

## Fractional-time quantum dynamics

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Application of the fractional calculus to quantum processes is presented. In particular, the quantum dynamics is considered in the framework of the fractional time Schrödinger equation (SE), which differs from the standard SE by the fractional time derivative:  $\partial/\partial t \rightarrow \partial^\alpha/\partial t^\alpha$ . It is shown that for  $\alpha=1/2$  the fractional SE is isospectral to a comb model. An analytical expression for the Green's functions of the systems are obtained. The semiclassical limit is discussed.

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Application of the fractional calculus to quantum processes is a new and fast developing part of quantum physics which studies nonlocal quantum phenomena [1–10]. It aims to explore nonlocal effects found for either long-range interactions or time-dependent processes with many scales [3,11–16]. Fractional calculus with a variety of applications [3,12–19], including applications to quantum processes [2,4,7–10,20–23], is a well-developed and well-established field that was extensively reviewed.

The concept of differentiation of noninteger orders rises from works of Leibniz, Liouville, Riemann, Grunwald, and Letnikov, see, e.g., [18,19]. Its application is related to random processes with power-law distributions. This corresponds to the absence of characteristic average values for processes exhibiting many scales [13,24]. A continuously increasing list of applications in many sciences has developed: it includes material science [12,25], physical kinetics [14], and anomalous transport theory with a variety of applications in solid-state physics [11,13,24] and in nonlinear dynamics [14,15].

In quantum physics, the fractional concept can be introduced by means of the Feynman propagator for nonrelativistic quantum mechanics as for Brownian path integrals [26]. Equivalence between the Wiener and the Feynman path integrals, established by Kac [27], indicates some relation between the classical diffusion equation and the Schrödinger equation. Therefore, an appearance of the space fractional derivatives in the Schrödinger equation is natural since both the standard Schrödinger equation and the space fractional one obey the Markov process. As shown in the seminal papers [2,7], it relates with 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 (FSE) [2,7].

A fractional time derivative can be introduced in the quantum mechanics by analogy with the fractional Fokker-Planck equation (FFPE), as well, by means of the Wick rotation of time  $t \rightarrow -it/\hbar$  [8]. However its physical interpretation is still vague: for example, a phase of the wave function as well as the semiclassical approximation should be understood. The fractional time Schrödinger equation was first considered in [8]. Its generalization to space-time fractional quantum dynamics [20,21] was performed and a relation to the fractional uncertainty [22] was studied as well. Exact solutions were also obtained for the time fractional nonlinear Schrödinger equation [28]. It is worth noting that,

contrary to the space fractional derivative, the fractional time Schrödinger equation describes non-Markovian evolution with a memory effect.

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

$$(i\hbar)^\alpha \frac{\partial^\alpha \psi(\mathbf{x}, t)}{\partial t^\alpha} = \hat{H} \psi(\mathbf{x}, t), \quad (1)$$

where  $\alpha \leq 1$ . For concordance of the dimension in Eq. (1) all variables and parameters are considered dimensionless, and  $\tilde{\hbar}$  is the dimensionless Planck constant, see also [8,20]. 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 [29]

$$\frac{\partial^\alpha \psi(t)}{\partial t^\alpha} \equiv I_t^{1-\alpha} \frac{\partial \psi(t)}{\partial t} = \int_0^t \frac{(t-\tau)^{-\alpha}}{\Gamma(1-\alpha)} \frac{\partial \psi(\tau)}{\partial \tau} d\tau, \quad (2)$$

which is known as the Caputo fractional derivative [17], and  $\Gamma(z)$  is a gamma function. This definition makes it possible to carry out the Laplace transform of the fractional derivative. Introducing the Laplace image  $\tilde{\psi}(s) = \hat{\mathcal{L}} \psi(t)$ , one obtains

$$\hat{\mathcal{L}} \left[ \frac{\partial^\alpha \psi(t)}{\partial t^\alpha} \right] = s^\alpha \tilde{\psi}(s) - s^{\alpha-1} \psi(0). \quad (3)$$

