



# Analytic and Numerical Solutions of Time-Fractional Linear Schrödinger Equation

Research Article

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**Abstract.** Fractional Schrödinger equation is a basic equation in fractional quantum mechanics. In this paper, we consider both analytic and numerical solutions of time-fractional linear Schrödinger Equations. This is done via a proposed semi-analytical method upon the modification of the classical *Differential Transformation Method* (DTM). Some illustrative examples are used; the results obtained converge faster to their exact forms. This shows that this modified version is very efficient, and reliable; as less computational work is involved, even without given up accuracy. Therefore, it is strongly recommended for both linear and nonlinear time-fractional *partial differential equations* (PDEs) with applications in other areas of applied sciences, management, and finance.

**Keywords.** Time-fractional differential equations; Modified DTM; Schrödinger Equations; Analytical solutions

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## 1. Introduction

Schrödinger equation is a *partial differential equation* (PDE) used in quantum mechanics for the description of how the quantum state of a physical system changes with respect to time. This appears in two forms: the *time dependent Schrödinger wave equation* (TDSWS) and the *time independent Schrödinger equation* (TISE) [15].

The application of Schrödinger equation is of great interest in Physics and other aspects of applied science [12]. Meanwhile, fractional Schrödinger equation is a basic equation of fractional

quantum mechanics, as discovered and coined by Laskin [8, 9]. It is a generalization of the classical quantum mechanics.

The time-fractional Schrödinger equation is of the form:

$$i \frac{\partial^\alpha u}{\partial t^\alpha} + \lambda \frac{\partial^2 u}{\partial x^2} + p(x)u + \xi |u|^2 u = 0 \quad (1.1)$$

with an initial condition:

$$h(x) = u(x, 0), \quad i^2 = -1, \quad (1.2)$$

where the function  $u = u(x, t)$  is complex,  $\lambda$  and  $\xi$  are constants and  $p(x)$  is a function of  $x$ .

A special case of (1.1) based on some conditions will be considered for the linear forms of (1.1).

In recent years, regard has been given to the study of fractional calculus; it appears most suitable for the generalization of fractional differential equations [13, 18]. Fractional differential equations are seen as alternative methods to non-linear differential equations [14].

In this work, a relatively new version of the modification referred to as *modified differential transform method* (MDTM) will be applied to linear Schrödinger equations for exact and numerical solutions. It is noteworthy to say here that the MDTM has advantages over the decomposition methods and the classical DTM as the computational time required is minimal, and for ease and simplicity of usage.

## 2. Fractional Calculus: Preliminaries and Notations

In this section, we give a brief introduction of fractional calculus with regards to its preliminaries, basic definitions and notations [1, 2, 10].

In fractional calculus, the power of the differential operator is considered a real or complex number. Hence, the following definitions:

**Definition 2.1** (Fractional derivative in gamma sense). Suppose  $D = \frac{d(\cdot)}{dx}$  and  $J$  are differential and integration operators respectively, such that, the gamma function of  $h(x)$  is defined as:

$$\Gamma(n) = \int_0^\infty e^{-x} t^{n-1} dt, \quad \text{Re}(n) > 0, \quad \Gamma(n+1) = n!, \quad \Gamma(1/2) = \sqrt{\pi}. \quad (2.1)$$

Equation in terms of gamma sense is expressed as:

$$D^\alpha h(x) = \frac{d^\alpha h(x)}{dx^\alpha} = \frac{\Gamma(k+1)}{\Gamma(k-\alpha+1)} x^{k-\alpha}. \quad (2.2)$$

We referred to as a fractional derivative of  $h(x)$ , of order  $\alpha$ , if  $\alpha \in \mathbb{R}$ .

