Generalized Space Fractional Variable-Order Schrödinger Equation

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Abstract: The Schrödinger equation is a partial differential equation that describes how the quantum state of some physical system changes with time. In this paper we generalize Schrödinger equation by including fractional variable. We solve the evolution equation numerically via the Crank-Nicholson scheme. The stability and the convergence of numerical scheme are highlighted.

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1. Introduction

Schrödinger equation is an evolution equation that describes how the quantum state of some physical system evolves with time. It was formulated in late 1925, and published in 1926, by the Austrian physicist Erwin Schrodinger. It is used to describe several processes in mathematical physics. In the field of classical mechanics, the equation of motion is known as Newton's second law, and equivalent formulations are the Euler-Lagrange equations and Hamilton's equations All of these formulations are used to solve for the motion of a mechanical system and mathematically predict what the system will do at any time beyond the initial settings and configuration of the system. In quantum mechanics, the analogue of Newton's law is Schrödinger's equation for a quantum system (usually atoms, molecules, and subatomic particles whether free, bound, or localized). It is not a simple algebraic equation, but (in general) a linear partial differential equation. The differential equation describes the wave function of the system, also called the quantum state or state vector of the system. The equation is derived by partially differentiating the standard wave equation and substituting the relation between the momentum of the particle and the wavelength of the wave associated with the particle in De Broglie's hypothesis [2].

In the standard interpretation of quantum mechanics, the wave function is the most complete description that can be given to a physical system. Solutions to Schrödinger's evolution equation describe not only molecular, atomic, and subatomic systems, but also macroscopic systems, possibly even the whole world. Like Newton's Second law, the Schrödinger equation can be mathematically transformed into other formulations such as Wemer Heisenberg's matrix mechanics, and Richard Feynman's path integral formulation. Also like Newton's Second law, the Schrödinger evolution equation describes time in a way that is inconvenient for relativistic measures, a problem that is not as severe in matrix theory and completely absent in the path integral expressions [2]. In this paper we are interested in extending this equation by considering fractional differentiation. We are going to allow possible perturbation on our evolution systems and consider non-smooth initial conditions. This will render the problem very complex and the exact solution as in the case of the normal shrodinger equation will be almost impossible to be determined analytically. We will rely on several numerical methods in order to investigate the problem with fractional powers. We will use the theory of approximation of nonlinear operators to ascertain that our problem is well-posed. Techniques used will also include the perturbation of nonlinear operators in Banach spaces. The fractional evolution equation will display some physical characteristics that are not found in the case of integer derivatives. We will rely on Crank Nicholson methods and we will show that our numerical scheme converges to the solution of the evolution equation with fractional powers. Furthermore we will describe how our fractional solutions depend continuously upon the fractional powers of the evolution equations. This paper will be subdivided as follows: In the first part we will introduce fractional powers on the evolution equations and provide physical interpretations to the new problem [1-3]. Then we will proceed to test whether the problem will be sensitive to the changes in the initial conditions. We will then define the spaces we will work in and give a full display of the general version of our fractional evolution equation. Then we will proceed to cover the preliminaries where we will expose the methods that we are going to use in this paper, we will in particular discuss the Crank Nicholson numerical scheme and show how it can be applicable to the system under consideration. This will be the end of section 2 and we will the move to section 3 where we provide a full analysis of the given problem. In section 4 we will show that our numerical scheme converges and we will provide some numerical simulations to our problem. In section 5 we will provide a conclusion to our probl em.