Another interesting property of the FSE is time evolution in the form of the Mittag-Leffler function. For the time-independent Hamiltonian, the eigenvalue equation (with corresponding boundary conditions) is  $H \phi_\lambda = \lambda \phi_\lambda$ . Therefore one obtains the Green's function in the term of the Mittag-Leffler function  $E_{\alpha,1}(z) \equiv E_\alpha(z) = \sum_{j=0}^{\infty} z^j / \Gamma(j\alpha + 1)$  [8,13]:

$$G(\mathbf{x}, t; \mathbf{x}') = \sum_{\lambda} \phi_{\lambda}^*(\mathbf{x}') \phi_{\lambda}(\mathbf{x}) E_{\alpha} \left( \lambda \left[ \frac{t}{i\hbar} \right]^{\alpha} \right), \quad (4)$$

which is a fractional generalization of the Green's function. It is worth noting that this solution for the Green's function in the form of the Mittag-Leffler function does not satisfy Stone's theorem on one-parameter unitary groups [30].

In the general case, when the eigenvalue problem cannot be solved rigorously, the analysis of the fractional Green's function meets serious deficiencies. For a example, the semiclassical analysis of the FSE leads to a much more complicated form for the wave function than the physically trans-

parent expression for the local wave function  $\psi(x,t) \sim e^{iS(t,x)/\hbar}$ . Moreover, the classical action  $S(t,x)$  is not defined anymore for the FSE. Another important question could be addressed to both FSE (1) and Eq. (4): for the fractional Fokker-Planck equation, the fractional time derivative is an asymptotic description of a continuous time random walk, and it describes subdiffusion. Therefore, what is the physical meaning of the fractional time derivative in quantum processes when a concept of a multiscale continuous time random walk is absent?

To shed light on this situation, we consider a case with  $\alpha=1/2$  when fractional quantum dynamics can be modeled by means of the conventional quantum mechanics in the framework of a comb model. The comb model is an analog of a one-dimensional (1D) medium where fractional diffusion has been observed [31,32]. It is a particular example of a non-Markovian phenomenon, explained in the framework of a so-called continuous time random walk [13,24,31]. This model is also known as a toy model for a porous medium used for exploration of low dimensional percolation clusters [33].

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

$$i\hbar \frac{\partial \Psi}{\partial t} = \delta(y) \hat{H}(\mathbf{x}) \Psi - \frac{\hbar^2}{2} \frac{\partial^2 \Psi}{\partial y^2}, \quad (5)$$

where the Hamiltonian is the same as in Eq. (1) and  $\hat{H} = \hat{H}(\mathbf{x}) = (\hbar^2/2) \nabla^2 + V(\mathbf{x})$  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 [34]. We will study an initial value problem with the initial condition  $\Psi(t=0) = \Psi_0(\mathbf{x}, y)$ . It is worth noting that the semiclassical asymptotic expansion in  $\hbar$  of the wave function is impossible since the  $\delta$  potential in the  $y$  direction “cannot have a sensible semiclassical limit” [35,36] and degrees of freedom cannot easily be separated. Using the eigenvalue problem

$$\hat{H}(\mathbf{x}) \psi_\lambda(\mathbf{x}) = \lambda \psi_\lambda(\mathbf{x}), \quad (6)$$

we present the wave function in Eq. (5) as the expansion  $\Psi(\mathbf{x}, y, t) = \sum_\lambda \phi_\lambda(y, t) \psi_\lambda(\mathbf{x})$ , 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

$$i\hbar \frac{\partial \phi_\lambda}{\partial t} = \frac{\hbar^2}{2} \frac{\partial^2 \phi_\lambda}{\partial y^2} + \lambda \delta(y) \phi_\lambda. \quad (7)$$

The Green’s function for this Schrödinger equation has been obtained in [35,37];

$$G_\lambda(y, t; y') = G_0(y, t; y') + \left[ -\frac{\lambda}{\hbar} \int_0^\infty du G_0(|y| + |y'| + u, t; 0) \exp(-u\lambda/\hbar) \right], \quad (8)$$

where  $G_0(y, t; y') = 1/\sqrt{2\pi i \hbar t} \exp[i(y-y')^2/2\hbar t]$  is the free particle propagator. Using this result, we obtain for the wave function of Eq. (5)

$$\Psi(\mathbf{x}, y, t) = \int dy' G_0(y, t; y') \Psi_0(\mathbf{x}, y') + \left[ - \int dy' du G_0(|y| + |y'| + u, t; 0) e^{-u\lambda/\hbar} \frac{\hat{H}}{\hbar} \Psi_0(\mathbf{x}, y') \right]. \quad (9)$$

