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Comb Model: Non-Markovian versus Markovian

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Abstract: Combs are a simple caricature of various types of natural branched structures, which belong to the category of loopless graphs and consist of a backbone and branches. We study two generalizations of comb models and present a generic method to obtain their transport properties. The first is a continuous time random walk on a many dimensional $m + n$ comb, where m and n are the dimensions of the backbone and branches, respectively. We observe subdiffusion, ultra-slow diffusion and random localization as a function of n. The second deals with a quantum particle in the $1 + 1$ comb. It turns out that the comb geometry leads to a power-law relaxation, described by a wave function in the framework of the Schrödinger equation.

Keywords: comb model; continuous time random walk; fractional Fokker-Planck equation; subdiffusion; Fox H-function; fractional Schrödinger equation

1. Introduction

We consider realistic models of non-Markovian transport that takes place in a comb geometry. A comb model is a simple caricature of various types of natural branched structures, see Figure 1, where random walks on comb structures provide a geometrical explanation of anomalous diffusion. The comb model was introduced to understand anomalous transport in percolation clusters [1–3]. Now, comb-like models are widely employed to describe various experimental applications. These models have proven useful for describing the transport along spiny dendrites [4–6], diffusion of drugs in the circulatory system [7], anomalous diffusion in cold atoms [8,9], and diffusion in crowded media [10,11] and many other interdisciplinary applications. Another example is the occupation time statistics for random walkers on combs where the branches can be regarded as independent complex structures, namely fractal or other ramified branches [12]. In this context we include also a Langevin approach for fractional Brownian walks [13,14]. Finally, we would like to mention studies to understand the diffusion mechanism along a variety of branched systems where scaling arguments, verified by numerical simulations, have been able to predict how the mean squared displacement (MSD) grows with time [15]. An extended review of a variety of realizations of comb models can be found in Reference [16].

We consider two realizations of non-Markovian dynamics in comb models. The first model is continuous time random walks on a many dimensional $m + n$ comb, where m and n are dimensions of the backbone and branches (or fingers), respectively. We observe subdifusion, ultra-slow diffusion and random localization as a function of n. The second example concerns a quantum particle in the 1 + 1 comb. Here we obtain that the comb geometry leads to a power-law relaxation, described by a wave function in the framework of the Schrödinger equation.

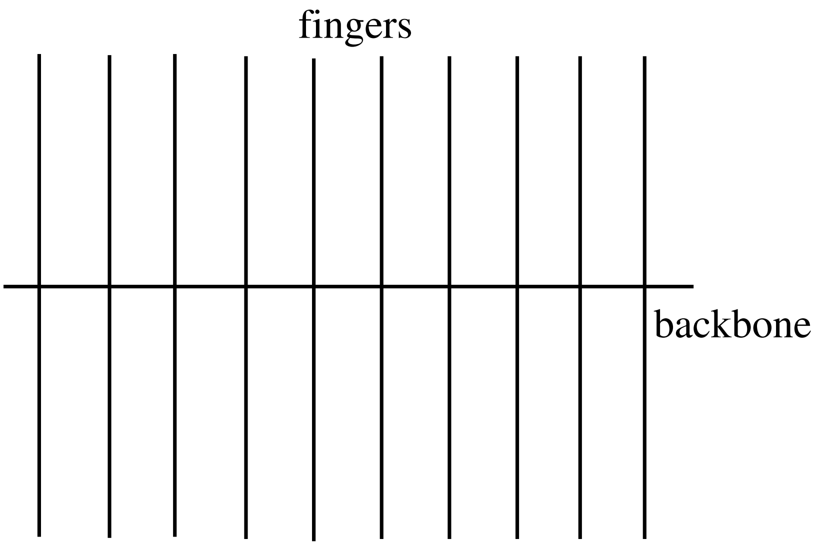

Figure 1. Comb structure consisting of a backbone and continuously distributed branches/fingers.

1.1. Preliminaries I: Subdiffusion versus Diffusion

Diffusion on comb structures has also been studied by macroscopic approaches, based on Fokker-Planck equations [3]. We consider a standard two dimensional (2D) diffusion equation, which describes Brownian motion in the specific comb geometry shown in Figure 1. The comb geometry implies that the displacement in the x-direction is possible only along the structure axis, that is, the x-axis at $y = 0$. Diffusion in the x-direction is highly inhomogeneous and the diffusion coefficient is given by $D_{xx} = D_x\delta(y)$, while the diffusion coefficient in the y-direction, the side-branch direction, also called teeth or fingers, is a constant, namely $D_{yy} = D_y$. The diffusion equation on the comb structure reads

$$\frac{\partial}{\partial t}P(x,y,t) = D_x\delta(y)\frac{\partial^2}{\partial x^2}P(x,y,t) + D_y\frac{\partial^2}{\partial y^2}P(x,y,t), \tag{1}$$

where $P(x,y,t)$ is the probability density function (PDF) of finding a diffusing particle at time t at the position with coordinates (x,y) in the 2D comb space. The initial condition is $P(x,y,t=0) = \delta(x)\delta(y)$ and natural boundary conditions are chosen at infinity, that is, $P(x,y,t) = \partial_x P(x,y,t) = \partial_y P(x,y,t) = 0$ for either $x = \pm\infty$ or $y = \pm\infty$.