2. Preliminaries

We consider the modified fractional nonrelativistic Schrödinger equation for a single particle moving in an electric field as given below.

$$i\frac{h}{2\pi}\frac{\partial^{\alpha}\Psi(x,t)}{\partial t^{\alpha}}=\left[-\frac{\left[\frac{h}{2\pi}\right]^2}{2m}\nabla^2+V(x,t)\right]\Psi(x,t)-p(x,t),$$

where m is the particle's mass, V is its potential energy, ∇^2 is the Laplacian, and Ψ is the wave-function and $p(x,t)$ is the nonlinear excitation term. The Crank–Nicholson scheme for the modified equation can be stated as follows:

(2.2)

$$\frac{\partial^{\alpha_l^{k+1}}u(x_l,t_{k+1})}{\partial t^{\alpha_l^{k+1}}}=\frac{\tau^{-\alpha_l^{k+1}}}{\Gamma(2-\alpha_l^{k+1})}\Bigg(u(x_l,t_{k+1})-u(x_l,t_k)+\sum_{j=1}^{k}\left[u(x_l,t_{k+1-j})-u(x_l,t_{k-j})\right]\left[(j+1)^{1-\alpha_l^{k+1}}-(j)^{1-\alpha_l^{k+1}}\right]+\sum_{j=1}^{k}\left[u(x_{l+1},t_{k+1-j})-u(x_{l-1},t_{k-j})\right]\left[(j+1)^{2+k}-(j)^{1+2k}\right]\Bigg).$$

Then we will proceed to cover the preliminaries where we will expose the methods that we are going to use in this paper, we will in particular discuss the Crank Nicholson numerical scheme and show how it can be applicable to the system under consideration. The Crank–Nicholson scheme for the the modified equation can be stated as follows: (2.2)

$$\frac{\partial^{\alpha_l^{k+1}}u(x_l,t_{k+1})}{\partial t^{\alpha_l^{k+1}}}=\frac{\tau^{-\alpha_l^{k+1}}}{\Gamma(2-\alpha_l^{k+1})}\Bigg(u(x_l,t_{k+1})-u(x_l,t_k)+\sum_{j=1}^{k}\left[u(x_l,t_{k+1-j})-u(x_l,t_{k-j})\right]\left[(j+1)^{1-\alpha_l^{k+1}}-(j)^{1-\alpha_l^{k+1}}\right]+\sum_{j=1}^{k}\left[u(x_{l+1},t_{k+1-j})-u(x_{l-1},t_{k-j})\right]\left[(j+1)^{2+k}-(j)^{1+2k}\right]\Bigg).$$

Now replacing equations (2.1) and (2.2 in (1.1) we obtain the following: (2.3)

$$\left[\frac{S\tau^{-\alpha_l^{k+1}}}{\Gamma(2-\alpha_l^{k+1})}\left(u(x_l,t_{k+1})-u(x_l,t_k)+\sum_{j=1}^{k}\left[u(x_l,t_{k+1-j})-u(x_l,t_{k-j})\right]\left[(j+1)^{1-\alpha_l^{k+1}}-(j)^{1-\alpha_l^{k+1}}\right]\right)\right]$$
$$=T\left[\frac{1}{2}\left(\left(\frac{u(x_{l+1},t_{k+1})-2u(x_l,t_{k+1})+u(x_{l-1},t_{k+1})}{(h)^2}\right)+\left(\frac{u(x_{l+1},t_k)-2u(x_l,t_k)+u(x_{l-1},t_k)}{(h)^2}\right)\right)\right]$$
$$+\frac{1}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_{l+1},t_{k+1})-u(x_{l-1},t_{k+1})}{2(h)}\right)+\left(\frac{u(x_{l+1},t_k)-u(x_{l-1},t_k)}{2(h)}\right)\right)\right]$$
$$+\frac{3}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_l,t_{k+1})-u(x_l,t_{k+1})}{2(h)}\right)+\left(\frac{u(x_l,t_k)-u(x_l,t_k)}{2(h)}\right)\right)\right]$$
$$+\frac{1}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_l,t_{k+1})-u(x_l,t_k)}{2(h)}\right)+\left(\frac{u(x_l,t_k)-u(x_l,t_{k-1})}{2(h)}\right)\right)\right]$$

