Fractional-Time Schrödinger Equation: Fractional Dynamics on a Comb

Alexander Iomin

Department of Physics, Technion, Haifa, 32000, Israel

Abstract

The physical relevance of the fractional time derivative in quantum mechanics is discussed. It is shown that the introduction of the fractional time Schrödinger equation (FTSE) in quantum mechanics by analogy with the fractional diffusion $\frac{\partial}{\partial t} \rightarrow \frac{\partial^\alpha}{\partial t^\alpha}$ can lead to an essential deficiency in the quantum mechanical description, and needs special care. To shed light on this situation, a quantum comb model is introduced. It is shown that for $\alpha = 1/2$, the FTSE is a particular case of the quantum comb model. This exact example shows that the FTSE is insufficient to describe a quantum process, and the appearance of the fractional time derivative by a simple change $\frac{\partial}{\partial t} \rightarrow \frac{\partial^\alpha}{\partial t^\alpha}$ in the Schrödinger equation leads to the loss of most of the information about quantum dynamics.

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1. Introduction

In quantum physics, the fractional concept can be introduced by means of the Feynman propagator for non-relativistic quantum mechanics as for Brownian path integrals [1]. Equivalence between the Wiener and the Feynman path integrals, established by Kac [2], indicates some relation between the classical diffusion equation and the Schrödinger equation. Therefore, the appearance of the space fractional derivatives in the Schrödinger equation is natural, since both

Email address: iomin@physics.technion.ac.il (Alexander Iomin)

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the standard Schrödinger equation and the space fractional one obey the Markov process. As shown in the seminal papers [3, 4], it relates to the path integrals approach. As a result of this, the path integral approach for Lévy stable processes, leading to the fractional diffusion equation, can be extended to a quantum Feynman-Lévy measure which leads to the space fractional Schrödinger equation [3, 4].

The fractional time Schrödinger equation (FTSE) was first considered in [5], where a fractional time derivative was introduced in the quantum mechanics by analogy with the fractional Fokker-Planck equation (FFPE), by means of the Wick rotation of time $t \rightarrow -it/\hbar$. The dynamics does not correspond to the unitary transformation: the Green function is found in the form of the Mittag-Leffler function and does not satisfy Stone’s theorem on one-parameter unitary groups [6]. A generalization for the space-time fractional quantum dynamics [7, 8] was performed and a relation to the fractional uncertainty [9] was studied as well. It was also shown that the FTSE introduces new nonlinear phenomena in the semiclassical limit, and this semiclassical approach differs from those described in the framework of the standard Schrödinger equation [10].

The fractional time quantum dynamics with the Hamiltonian $\hat{H}(x)$ is described by the FTSE

$$\hat{H}\psi(x,t) = \psi(x,t),$$

where $\alpha \leq 1$. For agreement of the dimension in Eq. (1), all variables and parameters are considered dimensionless, and $\hbar$ is the dimensionless Planck constant, see also [5, 7]. For $\alpha = 1$, Eq. (1) is the ”conventional” (standard) Schrödinger equation. For $\alpha < 1$ the fractional derivative is a formal notation of an integral with a power law memory kernel of the form

$$\frac{\partial^\alpha \psi(t)}{\partial t^\alpha} = I^1_{t} - \alpha \frac{\partial \psi(t)}{\partial t} = \int_0^t \frac{(t - \tau)^{-\alpha}}{\Gamma(1 - \alpha)} \frac{\partial \psi(\tau)}{\partial \tau} d\tau,$$

which is the Caputo fractional derivative: $\frac{\partial^\alpha \psi(t)}{\partial t^\alpha} \equiv D^\alpha_0 \psi(t)$ (see Appendix).

In this paper we present an exact example where the fractional time derivative is naturally introduced and has a well defined physical meaning. We con-
Consider a case with $\alpha = 1/2$, when fractional quantum dynamics can be modelled by means of the conventional quantum mechanics in the framework of a comb model, and the FFPE for $\alpha = 1/2$ is a particular case of the quantum comb model which is a quantum counterpart of a diffusive comb model \[11, 12\]. We also show that the FTSE \[2\] is insufficient to describe a quantum process, and the appearance of the fractional time derivative leads to the loss of most of the information about quantum dynamics. The main idea is to show that Eq. \[1\] is a result of a projection of the two-dimensional $(x, y)$ comb dynamics in the one-dimensional configuration space. For diffusion, which is described by the Fokker-Planck equation, this projection is a simple integration over the $y$ space.

