Int J Theor Phys (2010) 49: 1746–1752
DOI 10.1007/s10773-010-0354-x

A Fractional Schrödinger Equation and Its Solution

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Received: 8 February 2010 / Accepted: 8 April 2010 / Published online: 8 May 2010

Abstract This paper presents a fractional Schrödinger equation and its solution. The fractional Schrödinger equation may be obtained using a fractional variational principle and a fractional Klein-Gordon equation; both methods are considered here. We extend the variational formulations for fractional discrete systems to fractional field systems defined in terms of Caputo derivatives to obtain the fractional Euler-Lagrange equations of motion. We present the Lagrangian for the fractional Schrödinger equation of order α. We also use a fractional Klein-Gordon equation to obtain the fractional Schrödinger equation which is the same as that obtained using the fractional variational principle. As an example, we consider the eigensolutions of a particle in an infinite potential well. The solutions are obtained in terms of the sines of the Mittag-Leffler function.

Keywords Lagrangian and Hamiltonian approach

1 Introduction

Schrödinger equation represents a fundamental equation in quantum field theory. This equation is not derived from a conical set of axioms. For example Schrödinger, himself arrived at

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the equation named after him by simply inserting de Broglies relation into a classical wave equation [1]. Another attempt to derive Schrödinger equation from classical physics was using Nelson's stochastic theory [2, 3], which includes a mathematical arbitrariness of the definition of the acceleration and this has not been accepted as a basis of quantum theory. Hall and Reginatta [4], showed that the Schrödinger equation can be derived from "exactly uncertainty principle". It is worthwhile to mention that the above treatments leads to the regular kind of Schrödinger equations which are solved by the regular calculus (integro and differential equation). Fractional calculus generalized the classical calculus and it has many important applications in various fields of science and engineering [5–18]. These applications include classical and quantum mechanics, field theory, and optimal control [5–18] formulated mostly in terms of Riemann-Liouville (RL) and Caputo fractional derivatives. In contrast with RL derivative, Caputo derivative of a constant is zero, and for a fractional differential equation defined in terms of Caputo derivatives the standard boundary conditions are well defined. Therefore, this kind of fractional derivative gained importance among engineers and scientists.

The fractional Schrödinger equation (*FSE*) which contains fractional derivative terms (Caputo or Riesz derivatives) [19–21] was proposed by many authors. For example, Dong and Xu [19], solved the *FSE* using the quantum Riesz fractional operator introduced by Laskin [22, 23]. Naber [20] showed a time Caputo *FSE*. Wang and Xu [21] generalized the fractional Schrödinger equation to construct a space- time *FSE* equation. Even though of the recent progress in the filed of fractional calculus, the *FSE* was proposed without any derivation.

At this stage, it should be pointed out that several definitions have been proposed of a fractional derivative, among those Riemann-Liouville and Caputo fractional derivatives are most popular. The differential equations defined in terms of Riemann-Liouville derivatives require fractional initial conditions whereas the differential equations defined in terms of Caputo derivatives require regular boundary conditions. For this reason, Caputo fractional derivatives are popular among scientists and engineers. Accordingly, we shall use the formulations developed in [24] to obtain the Lagrangian formulation of field systems with Caputo and Riemann-Liouville fractional derivatives.

In this paper, we would like to derive Schrödinger equation from the fractional variational principle point of view and as well as from the fractional Klein-Gordon equation.

The plan of this paper is as follows:

In Sect. 2, we present the Euler-Lagrange equations for a fractional field. In Sect. 3, we define a fractional Lagrangian density function and use the theories developed in Sect. 2 to derive the *FSE*. In Sect. 4, we derive the *FSE* from a fractional Klein-Gordon equation. In Sect. 5, we present the eigensolutions of the *FSE*. Finally, Sect. 6 is devoted to our conclusions.

