Central FD				Compact FD			
	p		q		p		q	
	error	*Rate*	error	*Rate*	error	*Rate*	error	*Rate*
n_x								
10	6.0407e-03	–	2.1022e-02	–	2.7723e-04	–	1.0417e-03	–
20	1.5833e-03	1.932	5.6639e-03	1.892	4.1847e-05	2.728	7.5826e-05	3.780
40	3.9739e-04	1.994	1.4456e-03	1.970	3.1408e-06	3.736	5.1359e-06	3.884
80	9.9348e-05	2.000	3.6328e-04	1.992	2.1760e-07	3.851	3.3588e-07	3.935
160	2.4839e-05	2.000	9.0894e-05	2.000	1.4329e-08	3.925	2.1412e-08	3.971
320	6.2132e-06	1.999	2.2735e-05	1.999	9.1208e-10	3.974	1.3511e-09	3.986

Example 5.3. The third problem is the ST-FS equation as:

$$i\,{}_0^C D_t^{\alpha} u(x,t) - (-\Delta)^{\gamma/2} u(x,t) + u(x,t) = f(x,t), \quad x \in (0, 4\pi). \tag{45}$$

For this case, the RHS is given as below

$$f(x,t) = i\frac{\Gamma(1+\beta)}{\Gamma(1+\beta-\alpha)} t^{\beta-\alpha}\left(\psi_0(x) + i\phi_0(x)\right) - t^{\beta}\left(\psi_\gamma(x) + i\phi_\gamma(x)\right) + t^{\beta}\left(\psi_0(x) + i\phi_0(x)\right), \tag{46}$$

and the Laplace transform of its real and imaginary parts are

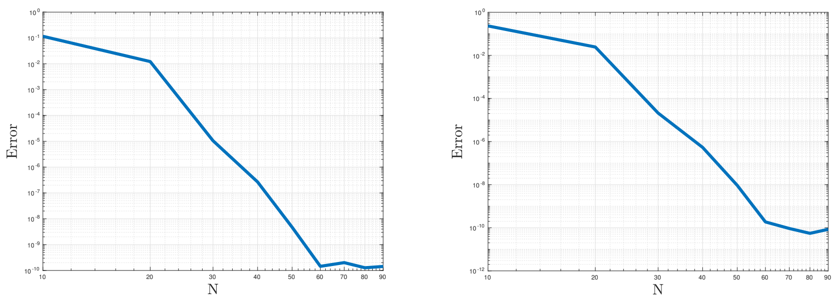
$$\mathcal{F}_1(x,s) = \Gamma(1+\beta)\left[-\frac{\phi_0(x)}{s^{1+\beta-\alpha}} - \frac{\psi_\gamma(x)}{s^{1+\beta}} + \frac{\psi_0(x)}{s^{1+\beta}}\right], \tag{47a}$$

$$\mathcal{F}_2(x,s) = \Gamma(1+\beta)\left[\frac{\psi_0(x)}{s^{1+\beta-\alpha}} - \frac{\phi_\gamma(x)}{s^{1+\beta}} + \frac{\phi_0(x)}{s^{1+\beta}}\right]. \tag{47b}$$

Table 3: Errors in maximum norm and computational order obtained for the third problem with $M = 150$, $\beta = 4 - \frac{\alpha}{2}$, $\alpha = 0.5$ and $\gamma = 1.75$.

	Central FD				Compact FD			
	p		q		p		q	
	error	*Rate*	error	*Rate*	error	*Rate*	error	*Rate*
n_x								
10	5.8954e-03	–	2.0181e-02	–	2.4002e-04	–	1.0139e-03	–
20	1.5231e-03	1.953	5.5076e-03	1.874	3.6066e-05	2.734	7.1625e-05	3.823
40	3.8288e-04	1.992	1.3898e-03	1.987	2.7920e-06	3.691	4.8715e-06	3.878
80	9.5801e-05	1.999	3.5019e-04	1.989	1.8606e-07	3.907	3.1204e-07	3.965
160	2.3990e-05	1.998	8.7591e-05	1.999	1.2117e-08	3.941	1.9742e-08	3.982
320	5.9976e-06	2.000	2.1900e-05	2.000	7.6598e-10	3.984	1.2403e-09	3.992

For all three cases, the final time is $T = 1$. The LTM is combined with central and compact FD methods. In Tables 1 to 3, we show the maximum norm of the errors and the computational orders of accuracy for the standard, time fractional and time-space fractional Schrödinger equations, respectively . Two different FD methods are implemented and yield the second- and fourth-order accurate results, as we expected. Figure 1 demonstrates the temporal convergence of the scheme for the third example, which shows that the errors decay exponentially.



(a) real part (p). (b) imaginary part (q).

Figure 1: Convergence plots of LTM with $M = 10, \ldots, 90$ and $n_x = 800$.