Suppose  $h(x) = x^k$  (a monomial, of degree  $k$ , not necessarily a fraction), then:

$$Dh(x) = \frac{dh(x)}{dx} = kx^{k-1}, \quad D^2h(x) = \frac{d^2h(x)}{dx^2} = k(k-1)x^{k-2} = \frac{k!}{(k-2)!} x^{k-2}. \quad (2.3)$$

In general,

$$\frac{d^m h(x)}{dx^m} = \frac{k!}{(k-m)!} x^{k-m}. \quad (2.4)$$

**Definition 2.2.** Suppose  $h(x)$  is defined for  $x > 0$ , then:

$$(Jh)(x) = \int_0^x h(s)ds \quad (2.5)$$

and as such, an arbitrary extension of (2.5) (i.e. Cauchy formula for repeated integration) yields:

$$(J^n h)(x) = \frac{1}{(n-1)!} \int_0^x (x-s)^{n-1} h(s)ds. \quad (2.6)$$

Thus, the gamma sense of (2.6) is:

$$(J^\alpha h)(x) = \frac{1}{\Gamma(\alpha)} \int_0^x (x-s)^{\alpha-1} h(s)ds, \quad \alpha > 0, t > 0. \quad (2.7)$$

Equation (2.7) is the Riemann-Liouville fractional integration of order  $\alpha$ .

**Definition 2.3** (Riemann-Liouville fractional derivative).

$$D^\alpha h(x) = \frac{d^\phi(J^{\phi-\alpha} h(x))}{dx^\phi}. \quad (2.8)$$

**Definition 2.4** (Caputo fractional derivative).

$$D^\alpha f(x) = \frac{J^{\phi-\alpha}(d^\phi f(x))}{dx^\phi}, \quad \phi - 1 < \alpha < \phi, \phi \in \mathbb{N}. \quad (2.9)$$

**Note 2.1.** In (2.8), Riemann-Liouville compute first, the fractional integral of the function and thereafter, an ordinary derivative of the obtained result but the reverse is the case in Caputo sense of fractional derivatives; this allows the inclusion of the traditional initial and boundary conditions in the formulation of the problem.

**Note 2.2.** The link between the Riemann-Liouville operator and the Caputo fractional differential operator (see [16, Lemma 4]) is:

$$(J^\alpha D_t^\alpha)h(t) = (D_t^{-\alpha} D_t^\alpha)h(t) = h(t) - \sum_{k=0}^{n-1} h^k(0) \frac{t^k}{k!}, \quad n-1 < \alpha < n, n \in \mathbb{N}. \quad (2.10)$$

As such,

$$h(t) = (J^\alpha D_t^\alpha)h(t) + \sum_{k=0}^{n-1} h^k(0) \frac{t^k}{k!}. \quad (2.11)$$

**Definition 2.5** (The Mittag-Leffler Function). The Mittag-Leffler function,  $E_\alpha(z)$  valid in the whole complex plane is defined and denoted by the series representation as:

$$E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(1+\alpha k)}, \quad \alpha \geq 0, z \in \mathbb{C}. \quad (2.12)$$

**Remark 2.1.** For  $\alpha = 1$ , the Mittag-Leffler function,  $E_\alpha(z)$  in (2.12) becomes:

$$E_{\alpha=1}(z) = e^z. \quad (2.13)$$

### 3. A Two-dimensional DTM

Let  $\varpi(x, y)$  be a two-variable function analytic at  $(x_*, y_*)$  in the Domain,  $D$ , then, the differential transform of  $\varpi(x, y)$  is defined and denoted as:

$$\Psi(k, h) = \frac{1}{k!h!} \left[ \frac{\partial^{k+h} \varpi(x, y)}{\partial x^k \partial y^h} \right]_{(x,y)=(x_*,y_*)} \quad (3.1)$$

where the differential inverse transform of  $\Psi(k, h)$  is:

$$\varpi(x, y) = \sum_{k=0}^{\infty} \sum_{h=0}^{\infty} \Psi(k, h)(x - x_*)^k (y - y_*)^h. \quad (3.2)$$

The *differential transformation method* (DTM) has been studied by many researchers and showed to be easier in terms of application when solving both linear and nonlinear differential equations as it converts the said problems to their equivalents in algebraic recursive forms. This is unlike other semi-analytical methods: ADM, VIM, HAM and so on that require the determination of a successive term only by integrating a previous component (term) [5, 7, 11, 17].

