Approximation of time-fractional diffusion with central drift by difference schemes

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Abstract

By generalization of Ehrenfest's urn model, we obtain discrete approximations to spacially one-dimentional time fractional diffusion processes with drift towards the origin. These discrete approximations can be interpreted (a) as difference schemes for the relevant time-fractional partial differential equation, (b) as random walk models. The relevant convergence questions as well as the behaviour for time tending to infinity are discussed, and results of numerical case studies are displayed.

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1 Introduction

In recent years there has been growing interest in diffusion in various fields of physics, chemistry, and related sciences. It is well known that the fundamental solution (or Green function) of the classical diffusion (or heat) equation can be interpreted as a Gaussian normal probability density function (pdf) in space evolving in time.

Robert Brown in 1827 was the first interested in diffusion in fluids. He noticed that small particles suspended in fluids perform peculiarly erratic movements. This phenomenon, which can also be observed in gases, is referred to as Brownian motion. It later became clear that Brownian motion is an outward manifestation of the molecular motion postulated by kinetic theory of matter. In 1905 Albert Einstein was the first to develop a satisficatory theory. Then the theory was considerably generalized and extended by Marjan Smoluchowski, Fokker, Planck, Burger,Wiener and others. Einstein considered the case of the free particle that is, a particle on which no forces other than those due to the molecules of the surrounding medium are acting. This motion was modelled by the classical diffusion equation [26] [33],[28]

$$\frac{\partial u(x,t)}{\partial t} = a\frac{\partial^2 u(x,t)}{\partial x^2}\ , a>0\ x\in\mathbb{R},\ t>0\,. \tag{1.1}$$

The solution $u(x,t)$ of this equation with the initial condition $u(x,0)=\delta(x-\xi)$ is well known as the corresponding *Green function* or the *fundamental solution.* $u(x,t)$ represents the probability density function of a particle being at the point x in the time instant t when it initially (at the time $t=0$) is at the point $x=\xi$:

$$u(x,t) = \frac{1}{2\sqrt{\pi a t}}\, e^{-(x-\xi)^2/(4at)}\ .$$

Here a is a positive constant depending on the temperature, the friction coefficient, the universal gas constant, and finally on the Avogadro number. The free motion of the particle modelled by Eq.(1.1) has met great interest among mathematicians, physicists, and others, and it has found many generalizations. Approximative random walks of the particle have also been studied by many authors, see for example, [5], [15]. As soon as the theory for the free particle was established, many modifications in order to take into consideration the external outside force were devised. Assuming the external outside forces acting towards the origin $x=0$ and being proportional to the distance of the particle from the origin Smoluchowski [26] has shown that Eq.(1.1) should be augmented by a drift term:

$$\frac{\partial u(x,t)}{\partial t} = a\frac{\partial^2 u(x,t)}{\partial x^2} + \frac{\partial}{\partial x}(bxu(x,t))\ , b>0\,. \tag{1.2}$$

Again we assume that the initial condition is $u(x,0)=\delta(x-\xi)$. The solution of this equation is [21], [20], [16]

$$u(x,t) = p(\xi;x,t) = \frac{1}{\sqrt{2\pi}\sigma(t)}\, e^{\frac{-(x-m(t))^2}{2\sigma^2}}\ , \tag{1.3}$$

where $m(t) = \xi\, e^{-bt}$, $\sigma^2 = \frac{a}{b}(1 - e^{-2bt})$, and $a > 0, b > 0$. As a more general situation, we consider the equation

$$\frac{\partial u(x,t)}{\partial t} = a\frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial}{\partial x}(F(x)u(x,t)) \ , a > 0 \tag{1.4}$$

assuming the force $F(x) = -\frac{dU(x)}{dx}$, $U(x)$ to be defined as a symmetric differentiable potential, increasing for $x > 0$, $U(x) = U(-x)$. In this general situation of a *potential well*, the drift is directed towards the origin. We pay special attention to the following examples (with $b > 0$):

(a) $U(x) = \frac{bx^2}{2}$, the harmonic diffusive oscillator

(b) $U(x) = \frac{bx^4}{4}$, the quartic diffusive oscillator,

(c) $U(x) = (\frac{dx^2}{2} + \frac{bx^4}{4})\, , d > 0$, anharmonic diffusive oscillator,

(d) $U(x) = \frac{bx^{2m+2}}{(2m+2)}$, $m = 1, 2, \ldots$, the strongly non-linear diffusive oscillator.

Therefore, Eq.(1.2) can be interpreted as modelling the diffusion of a particle under the action of the external outside force $F(x) = -bx, b > 0$.

In this moment, we should mention the work of A. Chechkin et al. [3]. These authors deal with the above forms of the potential well for the diffusion fractional in space, in which $\frac{\partial^2 u(x,t)}{\partial x^2}$ is replaced by a symmetric fractional (in space) derivative.

In our paper, we consider another important generalization of Eq.(1.2), namely we shall discuss the diffusion fractional in time under various forms of forces. By fractional in time, we mean that the first-order time derivative is replaced by the Caputo derivative of order $\beta \in (0, 1]$. In this case Eq.(1.2) goes over into

$$\frac{\partial^\beta u(x,t)}{\partial t^\beta} = a\frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial}{\partial x}(F(x)u(x,t)) \ , \ 0 < \beta \le 1 \ , a > 0 \ . \tag{1.5}$$

Here we take $(-F(x))$ as a differentiable odd function of x, positive for $x > 0$. The use of the Caputo derivative (see Gorenflo, Mainardi [9], [8], [10], and the appendix) allows us to take in a natural way into account an initial condition $u(x, 0) = f(x)$ and then consider the evolution of $u(x, t)$ for $x \in \mathbb{R},\ t > 0$.

We shall present a discrete method of solving approximately Eq.(1.5) with linear drift and, by analogy, give the results for the other types of $F(x)$. We shall devise both explicit and implicit differences schemes for $\beta = 1$ and for $0 < \beta < 1$. Then, we shall discuss questions of convergence in particular for t tending to infinity, and compare the result with the continuous stationary solution of Eq.(1.5). Finally, approximating random walks will be simulated and interpreted.

Before proceeding, let us return to Eq.(1.2) with initial condition $u(x, 0) = \delta(x - \xi)$ and its solution Eq.(1.3). Denoting by $\langle x(t)\rangle = \int\limits_{-\infty}^{\infty} xu(x,t)dx$ the mean position of a corresponding diffusing particle, we see that

$$\langle x(t)\rangle = m(t) = \xi e^{-bt} \quad . \tag{1.6}$$

Now, not going into the details of constructing a solution formula for the more general Eq.(1.5) with $F(x) = -bx$, $u(x,0) = \delta(x-\xi)$ we remark that we still can calculate the function$\langle x(t)\rangle$. Multiplying Eq.(1.5) by x and integrating over $x \in \mathbb{R}$, using the natural properties $u(x,t) \to 0$ and $x^n u(x,t) \to 0$ for all $n \geq 1$ as $|x| \to \infty$, we get the initial value problem

$$\frac{d^\beta \langle x(t)\rangle}{dt^\beta} = -b\langle x(t)\rangle,\ 0 < \beta < 1,\ \langle x(0)\rangle = \xi\ ,$$

whose solution is (see [11])

$$\langle x(t)\rangle = \xi E_\beta(-bt^\beta)\,. \tag{1.7}$$

Here $E_\beta(z) = \sum\limits_{n=0}^{\infty} \frac{z^n}{\Gamma(1+n\beta)}$ is the Mittag-Leffler function (see Vol. 3 of [4]). It is important to compare the asymptotic behaviour in the cases $0 < \beta < 1$ and $\beta = 1$. For $\beta = 1$ we have Eq.(1.6), whereas for $0 < \beta < 1$ we have a power-law decay [11]

$$E_\beta(-bt^\beta) \approx \frac{sin(\beta\pi)}{\pi}\frac{\Gamma(\beta)}{bt^\beta} \quad ,t \to \infty, b > 0 \quad .$$