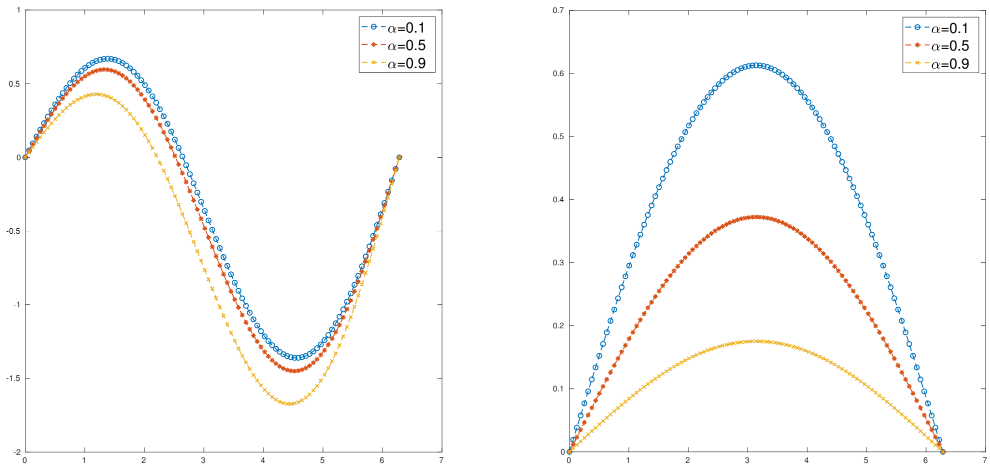
Example 5.4. Consider the following ST-FS equation as:

$$i{}_0^C D_t^\alpha u(x,t) - (-\Delta)^{\gamma/2} u(x,t) + u(x,t) = 0, \quad x \in (0, 2\pi), \tag{48}$$

with following initial condition

$$u(x,0) = \sin(x) + i\sin(x/2). \tag{49}$$

Figure 2 shows the approximation solution of LTM-(compact) FD method for a fix β and various α and Figure 3 reflect the behavior of the numerical solutions in terms of a fix α and different values of β.



(a) $p(x, 2)$ (b) $q(x, 2)$

Figure 2: Numerical solutions of Example 5.4 for $\beta = 1.75$ and $\alpha = 0.1,\ 0.5,\ 0.9$.

6 Conclusion

In this work, we solve the time/ time-space fractional Schrödinger equation. For time discretization the Laplace transform method has been utilized. Spectral fractional Laplacian operators have been considered as the fractional differential operator. Here, we have dealt with the definition of the spectral fractional Laplacian operator $(-\Delta)^{\gamma/2}$. For space discretization of the time-fractional Schrödinger equation, the central and compact finite difference schemes have been used. For discretizing the space fractional term, we use matrix transformation technique. In this technique the fractional Laplacian operator $(-\Delta)^{\gamma/2}$ is approximated by fractional power of $\mathcal{A}$ which is the spatial discretization of the Laplacian operator $(-\Delta)$. The results of the presented examples express the applicability of the approach. For a given time/time-space fractional Schrödinger equation, the error convergence rate using the central finite difference method is equal to two, whereas, by using the compact finite difference method, the error convergence rate is four.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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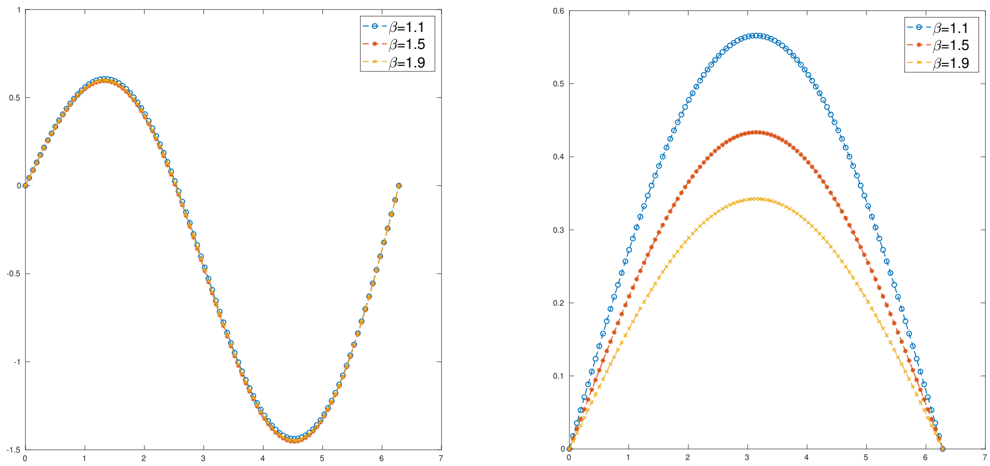

(a) $p(x, 2)$ (b) $q(x, 2)$

Figure 3: Numerical solutions of Example 5.4 for $\alpha = 0.5$ and $\beta = 1.1,\ 1.5,\ 1.9$.

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