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Now replacing equations (2.1) and (2.2 in (1.1) we obtain the following: (2.3)

$$\begin{aligned}
&\Bigg[\frac{S\,\tau^{-\alpha_l^{k+1}}}{\Gamma(2-\alpha_l^{k+1})}\Bigg(u(x_l,t_{k+1})-u(x_l,t_k)\\
&\quad+\sum_{j=1}^{k}\left[u(x_l,t_{k+1-j})-u(x_l,t_{k-j})\right]\left[(j+1)^{1-\alpha_l^{k+1}}-(j)^{1-\alpha_l^{k+1}}\right]\Bigg)\Bigg]\\
&\quad=T\Bigg[\frac{1}{2}\Bigg(\left(\frac{u(x_{l+1},t_{k+1})-2u(x_l,t_{k+1})+u(x_{l-1},t_{k+1})}{(h)^2}\right)\\
&\quad+\left(\frac{u(x_{l+1},t_k)-2u(x_l,t_k)+u(x_{l-1},t_k)}{(h)^2}\right)\Bigg)\Bigg]\\
&\quad+\frac{1}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_{l+1},t_{k+1})-u(x_{l-1},t_{k+1})}{2(h)}\right)+\left(\frac{u(x_{l+1},t_k)-u(x_{l-1},t_k)}{2(h)}\right)\right)\right]\\
&\quad+\frac{3}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_l,t_{k+1})-u(x_l,t_{k+1})}{2(h)}\right)+\left(\frac{u(x_l,t_k)-u(x_l,t_k)}{2(h)}\right)\right)\right]\\
&\quad+\frac{1}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_l,t_{k+1})-u(x_l,t_k)}{2(h)}\right)+\left(\frac{u(x_l,t_k)-u(x_l,t_{k-1})}{2(h)}\right)\right)\right]
\end{aligned}$$

The Crank–Nicholson scheme for the modified equation can be stated as follows: (2.2)

$$\begin{aligned}
&\frac{\partial^{\alpha_l^{k+1}}u(x_l,t_{k+1})}{\partial t^{\alpha_l^{k+1}}}\\
&\quad=\frac{\tau^{-\alpha_l^{k+1}}}{\Gamma(2-\alpha_l^{k+1})}\Bigg(u(x_l,t_{k+1})-u(x_l,t_k)\\
&\quad+\sum_{j=1}^{k}\left[u(x_l,t_{k+1-j})-u(x_l,t_{k-j})\right]\left[(j+1)^{1-\alpha_l^{k+1}}-(j)^{1-\alpha_l^{k+1}}\right]\\
&\quad+\sum_{j=1}^{k}\left[u(x_{l+1},t_{k+1-j})-u(x_{l-1},t_{k-j})\right]\left[(j+1)^{2+k}-(j)^{1+2k}\right]\Bigg).
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&\quad+\sum_{j=1}^{k}\left[u(x_l,t_{k+1-j})-u(x_l,t_{k-j})\right]\left[(j+1)^{1-\alpha_l^{k+1}}-(j)^{1-\alpha_l^{k+1}}\right]\\
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&\quad=T\Bigg[\frac{1}{2}\Bigg(\left(\frac{u(x_{l+1},t_{k+1})-2u(x_l,t_{k+1})+u(x_{l-1},t_{k+1})}{(h)^2}\right)\\
&\quad+\left(\frac{u(x_{l+1},t_k)-2u(x_l,t_k)+u(x_{l-1},t_k)}{(h)^2}\right)\Bigg)\Bigg]\\
&\quad+\frac{1}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_{l+1},t_{k+1})-u(x_{l-1},t_{k+1})}{2(h)}\right)+\left(\frac{u(x_{l+1},t_k)-u(x_{l-1},t_k)}{2(h)}\right)\right)\right]\\
&\quad+\frac{3}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_l,t_{k+1})-u(x_l,t_{k+1})}{2(h)}\right)+\left(\frac{u(x_l,t_k)-u(x_l,t_k)}{2(h)}\right)\right)\right]\\
&\quad+\frac{1}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_l,t_{k+1})-u(x_l,t_k)}{2(h)}\right)+\left(\frac{u(x_l,t_k)-u(x_l,t_{k-1})}{2(h)}\right)\right)\right]
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The Crank–Nicholson scheme for the modified equation can be stated as follows: (2.2)