Following standard procedures of the Fourier transformation in space and the Laplace transformation in time $\mathcal{L}\mathcal{F}_x[P(x,y,t)] = \hat{\tilde{P}}(k,y,s)$, particular solutions of the comb equation can be obtained. In Fourier-Laplace space, Equation (1) reads

$$s\hat{\tilde{P}}(k,y,s) = -D_x\delta(y)k^2\hat{\tilde{P}}(k,y,s) + D_y\frac{\partial^2}{\partial y^2}\hat{\tilde{P}}(k,y,s) + \delta(y), \tag{2}$$

where s is the Laplace variable and k is the Fourier variable. We look for solutions in the form

$$\hat{\tilde{P}}(k,y,s) = f(k,s)g(y,s) = f(k,s)\exp\left[-\sqrt{s/D_y}|y|\right], \tag{3}$$

where $f(k,s) = \hat{\tilde{P}}(k,y=0,s)$ describes diffusion along the backbone in Laplace space. Substituting solution (3) into Equation (2) and integrating over y, we obtain an equation for $f(k,s)$,

$$f(k,s) = \frac{1}{2\sqrt{sD_y} + D_xk^2}. \tag{4}$$

Analytical solutions of the distribution functions can be represented in the form of the Mittag-Leffler and the Fox H functions, presented in Appendix B.

It turns out that the transport along the backbone is subdiffusive, while normal diffusion occurs along the side-branched fingers. To show this, we calculate the MSDs and Equations (3) and (4) yield indeed subdiffusion in the x-direction,

$$\langle x^2(t)\rangle = \mathcal{L}^{-1}\left[\int_{-\infty}^{\infty} g(y)dy\Big(-\frac{d^2 f}{dk^2}(k=0,s)\Big)\right] = \frac{D_x}{\sqrt{D_y}}\frac{\sqrt{t}}{\Gamma(3/2)}, \tag{5}$$

and normal diffusion in the fingers,

$$\langle y^2(t)\rangle = \mathcal{L}^{-1}\left[\int_{-\infty}^{\infty} y^2 g(y)dy f(k=0,s)\right] = 2D_y t. \tag{6}$$

Here $\Gamma(z+1) = z\Gamma(z)$ is the gamma function.

1.2. Preliminaries II: Fractional Fokker-Planck Equation

Equation (6) implies that for $y \neq 0$ the comb diffusion equation (1) reduces to the normal diffusion equation. The same result is obtained by integrating Equation (1) with respect to x, taking into account the boundary conditions. However, integration with respect to y leads to a completely different equation for the marginal distribution $P_1(x,t) = \int_{-\infty}^{\infty} P(x,y,t)dy$:

$$\frac{\partial}{\partial t}P_1(x,t) = D_x\frac{\partial^2}{\partial x^2}P(x,y=0,t), \tag{7}$$

where $\hat{P}(x,y=0,s) = f(x,s)$. To obtain this equation in closed form, we return to Equation (3) in (x,y)-space,

$$\hat{P}(x,y,s) = \hat{P}(x,y=0,s)\exp\left[-\sqrt{s/D_y}|y|\right], \tag{8}$$

and integrate it with respect to y. This yields the relation $\hat{P}(x,y=0,s) = \sqrt{s/4D_y}\hat{P}_1(x,s)$. Using this relation and Laplace transforming Equation (7), we find

$$s^{\frac{1}{2}}\hat{P}_1(x,s) - \delta(x)s^{-\frac{1}{2}} = \frac{D_x}{2\sqrt{D_y}}\frac{\partial^2}{\partial x^2}\hat{P}_1(x,s). \tag{9}$$

Performing the Laplace inversion, we obtain the integro-differential equation

$${}^{C}_{0}\mathcal{D}_t^{\frac{1}{2}}P_1(x,t) = \frac{D_x}{2\sqrt{D_y}}\frac{\partial^2}{\partial x^2}P_1(x,t). \tag{10}$$

The integro-differential operator ${}^{C}_{0}\mathcal{D}_t^{\alpha} \equiv {}^{C}\mathcal{D}_t^{\alpha}$ is the so-called Caputo fractional derivative, see Appendix A,

$${}^{C}\mathcal{D}_t^{\alpha}P_1(t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{1}{(t-t')^{\alpha}}\frac{d\,P_1(t')}{d\,t'}dt', \quad 0<\alpha<1, \tag{11}$$

while Equation (10) is called the fractional Fokker-Planck equation (FFPE). Instead of the Caputo derivative, it is possible to employ the Riemann-Liouville fractional derivative,

$$\mathcal{D}_t^{\alpha}P_1(t) \equiv {}^{RL}_{0}\mathcal{D}_t^{\alpha}P_1(t) = \frac{1}{\Gamma(1-\alpha)}\frac{d}{d\,t}\int_0^t \frac{P_1(t')dt'}{(t-t')^{\alpha}}, \quad 0<\alpha<1, \tag{12}$$

which leads to a different form of the FFPE [17],

$$\frac{\partial}{\partial t}P_1(x,t) = \frac{D_x}{2\sqrt{D_y}}\mathcal{D}_t^{1-\alpha}\frac{\partial^2}{\partial x^2}P_1(x,t)\,, \tag{13}$$

where $\alpha = 1/2$. For arbitrary $0 < \alpha < 1$, this equation is a general form of the FFPE with the solution (A17)

$$P_1(x,t) = \frac{1}{\sqrt{D_\alpha t^\alpha}}H_{1,1}^{1,0}\left[\frac{x^2}{D_\alpha t^\alpha}\,\middle|\,\begin{matrix}(1-\frac{\alpha}{2},\alpha)\\(0,2)\end{matrix}\right]. \tag{14}$$

In that case, the diffusion coefficient must be generalized as well, $D_x/(2\sqrt{D_y}) = D_{\frac{1}{2}} \to D_\alpha$.