2 Relation to the Ehrenfest model

We describe a random walk model approximating the diffusion Eq.(1.2) with drift towards the origin. We descretize space and time by a grid $\{(x_j,t_n) \mid j \in \mathbb{Z}\,, n \in \mathbb{N}_0\}$ with $x_j = jh$, $t_n = n\tau$. Here $h > 0$, and $\tau > 0$ are the steps in space and in time, respectively. Treating $u(x,t)$ as density of an extensive quantity (like mass, charge, or probability) we want to approximate the collected quantity $\int_{x_j-\frac{h}{2}}^{x_j+\frac{h}{2}} u(x,t_n)\,dx$ present in a spatial cell $x_j - \frac{h}{2} < x \leq x_j + \frac{h}{2}$ at the instant $t = t_n$ by a clump $y_j^{(n)}$,

$$y_j^{(n)} \approx \int_{x_j-\frac{h}{2}}^{x_j+\frac{h}{2}} u(x,t_n)\,dx \quad . \tag{2.1}$$

Let us henceforth consider the extensive quantity as probability. Then we will find by symmetric discretization in space and forward differencing in time an approximating random walk model, having the form of an explicit difference scheme

$$\frac{y_j^{(n+1)} - y_j^{(n)}}{\tau} = a\,\frac{y_{j+1}^{(n)} - 2y_j^{(n)} + y_j^{(n)}}{h^2} + \frac{b}{2h}\left(x_{j+1}y_{j+1}^{(n)} - x_{j-1}y_{j-1}^{(n)}\right)\ , \tag{2.2}$$

which we subject to a scaling relation $0 < \mu = \frac{\tau}{h^2}$, as is natural for diffusion problems and is known from numerical analysis, see [25]. Eq.(2.2) is equivalent to the equation

$$y_j^{(n+1)} = \gamma y_j^{(n)} + \lambda_{j+1} y_{j+1}^{(n)} + \rho_{j-1} y_{j-1}^{(n)} \ , \tag{2.3}$$

with

$$\gamma = (1-2a\mu),\ \lambda_j = \mu(a+\frac{j}{R}),\ \rho_j = \mu(a-\frac{j}{R}) \text{ and } R = \frac{2a}{bh^2} \ .$$

Our intention that Eq.(2.3) should describe a random walk with sojourn probability $y_j^{(n)}$ of a particle being in point x_j at instant t_n (so that Eq.(2.3) describes the transition from instant t_n to t_{n+1}) requires that $\gamma \geq 0$ and all occuring $\lambda_j \geq 0$, $\rho_j \geq 0$, hence $0 < \mu \leq \frac{1}{2a}$ and the restriction of the index j to the set $(-R, -R+1, -R+2, \ldots, R-2, R-1, R)$ of integers with the convenient stipulation that R should be a natural number. We then take $y_j^{(n)} = 0$ for $|j| \geq R+1$. *We keep this in mind for all our discrete schemes.*

An objection could be raised against this model. Namely whereas in Eq.(1.2) $-\infty < x < \infty$, we consider Eq.(2.3) by the restriction $-R \leq j \leq R$ only in grid points $x_j = jh$ with $-Rh \leq x_j \leq Rh$. However, as usual in the theory of difference schemes we let $h \to 0$ and by the scaling $\tau = \mu h^2$ also $\tau \to 0$. Then $Rh = \frac{2a}{bh} \to \infty$, and thus in the limit the whole real axis $-\infty < x < \infty$ is covered. In this sense the difference scheme Eq.(2.2) with $|j| \leq R$ is consistent to Eq.(1.2). Now as we have the transition probabilities λ_j, ρ_j, and γ of jumping one step of length h to the left, to the right, or staying in place respectively, being non negative and summing up to 1, i.e., $\lambda_j + \rho_j + \gamma = 1$, we can view our discrete model as a Markov chain with a transition matrix $P = (p_{i,j})$ where $p_{i,j} = 0 \ \forall\, |i-j| > 1$.

Let us from now on for ease of writing and without loosing generality *assume*

$$a = 1 \text{ and } b = 1.$$

Then $R = \frac{2}{h^2}$ and the tridiagonal stochastic matrix takes the form

$$P = \begin{pmatrix} (1-2\mu) & 2\mu & 0 & \ldots & \ldots & \ldots & \ldots & 0 \\ \frac{\mu}{R} & (1-2\mu) & \mu(2-\frac{1}{R}) & \ldots & \ldots & \ldots & \ldots & 0 \\ 0 & \frac{2\mu}{R} & (1-2\mu) & \mu(2-\frac{2}{R}) & \ldots & \ldots & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ \ldots & \ldots & \ldots & 0 & \mu(2-\frac{2}{R}) & (1-2\mu) & \frac{2\mu}{R} & 0 \\ \ldots & \ldots & \ldots & \ldots & 0 & \mu(2-\frac{1}{R}) & (1-2\mu) & \frac{\mu}{R} \\ \ldots & \ldots & \ldots & \ldots & 0 & 0 & 2\mu & (1-2\mu) \end{pmatrix}$$

Eq.(2.3) can be written in the condensed form

$$y^{(n+1)} = P^T . y^{(n)} \ , \tag{2.4}$$

with the column vector, $y^{(k)} = \{y_{-R}^{(k)}, y_{-R+1}^{(k)}, \ldots, y_R^{(k)}\}^T \ , k \in \mathbb{N}$. For the interpretation of $y^{(n)}$ as a vector of probabilities, we require $y^{(0)}$ likewise to be such column vector, namely $y_j^{(0)} \geq 0$ and $\sum_{j=-R}^{R} y_j^{(0)} = 1$. Then all $y^{(n)}$ for $n = 1, 2, 3, \dots$ are non-negative. Furthermore,

$$\sum_{j=-R}^{R} y_j^{(n)} = 1 \, \forall n \in \mathbb{N}_0 \quad ,$$

as is easily shown by induction. Actually, the evolution of $y^{(n)}$ is that of a Markov chain [5] with possible states $(x_{-R}, x_{-R+1}, \dots, x_{R-1}, x_R)$.

We compare this discrete model with the generalized Ehrenfest model described by Vincze [31]. Vincze considers N balls, numbered from 1 to N, k of them in an urn U_1, $N-k$ in an urn U_2. In an urn U_0 there are $N+s$ slips of paper ($s \geq 0$) each of them having probability $(N+s)^{-1}$ of being randomly drawn. N of the slips are numbered from 1 to N, the other s slips are not numbered. We repeat indefinitely the following experiment.

We draw a slip from the urn U_0. If it carries a number we move the ball which has the same number from the urn (U_1 or U_2) in which it is lying to the other urn (U_2 or U_1). If the slip is not numbered, we leave the ball in its urn. Then we put the slip back into the urn U_0.