2 Lagrangian Formulation of Field Systems with Fractional Derivatives

In this section, we will review the Lagrangian formulation of field systems with fractional derivatives [24]. Consider a function f depending on n variables, $x_1, \dots, x_n$ defined over the domain $\Omega = [a_1, b_1] \times \cdots \times [a_n, b_n]$. Following the convention used in physics, we defined the left and the right partial Riemann-Liouville and Caputo fractional derivatives of order α_k, $0 < \alpha_k < 1$ with respect to x_k as

$$({}_+\partial_k^{\alpha} f)(x) = \frac{1}{\Gamma(1-\alpha_k)} \partial x_k \int_{a_k}^{x_k} \frac{f(x_1, \dots, x_{k-1}, u, x_{k+1}, \dots, x_n)}{(x_k - u)^{\alpha_k}} du, \tag{1}$$

$$({}_{-}\partial_k^\alpha f)(x) = \frac{-1}{\Gamma(1-\alpha_k)}\partial x_k \int_{x_k}^{b_k} \frac{f(x_1,\dots,x_{k-1},u,x_{k+1},\dots,x_n)}{(u-x_k)^{\alpha_k}}du, \tag{2}$$

$$({}_{+}^{C}\partial_k^\alpha f)(x) = \frac{1}{\Gamma(1-\alpha_k)}\int_{a_k}^{x_k} \frac{\partial_u f(x_1,\dots,x_{k-1},u,x_{k+1},\dots,x_n)}{(x_k-u)_k^{\alpha}}du, \tag{3}$$

and

$$({}_{-}^{C}\partial_k^\alpha f)(x) = \frac{-1}{\Gamma(1-\alpha_k)}\int_{x_k}^{b_k} \frac{\partial_u f(x_1,\dots,x_{k-1},u,x_{k+1},\dots,x_n)}{(u-x_k)^{\alpha_k}}du, \tag{4}$$

where $\partial x_k g$ is the partial derivatives of g with respect to the variable x_k. Here, in ${}_{+}\partial_k^\alpha$, ${}_{-}\partial_k^\alpha$, ${}_{+}^{C}\partial_k^\alpha$, and ${}_{-}^{C}\partial_k^\alpha$, the meaning of various subscripts and superscripts need to be made clear. The subscript k and the superscript α indicate that the derivative is taken with respect to the variable x_k and it is of order α_k (note that we write only α for α_k, and the subscript k to ∂ also represents the subscript to α), the subscripts $+$ and $-$ prior to the symbol ∂ represent the left and the right fractional derivatives respectively, and accordingly the limits of integrations are taken as $[a_k, x_k]$ and $[x_k, b_k]$. Further, no superscript and the superscript C prior to the symbol ∂ represent the Riemann-Liouville fractional derivative and the Caputo fractional derivative, respectively. Superscript α is necessary here as a reminder that the operator ∂^α represents a fractional derivative. When α is equal to 1, the superscript α can be neglected. Although, our aim in this section is to present the action principle for systems defined in terms of Caputo fractional derivatives, the Riemann-Liouville fractional derivatives are also defined here because they naturally arise in the formulation.

To develop the action principle for field systems described in terms of fractional derivatives, define a functional $S(\phi)$ as

$$S(\phi) = \int \mathcal{L}\big(\phi(x_k), ({}_{+}^{C}\partial_k^\alpha)\phi(x_k), ({}_{-}^{C}\partial_k^\beta)\phi(x_k), x_k\big)(dx_k), \tag{5}$$

where $\mathcal{L}(\phi(x_k), ({}_{+}^{C}\partial_k^\alpha)\phi(x_k), ({}_{-}^{C}\partial_k^\beta)\phi(x_k), x_k)$ is a Lagrangian density function. Here we have used Goldstein's [25] notation. Accordingly, x_k represents n variables x_1 to x_n, $\phi(x_k) \equiv \phi(x_1,\dots,x_1)$, $\mathcal{L}(*, {}_{+}^{C}\partial_k^\alpha, *, *) \equiv \mathcal{L}(*, {}_{+}^{C}\partial_1^\alpha, \dots, {}_{+}^{C}\partial_n^\alpha, *, *)$, $(dx_k) \equiv dx_1 \cdots dx_n$, and the integration is taken over the entire domain Ω. Other terms are defined accordingly.