Concluding this introduction, it is worth mentioning, that the comb model in Equation (1) describes anomalous transport in homogeneous media. Natural phenomenological extensions of the comb model (1) consist of a generalization of the time process, by generalizing the memory kernel in Equation (11), as well as the space inhomogeneous (fractal) geometry, by introducing the power-law density of fingers [18,19]. This modification of the comb model leads to a so-called fractal comb model, where the solution for the PDF (14) has been obtained in terms of the Fox H-functions as a special case in Reference [19], as well.

2. Non-Markovian Diffusion in $m + n$ Space

We can extend the geometrical picture of the two-dimensional comb to a geometry where the backbone dynamics takes place in m-dimensional space, while diffusion in fingers takes place in n-dimensional space. The generalization of (1) for the $1+1$ comb to the $m+n$ comb model reads

$$\partial_t P(\mathbf{x},\mathbf{y},t) = \delta^{(n)}(\mathbf{y})\partial_{\mathbf{x}}^2 P(\mathbf{x},\mathbf{y},t) + D\partial_{\mathbf{y}}^2 P(\mathbf{x},\mathbf{y},t), \tag{15}$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_m)$ and $\mathbf{y} = (y_1, y_2, \ldots, y_n)$ are m and n dimensional vectors, while $\partial_{\mathbf{x}}^2 \equiv \partial_{x_1}^2 + \cdots + \partial_{x_m}^2$ and $\partial_{\mathbf{y}}^2 \equiv \partial_{y_1}^2 + \cdots + \partial_{y_n}^2$ are the corresponding Laplacians, and $\delta^{(n)}(\mathbf{y}) = \delta(y_1)\delta(y_2)\cdots\delta(y_n)$. Note that Equation (15) is written for dimensionless x and y variables and D is an effective dimensionless diffusivity parameter, see Reference [20]. In this case, we rescale the time and space variables in Equation (1) as follows. For the time and backbone we use $t\frac{D_y^3}{D_x^2} \to t$ and $x\frac{D_y}{D_x} \to x$. For the fingers we have an additional scaling parameter D, which yields $y\frac{D_y}{D_x} \to y/\sqrt{D}$. After this variable change of Equation (1) in the $1+1$ space, we arrive at Equation (15) in the $m+n$ space.

In the following we simplify the notations as $\mathbf{x} \equiv x$ and $\mathbf{y} \equiv y$. Since the y-space of branches is the complement of the backbone x-space, their overlapping region has a point of zero measure. Therefore, a formal solution of Equation (15) can be written in the same convolution form as for Equation (1), namely

$$P(x,y,t) = \int_0^t G(y,t-t')F(x,t')dt'. \tag{16}$$

Here $G(y,t)$ describes n-dimensional diffusion in the side-branches, while $F(x,t)$ is a solution for the m-dimensional backbone. Diffusion in the n-dimensional space is described by the solution

$$G(y,t) = \left[4\pi Dt\right]^{-\frac{n}{2}}\exp\left(-\frac{|y|^2}{4Dt}\right), \tag{17}$$

where $|y|^2 = y_1^2 + y_2^2 + \cdots + y_n^2$. To obtain the MSD in the x-direction, we need to find the marginal distribution $P_1(x,t)$ by integrating the formal solution (16) with respect to the y coordinates. Taking into account that the solution for the side-branch diffusion is normalized, we find

$$P_1(x,t) = \int_{-\infty}^{\infty} P(x,y,t)d^n y = \int_0^t F(x,t')dt' \,. \tag{18}$$

In Laplace space, this expression establishes a relation between $\hat{P}_1(x,s) = \mathcal{L}[P_1(x,t)]$ and $\hat{F}(x,s) = \mathcal{L}[F(x,t)]$, which reads

$$\hat{F}(x,s) = s\hat{P}_1(x,s). \tag{19}$$

The initial condition for the marginal distribution is $P_1(x,t=0) = \delta^{(m)}(x)$. Relation (19) leads to an equation for $\hat{P}_1(x,t)$. Integrating Equation (15) over y, we use

$$\int_{-\infty}^{\infty} P(x,y,t)\delta^{(n)}(y)d^n y = \int_0^t \left[\frac{(t-t')^{-1}}{4\pi D}\right]^{\frac{n}{2}} F(x,t')dt'. \tag{20}$$

For $n > 2$ this integral with respect to time diverges and a regularization procedure is performed in the Caputo form [21], which is the most convenient for the present calculations,

$$\int_{-\infty}^{\infty} P(x,y,t)\delta^{(n)}(y)d^n y = \left[\frac{1}{4\pi D}\right]^{\frac{n}{2}} \cdot \frac{\Gamma\left(1-\frac{n}{2}\right)}{\Gamma\left(N+1-\frac{n}{2}\right)} \int_0^t (t-t')^{N-\frac{n}{2}} \partial_{t'}^N F(x,t')dt', \tag{21}$$

where $N < \frac{n}{2} < N+1$. Now the Laplace transform can be carried out. Denoting $\nu = \frac{n}{2} - 1$, this yields

$$s^{\nu}\hat{F}(x,s) - \sum_{j=0}^{N-1} F^{(j)}(x,0)s^{\nu-j-1} \equiv \mathcal{L}[t^{-\frac{n}{2}}]_C \hat{F}(x,s) + \mathrm{O}(n>2, t=0)\,, \tag{22}$$

where index C means the regularization in the Caputo form. For $n \leq 2$, the Laplace transformation is a straightforward procedure, while for $n > 2$ the regularization of the integration is necessary before performing the Laplace transformation. Under these conditions the Laplace transform exists. Taking into account Equations (16), (17), (19) and (22), we obtain

$$s\hat{P}_1(x,s) = \frac{1}{[4\pi D]^{\frac{n}{2}}}\partial_x^2 \mathcal{L}[t^{-\frac{n}{2}}]_C s\hat{P}_1(x,s) + \delta^{(m)}(x) + \frac{1}{[4\pi D]^{\frac{n}{2}}}\partial_x^2 \mathrm{O}(n>2, t=0). \tag{23}$$