If we record the states as the number of balls in the urn U_1, then there are three probabilities: $\frac{k}{N+s}$ for the next state to be $k-1$, $\frac{N-k}{N+s}$ for the next state to be $k+1$, and finally $\frac{s}{N+s}$ for the next state to be k again. In the special case ($s = 0$) we have the classical Ehrenfest model described by many authors (see [23], [15],[1], [7], [29], and [2]). In other words, if $x_n^{(s)} = k$ is the number of balls in urn U_1 after n steps, then the transition probabilities are

$$q_{k,k} = P(x_{n+1}^{(s)} = k | x_n^{(s)} = k) = \tfrac{s}{s+N}, \;\; k = 0, 1, \dots, N \quad ,$$

$$q_{k,k-1} = P(x_{n+1}^{(s)} = k-1 | x_n^{(s)} = k) = \tfrac{k}{s+N}, \;\; k = 1, 2, \dots, N \quad ,$$

$$q_{k,k+1} = P(x_{n+1}^{(s)} = k+1 | x_n^{(s)} = k) = \tfrac{N-k}{s+N}, \;\; k = 0, 1, 2, \dots, N-1 \quad ,$$

and

$$q_{k,k} + q_{k,k-1} + p_{k,k+1} = 1 \qquad \forall k = 0, 1, 2, \dots, N \; , \; q_{k,k\pm j} = 0 \qquad \forall j > 1 \quad .$$

This model is also called the modified Ehrenfest model. In the special case $s = 0$, its states can only change by moving one ball from U_1 to U_2 with the probability ($q_{k,k-1}$) or to move one ball from U_2 to U_1 with the probability ($q_{k,k+1}$). In the general case $s \geq 0$ the transition probabilities $q_{i,j}$, $0 \leq i \leq N, 0 \leq j \leq N$ form a tridiagonal stochastic matrix

$$Q_s = \begin{pmatrix} \frac{s}{s+N} & 1-\frac{s}{s+N} & 0 & \dots & \dots & \dots & \dots & 0 \\ \frac{1}{s+N} & \frac{s}{s+N} & 1-\frac{s+1}{s+N} & \dots & \dots & \dots & \dots & 0 \\ 0 & \frac{2}{s+N} & \frac{s}{s+N} & 1-\frac{s+2}{s+N} & \dots & \dots & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & 0 & \frac{N-2}{s+N} & \frac{s}{s+N} & 1-\frac{s+N-2}{s+N} & 0 \\ \dots & \dots & \dots & \dots & 0 & \frac{N-1}{s+N} & \frac{s}{s+N} & 1-\frac{s+N-1}{s+N} \\ \dots & \dots & \dots & \dots & 0 & 0 & \frac{N}{s+N} & \frac{s}{s+N} \end{pmatrix} .$$

This matrix coincides with the matrix P, if N is an even number (i.e.$N \in 2\mathbb{N}$), $R = \frac{N}{2}$ and $\mu = \frac{N}{2(s+N)}$. The position $x = 0$ corresponds to $N/2$ balls in U_1, the position $x = Rh$ to N balls in urn U_1, and the position $x = -Rh$ to 0 balls in urn U_1. Let us denote the probability for finding k balls in urn U_1 after n steps by $q_k^{(n)}$, $n = 0, 1, 2, 3, \cdots$. Then

$$q_k^{(n+1)} = q_{k-1}^{(n)} \frac{N-k+1}{s+N} + q_k^{(n)} \frac{s}{s+N} + q_{k+1}^{(n)} \frac{k+1}{s+N}, k = 0, 1, \ldots, N-1 \,. \quad (2.5)$$

This equation can be interpreted as a discrete approximation to a diffusion process with central force. It seems that Schrödinger and Kohlrausch were the first to point out the connection between the discrete Ehrenfest model and Brownian motion of an elastically bound particle. Smoluchowski [26] showed that this model approximates the partial differential Eq.(1.2). This equation describes also the so called Ornstein-Uhlenbeck process [28].

Note the following: In the sense of the urn model s should be an integer, however for Eq.(2.5)to describe a Markov chain, s is only required to be a non-negative real number.

3 Discrete approximation of the time fractional diffusion with central linear drift

In this section we will consider the approximate solution of the Eq.(1.5) with $F(x) = -bx$ obtained by discretizing it by the explicit finite-difference method.

$$\underset{\tau\ *}{D}^{\beta}\, y_j^{(n+1)} = a\, \frac{y_{j+1}^{(n)} - 2y_j^{(n)} + y_{j-1}^{(n)}}{h^2} + \frac{b}{2h} \left(x_{j+1} y_{j+1}^{(n)} - x_{j-1} y_{j-1}^{(n)} \right), 0 < \beta \leq 1 \,. \quad (3.1)$$

We restrict here $R = \frac{2a}{bh^2}$, as in Section 2, and the index j to the range $(-R, -R+1, -R+2, \ldots, R-2, R-1, R)$, adjusting the spatial step h so that $R \in \mathbb{N}$. We complement Eq.(3.1) by prescribing the non-negative initial values $y_j^{(0)}$ obeying $\sum\limits_{j=-R}^{R} y_j^{(0)} = 1$, and for convenience, all $y_j^{(n)} = 0$ for $|j| \geq R+1$, $n = 0, 1, 2, \ldots$. In Eq.(3.1) the difference operator $\underset{\tau\ *}{D}^{\beta}$ denotes the discretization of the *Caputo time derivative* (see the Appendix, [12], [19], [22] and [18]). For $\beta = 1$, Eq.(3.1) is reduced to Eq.(1.2). For discretizing the Caputo time derivative, we use, as in [13] a backward *Grünwald- Letnikov* scheme in time (starting at level $t = t_{n+1}$) which reads

$$\underset{\tau\ *}{D}^{\beta}\, y_j^{(n+1)} = \sum_{k=0}^{n+1} (-1)^k \binom{\beta}{k} \frac{y_j^{(n+1-k)} - y_j^{(0)}}{\tau^\beta} \quad , \; 0 < \beta \leq 1 \,. \quad (3.2)$$

Observe that $\underset{\tau\ *}{D}^{1}\, y_j^{(n+1)} = \frac{1}{\tau} \left(y_j^{(n+1)} - y_j^{(n)} \right)$. Note that in case of sufficient smoothness the scheme(3.1) has order of accurecy $O(h^2 + \tau)$. By introducing the scaling parameter

$$\mu = \frac{\tau^\beta}{h^2}\ ,\ 0 < \mu \le \frac{\beta}{2}\ , \tag{3.3}$$

and solving Eq.(3.2) for $y_j^{(n+1)}$, $-R \le j \le R$, we get

$$\begin{aligned} y_j^{(n+1)} \ &= \sum_{k=0}^{n} (-1)^k \binom{\beta}{k} y_j^{(0)} \ + \sum_{k=1}^{n} (-1)^{k+1} \binom{\beta}{k} y_j^{(n+1-k)} \\ &\quad + y_{j+1}^{(n)} \left[\mu + \frac{\mu h^2}{2}(j+1)\right] - 2\mu y_j^{(n)} \ + y_{j-1}^{(n)} \left[\mu - \frac{\mu h^2}{2}(j-1)\right] . \end{aligned} \tag{3.4}$$

Again $y^{(n+1)}$ represents the probability column vector for where to find the particle at the time instant t_{n+1}. It depends on $y_{j-1}^{(n)}$, $y_j^{(n)}$, $y_{j+1}^{(n)}$, $y_j^{(n-1)}$,..., and back to $y_j^{(0)}$. This model, having the form of an explicit difference scheme, can be interpreted as a random walk with memory. Let

$$b_n = \sum_{k=0}^{n} (-1)^k \binom{\beta}{k}\ , n = 0, 1, 2, \ldots;\ c_k = (-1)^{k+1} \binom{\beta}{k}\ , k = 1, 2, \ldots\ .$$