Now our aim is to compare the Green’s function of this solution with the one of Eq. (4). Contrary to fractional diffusion, where the FFPE with  $\alpha=1/2$  is identical to the comb model, the FSE (1) is not identical to the quantum comb model of Eq. (5). Nevertheless, the models have some features in common, namely, there are the some singularities of the Green’s functions which determine the spectrum. To show this, let us present both Eqs. (4) and (9) in the form of the inverse Laplace transform. For simplicity we consider the one-dimensional  $x$  space. First, we consider Eq. (9). Presenting the wave function as the Laplace inversion and carrying out integration on  $u$  in the second part, we have for the Green’s function

$$\hat{G}(x, y, t; x', y') = G_0(y, t; y') \delta(x - x') - \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} \sum_\lambda \frac{\exp(st + \sqrt{-2is/\hbar}(|y| + |y'|)) ds}{\sqrt{i\hbar s}(\sqrt{-2is/\hbar} - \lambda/\hbar)} \Psi_\lambda^*(x') \Psi_\lambda(x), \quad (10)$$

where the eigenvalue problem of Eq. (6) is used. Using integral presentation of the Mittag-Leffler function [38], we rewrite the Green’s function of the FSE in Eq. (4) as follows:

$$G(x, t; x') = \sum_\lambda \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} \frac{\psi_\lambda^*(x') \psi_\lambda(x) e^{st} ds}{\sqrt{s}(\sqrt{s} - \lambda/\sqrt{2i\hbar})}. \quad (11)$$

Therefore, disregarding the free propagator in Eq. (10), one obtains the same spectral properties of both systems since the spectral decompositions of the evolution operators are the same.

In what follows we consider the dynamics of the FSE in the framework of the Green’s function [Eq. (11)]. There are two contributions to this integral from a pole at  $s_0 = \lambda^2/2i\hbar$

and from a branch point at  $s=0$  with a branch cut from  $-\infty$ . Carrying out this integration (see [8]), we present the wave function in the following operator form [see Eq. (4)]:

$$\begin{aligned} \psi(x,t) &= E_{1/2} \left( \hat{H} \left[ \frac{t}{2i\tilde{h}} \right]^{1/2} \right) \psi_0(x) \\ &= \left[ 2e^{-i\hat{H}^2 t/2\tilde{h}} - \frac{\hat{H}\sqrt{2i\tilde{h}}}{\pi} \int_0^\infty \frac{e^{-rt} dr}{\sqrt{r(2i\tilde{h}r + \hat{H}^2)}} \right] \psi_0(x). \end{aligned} \quad (12)$$

It consists of two parts, the oscillatory one and the decay in time. This expression is convenient for studying the large time asymptotic  $t \gg 1$  when the decay term can be neglected.

The decay term is of the order of  $\sim \sqrt{\tilde{h}}$  and can be neglected in the semiclassical limit  $\tilde{h} \rightarrow 0$  as well. The evolution of the semiclassical wave function  $\psi_{\text{scl}}(x,t) = \psi(x,t)/2$  is due to the oscillatory term with the Hamiltonian  $\mathcal{H}_{\text{scl}} = \hat{H}^2/2$ . This semiclassical dynamics is essentially nonlinear.

As an example of the Hamiltonian, we take the same operator considered in Ref. [32] for Lévy walks on the comb. It is

$$\hat{H} = -2i\tilde{h}\omega \left( x \frac{\partial}{\partial x} + \frac{1}{2} \right), \quad (13)$$

where  $\omega$  is a dimensionless frequency. In the framework of the Fokker-Planck equation, it corresponds to the inhomogeneous convection. Here this Hamiltonian describes a one-dimensional motion near a hyperbolic point, and it has been studied in connection with the Riemann zeros and eigenvalue asymptotics [39–41], scattering of the inverted harmonic oscillator [42], and eigenstates near a hyperbolic point [43].