The Fourier transformation of Equation (23) yields

$$\hat{\bar{P}}_1(k,s) = \frac{\left[(4\pi D)^{\frac{n}{2}} + k^2 \mathrm{O}(n>2,t=0)\right]}{s\left([4\pi D]^{\frac{n}{2}} + k^2 \mathcal{L}[t^{-\frac{n}{2}}]\right)}. \tag{24}$$

Here $k^2 = \sum_{i=1}^m k_i^2$. This yields the MSD in the form

$$\begin{aligned} \langle x^2(t)\rangle &= \mathcal{L}^{-1}\Big[-\sum_{i=1}^m \frac{d^2}{d\,k_i^2}\bar{\hat{P}}_1(k,s)\Big]_{k=0} \\ &= \frac{2}{[4\pi D]^{\frac{n}{2}}}\mathcal{L}^{-1}\left[s^{-1}\mathcal{L}[t^{-\frac{n}{2}}]_C\right] + \mathcal{L}^{-1}\left[\sum_{j=0}^{N-1} s^{\frac{n}{2}-j-3}\bar{F}^{(j)}(0,0)\right]. \end{aligned} \tag{25}$$

From a physical point of view, it is reasonable to set the last term in Equation (25) to zero, since $\bar{F}^{(j)}(k=0,t=0) = 0$ without any restriction of generality. Let us consider three cases:

(i) We start with $n = 1$. Then Equation (25) yields

$$\langle x^2(t)\rangle = \frac{1}{\sqrt{\pi D}}\mathcal{L}^{-1}\left[s^{-\frac{n}{2}}\right] = \frac{t^{\frac{1}{2}}}{\sqrt{\pi D}}. \tag{26}$$

(ii) The case $n = 2$ corresponds to ultra-slow diffusion [22]. To see this, we present Equation (25) in the explicit form,

$$\langle x^2(t)\rangle = \frac{1}{2\pi D}\int_{-i\infty}^{+i\infty}\mathcal{L}[t^{-1}]\frac{e^{st}ds}{s} = \frac{1}{2\pi D}\int^t dt\int_{-i\infty}^{+i\infty}\mathcal{L}[t^{-1}]e^{st}ds. \tag{27}$$

Here, we take into account that $\mathcal{L}^{-1}\mathcal{L}\left[t^{-1}\right] \equiv t^{-1}$ and $e^{st}/s = \int^t e^{st}dt + C$, where C is an integration constant of the indefinite integration, and the Laplace transform of t^{-1} exists as a principal value integral [23]. In the class of entire functions, this Laplace transformation does not exists, $\mathcal{L}\left[t^{-1}\right] = \Gamma(0)$, however it does exist in the class of distributions or generalized functions, with $\mathcal{L}\left[t^{-1}\right] = -\ln(s) - \gamma$ [24], where $\gamma = 0.577216$ is the Euler constant. Therefore, Equation (27) yields

$$\langle x^2(t)\rangle = \frac{1}{2\pi D}\ln(t) + \frac{C}{2\pi D\,t} \approx \frac{1}{2\pi D}\ln(t), \quad \text{as} \quad t \to \infty, \tag{28}$$

confirming that for large times ultra-slow diffusion takes place, with the MSD growing as $\ln(t)$.

(iii) For $n > 2$, Equation (25) yields

$$\begin{aligned}\langle x^2(t)\rangle &= \frac{2}{[4\pi D]^{\frac{n}{2}}}\mathcal{L}^{-1}\left\{\frac{1}{s}\mathcal{L}[t^{-\frac{n}{2}}]_C\right\} = \frac{2\Gamma\left(1-\frac{n}{2}\right)}{[4\pi D]^{\frac{n}{2}}}\mathcal{L}^{-1}\left[s^{\frac{n}{2}-2}\right] \\ &= \frac{2\Gamma\left(1-\frac{n}{2}\right)}{[4\pi D]^{\frac{n}{2}}}\left[s^{N-1}s^{-(N-\frac{n}{2}+1)}\right] = \frac{2\Gamma\left(1-\frac{n}{2}\right)}{[4\pi D]^{\frac{n}{2}}}\left(\frac{d}{dt}\right)^{N-1}\Gamma\left(N-\tfrac{n}{2}+1\right)t^{N-\frac{n}{2}} \\ &= \frac{2}{[4\pi D]^{\frac{n}{2}}}\frac{\Gamma\left(N+1-\frac{n}{2}\right)}{\Gamma\left(N+1-\frac{n}{2}\right)}t^{1-\frac{n}{2}} = \frac{2}{[4\pi D]^{\frac{n}{2}}}t^{1-\frac{n}{2}} \to 0, \quad \text{as} \quad t \to \infty. \end{aligned} \tag{29}$$

In other words, there is no transport for $n > 2$; the MSD vanishes asymptotically for $t \to \infty$. This random localization follows from the fact that for $n > 2$ the random walk in fingers is not recurrent.

3. Quantum Comb and Fractional Schrödinger Equation

The concept of fractional calculus has also been introduced in quantum mechanics [25–27]. However its physical relevance remains an open question at this time. The quantization of the comb model is pertinent in this context. Note that the Wick rotation $t \to it$ in Equation (1) is a well defined procedure, which translates the diffusion problem into quantum mechanics. In this case, a quantum particle is described by a wave function $\Psi = \Psi(x, y, t)$, which is governed by the Schrödinger equation

$$\frac{\partial\Psi}{\partial t} = \delta(y)\frac{i\hbar_{\text{eff}}}{2m_x}\frac{\partial^2\Psi}{\partial x^2} + \frac{i\hbar_{\text{eff}}}{2m_y}\frac{\partial^2\Psi}{\partial y^2}, \tag{30}$$

where $\hbar_{\text{eff}}$ is an effective Planck constant, while $\delta(y)/m_x$ and $1/m_y$ are the diagonal components of the inverse mass tensor, which can be introduced by analogy with a quasi-particle mass on the Fermi surface [28].