In quantum mechanics this projection is performed by means of the Fourier transform $\Psi(x, y) \rightarrow \tilde{\Psi}_l(x) = \mathcal{F}_y \Psi(x, y)$, where $l$ is the Fourier index. For the comb model this procedure can be treated exactly, and we shall show that Eq. \[1\] is valid only for the zero Fourier component $\psi(x) \equiv \tilde{\Psi}_0(x)$. All other components are not described by the FTSE \[1\] and lost in the framework of this equation. The diffusive comb model is an analogue of a 1d medium where fractional diffusion has been observed \[11, 12\]. It is a particular example of a non-Markovian phenomenon, explained in the framework of the so-called continuous time random walks (CTRW) \[11, 13, 14\]. This model is also known as a toy model for a porous medium used for exploring of low dimensional percolation clusters \[15\].

2. Quantum Comb Model and FTSE

A special quantum behavior of a particle on the comb can be defined as the quantum motion in the $d+1$ configuration space $(x, y)$, such that the dynamics in the $d$ dimensional configuration space $x$ is possible only at $y = 0$, and motions in the $x$ and $y$ directions commute. Therefore the quantum dynamics is described by the following Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \delta(y)\hat{H}(x)\Psi - \frac{\hbar^2}{2} \frac{\partial^2 \Psi}{\partial y^2},$$

\[3\]
where the Hamiltonian \( \hat{H} \equiv \hat{H}(\mathbf{x}) = -\frac{\hbar^2}{2} \nabla^2 + V(\mathbf{x}) \) can be different from \( c\hbar H \) in Eq. (1). It governs the dynamics with a potential \( V(\mathbf{x}) \) in the \( \mathbf{x} \) space, while the \( y \) coordinate corresponds to the 1d free motion. All the parameters and variables are dimensionless 1.

By analogy with the diffusion (classical) comb model, we are concerned with the dynamics in the \( \mathbf{x} \) space. But simple integration of the wave function over the \( y \) coordinate is not valid. Therefore, one carries out the Fourier transform in the \( y \) space \( \mathcal{F}_y \Psi(x, y, t) = \tilde{\Psi}(x, l, t) \equiv \Psi_l \), and as a result of this, Eq. (3) reads

\[
i\hbar \frac{\partial \Psi_l}{\partial t} = \hat{H}(\mathbf{x})\Psi(x, 0, t) + \frac{\hbar^2}{2} \Psi_l.
\] (4)

To obtain this equation in a closed form, one needs to express the wave function at \( y = 0 \) \( \Psi(x, 0, t) \) by the Fourier image \( \Psi_l \). To this end the Laplace transform of Eq. (3) is performed

\[
\mathcal{L}[\Psi(x, y, t)] = \tilde{\Psi}(s, y).
\]

The solution in the Laplace domain reads

\[
\tilde{\Psi}_s(x, y) = \tilde{\Psi}_s(x, 0) \exp \left[i(1+i)\sqrt{s/\hbar}|y|\right],
\] (5)

where we used \( \sqrt{2i} = (1 + i) \). Performing the Fourier transform \( \tilde{\Psi}_{s,l}(x) = \mathcal{F}[\tilde{\Psi}_s(x, y)] \) one obtains from Eq. (5)

\[
\tilde{\Psi}_{s,l}(x) = \tilde{\Psi}_s(x, 0) \mathcal{F}_y e^{i(1+i)\sqrt{s/\hbar}|y|} = \frac{2i(1+i)\sqrt{s/\hbar}}{l^2 - 2is/\hbar} \tilde{\Psi}_s(x, 0).
\] (6)

Finally, the Laplace inversion for \( \tilde{\Psi}_s(x, 0) \) determines the wave function at \( y = 0 \)

\[
\Psi(x, 0, t) = \mathcal{L}^{-1}\left[\tilde{\Psi}_{s,l}(x) \frac{l^2 - 2is/\hbar}{2i(1+i)\sqrt{s/\hbar}}\right].
\] (7)