Then $b_0 = 1$, and all $c_k \ge 0$, $b_n \ge 0$, $\sum\limits_{k=1}^{\infty} c_k = 1$. In the case $0 < \beta < 1$ (see [10], [12]) we have $c_1 = \beta > c_2 > c_3 > \ldots$, and finally the relation

$$b_n + \sum_{k=1}^{n} c_k = 1\ . \tag{3.5}$$

By aid of the coefficients b_n and c_k in Eq.(3.4) the expression

$$\sum_{k=1}^{n} c_k y_j^{(n+1-k)} \ + b_n y_j^{(0)}\ ,$$

represents the dependence on the past (the memory part) and the expression

$$y_{j+1}^{(n)} \left[\mu + \frac{\mu h^2}{2}(j+1)\right] - 2\mu y_j^{(n)} \ + y_{j-1}^{(n)} \left[\mu - \frac{\mu h^2}{2}(j-1)\right]\ ,$$

represents the diffusion part, the particle going one step to the right or one step to the left or remaining in its position. For $\beta = 1$, all these coefficients will vanish and we have the natural discretization of Eq.(1.2). In Eq.(3.4), $y_j^{(n+1)}$ represents the probability of finding the position of the particle at point x_j at the time instant t_{n+1}. Therefore $y_j^{(n+1)}$ must be non-negative because as initial probabilities all $y_j^{(0)} \ge 0$, and the summation of $y_j^{(n)}$ over the index j at any time t_n must give one. In other words, we want

$$s_n = \sum_{j=-R}^{R} y_j^{(n)} = 1 \ \ \forall n \in \mathbb{N}\ .$$

We prove that this holds by induction. It is true for the initial index $n = 0$. So, as $b_0 = 1$, then

$$y_j^{(1)} = (1-2\mu)y_j^{(0)} + y_{j+1}^{(0)}[\mu + \frac{\mu h^2}{2}(j+1)] \; + \; y_{j-1}^{(0)}\,[\mu - \frac{\mu h^2}{2}(j-1)] \; . \quad (3.6)$$

Assuming $0 < \mu \leq \beta/2$ and taking the stochastic matrix P, as in Section 2, we represent this equation in matrix-vector form:

$$y^{(1)} = P^T . y^{(0)} \quad . \quad (3.7)$$

Now, summing both sides of Eq.(3.6) over j from $-R$ to R, we get

$$s_1 = (1-2\mu)s_0 + \mu s_0 + \sum_j \frac{j+1}{R} y_{j+1}^{(0)} + \mu s_0 - \sum_j \frac{j-1}{R} y_{j-1}^{(0)} = s_0 \; .$$

For $n = 1$:

$$y_j^{(2)} = b_1 y_j^{(0)} + (c_1 - 2\mu)y_j^{(1)} + y_{j+1}^{(1)}[\mu + \frac{\mu h^2}{2}(j+1)] + y_{j-1}^{(1)}[\mu - \frac{\mu h^2}{2}(j-1)] \; .$$

Here the dependence on the past appears and by the summation we get

$$s_2 = b_1 s_0 + (c_1 - 2\mu)s_1 + \mu s_1 + \sum_j \frac{j+1}{R} y_{j+1}^{(1)} + \mu s_1 - \sum_j \frac{j-1}{R} y_{j-1}^{(1)} \; ,$$

and because of $b_1 + c_1 = 1$, $s_1 = s_0$ we obtain $s_2 = s_0$. Now assuming that $s_n = 1$, $n \geq 2$, then to prove that $s_{n+1} = 1$, we write Eq.(3.4)in the form

$$\begin{aligned} y_j^{(n+1)} \;&=\; b_n y_j^{(0)} \; + \sum_{k=1}^{n} c_k y_j^{(n+1-k)} \; - \; 2\mu y_j^{(n)} + \\ &\quad + \; \mu\left(1 + \frac{j+1}{R}\right) y_{j+1}^{(n)} \; + \; \mu\left(1 - \frac{j-1}{R}\right) y_{j-1}^{(n)} \; . \quad (3.8) \end{aligned}$$

Summing here over j at both sides and using the relation (3.5), we get $s_{n+1} = 1$. So far, we have proved that our difference scheme is conservative and non negative inspite of its dependence on the past. In fact, $y_j^{(n+1)}$ is a linear combination of all $y_j^{(k)}$ with $-R \leq j \leq R$, $0 \leq k \leq n$, with coefficients whose sum is 1.

3.1 The solution of the explicit difference scheme

Let us now, in preparation of the next section, treat Eq.(3.4) in a matrix-vector notation. Therfore we must proceed in two steps, considering the step from n to $n + 1$, separately for $n = 0$ and $n \geq 1$. For $n = 0$, transposing the matrix Eq.(3.7) and adopting the notation

$$(y^{(n)})^T = z^{(n)} \;\; \forall n \in \mathbb{N} \;\; , z^{(n)} = (z_{-R}^{(n)}, z_{-R+1}^{(n)}, \ldots, z_R^{(n)}) \;\; ,$$

we find

$$z^{(1)} = z^{(0)}.P \ . \tag{3.9}$$

Here P is the stochastic matrix defined in Section 2 whose rows sum to one and $z^{(n)}$ is a row vector. It is convienent to write P in the form

$$P = I + \mu H \ ,$$

with I a unit matrix and H a matrix whose rows sum to zero:

$$H = \begin{pmatrix} -2 & 2 & 0 & \dots & \dots & \dots & \dots & 0 \\ \frac{1}{R} & -2 & (2-\frac{1}{R}) & \dots & \dots & \dots & \dots & 0 \\ 0 & \frac{2}{R} & -2 & (2-\frac{2}{R}) & \dots & \dots & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & 0 & (2-\frac{2}{R}) & -2 & \frac{2}{R} & 0 \\ \dots & \dots & \dots & \dots & 0 & (2-\frac{1}{R}) & -2 & \frac{1}{R} \\ \dots & \dots & \dots & \dots & \dots & 0 & 2 & -2 \end{pmatrix} .$$

Now, for $n \geq 1$, we define the matrix $Q = c_1 I + \mu H$, and write equation(3.4) as

$$z^{(n+1)} = b_n z^{(0)} + \sum_{k=2}^{n} c_k z^{(n+1-k)} + z^{(n)}.Q \ . \tag{3.10}$$

Observe that the matrix Q is stochastic only if $c_1 = 1$ which is equivalent to $\beta = 1$. The restriction for μ in Eq.(3.3) implies that Q is non negative.