The initial condition is $\Psi(x, y, t = 0) = \Psi_0(x, y)$, and boundary conditions at infinity are imposed. It is worth noting that contrary to the relaxation Equation (1), a quantum particle can be free at infinity as well, which corresponds to a scattering problem [29,30]. Another essential difference is that integration with respect to y has no physical meaning and cannot be performed for the wave function. The marginal PDF can be defined only for the probability amplitude $|\Psi(x, y, t)|^2$. This leads to fundamental complications for the analysis and the form of the fractional Schrödinger equation (It is tempting to carry out the Wick rotation of the time in FFPE (10), however this procedure is vague and needs additional justification [31]. Note also that the Schrödinger equation is a quantum mechanical axiomatic equation. In contrast, a Fokker-Planck equation is an asymptotic (diffusive) limit of the Master equation).

The evolution of the wave function is determined by the Green's function $G = G(x, y, t)$,

$$\Psi(x, y, t) = \int G(x - x', y - y', t)\Psi_0(x', y')dx'dy', \tag{31}$$

with the initial condition $G_0(x, y) = \delta(x)\delta(y)$. For $t > 0$, the Green's function obeys the equation

$$\frac{\partial G}{\partial t} = \delta(y)\frac{i\hbar_{\text{eff}}}{2m_x}\frac{\partial^2 G}{\partial x^2} + \frac{i\hbar_{\text{eff}}}{2m_y}\frac{\partial^2 G}{\partial y^2}. \tag{32}$$

We make the ansatz

$$G(x, y, t) = \int_0^t G_y(y, t - t')G_x(x, t')dt'. \tag{33}$$

It is tempting to consider $G_y(y, t - t')$ as a free particle propagator. However, the $\delta(y)$-potential on the backbone leads to some correction. The Green's function $G_y(y, t)$ is represented in analogy with the diffusive comb in Equation (3) as the inverse Laplace transform,

$$G_y(y, t) = \mathcal{L}^{-1}\left[\exp\left(-|y|\sqrt{2sm_y/i\hbar_{\text{eff}}}\right)\right](t), \tag{34}$$

and the Green's function (33) reads,

$$G(x, y, t) = \frac{1}{2\pi}\int_0^t dt' G_x(x, t')\mathcal{L}^{-1}\left[\exp\left(-|y|\sqrt{2sm_y/i\hbar_{\text{eff}}}\right)\right](t - t'). \tag{35}$$

Performing the Laplace and Fourier transformations of Equation (32), taking into account the solution (35) and combining terms at $\delta(y)$, we arrive at the solution for $\hat{\tilde{G}}(k, s)$ in the form of Equation (4), which now reads

$$\hat{\tilde{G}}_x(k, s) = \frac{\sqrt{m_y/2i\hbar_{\text{eff}}}}{D_Q k^2 + \sqrt{s}}, \tag{36}$$

where $D_Q = (1 + i)\frac{\sqrt{\hbar_{\text{eff}} m_y}}{4m_x}$ and $\sqrt{2i} = 1 + i$. Performing the Laplace inversion, we obtain the solution in Fourier k-space,

$$\hat{G}_x(k, t) = \frac{m_y}{2i\hbar_{\text{eff}}}t^{-\frac{1}{2}}E_{\frac{1}{2},\frac{1}{2}}\left(-D_Q k^2 t^{\frac{1}{2}}\right), \tag{37}$$

which definitely does not correspond to unitary dynamics (This solution corresponds to relaxation in the open quantum system (on the backbone). The asymptotic solution for $t \to \infty$ is presented in Appendix C, see also Appendix A). Therefore, the quantum dynamics on the x-axis, the backbone, is not unitary. It consists of two parts, one which corresponds to an oscillatory process, that is, is unitary and one which represents a decay process. Introducing the effective Hamiltonian $D_Q k^2 \to \mathbf{H} = -D_Q\frac{\partial^2}{\partial x^2}$ of the quantum backbone dynamics, we obtain from Equation (37) the Green's function of the x-dynamics,

$$G_x(x - x', t) = \langle x' \mid G_x(\mathbf{H}(x), t) \mid x\rangle = \int_{-\infty}^{\infty} e^{i(x-x')k}G_x(k, t)dk, \tag{38}$$

where $G_x(\mathbf{H}(x), t)$ is the operator form of the Green's function,

$$\mathbf{G}_x \equiv G_x(\mathbf{H}(x), t) = \frac{m_y}{2i\hbar_{\text{eff}}} t^{-\frac{1}{2}} E_{\frac{1}{2},\frac{1}{2}} \left[-\mathbf{H}(x) t^{\frac{1}{2}} \right], \tag{39}$$

and $\mathbf{H}(x)$ is itself a non-Hermitian operator.