1 Analogously to the FTSE, following Ref. 4, one introduces the Planck length \( L_P = \sqrt{\hbar G/c^3} \), time \( T_P = \sqrt{\hbar G/c^3} \), mass \( M_P = \sqrt{\hbar c/G} \), and energy \( E_P = M_P c^2 \), where \( \hbar, G, \) and \( c \) are the Planck constant, the gravitational constant and the speed of light, respectively. Therefore, quantum mechanics of a particle with mass \( m \) is described by the dimensionless units \( x/L_P \to x, y/L_P \to y, t/T_P \to t \), while the dimensionless Planck constant is defined as the inverse dimensionless mass \( \hbar = M_P/m \). Note, that the dimensionless potential is now \( V(x) \to V(x)/M_P c^2 \).
Let us, first, consider a simple case with \( l = 0 \). We have from Eq. (7) \( \tilde{\Psi}_s(x,0) = -\sqrt{s/2} \tilde{\psi}_{s,0} \). Then we define \( \tilde{\Psi}_0(x,t) = \psi(x) \), and, carrying out the Laplace transform in Eq. (4), we arrive at the definition of the Caputo fractional derivative (2) in the Laplace domain (see Appendix) \( \mathcal{L}[\partial^1/2_t \tilde{\psi}(t)] = s^{1/2} \tilde{\psi}(s) - s^{-1/2} \psi(0) \). Finally, carrying out the inverse Laplace transform and redefining \( \tilde{\mathcal{H}} \rightarrow \mathcal{H} \), one obtains the FTSE which coincides exactly with Eq. (1) for \( \alpha = 1/2 \).

Repeating this procedure for an arbitrary \( l \), one performs the Laplace transform of the term proportional to \( l^2/\sqrt{s} \) in Eq. (7). Performing simple operations of fractional calculus and taking into account Eqs. (A. 3) and (A. 9), one obtains

\[
(i\hbar) \frac{\partial^2 \Psi_l}{\partial t^2} = -\frac{l^2}{2\sqrt{2}} \partial_y \mathcal{H}(x) \Psi_l + \frac{i}{\sqrt{2\hbar}} \mathcal{H} \Psi_l + \frac{\hbar l^2}{2} \Psi_l. \tag{8}
\]

This comb FTSE describes the quantum dynamics in the \( x \) configuration space. The index \( l \) corresponds to an effective interaction of a quantum system with an additional degree of freedom, while the fractional time derivatives, with \( \alpha = 1/2 \), reflect this interaction in the form of non-Markov memory effects.

3. Green’s Function

The initial value problem with the initial condition \( \Psi(t = 0) = \Psi_0(x,y) \) is described by Green’s function. For the complete analogy with the classical comb model and fractional diffusion [12, 16], the boundary conditions for the \( y \) direction defined at infinities \( y = \pm \infty \) are \( \Psi(x,t) = \partial \Psi(x,t)/\partial y = 0 \). Using the eigenvalue problem

\[
\hat{H}(x) \psi_\lambda(x) = \lambda \psi_\lambda(x), \tag{9}
\]

we present the wave function in Eq. (3) as the expansion \( \Psi(x,y,t) = \sum_\lambda \phi_\lambda(y,t) \psi_\lambda(x) \), where \( \sum_\lambda \) also supposes integration on \( \lambda \) for the continuous spectrum. For the fixed \( \lambda \) we arrive at the dynamics of a particle in the \( \delta \) potential

\[
(i\hbar) \frac{\partial \phi_\lambda}{\partial t} = -\frac{\hbar l^2}{2} \frac{\partial^2 \phi_\lambda}{\partial y^2} + \lambda \delta(y) \phi_\lambda. \tag{10}
\]
Taking into account that the Green function of Eq. (3) has the spectral decomposition,

\[ G(x, y, t; x', y') = \sum_{\lambda} G_{\lambda}(y, t; y') \psi_{\lambda}^*(x) \psi_{\lambda}(x'), \]

we obtain that the Schrödinger equation for the Green function \( G_{\lambda}(y, t; y') \) reads

\[ \frac{\tilde{\hbar} \partial G_{\lambda}}{\partial t} = -\frac{\tilde{\hbar}^2}{2} \frac{\partial^2 G_{\lambda}}{\partial y^2} + \lambda \delta(y) G_{\lambda} + i \tilde{\hbar} \delta(y) \delta(t). \]  