4 The implicit scheme (Θ-method)

The idea of the θ- method (also known as the weighted method) is to replace $y_j^{(n)}$ in the right hand side of Eq.(3.1) by $(\theta y_j^{(n+1)} + (1-\theta) y_j^{(n)})$ where $0 < \theta \leq 1$. With $\theta = 0$, we have the explicit scheme. Again, we shall discuss separately the cases $n = 0$ and $n \geq 1$. For convenience, we set $\bar{\theta} = (1-\theta)$. For $n = 0$, we rewrite Eq.(3.9) in the form

$$z^{(1)}.(I - \mu\theta H) = z^{(0)}.(I + \mu\bar{\theta} H) \ . \tag{4.1}$$

Then

$$z^{(1)} = z^{(0)}.(I + \mu\bar{\theta} H).(I - \mu\theta H)^{-1} \ . \tag{4.2}$$

We want the matrix $P_\theta = (I + \mu\bar{\theta}H).(I - \mu\theta H)^{-1}$ to be a stochastic matrix. This wish leads us to conditions for μ depending on θ. First, P_θ must be non-negative. Obviously, $(I - \mu\theta H)$ is a strictly diagonally dominant M-matrix, hence its inverse is non-negative. $(I + \mu\bar{\theta}H)$ is non-negative if $(1 - 2\mu\bar{\theta}) \geq 0$. So we arrive, with $r = 1$ (below to be modified to $r = \beta$), at the conditions [14], [30]

$$0 < \mu \leq r/2 \ \text{ if } \ \theta = 0 \ , 0 < \mu \leq \frac{r}{2(1-\theta)} \ \text{ if } \ 0 < \theta < 1 \ , 0 < \mu < \infty \ \text{ if } \ \theta = 1 \ .$$

Second, the rows of P_θ must sum to 1. So, we require $P_\theta.\ \eta\ =\ \eta$, with the column vector η all of whose $2R+1$ components have the value 1, i.e., $\eta\ =\ (1,1,\ldots,1)^T$. Since the rows of H are all summing to zero, we have $(H.\eta = 0)$. This leads to $(I-\mu\theta H).\eta = \eta$ and $(I+\mu\bar{\theta}H).\eta = \eta$. Therefore

$$\eta = (I+\mu\bar{\theta}H).\eta = (I+\mu\bar{\theta}H).(I-\mu\theta H).\eta = P_\theta.\eta\ \ .$$

Now, we shall prove $\sum\limits_j y_j^{(n)} = 1\,\forall n$ which is equivalent to $\sum\limits_j z_j^{(n)} = 1\,\forall n$.

To this purpose, we shall use the following rule: $w\ =\ (w_1, w_2, \cdots)^T$ is a probability column vector iff $w_i \geq 0,\ \ i = 1,2,\cdots$ and $w^T.\eta = 1$.

Now, we know that $(I-\mu\theta H)^{-1}$ and P_θ are stochastic matrices. Hence $z^{(0)}.\eta\ =\ 1$ and hence Eq.(4.2) implies that $z^{(1)}.\eta\ =\ z^{(0)}.(P_\theta.\eta)\ =\ z^{(0)}.\eta\ =\ 1$, Hence the desired relation is true for $n = 0$. For $n \geq 1$, let us rewrite Eq.(3.10) as

$$z^{(n+1)} = b_n z^{(0)} + \sum_{k=1}^{n} c_k z^{(n+1-k)}\ +\mu\, z^{(n)}.H\ \ . \tag{4.3}$$

Replacing $z^{(n)}$ in $(\mu z^{(n)}.H)$ by $(\theta z^{(n+1)} + \bar{\theta} z^{(n)})$ and solving for $z^{(n+1)}$ gives

$$z^{(n+1)} = \left[b_n z^{(0)} + \sum_{k=1}^{n} c_k z^{(n+1-k)}\ +\ \mu\,\bar{\theta}\, z^{(n)}.H\right].[I-\mu\theta H]^{-1}\ \ . \tag{4.4}$$

Here $(I-\mu\theta H)^{-1}$ is a non-negative matrix and also all b_n and c_k are also non-negative. The consideration of the index $k\ =\ 1$ in Eq. (4.4) however, forces us to sharpen our restriction on μ by taking $r\ =\ \beta\ =\ c_1$. Hence, assuming $\sum\limits_j z_j^{(n)}\ =\ 1$ (i.e., $z^{(n)}.\eta = 1$), then multiplying each side of Eq.(4.4) by η, and using the important Eq.(3.5), we get $z^{(n+1)}.\eta = 1$. Thus, $z^{(n+1)}$ is a probability row vector. So the relation $(z^{(n)}.\eta = 1)$ is true for all values of n. As a matter of fact, the implicit scheme allows us to predict the future faster than the explict scheme, because μ and τ depend on each other by the scaling relation (3.3) and the bound for μ is increasing (up to ∞) if θ is increasing from 0 to 1.

5 The convergence to the stationary solution of the model

Both Vincze, Fritz and Kac (see [31], [6] and [15]) showed that the elements of the iterated stochastic matrix Q_s^n of the generalized discrete Ehrenfest model (urn model) converge to the binomial distribution at $n \to \infty$. This means:

$$\lim_{n\to\infty} Q_s^n = \begin{pmatrix} p_0 & p_1 & \cdots & p_N \\ \vdots & \vdots & & \vdots \\ p_0 & p_1 & \cdots & p_N \end{pmatrix}$$

with

$$p_k = 2^{-N}\binom{N}{k},\ k = 0, 1, \ldots, N \ ,$$

exists. N is the total number of balls. The vector $p = \{p_0, \ldots, p_N\}$ satisfying $\sum_{k=0}^{N} p_k = 1$ represents the stationary distribution of the Markov chain whose matrix is Q_s(see Section 2).

Both the probability of finding k balls in the urn U_1 after $n+1$ steps equation (2.5) and the probability of finding the particle at the point x_j at the time instant t_{n+1} Eq.(2.3) are interpreted as the discrete approximation to a diffusion with central linear force. Therefore, by taking the limit as $Rh \to \infty$ in Eq.(2.3), it can be represented as the partial differential Eq.(1.2) [26]. Since, the stochastic matrix P representing the random walk approach of equation (2.3) and the stochastic matrix Q_s representing the random walk approach of equation (2.5) are related to each other by some relations (see section 2), then the matrix P has a similar limit as $n \to \infty$. So far, to show the behaviour of this model represented by Eq.(1.2) as $t \to \infty$ (i.e., for $\beta = 1$), We form a vector $\bar{y}$ with components

$$\bar{y}_j = 2^{-2R}\binom{2R}{j+R} \ , \ -R \le j \le R \ , \tag{5.1}$$

and a sequence of numbers $q = \{q(t_1, q(t_2), \cdots\}$, where $0 < t_1 < t_2 < \cdots \to \infty$. The number $q(t_i)$ is defined as

$$q(t_i) = \sum_{j=-R}^{R} |y_j(t_i) - \bar{y}_j| \ , i = 1, 2, \ldots \ . \tag{5.2}$$

The iteration index n is calculated from the relation $n\tau = t_i$, $t_i = 1, 2, \cdots \to \infty$ while τ is calculated from the scaling parameter (3.3). The simulation of the vector q shows that it approximates an exponential function

$$q \approx c\, e^{-at} \ , \tag{5.3}$$

where a and c are constants and a is called the rate of exponential convergence. Such exponential convergence is a general property of an ergodic Markov chain (see Feller [5]). The numerical estimation of a shows that a tends to 1 as t tends to infinity.