Let us show that the solution (39) corresponds to a fractional differential equation, namely the Fractional Time Schrödinger Equation (FTSE) with the fractional time derivative in the Riemann-Liouville form (12),

$${}^{RL}_{0}\mathcal{D}_t^{\frac{1}{2}} \mathbf{G}_x \equiv \mathcal{D}_t^{\frac{1}{2}} \mathbf{G}_x = \mathbf{H}\, \mathbf{G}_x. \tag{40}$$

To this end we perform a small fractional calculus exercise. First, we carry out the Laplace transformation of Equation (40), using the general property

$$\mathcal{L}\left[\mathcal{D}_t^{\alpha} f(t)\right] = s^{\alpha} f(s) - \sum_{k=0}^{n-1} s^k [\mathcal{D}_t^{\alpha-k-1} f(t)]\,|_{t=0}\,, \tag{41}$$

where $n-1 < \alpha < n$ and in our case $\alpha = 1/2$ and $k = 0$. If we take $f(t) = t^{\beta-1} E_{\alpha,\beta}\left(\lambda t^{\alpha}\right)$ then the fractional integration yields, see, for example, Reference [32],

$$\mathcal{D}_t^{-\nu} f(t) = \frac{1}{\Gamma(\nu)} \int_0^t (t-\tau)^{\nu-1} \tau^{\beta-1} E_{\alpha,\beta}\left(\lambda \tau^{\alpha}\right) = t^{\nu+\beta-1}. \tag{42}$$

Taking into account that $\alpha = \beta = \nu = 1/2$, we obtain

$$\mathcal{D}_t^{-\frac{1}{2}} f(t)\,|_{t=0} = E_{\frac{1}{2},1}(0) = 1. \tag{43}$$

This establishes that Equation (39) is indeed the solution of the FTSE (40).

Quantum Friction Due to Fingers

We have obtained an exact fractional quantum mechanics with an effective Hamiltonian, which is a non-Hermitian operator. It describes the initial wave packet spreading along the backbone x-axis in the presence of the decay due to the interaction with the fingers y-degree of freedom. The survival probability is not conserved, $\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx \neq 1$, and it is a decreasing function in complete analogy with fractional diffusion.

The second argument on the fractional time derivative in the FTSE (40) relates to the memory effect that results from the quantum dynamics in fingers as in classical diffusion. However, fractional quantum dynamics differs drastically from classical subdiffusion. Technically, the memory effect results from the Green's function $G_y(y-y_0,t)$, which describes the evolution of the wave function $\Psi_y(y,t)$ of a quantum particle but not its PDF $|\Psi_y(y,t)|^2$. Another important point is that the quantum recurrence takes place in the Hilbert space. Therefore, it is defined by the PDF $\mathcal{P}(t)$ to find a particle in the initial state $\Psi_y(y,t=0) = |y_0\rangle$ at time t. This yields

$$\mathcal{P}(t) = \left|\langle y_0|\Psi_y(y,t)\rangle\right|^2 = \left|G_y(y-y_0,t)\right|^2. \tag{44}$$

Taking into account Equation (34), we obtain $\mathcal{P}(t) \sim 1/t$. Note that it is also the survival probability of a quantum particle in fingers at time t. Therefore

$$\mathcal{P}(t) = \int_t^{\infty} p(\tau) d\tau, \tag{45}$$

where $p(t)$ is a quantum analog of the classical waiting time PDF, which decays as $1/t^2$. Correspondingly, the mean waiting time diverges: $\int tp(t)dt = \infty$. Therefore, this comb dynamics determines a quantum friction, which leads to the FTSE. An alternative approach to the problem has been developed in Reference [31].

4. Conclusions

As far as comb models are concerned, we have arrived at a very interesting conclusion on the impact of geometry on Markov properties of both diffusive and quantum dynamics. The standard Markov property implies a chain rule for the Green's function

$$G(x,t|x_0,t_0) = \int G(x,t|x',t')G(x',t'|x_0,t_0)dx' \,, \tag{46}$$

where $x \in \mathbb{R}^m$. As we have seen, the dimensionality of the backbone m does not affect the transport exponent. However, if we add additional degrees of freedom $y \in \mathbb{R}^n$ to form a comb, then the Markov process in fingers or branches leads to a memory effect in the x-space, which destroys the Markov property (46). This memory effect in the MSD given by the main result (25) is due to the term $[\mathcal{L}t^{-\frac{n}{2}}]_C$, where the power law function of time is considered as the generalised function in the Caputo regularization [24]. For $n = 0$ (no fingers), we obtain normal diffusion, while for $n > 0$, subdiffusion, ultra-slow diffusion and random localization are obtained in Equations (26), (28) and (29), respectively.

In quantum mechanics, quantum Markov evolution in fingers destroys the Markov chain rule (46) in the backbone as well. The nature of the memory effect is not completely understood, in contrast to the classical random walk theory. We explain the memory effect due to quantum diffusion in fingers. In our case, the FFPE (40) is a realistic model, where the fractional time derivative is due to the comb geometry The latter leads to the quantum analog of a classical waiting time PDF, which decays as $1/t^2$. Correspondingly, the mean waiting time diverges logarithmically. Therefore, this comb dynamics determines a quantum friction, which leads to the FTSE. This issue has been the focus of extensive studies, reflected in recent reviews [16,33,34].

Another important result of the non-Markovian dynamics is the non-Hermitian operator H(x). In the FTSE (40), the dynamics is no longer Hamiltonian. This property is caused by the comb geometry, which makes it possible to describe the process of relaxation in the framework of the FTSE (40). This non-Hamiltonian description of quantum relaxation is an important and new approach to open quantum systems [35].