(11)

Here the initial condition is already taken into account. The Green function for this Schrödinger equation has been obtained in [17, 19], for free boundary conditions at infinities. For the chosen boundary conditions it is instructive to employ Eq. (5) in the Laplace domain. Then replacing the eigenvalues \( \lambda \) by the Hamiltonian \( \hat{H}(x) \), one obtains the Green’s function in the form of the inverse Laplace transform

\[ G[\hat{H}(x), y, t] = L^{-1} \left[ \frac{i \tilde{\hbar} e^{i(1+i)\sqrt{s/\tilde{\hbar}|y|}}}{\hat{H}(x) - i(1+i)\sqrt{s/\tilde{\hbar}|y|}} \right]. \]  

(12)

One performs the inverse Laplace transform, using the following presentation for the denominator

\[ \int_0^\infty \exp \left\{ -u[\hat{H}(x) - i(1+i)\sqrt{\tilde{\hbar}s}] \right\} du. \]

This presentation is valid for any spectrum \( \lambda \) due to the second term in the exponential. Therefore, the Green function reads

\[ G[\hat{H}(x), y, t] = \frac{\sqrt{\tilde{\hbar}}}{\sqrt{2\pi i}} \int_0^\infty (|y|+\tilde{\hbar}^2 u) \exp \left[ -u[\hat{H}(x) - \frac{i(|y|+\tilde{\hbar}^2 u)^2}{2\tilde{\hbar}}] \right] du. \]

(13)

Using the Fourier transform for the exponential

\[ \exp \left[ \frac{i(|y|+\tilde{\hbar}^2 u)^2}{2\tilde{\hbar}} \right] = \sqrt{\frac{\tilde{\hbar}}{2\pi i}} \int_{-\infty}^{\infty} e^{i\tilde{\hbar} \xi^2/2} e^{-i\xi(|y|+\tilde{\hbar}^2 u)} d\xi, \]

one presents the Green function in the following convenient form

\[ G(x, y, t; x') = \frac{\hbar}{2\pi i} \int_{-\infty}^{\infty} \left\{ e^{i\tilde{\hbar} \xi^2/2} \left( i \frac{\partial}{\partial \xi} \right) \int_0^\infty \exp \left[ -u\hat{H}(x) - i\xi(|y|+\tilde{\hbar}^2 u) \right] du \right\} d\xi. \]

(14)

This expression is convenient for further analysis in the framework of the path integral.
4. Path Integral Presentation

As an example, it is instructive to consider a free particle, because it has a straightforward relation to the original diffusive comb model [11, 12]. Therefore, we find the Green function along the structure x axis in the coordinate space

\[ G(x, y, t; x') = \langle x'|G[\hat{H}(x), y, t]|x \rangle \]

for a free particle of a unit mass with the Hamiltonian \( \hat{H} = \frac{p^2}{2} \). Expressing the exponential \( \langle x'|e^{-u\hat{H}}|x \rangle \) in the path integral form, \( \frac{1}{\sqrt{2\pi \tilde{h}^2 u}} e^{-\frac{(x-x')^2}{2\tilde{h}^2 u}} \), one obtains from Eq. (14):

\[ G(x, y, t; x') = \frac{1}{t} \sqrt{\frac{2\pi}{(2\pi)^3}} \int_{-\infty}^{\infty} \left\{ e^{i\tilde{ht}\xi^2/2} \left( \frac{\partial}{\partial \xi} \right) \int_{0}^{\infty} \exp \left[ -\left( \frac{x-x'}{\tilde{h}^2 u} - i\xi(|y| + \tilde{h}^2 u) \right) \frac{du}{\sqrt{u}} \right] d\xi \right\}.
\]