For estimating the convergence as $0 < \beta < 1$, i.e. for the non Markovian chain and under the action of the other types of forces (b), (c) and (d), defined in Section 1, we shall apply the more general method for calculating the discrete stationary solution of Eq.(1.5). This is made by omitting the dependence on the time. First, for $0 < \beta < 1$ and $F(x) = -x$, we shall omit the dependence on the time at Eq.(4.3). To this purpose, we replace all the indices$(n+1), (0)$ and $(n+1-k)$ by simply (n). Then Eq.(4.3) converges to $z.H = 0$ which is equivalent to $H^T.y = 0$. The last matrix equation is valid for both $\beta = 1$ and $0 < \beta < 1$ and it has an eigenvector y^* of eigenvalue zero. From the properties of the matrices, we can construct a vector $\bar{y}$ such that $\bar{y} = cy^*$, and the constant c is obtained from the relation $c = 1/\sum\limits_{j=-R}^{R} y_j^*$. By this normalization, we obtain a normalized vector $\bar{y}$ whose elements sum to 1 and its elements are the same as in Eq.(5.1). Again, we construct a sequence of numbers

$$d = \{d(t_1), d(t_2), \dots\} \ , \tag{5.4}$$

as in Eq.(5.2). The numerical estimation of the sequence d shows that it behaves as the behaviour of the vector q (Eq.(5.3) for $\beta = 1$).The simulation of the sequence d equation (5.4) for $0 < \beta < 1$ shows that it approximates a power function

$$d \approx c\,t^{-\omega} \ , \tag{5.5}$$

where c and ω are also constants and ω is called the rate of algebric convergence. The numerical estimation shows that ω tends to β faster than in the case $\beta =$ 1. The implicit scheme allows us to calculate the vector d so fast because the number of steps in this case is less than that of the explicit scheme. For estimating the convegence of the model under the action of the cubic function $F(x) = -x^3$, we apply the same method. The only difference is that we replace the transition probabilities ρ_j and λ_j constituting the matrix P by

$$\rho'_j = \mu(1 - \frac{j^3}{R^3}) \ , \lambda'_j = \mu((1 + \frac{j^3}{R^3}) \ , \tag{5.6}$$

with $-R \leq j \leq R$ and $R = (\frac{2}{h^4})^{1/3}$. The probability γ of the particle to its position remains unchanged. The elements q_i and d_i are so small, so that we shall plot their logarithms against t. By using the relation (2.1), we find that the vector $\bar{y}/h$ approximates the normalized exact analytic solution $u(x)$ of the stationary equation of the model (i.e., as $t \to \infty$). To obtain the stationary solution, we replace $u(x,t)$ by $u(x)$ in Eqs.(1.2 and 1.5). That means, we omit the dependence on the time t . In Eq.(1.5) the fractional time derivative $\frac{\partial^\beta u(x,t)}{\partial t^\beta}$ is the *Caputo fractional derivative* (see the appendix). The *Caputo fractional derivative* of a constant is zero. Then Eq.(1.5) as well as Eq.(1.2) tends to the equation

$$\frac{\partial^2 u(x)}{\partial x^2} - \frac{\partial\,(F(x)u(x))}{\partial x} = 0 \ , \tag{5.7}$$

as $t \to \infty$ whose solution is

$$u(x) = C\ e^{-U(x)} \ , \tag{5.8}$$

C being the constant of integration. Since $u(x)$ represents a probability density function, we can determine the constant C from the normalization condition $\int\limits_{-\infty}^{+\infty} u(x)dx = 1$. Therefore,the solution of the stationary Eq.(1.5) for a linear force $-x$ is

$$u(x) = \frac{1}{\sqrt{2\pi}}\, e^{-x^2/2} \ , \tag{5.9}$$

and the stationary solution for the cubic force $-x^3$ is

$$u(x) = \frac{\sqrt{2}}{\Gamma(1/4)} e^{-x^4/4} . \tag{5.10}$$

6 Random walk simulation

We now discuss the discrete random walk model of the elastically bound particle (diffusion under the action of the force $-x$, namely the generalized Ehrenfest model). We shall discuss this model separately for $\beta = 1$ and for $0 < \beta < 1$ to see the effect of the memory part. Firstly,we shall discuss the case $\beta = 1$, namely Eq.(1.2) considered as a Markov chain. If we assume that the particle is sitting at the point x_j at the time instant t_n, then as the time proceeds to the instant t_{n+1} the particle jumps either to the point x_{j-1} with probability λ_j, x_{j+1} with probability ρ_j, or remains in its position with probability γ. The transition probabilities λ_j, ρ_j, and γ are defined in section 2. The past history before the instant t_n is completely forgotten. The sketch of transitions of this case is at Fig. [31].

In the case $0 < \beta < 1$ we must keep in mind the whole past history of the wandering particle. Its history consists of its positions at the times $t_0, t_1, \cdots$ and up to t_n. That means, the path of the particle is $x_j(t_o), x_j(t_1), \ldots, x_j(t_n)$. The initial position of the particle $x_j(t_0)$ may be any grid point inside the interval $[-Rh, Rh]$. As we have done in the previous sections, we shall distinguish the cases corresponding to $n = 0$ and $n \geq 1$ in the simulation. For $n = 0$, the random walk of the Eq.(3.6) is Markov-like. For $n \geq 1$, we rewrite Eq.(3.8) in the form

$$\begin{aligned} y_j^{(n+1)} = & \left(1 - \sum_{k=1}^{n} c_k\right) y_j^{(0)} + c_n y_j^{(1)} + c_{n-1} y_j^{(2)} + \cdots + c_2 y_j^{n-1} \\ & + (c_1 - 2\mu) y_j^{(n)} + \mu \left(1 + \frac{j+1}{R}\right) y_{j+1}^{(n)} + \mu \left(1 - \frac{j-1}{R}\right) y_{j-1}^{(n)} \end{aligned} \tag{6.1}$$

Clearly all the coefficients $c_1, c_2, \ldots, c_n, (1 - \sum\limits_{k=1}^{n} c_k)$ are non-negative. The idea of simulation is analogous to that of [13]. Assuming the particle sitting at the grid point $x_j \in [-Rh, Rh]$ at instant $t_n, n \geq 1$, then its position at the next instant t_{n+1} is obtained as follows. We set $s_k = \sum\limits_{i=1}^{k} c_i$ for $k = 1, 2, \ldots, n$ and generate a uniformly in $[0, 1)$ distributed random number u. Then we test successively into which one of the intervals $[0, s_1), [s_1, s_2), [s_2, s_3), \ldots, [s_n, 1)$ u falls. The length of these intervals are respectively $c_1, c_2, \ldots, c_n$ and $b_n = 1 - s_n$. We subdivide the first interval ($[0, s_1) = [0, c_1)$) into three sub-intervals of lengthsλ_j, γ' and ρ_j where $\gamma' = (c_1 - 2\mu)$. Now if $u \in [0, c_1)$, we move the particle from its position $x(t_n) = x_j$ to the point x_{j-1}, x_j or x_{j+1} depending on whether u is in the subinterval of length λ_j, γ' or ρ_j, respectively. If $u \in [s_{k-1}, s_k)$ with

$2 \leq k \leq n$, we move the particle from its position $x(t_n)$ back to its previous position $x(t_{n+1-k})$. In the case $u \in [s_n, 1)$ we move it back to its initial position $x(t_0) = x(0)$. The diagram of transitions is given in Section 8 (Fig.[32]).

For the actual simulations let us note the following: for a more general force $F(x)$, we must replace the term $\frac{b}{2h}\left(x_{j+1}y_{j+1}^{(n)} - x_{j-1}y_{j-1}^{(n)}\right)$ in Eqs.[(2.2) and (3.1)] by $\frac{-1}{2h}\left(F(x_{j+1})y_{j+1}^{(n)} - F(x_{j-1})y_{j-1}^{(n)}\right)$ and take into account all the other resulting changes in discretization.