To find the necessary condition for extremum of the action functional defined above, consider a one parameter family of possible functions $\phi(x_k;\epsilon)$ as follows,

$$\phi(x_k;\epsilon) = \phi(x_k;0) + \epsilon\eta(x_k), \tag{6}$$

where $\phi(x_k;0)$ is the correct function which satisfies the Hamilton's principle for the fractional system, $\eta(x_k)$ is a well-behaved function that vanishes at the endpoints, and ϵ is an arbitrary parameter. Note that $S[\phi(x_k;\epsilon)]$ is extremum at $\epsilon = 0$. Substituting (6) into (5), differentiating the resulting expression with respect to ϵ, and then setting ϵ to 0, we obtain,

$$\left.\frac{dS}{d\epsilon}\right|_{\epsilon=0} = \int \left[\frac{\partial\mathcal{L}}{\partial\phi}\eta + \sum_{k=1}^{n}\frac{\partial\mathcal{L}}{\partial({}_{+}^{C}\partial_k^\alpha\phi)}({}_{+}^{C}\partial_k^\alpha\eta) + \sum_{k=1}^{n}\frac{\partial\mathcal{L}}{\partial({}_{-}^{C}\partial_k^\beta\phi)}({}_{-}^{C}\partial_k^\beta\eta)\right](dx_k) = 0. \tag{7}$$

Finally, using the formula for integration by part [15], the fact that $\eta(x_k)$ is zero at the boundary, and a lemma from Calculus of Variations, we obtain [24]

$$\frac{\partial\mathcal{L}}{\partial\phi} + \sum_{k=1}^{n}{}_{-}\partial_k^\alpha\frac{\partial\mathcal{L}}{\partial({}_{+}^{C}\partial_k^\alpha\phi)} + \sum_{k=1}^{n}{}_{+}\partial_k^\beta\frac{\partial\mathcal{L}}{\partial({}_{-}^{C}\partial_k^\beta\phi)} = 0. \tag{8}$$

Equation (8) is the Euler-Lagrange equation for the fractional field system. For $\alpha_k, \beta_k \to 1$, (8) gives the usual Euler-Lagrange equations for classical fields.

The above treatment can also lead us to the Euler-Lagrange equations for functional defined in terms of mixed Caputo and Riemann-Liouville derivatives as

$$\frac{\partial \mathcal{L}}{\partial \phi} + \sum_{k=1}^{n} {}_{-}\partial_k^{\alpha} \frac{\partial \mathcal{L}}{\partial ({}_{+}^{C}\partial_k^{\alpha}\phi)} + \sum_{k=1}^{n} {}_{+}\partial_k^{\beta} \frac{\partial \mathcal{L}}{\partial ({}_{-}^{C}\partial_k^{\beta}\phi)}$$
$$+ \sum_{k=1}^{n} {}_{+}^{C}\partial_k^{\alpha}\phi \frac{\partial \mathcal{L}}{\partial ({}_{-}\partial_k^{\alpha})} + \sum_{k=1}^{n} {}_{-}^{C}\partial_k^{\beta}\phi \frac{\partial \mathcal{L}}{\partial ({}_{+}\partial_k^{\beta})} = 0. \tag{9}$$

3 Schrödinger Equation with Fractional Derivatives

We will now apply the Lagrangian formulation developed in Sect. 2, to derive *FSE*. We shall limit our discussion to four dimensional system (the three spatial coordinates, x_1, x_2 and x_3, and the zeroth for time, $x_0 = it$, where i is the imaginary unit. Note that we are considering the units that takes the speed of light equal to 1). The Greek indices μ, λ, ν etc. will range from 0 to 3, the Roman indices i, j, k etc. will range from 1 to 3, and unless specifically stated, the repeated indices will represent summation. Following this convention, we propose the following Lagrangian density field

$$\mathcal{L} = \frac{i\hbar^{\alpha}}{2}\left[\psi^{\dagger}\, {}_{+}^{C}\partial_0^{\alpha} + \psi\, {}_{-}\partial_0^{\alpha}\psi^{\dagger}\right] + \frac{\hbar^{2\alpha}}{2m^{\alpha}}\left[{}_{+}^{C}\partial_k^{\alpha}\psi\, {}_{-}\partial_k^{\alpha}\psi^{\dagger}\right] - V\, \psi\psi^{\dagger} \tag{10}$$