The standard quantum dynamics with the Hamiltonian of Eq. (13) is linear and coincides with semiclassical one. The wave functions and expectation values are well-behaved values. For example, evolution of the wave function is an explicit function of the initial condition

$$\Psi_{\hat{H}}(x,t) = e^{-i\hat{H}t/\tilde{h}} \psi_0(x) = e^{-t/2\tilde{h}} \psi_0(xe^{-t/\tilde{h}}), \quad (14)$$

and defining  $y = xe^{-t/\tilde{h}}$ , one obtains for the second moment

$$\langle \hat{x}^2(t) \rangle = e^{2t/\tilde{h}} \int y^2 \psi_0^*(y) \psi_0(y) dy < \infty. \quad (15)$$

Contrary to this, the semiclassical dynamics of the system described by the FSE (and on the comb, respectively) is non-

linear and the expectation values can diverge for the same initial condition  $\psi_0(x)$ :

$$\psi_{\text{scl}}(x,t) = \sqrt{\frac{\tilde{h}}{2\pi it}} \int_{-\infty}^{\infty} du e^{i\tilde{h}u^2/2t - u^2} \psi_0(e^{-u}x), \quad (16)$$

$$\langle \hat{x}^2(t) \rangle = \int y^2 \psi_0^*(y) \psi_0(y) dy. \quad (17)$$

For example, for the Gaussian initial condition  $\psi_0(x) = e^{-x^2/\sqrt{\pi}}$  the expectation value in Eq. (17) diverges at  $t = \tilde{h}\pi/4$ . This result was observed in Ref. [44] where the quantum motion near the separatrix was studied.

We can conclude 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. As already mentioned, the  $y$  direction in the comb model was introduced to model the time fractional derivative  $\partial^{1/2}/\partial t^{1/2}$  by analogy with the continuous time random walk, where delay times of escapes from the motion in the  $x$  space are distributed by the power law  $\sim t^{-3/2}$  [31–33]. It is worth noting that in the subdiffusive case with  $\alpha=1/2$  the fractional Fokker-Planck equation is identical to the diffusion comb model [32]. In the quantum case the situation differs essentially from fractional diffusion. First of all, the quantum comb model and FSE are not identical. As shown here the systems are isospectral: they have the same singularities for the Green's functions. In the quantum case a “random entrapping” is due to the reversible leakage probability of the wave function. The decay term in the Green's function of Eq. (12) is the specific property of the FSE which violates the Hermitian property of Hamiltonian  $\hat{H}$ . For the quantum comb, the  $y$  space is the environment. In this connection, an interesting question arises: how does the time fractional derivative, which describes a specific interaction with the environment, relate to a possible description in the framework of the Lindblad equation [45,46]? Both the quantum motion on the comb and the FSE introduce nonlinear phenomena in the semiclassical limit, and this semiclassical approach differs from one described in the framework of the standard Schrödinger equation.

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- [29] 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., [3,13–15,18,19])  ${}_a I_x^\alpha f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x f(y)(x-y)^{\alpha-1} dy$ , where  $\alpha > 0$ ,  $x > a$ , and  $\Gamma(z)$  is the Gamma function. Therefore, the fractional derivative is the inverse operator to  ${}_a I_x^\alpha$  as  ${}_a D_x^\alpha f(x) = {}_a I_x^{-\alpha}$  and  ${}_a I_x^\alpha = {}_a D_x^{-\alpha}$ . Its explicit form is  ${}_a D_x^{-\alpha} = \frac{1}{\Gamma(-\alpha)} \int_a^x f(y)(x-y)^{-1-\alpha} dy$ . For arbitrary  $\alpha > 0$  this integral diverges, and as a result of a regularization procedure, there are two alternative definitions of  ${}_a D_x^{-\alpha}$ . For an integer  $n$  defined as  $n-1 < \alpha < n$ , one obtains the Riemann-Liouville fractional derivative of the form  ${}_a D_{RL}^\alpha f(x) = (d^n/dx^n) {}_a I_x^{n-\alpha} f(x)$  and fractional derivative in the Caputo form  ${}_a D_C^\alpha f(x) = d^n/dx^n f(x)$ . [For  $n=1$  see Eq. (2).] There is no constraint on the lower limit  $a$ . For example, when  $a=0$ , one has  ${}_0 D_{RL}^\alpha x^\beta = x^{\beta-\alpha} \Gamma(\beta+1)/\Gamma(\beta+1-\alpha)$  and  ${}_a D_C^\alpha f(x) = {}_0 D_{RL}^\alpha f(x) - \sum_{k=0}^{n-1} f^{(k)}(0^+) x^{k-\alpha}/\Gamma(k-\alpha+1)$ , and  ${}_a D_C^\alpha[1] = 0$ , while  ${}_0 D_{RL}^\alpha[1] = x^{-\alpha}/\Gamma(1-\alpha)$ .
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