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Appendix A. A Brief Survey on Fractional Integration

Extended reviews of fractional calculus can be found for example, in References [32,36,37]. Fractional integration of the order of α is defined by the operator

$${}_a\mathcal{I}_x^\alpha f(x) = \frac{1}{\Gamma(\alpha)} \int_a^x f(y)(x-y)^{\alpha-1}dy \,, \tag{A1}$$

where $\alpha > 0$, $x > a$ and $\Gamma(z)$ is the Gamma function. Fractional derivation was developed as a generalization of integer order derivatives and is defined as the inverse operation to the fractional integral. Therefore, the fractional derivative is defined as the inverse operator to ${}_a\mathcal{I}_x^\alpha$, namely ${}_a\mathcal{D}_x^\alpha f(x) = {}_a\mathcal{I}_x^{-\alpha} f(x)$ and ${}_a\mathcal{I}_x^\alpha = {}_a\mathcal{D}_x^{-\alpha}$. Its explicit form is

$${}_a\mathcal{D}_x^\alpha f(x) = \frac{1}{\Gamma(-\alpha)} \int_a^x f(y)(x-y)^{-1-\alpha}dy \,. \tag{A2}$$

This integral diverges for arbitrary $\alpha > 0$ and a regularization procedure is introduced with two alternative definitions of ${}_a\mathcal{D}_x^\alpha$. For an integer n defined as $n-1 < \alpha < n$, we obtain the Riemann-Liouville fractional derivative,

$$ {}^{RL}_{\ a}\mathcal{D}_x^\alpha f(x) \equiv {}_a\mathcal{D}_x^\alpha f(x) = \frac{d^n}{dx^n}\,{}_a\mathcal{I}_x^{n-\alpha} f(x)\,, \tag{A3} $$

and the Caputo fractional derivative,

$$ {}^{C}_{a}\mathcal{D}_x^\alpha f(x) = {}_a\mathcal{I}_x^{n-\alpha} \frac{d^n}{dx^n} f(x)\,. \tag{A4} $$

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

$$ {}^{RL}_{\ 0}\mathcal{D}_x^\alpha x^\beta = \frac{x^{\beta-\alpha}\Gamma(\beta+1)}{\Gamma(\beta+1-\alpha)}\,. \tag{A5} $$

This fractional derivation with the fixed lower 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 fractional integral is

$$ {}_x\mathcal{I}_a^\alpha f(x) = \frac{1}{\Gamma(\alpha)} \int_x^a (y-x)^{\alpha-1} f(y)dy\,. \tag{A6} $$

Another important property is $D^\alpha I^\beta = I^{\beta-\alpha}$, where subscripts are omitted for brevity. Note that the inverse combination is not valid. In general $\mathcal{I}^\beta\mathcal{D}^\alpha \neq \mathcal{I}^{\beta-\alpha}$, since it depends on the lower limits of the integrations [32]. We also use here a convolution rule for the Laplace transform for $0 < \alpha < 1$

$$ \mathcal{L}[\mathcal{I}_x^\alpha f(x)] = s^{-\alpha}\tilde{f}(s)\,. \tag{A7} $$

Note that for arbitrary $\alpha > 1$ the treatment of the Caputo fractional derivative by the Laplace transformation is more convenient than that of the Riemann-Liouville one.

Note that the solutions considered here can be obtained in the form of the Mittag-Leffler function by the Laplace inversion [32,38,39]

$$ E_{(\nu,\beta)}(zr^\nu) = \frac{r^{1-\beta}}{2\pi i} \int_{\mathcal{C}} \frac{s^{\nu-\beta}e^{sr}}{s^\nu - z} ds\,, \tag{A8} $$

where $\mathcal{C}$ is a suitable contour of integration, starting and finishing at $-\infty$ and encompassing a circle $|s| \leq |z|^{\frac{1}{\nu}}$ in the positive direction and $\nu, \beta > 0$.

Appendix B. Solution in the Form of the Fox *H* Function

The Fox H function is defined in terms of the Mellin-Barnes integral [39,40],

$$ H_{p,q}^{m,n}(z) = H_{p,q}^{m,n}\left[z \,\middle|\, \begin{array}{l} (a_1, A_1), \ldots, (a_p, A_p) \\ (b_1, B_1), \ldots, (b_q, B_q) \end{array} \right] = \frac{1}{2\pi i} \int_\Omega \Theta(s) z^{-s} ds\,, \tag{A9} $$

where

$$ \Theta(s) = \frac{\left\{ \prod_{j=1}^m \Gamma(b_j + sB_j) \right\} \left\{ \prod_{j=1}^n \Gamma(1 - a_j - sA_j) \right\}}{\left\{ \prod_{j=m+1}^q \Gamma(1 - b_j - sB_j) \right\} \left\{ \prod_{j=n+1}^p \Gamma(a_j + sA_j) \right\}}\,, \tag{A10} $$

with $0 \leq n \leq p$, $1 \leq m \leq q$ and $a_i, b_j \in C$, while $A_i, B_j \in R+$, for $i = 1, \ldots, p$ and $j = 1, \ldots, q$. The contour Ω starting at $\sigma - i\infty$ and ending at $\sigma + i\infty$, separates the poles of the functions $\Gamma(b_j + sB_j)$, $j = 1, \ldots, m$ from those of the function $\Gamma(1 - a_i - sA_i)$, $i = 1, \ldots, n$.