Using (9), (10), the Euler-Lagrange equations for the variable $\psi^{\dagger}$ and ψ are given as

$$\frac{\partial \mathcal{L}}{\partial \psi^{\dagger}} + {}_{+}^{C}\partial_0^{\alpha} \frac{\partial \mathcal{L}}{\partial ({}_{-}\partial_0^{\alpha}\psi^{\dagger})} + {}_{+}^{C}\partial_k^{\alpha} \frac{\partial \mathcal{L}}{\partial ({}_{-}\partial_k^{\alpha}\psi^{\dagger})} = 0, \tag{11}$$

$$\frac{\partial \mathcal{L}}{\partial \psi} + {}_{+}^{C}\partial_0^{\alpha} \frac{\partial \mathcal{L}}{\partial ({}_{-}\partial_0^{\alpha}\psi)} + {}_{+}^{C}\partial_k^{\alpha} \frac{\partial \mathcal{L}}{\partial ({}_{-}\partial_k^{\alpha}\psi)} = 0. \tag{12}$$

The *FSE* for $\psi^{\dagger}$ and ψ are obtained respectively as

$$i\hbar^{\alpha}\, {}_{+}^{C}\partial_0^{\alpha}\psi = -\frac{\hbar^{2\alpha}}{2m^{\alpha}}\, {}_{+}^{C}\partial_k^{\alpha}\, {}_{+}^{C}\partial_k^{\alpha}\psi + V\psi, \tag{13}$$

$$i\hbar^{\alpha}\, {}_{-}\partial_0^{\alpha}\psi^{\dagger} = -\frac{\hbar^{2\alpha}}{2m^{\alpha}}\, {}_{-}\partial_k^{\alpha}\, {}_{-}\partial_k^{\alpha}\psi^{\dagger} + V\psi^{\dagger}. \tag{14}$$

Equation (13) is the desired fractional Schrödinger equation with Caputo fractional derivatives and (14) is its adjoint form. For $\alpha = 1$, we obtain the standard Schrödinger equation.

In the next section, we derive the *FSE* from the fractional Klein-Gordon, find the eigen-solutions of the *FSE*, and discuss the resulting consequences.

4 Fractional Klein-Gordon and Schrödinger Equations

In this section we propose a fractional Klein-Gordon equation (FKGE) as

$$\left[({}_{+}^{C}\partial_{\mu}^{\alpha})({}_{+}^{C}\partial_{\mu}^{\alpha}) - m^{2\alpha}\right]\psi(\mathbf{x}, t) = 0. \tag{15}$$

Here we use Einstein's summation rule for μ only. Note that here we have defined the fractional derivative in the Caputo sense. For $\alpha = 1$, (15) reduces to the standard Klein-Gordon equation.

The fractional momenta operator p_α^μ is defined as

$$p_\alpha^\mu = -i\hbar^\alpha({}_{+}^{C}\partial_\mu^\alpha). \tag{16}$$

Hence, (15) can be written as

$$\left[p_\alpha^\mu p_\alpha^\mu + m^{2\alpha}\right]\psi(\mathbf{x}, t) = 0. \tag{17}$$

We obtain the following eigen value problem

$$i\hbar^\alpha\, {}_{+}^{C}\partial_0^\alpha \psi(\mathbf{x}, t) = \sqrt{\left(p_\alpha^k\right)^2 + m^{2\alpha}}\,\psi(\mathbf{x}, t). \tag{18}$$

For the non-relativistic limit, $(p_\alpha^k)^2 \ll m^{2\alpha}$, we deduce

$$i\hbar^\alpha\, {}_{+}^{C}\partial_0^\alpha \psi(\mathbf{x}, t) = m^\alpha\sqrt{1 + \frac{(p_\alpha^k)^2}{m^{2\alpha}}}\,\psi(\mathbf{x}, t) \approx \left(m^\alpha + \frac{(p_\alpha^k)^2}{2m^\alpha}\right)\psi(\mathbf{x}, t). \tag{19}$$

Equation (19) is the fractional non-relativistic wave equation, which is called as *FSE*.