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$$\left[\frac{S\,\tau^{-\alpha_l^{k+1}}}{\Gamma(2-\alpha_l^{k+1})}\Bigg(u(x_l,t_{k+1}) - u(x_l,t_k) + \sum_{j=1}^{k}\left[u(x_l,t_{k+1-j}) - u(x_l,t_{k-j})\right]\left[(j+1)^{1-\alpha_l^{k+1}} - (j)^{1-\alpha_l^{k+1}}\right]\Bigg)\right]$$

$$= T\left[\frac{1}{2}\left(\left(\frac{u(x_{l+1},t_{k+1}) - 2u(x_l,t_{k+1}) + u(x_{l-1},t_{k+1})}{(h)^2}\right) + \left(\frac{u(x_{l+1},t_k) - 2u(x_l,t_k) + u(x_{l-1},t_k)}{(h)^2}\right)\right)\right]$$
$$+\frac{1}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_{l+1},t_{k+1}) - u(x_{l-1},t_{k+1})}{2(h)}\right) + \left(\frac{u(x_{l+1},t_k) - u(x_{l-1},t_k)}{2(h)}\right)\right)\right]$$
$$+\frac{3}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_l,t_{k+1}) - u(x_l,t_{k+1})}{2(h)}\right) + \left(\frac{u(x_l,t_k) - u(x_l,t_k)}{2(h)}\right)\right)\right]$$
$$+\frac{1}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_l,t_{k+1}) - u(x_l,t_k)}{2(h)}\right) + \left(\frac{u(x_l,t_k) - u(x_l,t_{k-1})}{2(h)}\right)\right)\right]$$

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$$\left[\frac{S\,\tau^{-\alpha_l^{k+1}}}{\Gamma\left(2-\alpha_l^{k+1}\right)}\left(u(x_l,t_{k+1}) - u(x_l,t_k) + \sum_{j=1}^{k}\left[u(x_l,t_{k+1-j}) - u(x_l,t_{k-j})\right]\left[(j+1)^{1-\alpha_l^{k+1}} - (j)^{1-\alpha_l^{k+1}}\right]\right)\right]$$

$$= T\left[\frac{1}{2}\left(\left(\frac{u(x_{l+1},t_{k+1}) - 2u(x_l,t_{k+1}) + u(x_{l-1},t_{k+1})}{(h)^2}\right) + \left(\frac{u(x_{l+1},t_k) - 2u(x_l,t_k) + u(x_{l-1},t_k)}{(h)^2}\right)\right)\right]$$

$$+\frac{1}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_{l+1},t_{k+1}) - u(x_{l-1},t_{k+1})}{2(h)}\right) + \left(\frac{u(x_{l+1},t_k) - u(x_{l-1},t_k)}{2(h)}\right)\right)\right]$$

$$+\frac{3}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_l,t_{k+1}) - u(x_l,t_{k+1})}{2(h)}\right) + \left(\frac{u(x_l,t_k) - u(x_l,t_k)}{2(h)}\right)\right)\right]$$

$$+\frac{1}{r_l}\left[\frac{1}{2}\left(\left(\frac{u(x_l,t_{k+1}) - u(x_l,t_k)}{2(h)}\right) + \left(\frac{u(x_l,t_k) - u(x_l,t_{k-1})}{2(h)}\right)\right)\right]$$

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2. Conclusion

WE have studied a modified Schrödinger equation for a single particle moving in an electric field with a nonlinear nonhomogeneous term. We have been able to show the well-posedness of this equation and show that the solution depends continuously upon the order of the fractional derivative. The equation read as :

$$i\frac{h}{2\pi}\frac{\partial^{\alpha}\Psi(x,t)}{\partial t^{\alpha}} = \left[-\frac{\left[\frac{h}{2\pi}\right]^2}{2m}\nabla^2 + V(x,t)\right]\Psi(x,t) - p(x,t),$$

where m is the particle's mass, V is its potential energy, ∇^2 is the Laplacian, and Ψ is the wave-function and $p(x,t)$ is the nonlinear excitation term.

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