In spite of the many advantages of the DTM over other semi-analytical methods, some levels of difficulties are still met when dealing mainly with nonlinearity of differential equations. This again creates rooms for modification of the DTM in various forms by many authors and researchers [4, 6].

#### 3.1 The Overview of the Modified Differential Transform Method (MDTM)

Let  $v(x, t)$  be an analytic function at  $(x_*, t_*)$  in a domain  $D$ , then in considering the Taylor series of  $v(x, t)$ , regard is given to some variables  $s^{ov} = t$  instead of all the variables as in the classical DTM. Thus, the MDTM of  $v(x, t)$  with respect to  $t$  at  $t_*$  is defined and denoted by:

$$V(x, h) = \frac{1}{h!} \left[ \frac{\partial^h v(x, t)}{\partial t^h} \right]_{t=t_*} \quad (3.3)$$

and as such:

$$v(x, h) = \sum_{h=0}^{\infty} M(x, h)(t - t_*)^h. \quad (3.4)$$

Equation (3.4) is called the modified differential inverse transform of  $V(x, h)$  with respect to  $t$ .

##### 3.1.1 Basic Theorems and Properties of the MDTM [6]

**Theorem 3.1.** If  $v(x, t) = \alpha v_a(x, t) \pm \beta v_b(x, t)$ , then  $V(x, h) = \alpha V_a(x, h) \pm \beta V_b(x, h)$ .

**Theorem 3.2.** If  $v(x, t) = \frac{\alpha \partial^n v_*(x, t)}{\partial t^n}$ , then  $V(x, h) = \frac{\alpha(h+n)!}{h!} V_*(x, h+n)$ .

**Theorem 3.3.** If  $v(x, t) = \frac{\alpha \partial v_*(x, t)}{\partial t}$ , then  $V(x, h) = \frac{\alpha(h+1)! V_*(x, h+1)}{h!} = \alpha(h+1) V_*(x, h+1)$ .

**Theorem 3.4.** If  $v(x, t) = \frac{p(x) \partial^n v_*(x, t)}{\partial x^n}$ , then  $V(x, h) = \frac{p(x) \partial^n V_*(x, h)}{\partial x^n}$ .

**Theorem 3.5.** If  $v(x, t) = p(x)v_*^2(x, t)$ , then  $V(x, h) = p(x) \sum_{r=0}^h V_*(x, r)V_*(x, h-r)$ .

**Theorem 3.6** (PDTM of a fractional derivative). If  $f(x, t) = D_t^\alpha w(x, t)$ , then

$$\Gamma\left(1 + \frac{k}{q}\right)F(x, k) = \Gamma\left(1 + \alpha + \frac{k}{q}\right)W(x, k + \alpha q).$$

Consequently, we have:

$$\Gamma\left(1 + \alpha + \frac{k}{q}\right)W(x, k + \alpha q) = \Gamma\left(1 + \frac{k}{q}\right)F(x, k). \quad (3.5)$$

Setting  $\alpha q = 1$  in (3.5) gives:

$$W(x, k + 1) = \frac{\Gamma(1 + \alpha k)}{\Gamma(1 + \alpha(1 + k))}F(x, k). \quad (3.6a)$$

As such, for  $w(x, t)$ ,  $\alpha$ -analytic at  $x_0 = 0$

$$w(x, t) = \sum_{h=0}^{\infty} W(x, h)t^{\frac{h}{q}} = \sum_{h=0}^{\infty} W(x, h)t^{\alpha h}. \quad (3.6b)$$