Now let us solve FFPEs (10) and (13) in terms of the Fox H functions. Performing Fourier and Laplace transformations, we obtain the Montroll-Weiss equation in the form

$$\bar{\tilde{P}}_1(k,s) \equiv \mathcal{P}(k,s) = \frac{s^{\alpha-1}}{s^\alpha + D_\alpha k^2}\,, \tag{A11}$$

where we take $\bar{\tilde{P}}_0(k,s) = 1$. Then employing formula (A8) for the Mittag-Leffler function [32,38,39] one obtains

$$\mathcal{P}(k,t) \equiv \bar{P}_1(k,t) = E_{(\alpha,1)}\big(-D_\alpha k^2 t^\alpha\big)\,. \tag{A12}$$

The two parameter Mittag-Leffler function (A8) is a special case of the Fox H-function, which can be represented by means of the Mellin-Barnes integral (A9)

$$\begin{aligned} E_{(\alpha,\beta)}(-z) &= \frac{1}{2\pi i}\int_\Omega \frac{\Gamma(s)\Gamma(1-s)}{\Gamma(\beta-\alpha s)} z^{-s} ds = H^{1,1}_{1,2}\left[z \,\middle|\, \begin{matrix} (0,1) \\ (0,1),(1-\beta,\alpha) \end{matrix} \right] \\ &= \frac{1}{\delta} H^{1,1}_{1,2}\left[z \,\middle|\, \begin{matrix} (0,1/\delta) \\ (0,1),(1-\beta,\alpha/\delta) \end{matrix} \right]. \end{aligned} \tag{A13}$$

Fourier-cosine transformation of Equations (A12) and (A13) yields [16,39]

$$\begin{aligned} \mathcal{P}_\rho(x,t) &= \frac{1}{2\pi}\int_0^\infty dk k^{\rho-1}\cos(kx) H^{1,1}_{1,2}\left[\sqrt{D_\alpha t^\alpha}|k| \,\middle|\, \begin{matrix} (0,1/2) \\ (0,1),(0,\alpha/2) \end{matrix} \right] \\ &= \frac{1}{|x|^\rho} H^{2,1}_{3,3}\left[\frac{x^2}{D_\alpha t^\alpha} \,\middle|\, \begin{matrix} (1,1),(1,\alpha),(\frac{1+\rho}{2},1) \\ (1,2),(1,1),(\frac{1+\rho}{2},1) \end{matrix} \right]. \end{aligned} \tag{A14}$$

For $\rho = 1$ we obtain the solution of Equation (A11). Taking into account the properties of the Fox H function, we obtain

$$\frac{1}{|x|} H^{2,1}_{3,3}\left[\frac{x^2}{D_\alpha t^\alpha} \,\middle|\, \begin{matrix} (1,1),(1,\alpha),(1,1) \\ (1,2),(1,1),(1,1) \end{matrix} \right] = \frac{1}{|x|} H^{2,0}_{2,2}\left[\frac{x^2}{D_\alpha t^\alpha} \,\middle|\, \begin{matrix} (1,\alpha),(1,1) \\ (1,2),(1,1) \end{matrix} \right]. \tag{A15}$$

Use of property $x^\delta H^{m,n}_{p,q}\left[x \,\middle|\, \begin{matrix} (a_p,A_p) \\ (b_q,B_q) \end{matrix} \right] = H^{m,n}_{p,q}\left[x \,\middle|\, \begin{matrix} (a_p+\delta A_p,A_p) \\ (b_q+\delta B_q,B_q) \end{matrix} \right]$ reduces Equation (A14) to

$$P_1(x,t) \equiv \mathcal{P}(x,t) = \frac{1}{\sqrt{D_\alpha t^\alpha}} H^{2,0}_{2,2}\left[\frac{x^2}{D_\alpha t^\alpha} \,\middle|\, \begin{matrix} (1-\frac{\alpha}{2},\alpha),(\frac{1}{2},1) \\ (0,2),(\frac{1}{2},1) \end{matrix} \right]. \tag{A16}$$

Using property of Equation (A15) we obtain

$$P_1(x,t) = \frac{1}{\sqrt{D_\alpha t^\alpha}} H^{1,0}_{1,1}\left[\frac{x^2}{D_\alpha t^\alpha} \,\middle|\, \begin{matrix} (1-\frac{\alpha}{2},\alpha) \\ (0,2) \end{matrix} \right]. \tag{A17}$$

Appendix C. Asymptotic Forms of Green's Function

Equation (37) is the solution of the FTSE (40) for a particle in the backbone that interacts with fingers. Solution (38) can be represented in the form of the Fox H-function. For illustration purposes, we consider asymptotic solutions for small and large times. Using the property of the Mittag-Leffler functions [38]

$$E_{\alpha,\beta}(z) = \frac{1}{\Gamma(\beta)} + zE_{\alpha,\alpha+\beta}(z) \tag{A18}$$

and taking into account that the Mittag-Lefler function $E_{\alpha,1}(z) \equiv E_\alpha(z)$ for small arguments $|z| \ll 1$ and $\Re z < 0$ can be approximated by exponentials [38], we obtain

$$\hat{G}_x(k,t) \approx \frac{m_y}{2i\hbar_{\text{eff}}} \left[-D_Q k^2 \exp\left(-\frac{D_Q k^2 t^{\frac{1}{2}}}{\Gamma(3/2)} \right) + \frac{t^{-\frac{1}{2}}}{\Gamma(1/2)} \right], \tag{A19}$$

where $\Gamma(3/2) = (1/2)\Gamma(1/2) = \sqrt{\pi}/2$.

In the opposite case of large arguments, when $E_\alpha(z) \approx -z^{-1}/\Gamma(1-\alpha)$ [38], we have from Equation (A18)

$$\hat{G}_x(k,t) \approx \frac{m_y}{2i\hbar_{\text{eff}}} \frac{2t^{-\frac{1}{2}}}{\Gamma(1/2)}. \tag{A20}$$

Taking into account the term $\sim t^{-\frac{1}{2}}$, which is the dominant solution in both cases, the Green's function in Equation (38) $G_x(x-x',t) \sim t^{-\frac{1}{2}}\delta(x-x')$ describes relaxation in the open quantum system at the backbone. Eventually, the MSD $\langle x^2(t)\rangle \sim 1/t$ vanishes asymptotically for $t \to \infty$. This dynamical localization results from relaxation in the open quantum system. More complex examples of FTSEs are considered in References [16,31,34].

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