Integration over complex “time” \( u \) yields the following expression

\[ I(A, B) = \int_{0}^{\infty} \exp \left[ -\frac{A}{u} - Bu \right] \frac{du}{\sqrt{u}}, \quad (16)\]

where \( A = \frac{(x-x')^2}{2\tilde{h}^2} \) and \( B = -i\tilde{h}^2 \). Differentiation of Eq. (16) with respect to \( A \) and \( B \) yields the equation \( \frac{\partial^2 I(A, B)}{\partial A \partial B} = I(A, B) \). A solution of this equation is

\[ I(A, B) = \sqrt{\frac{\pi}{4\sqrt{AB}}} \exp[2\sqrt{AB}]. \]

Performing this integration, we arrive at integration over \( \xi \) that is carried out in the stationary phase approximation for the long time asymptotics \( \tilde{h}t \gg 1 \).

This yields

\[ \int_{-\infty}^{\infty} F(\xi) \exp[i\tilde{h}t\xi^2 - i\xi|y|] \approx \sqrt{\frac{\pi}{i\tilde{h}t}} F(\xi_0) \exp \left[ -i\frac{y^2}{4\tilde{h}t} \right], \quad (17)\]

where the stationary point is \( \xi_0 = \frac{|u|}{2\tilde{h}t} \). Taking integration (17) into account, we finally, obtain the Green function in the form

\[ G(x, y, t; x') \approx \frac{i^{1/4}}{4\sqrt{\pi t}} \left[ -\frac{i}{4} \left( \frac{|u|}{\tilde{h}t} \right)^{-\frac{3}{2}} + |y| - |x-x'| \sqrt{\frac{i\tilde{h}t}{2|y|}} \right] \times \exp \left[ -i\frac{y^2}{2\tilde{h}t} + i\sqrt{|i|y|/\tilde{h}|x-x'|} \right]. \]

This solution also satisfies the boundary conditions at \( x, y = \pm\infty \), where the Green function vanishes.
5. Conclusion

Physical relevance of the fractional time derivative in quantum mechanics is discussed. It is shown that the introduction of the fractional time Schrödinger equation in quantum mechanics by the change $\frac{\partial}{\partial t} \rightarrow \frac{\partial}{\partial \alpha t^\alpha}$ by an analogy with the fractional diffusion can lead to essential deficiency of the quantum mechanical description, and needs special care. To shed light on this situation, a quantum comb model is introduced. We observed that the fractional time derivative, at least for $\alpha = 1/2$, reflects an effective interaction of a quantum system with an additional degree of freedom. In the classical diffusion comb model, diffusion in the $y$ direction is responsible for traps that lead to subdiffusion along the $x$ structure axis, and this phenomenon is described by the time fractional derivative $\frac{\partial^\alpha}{\partial t^\alpha}$. This description in the framework of the fractional Fokker-Planck equation is identical to the diffusion comb model [12, 16]. In the quantum case the situation differs essentially from fractional diffusion. First of all, the quantum comb model (3) and the FTSE (1) are not identical. As shown here, the FTSE is an equation only for the zero Fourier component of the wave function, and this equation is insufficient to describe the complete dynamics in the $x$ space of the system. The FTSE is a particular and limiting case of the comb fractional time Schrödinger equation (8), obtained here, which describes the quantum dynamics in the $x$ configuration space, and the Fourier index $l$ corresponds to an effective interaction of the quantum Hamiltonian $\hat{H}(x)$ with an additional degree of freedom, while the fractional time derivatives, with $\alpha = 1/2$, reflect this interaction in the form of non-Markov memory effects. This equation can be readily solved by the Laplace transform and using the eigenvalue problem $\hat{H}(x)\psi_\lambda(x) = \lambda\psi_\lambda(x)$. Nevertheless, we obtained the Green function directly from the quantum comb model of Eq. (3) in a form suitable for the paths integral presentation. An example of $\hat{H}(x)$ that corresponds to a free particle is considered. Note also that this expression for the Green function is also suitable for the semiclassical treatment of more complicated Hamiltonian systems $\hat{H}(x)$.

In conclusion, we admit that this exact example shows that the FTSE (1) is
insufficient to describe a quantum process, and the appearance of the fractional time derivative by a simple change $\frac{\partial}{\partial t} \rightarrow \frac{\partial}{\partial t^\alpha}$ in the Schrödinger equation leads to loss of most of the information about quantum dynamics.