### 3.2 Analysis of the Fractional DTM

Consider the *nonlinear fractional differential equation* (NLFDE):

$$D_t^\alpha w(x, t) + L_{[x]}w(x, t) + N_{[x]}w(x, t) = q(x, t), \quad w(x, 0) = g(x), \quad t > 0, \quad (3.7)$$

where  $D_t^\alpha = \frac{\partial^\alpha}{\partial t^\alpha}$  is the fractional Caputo derivative of  $w = w(x, t)$ ; whose projected differential transform is  $W(x, h)$ ,  $L_{[.]}$  and  $N_{[.]}$  are linear and nonlinear differential operators with respect to  $x$  respectively, while  $q = q(x, t)$  is the source term.

We rewrite (3.7) as:

$$D_t^\alpha w(x, t) = -L_{[x]}w(x, t) - N_{[x]}w(x, t) + q(x, t), \quad w(x, 0) = g(x), \quad n - 1 < \alpha < n, \quad n \in \mathbb{R}. \quad (3.8)$$

Applying the inverse fractional Caputo derivative,  $D_t^{-\alpha}$  to both sides of (3.8) and with regard to (2.10) gives:

$$w(x, t) = g(x) + D_t^{-\alpha}[-L_{[x]}w(x, t) - N_{[x]}w(x, t) + q(x, t)], \quad w(x, 0) = g(x). \quad (3.9)$$

Thus, expanding the analytical and continuous function,  $u(x, t)$  in terms of fractional power series, the inverse projected differential transform of  $W(x, h)$  is given as follows:

$$w(x, t) = \sum_{h=0}^{\infty} W(x, h)t^{\alpha h} = w(x, 0) + \sum_{h=1}^{\infty} W(x, h)t^{\alpha h}, \quad w(x, 0) = g(x). \quad (3.10)$$

#### 4. Illustrative Examples and Applications

In this subsection, the proposed method is applied with some illustrative examples for the solutions of time-fractional linear Schrödinger equations resulting from (1.1) when  $\lambda = -1$ ,  $p(x) = 0$  and  $\xi = 0$ .

**Problem 4.1.** Consider the time-fractional linear Schrödinger Equation ([3, 11] for  $\alpha = 1$ ):

$$w_t^\alpha + iw_{xx} = 0 \quad \text{and} \quad w(x, 0) = e^{3ix}. \quad (4.1)$$

**Solution to Problem 4.1.** We take the *projected differential transform* (PDT) of (4.1) as follows:

$$\text{PDT} \left[ \frac{\partial^\alpha u}{\partial t^\alpha} + i \frac{\partial^2 u}{\partial x^2} = 0 \right] \quad \text{and} \quad \text{PDT}[w(x, 0) = e^{3ix}] \quad (4.2)$$

$$\Rightarrow \frac{\Gamma(1 + \alpha(1+k))}{\Gamma(1 + \alpha k)} W_{x,1+k} + i W_{x,k}'' = 0 \quad (4.3)$$

i.e.

$$W_{x,1+k} = \frac{-i\Gamma(1 + \alpha k) W_{x,k}''}{\Gamma(1 + \alpha(1+k))}, \quad k \geq 0, \quad W_{x,0} = e^{3ix} \quad \text{and} \quad W_{x,0}'' = -9e^{3ix}. \quad (4.4)$$

So, when  $k = 0$ ,

$$W_{x,1} = \frac{-\Gamma(1)}{\Gamma(1 + \alpha)} \{i W_{x,0}''\} \\ \Rightarrow W_{x,1} = \frac{9i}{\Gamma(1 + \alpha)} e^{3ix}. \quad (4.5)$$

Thus,

$$W_{x,1}'' = \frac{i(9i)^2 e^{3ix}}{\Gamma(1 + \alpha)} \quad (4.6)$$

when  $k = 1$ ,

$$W_{x,2} = \frac{-i\Gamma(1 + \alpha)}{\Gamma(1 + 2\alpha)} W_{x,1}'' \\ \Rightarrow W_{x,2} = \frac{(9i)^2}{\Gamma(1 + 2\alpha)} e^{3ix}. \quad (4.7)$$