7 Conclusion

The explicit difference scheme for the classical diffusion equation $\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$ can as is well known not only be used for approximating the density $u(x,t)$ but allows also re-interpretation and use as a random walk model for approximate simulation of the path of a particle whose sojourn probabilitiy density is $u(x,t)$. Analogous two-fold interpretation of explicit and implicit difference schemes is possible for various types of fractional diffusion problems. If fractionality is in the time variable then the difference scheme takes account of the whole past and consequently its stochastic interpretation yields a backword-oriented random walk in which the whole past history of a particle influences its future (in contrast to forward-oriented continuous or discrete time random walk in which after each jump the past is forgotten). We have here worked out the corresponding theory for time-fractional diffusion with symmetric drift towards the spatial origin and have shown its applicability by carrying out numerical case studies, for both possible uses of the difference schemes.

8 Numerical results

Figures [1-3] correspond to the explicit scheme for $F(x) = -x$ and $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$, the case where the particle starts its random walk at $x = 0$. Figures [4-6] correspond to the explicit scheme for $F(x) = -x$ and $y^{(0)} = \{\frac{1}{2R+1}, \cdots, \frac{1}{2R+1}, \cdots, \frac{1}{2R+1}\}$. Figures [7-11] correspond to the implicit scheme for $F(x) = -x$ and $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$. Figures [12-14] correspond to the implicit scheme for $F(x) = -x$ and $y^{(0)} = \{0, \cdots, 0, 1\}$. Figures [15,16] illustrate the convergence as $f(x) = -x$ and $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$. In these figures we have plotted *log d* against time t. Figures [17,18] show the approximate stationary solution and the approximate solution of the model of linear force.

Figures [19,20] correspond to the explicit scheme for $F(x) = -x^3$ and $y^{(0)} = \{0, \cdots, 0, 1\}$. Figures [21,22] correspond to the implicit scheme for $F(x) = -x^3$ and $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$. Figures [23,24] illustrate the convergence of the model for $F(x) = -x^3$ and $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$. We have plotted *log d* against time t. Figures [25,26] show the approximate stationary solution and the stationary analytic solution of the model for the cubic force $F(x) = -x^3$. Figures [27-30] exhibit the simulation of the random walk and its increments for $F(x) = -x$ and $x(0) = 0$ for $\beta = 1$ and $0 < \beta < 1$. In these figures, we have plotted x or Δx against the number of steps n. The results of all these figures are taken for $R = 10$. Observe the conspicuous flatness of the stationary solution as $x = 0$ in the case of the cubic force $-x^3$ in contrast to its form in the case of the linear force $-x$.

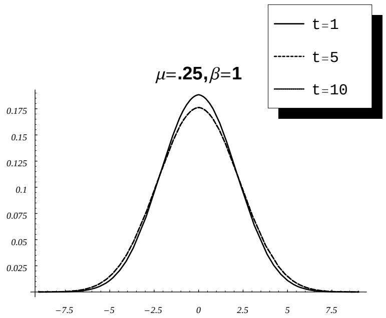


Figure 1:

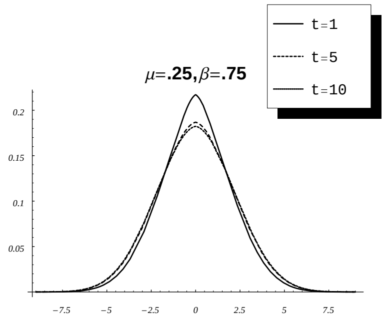
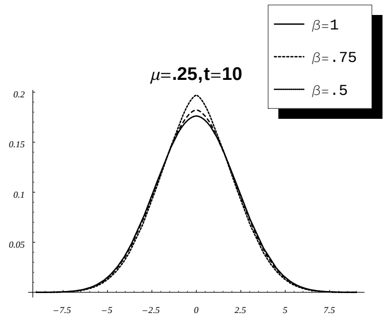


Figure 2:



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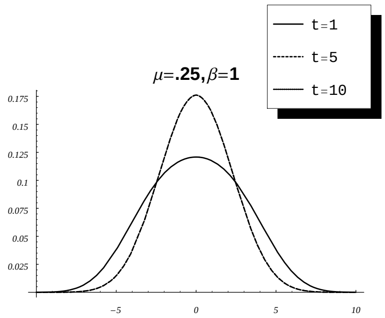

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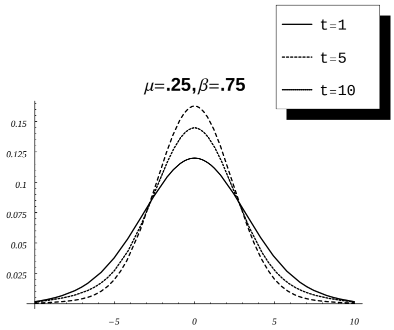

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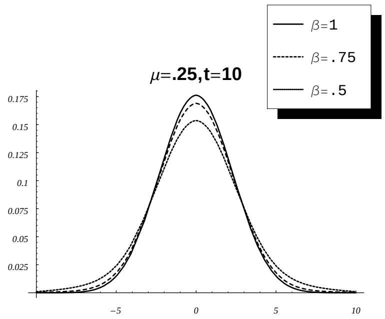

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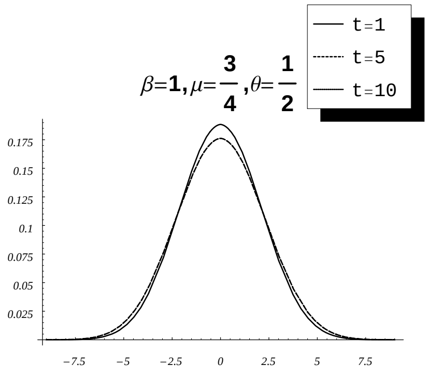

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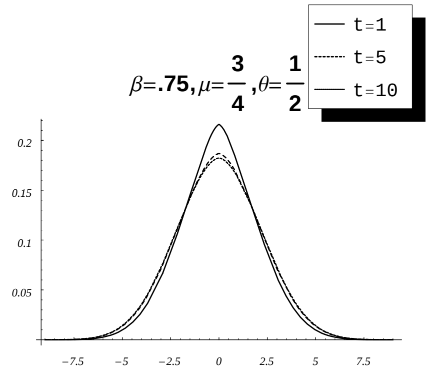

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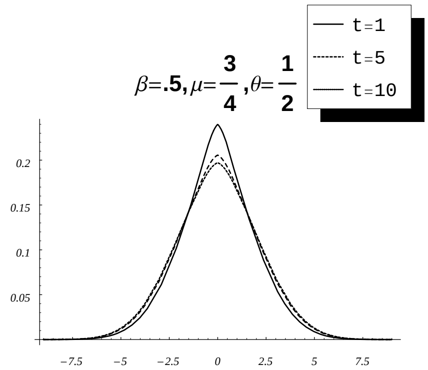

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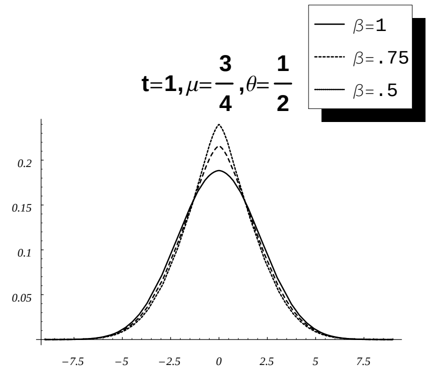