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Appendix: Fractional Calculus Tools

Fractional derivation was developed as a generalization of integer order derivatives and is defined as the inverse operation to the fractional integral. Fractional integration of the order of $\alpha$ is defined by the operator (see e.g., [14, 20, 21])

\[ aI^\alpha_x f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x f(y)(x-y)^{\alpha-1} dy, \]  

(A. 1)

where $\alpha > 0$, $x > a$ and $\Gamma(z)$ is the Gamma function. Therefore, the fractional derivative is defined as the inverse operator to $aI^\alpha_x$, namely $aD^\alpha_x f(x) = aI^{\alpha}_{-\alpha} f(x)$ and $aI^\alpha_x = aD^{-\alpha}_x$. Its explicit form is

\[ aD^\alpha_x f(x) = \frac{1}{\Gamma(-\alpha)} \int_a^x f(y)(x-y)^{-1-\alpha} dy. \]  

(A. 2)

For arbitrary $\alpha > 0$ this integral diverges, and as a result of this a regularization procedure is introduced with two alternative definitions of $aD^\alpha_x$. For an integer $n$ defined as $n - 1 < \alpha < n$, one obtains the Riemann-Liouville fractional derivative of the form

\[ aD^{\alpha}_{RL} f(x) = \frac{d^n}{dx^n} aI^{n-\alpha}_x f(x), \]  

(A. 3)

and fractional derivative in the Caputo form (see also [22])

\[ aD^{\alpha}_C f(x) = aI^{n-\alpha}_x f^{(n)}(x), \quad f^{(n)}(x) \equiv \frac{d^n}{dx^n} f(x). \]  

(A. 4)

There is no constraint on the lower limit $a$. For example, when $a = 0$, one has

\[ aD^{\alpha}_{RL} x^\beta = \frac{x^{\beta-\alpha}\Gamma(\beta + 1)}{\Gamma(\beta + 1 - \alpha)}. \]
We also have

\[ aD_0^\alpha f(x) = aD_0^{\alpha\RL} f(x) - \sum_{k=0}^{n-1} f^{(k)}(0^+) \frac{x^{k-\alpha}}{\Gamma(k - \alpha + 1)}, \]

and \( aD_0^\alpha[1] = 0 \), while \( aD_0^{\alpha\RL}[1] = x^{-\alpha}/\Gamma(1 - \alpha) \). When \( a = -\infty \), the resulting Weyl derivative is

\[ -\infty W^\alpha \equiv -\infty D_0^\alpha W = -\infty D_0^{\alpha\RL} = -\infty D_0^\alpha. \quad (A. 5) \]

One also has \( -\infty D_0^\alpha e^x = e^x \). This property is convenient for the Fourier transform

\[ \mathcal{F}[-\infty W^\alpha f(x)] = (ik)^\alpha \tilde{f}(k), \quad (A. 6) \]

where \( \mathcal{F}[f(x)] = \tilde{f}(k) \). This fractional derivation with the fixed low limit is also called the left fractional derivative. However, one can introduce the right fractional derivative, where the upper limit \( a \) is fixed and \( a > x \). For example, the right Weyl derivative is

\[ W_\infty^\alpha f(z) = \frac{1}{\Gamma(-\alpha)} \int_x^\infty \frac{f(y)dy}{(y-x)^{1+\alpha}}. \quad (A. 7) \]

The Laplace transform of the Caputo fractional derivative yields

\[ \mathcal{L}[aD_0^{\alpha\RL} f(x)] = s^\alpha \tilde{f}(s) - \sum_{k=0}^{n-1} f^{(k)}(0^+) s^{\alpha-1-k}, \quad (A. 8) \]

where \( \mathcal{L}[f(x)] = \tilde{f}(s) \), which is convenient for the present analysis, where the initial conditions are imposed in terms of integer derivatives. We also use here a convolution rule for \( 0 < \alpha < 1 \)

\[ \mathcal{L}[I_0^\alpha f(x)] = s^{-\alpha} \tilde{f}(s). \quad (A. 9) \]

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