Thus,

$$W_{x,2}'' = \frac{i(9i)^3 e^{3ix}}{\Gamma(1 + 2\alpha)} \quad (4.8)$$

when  $k = 2$ ,

$$W_{x,3} = \frac{-i\Gamma(1 + 2\alpha)}{\Gamma(1 + 3\alpha)} W_{x,2}'' \\ \Rightarrow W_{x,3} = \frac{(9i)^3}{\Gamma(1 + 3\alpha)} e^{3ix}. \quad (4.9)$$

In general, we have:

$$W_{x,n} = \frac{(9i)^n e^{3ix}}{\Gamma(1+n\alpha)} \quad (4.10)$$

therefore

$$\begin{aligned} w_{x,t} &= \sum_{h=0}^{\infty} W_{x,h} t^{\alpha h}, \quad qh = 1 \\ &= W_{x,0} + W_{x,1} t^{\alpha} + W_{x,2} t^{2\alpha} + W_{x,3} t^{3\alpha} + \dots \\ &= e^{3ix} + \frac{9it^{\alpha}}{\Gamma(1+\alpha)} e^{3ix} + \frac{(9i)^2 t^{2\alpha}}{\Gamma(1+2\alpha)} e^{3ix} + \frac{(9i)^3 t^{3\alpha}}{\Gamma(1+3\alpha)} e^{3ix} + \dots + \frac{(9i)^n t^{n\alpha}}{\Gamma(1+n\alpha)} e^{3ix} \\ &= e^{3ix} \left[ 1 + \frac{(9it^{\alpha})}{\Gamma(1+\alpha)} + \frac{(9it^{\alpha})^2}{\Gamma(1+2\alpha)} + \frac{(9it^{\alpha})^3}{\Gamma(1+3\alpha)} + \dots + \frac{(9it^{\alpha})^n}{\Gamma(1+n\alpha)} \right] \\ &= e^{3ix} \left[ \sum_{n=0}^{\infty} \frac{(9it^{\alpha})^n}{\Gamma(1+n\alpha)} \right]. \end{aligned} \quad (4.11)$$

Thus, by using Definition 2.5, we have that:

$$w_{x,t} = e^{3ix} E_{\alpha}(9it^{\alpha}). \quad (4.12)$$

**Note 4.1.** For  $\alpha = 1$ ,  $w(x,t) = e^{3i(x+3t)}$  is the exact solution as contained in [3, 11].

**Problem 4.2.** Consider the time-fractional linear Schrödinger Equation ([3, 11] for  $\alpha = 1$ ):

$$w_t^{\alpha} + iw_{xx} = 0 \quad \text{and} \quad w(x,0) = 1 + \cosh 2x. \quad (4.13)$$

**Solution to Problem 4.2.** We take the *projected differential transform* (PDT) of (4.13) as follows:

$$\text{PDT}[w_t^{\alpha} + iw_{xx} = 0] \quad \text{and} \quad \text{PDT}[w(x,0) = 1 + \cosh 2x] \quad (4.14)$$

$$\Rightarrow \frac{\Gamma(1+\alpha(1+k))}{\Gamma(1+\alpha k)} W_{x,1+k} + iW_{x,k}'' = 0, \quad W_{x,0} = 1 + \cosh 2x \quad \text{and} \quad W_{x,0}'' = 4 \cosh 2x \quad (4.15)$$

i.e

$$W_{x,1+k} = \frac{-i\Gamma(1+\alpha k)W_{x,k}''}{\Gamma(1+\alpha(1+k))}. \quad (4.16)$$