5 An Example

As an explicit example of the calculation of *FSE* and its solution of a classical particle in fractional quantum mechanics, we consider one-dimensional motion of a particle in an infinite potential square well. The potential well is given by

$$V(x) = \begin{cases} 0 & \text{for } 0 < x < L, \\ \infty & \text{elsewhere.} \end{cases} \tag{20}$$

The *FSE* reads as

$$i\hbar^\alpha\, {}_{+}^{C}\partial_0^\alpha \psi(x, t) = -\frac{\hbar^{2\alpha}}{2m^\alpha}\, {}_{+}^{C}\partial_k^\alpha\, {}_{+}^{C}\partial_k^\alpha \psi(x, t), \tag{21}$$

The wave function of this particle is satisfying the boundary condition $\psi(x = 0, t) = \psi(x = L, t) = 0$. In order to solve (21), we use the method of separation of variables as

$$\psi(x, t) = \phi(x) f(t). \tag{22}$$

This leads to the following separable equations

$${}_{+}^{C}\partial_0^\alpha f(t) = \frac{-iE}{\hbar^\alpha} f(t), \tag{23}$$

$$\frac{\hbar^{2\alpha}}{2m^\alpha}\, {}_{+}^{C}\partial_k^\alpha\, {}_{+}^{C}\partial_k^\alpha \phi(x) + E\phi(x) = 0. \tag{24}$$

Solution of (23) is given as

$$f(t) = E_\alpha\left(\frac{-iE}{\hbar^\alpha} t^\alpha\right), \tag{25}$$

where E_α is the Mittag-Leffler function defined as

$$E_\alpha(z) = \sum_{n=0}^{\infty} \frac{(z)^n}{\Gamma(\alpha n + 1)}, \tag{26}$$

which satisfy the following property

$${}_{+}^{C}\partial_0^\alpha E_\alpha\big(\lambda z^\alpha\big) = \lambda E_\alpha\big(\lambda z^\alpha\big). \tag{27}$$

To obtain the solution of (24), let us define $k^2 = \frac{2m^\alpha}{\hbar^{2\alpha}} E$, then (24) gives

$${}_{+}^{C}\partial_k^\alpha {}_{+}^{C}\partial_k^\alpha \phi(x) + k^2\phi(x) = 0. \tag{28}$$

The solutions of (28) are obtained in terms of the Mittag-Leffler function as

$$\phi(x) = E_\alpha\big(ikx^\alpha\big). \tag{29}$$

Noting that, the Mittag-Leffler function can be expressed as

$$E_\alpha\big(ikx^\alpha\big) = \sum_{n=0}^{\infty} \frac{(-1)^n (kx^\alpha)^{2n}}{\Gamma(2\alpha n + 1)} + i \sum_{n=0}^{\infty} \frac{(-1)^n (kx^\alpha)^{2n+1}}{\Gamma(\alpha(2n+1)+1)}, \tag{30}$$

$$= \cos_\alpha\big(kx^\alpha\big) + i \sin_\alpha\big(kx^\alpha\big). \tag{31}$$

Since, $\psi(x = 0, t) = \psi(x = L, t) = 0$, then the solution $\phi(x)$ is given as

$$\phi(x) = \sin_\alpha\big(kx^\alpha\big), \tag{32}$$

and the eigenvalues E_n^α is given by

$$E_n^\alpha = \frac{\hbar^{2\alpha}(k_n^\alpha)^2}{2m^\alpha}, \tag{33}$$

where k_n^α are the nth roots of the sine Mittag-Leffler function $\sin_\alpha(kx^\alpha)$. One should notice that as $\alpha \to 1$, we have the eigen solutions for the regular free Schrödinger equation.

6 Conclusions

In this paper, we have presented a fractional Schrödinger equations equation. We derived the fractional Schrödinger equations equation using two methods, first using a variational principle and then from the fractional Klein-Gordon equation. We demonstrated that both methods gives the same fractional Schrödinger equation. We obtained the eigen solutions of a free particle in an infinite potential well, and the solutions are obtained in terms of the sin's of Mittag-Leffler function.

Acknowledgements One of the authors (S.M.) would like to sincerely thank the Institute of International Education, New York, NY, and the Department of Mechanical Engineering and Energy Processes (MEEP) and the Dean of Graduate Studies at Southern Illinois University, Carbondale (SIUC), IL, for providing him the financial support and the necessary facilities during his stay at SIUC. Also he would like to thank the Deanship of Graduate studies at Al-Azhar University-Gaza for support. This work is partially supported by the Scientific and Technical Research Council of Turkey.

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