So, when  $k = 0$ ,

$$\begin{aligned} W_{x,1} &= \frac{-i\Gamma(1)}{\Gamma(1+\alpha(1+k))} W_{x,0}'' \\ \Rightarrow W_{x,1} &= \frac{4i \cosh 2x}{\Gamma(1+\alpha)}. \end{aligned} \quad (4.17)$$

Thus,

$$W''_{x,1} = \frac{-16i \cosh 2x}{\Gamma(1 + \alpha)}$$

when  $k = 1$ ,

$$W_{x,2} = \frac{-i\Gamma(1 + \alpha)}{\Gamma(1 + 2\alpha)} W''_{x,1}$$

$$\Rightarrow W_{x,2} = \frac{(4i)^2 \cosh 2x}{\Gamma(1 + 2\alpha)}. \quad (4.18)$$

Thus,

$$W''_{x,2} = \frac{(4i)^2 4 \cosh 2x}{\Gamma(1 + 2\alpha)} \quad (4.19)$$

when  $k = 2$ ,

$$W_{x,3} = \frac{-i\Gamma(1 + 2\alpha)}{\Gamma(1 + 3\alpha)} W''_{x,2}$$

$$\Rightarrow W_{x,3} = \frac{-(4i)^3 \cosh 2x}{\Gamma(1 + 3\alpha)}. \quad (4.20)$$

Therefore, the solution to Problem 4.2 is:

$$\begin{aligned} w_{x,t} &= \sum_{h=0}^{\infty} W_{x,h} t^{\alpha h}, \quad qh = 1 \\ &= W_{x,0} + W_{x,1} t^{\alpha} + W_{x,2} t^{2\alpha} + W_{x,3} t^{3\alpha} + \dots \\ &= \left\{ (1 + \cosh 2x) + \left( \frac{-4it^{\alpha} \cosh 2x}{\Gamma(1 + \alpha)} \right) + \left( \frac{(4i)^2 t^{2\alpha} \cosh 2x}{\Gamma(1 + 2\alpha)} \right) + \dots + \left( \frac{(4i)^n t^{n\alpha} \cosh 2x}{\Gamma(1 + n\alpha)} \right) \right\} \\ &= \left\{ 1 + \cosh 2x \left[ 1 + \frac{(-4it^{\alpha})}{\Gamma(1 + \alpha)} + \frac{(-4it^{\alpha})^2}{\Gamma(1 + 2\alpha)} + \frac{(-4it^{\alpha})^3}{\Gamma(1 + 3\alpha)} + \dots + \frac{(-4it^{\alpha})^n}{\Gamma(1 + n\alpha)} \right] \right\} \\ &= 1 + \cosh 2x \left[ \sum_{n=0}^{\infty} \frac{(-4it^{\alpha})^n}{\Gamma(1 + n\alpha)} \right]. \quad (4.21) \end{aligned}$$

Thus, by using Definition 2.5, we have that:

$$w_{x,t} = 1 + E_{\alpha}(-4it^{\alpha}) \cosh 2x. \quad (4.22)$$

**Remark 4.1.**  $w_{x,t} = 1 + e^{-4it} \cosh 2x$  is the exact solution of Problem 4.2 for  $\alpha = 1$ .

## 5. Concluding Remarks

We have considered in this work, both analytic and numerical solutions of time-fractional linear Schrödinger equations via a proposed semi-analytical method upon the modification of the



classical *Differential Transformation Method* (DTM). Some illustrative examples are used; the results obtained converge faster and rapidly to their exact forms. This shows that this modified version is very efficient, and reliable, as less computational work is involved, even without given up accuracy, and no linearization, perturbation or discretization is involved. The method is therefore, recommended for solving linear and nonlinear time-fractional *partial differential equations* (PDEs) with applications in other areas of applied sciences, management, and finance.

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## Competing Interests

The authors declare that they have no competing interests.

## Authors' Contributions

All the authors contributed significantly in writing this article. The authors read and approved the final manuscript.

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