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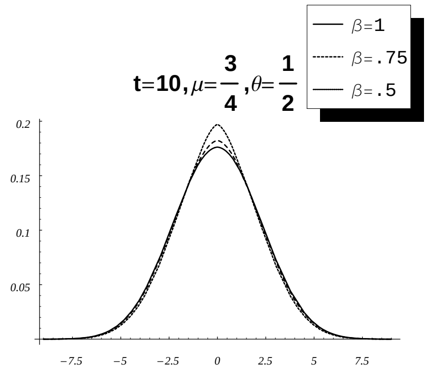

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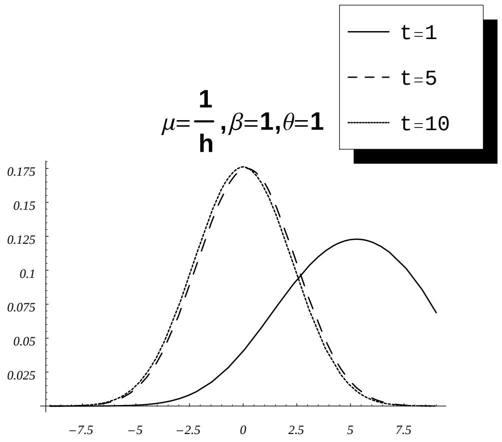

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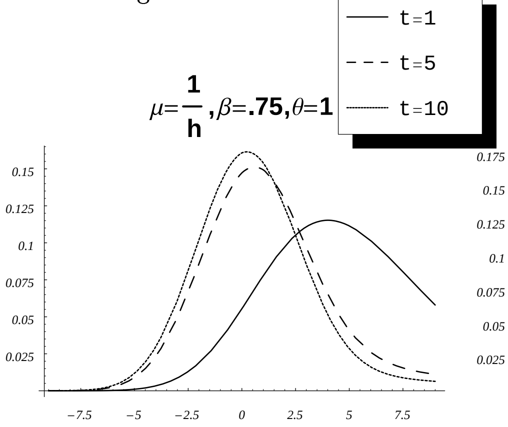

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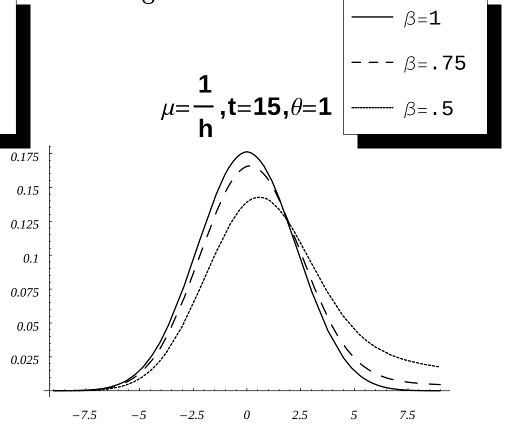

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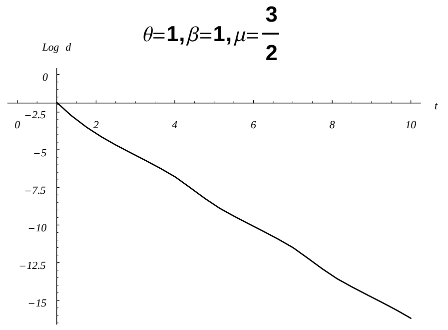

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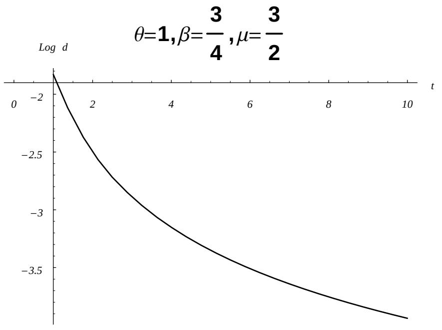

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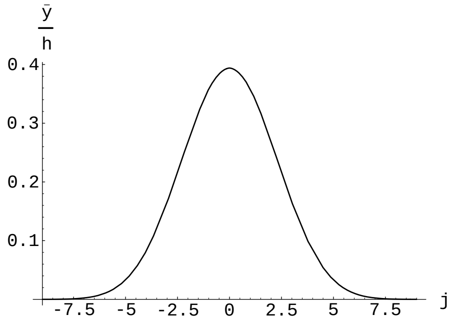

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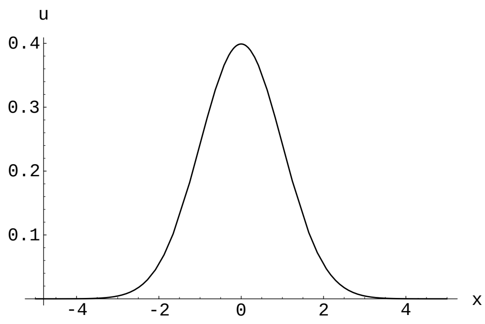

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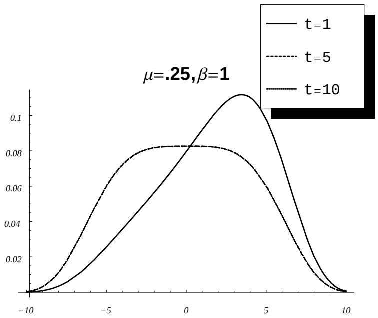

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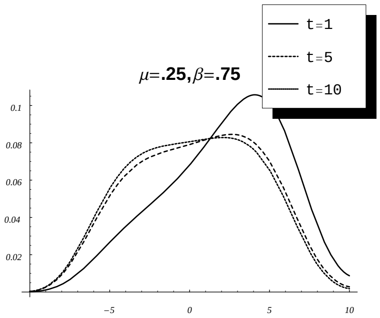

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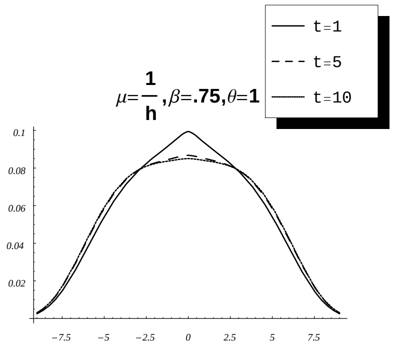

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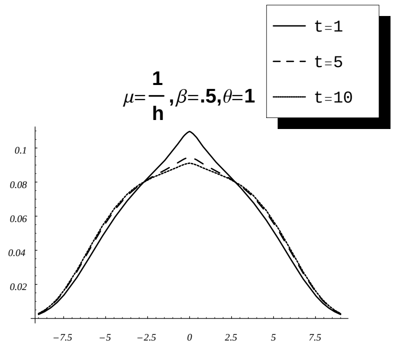

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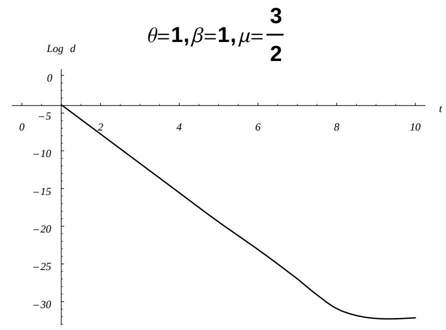

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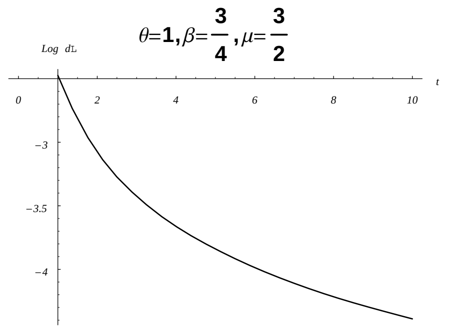

Figure 24:

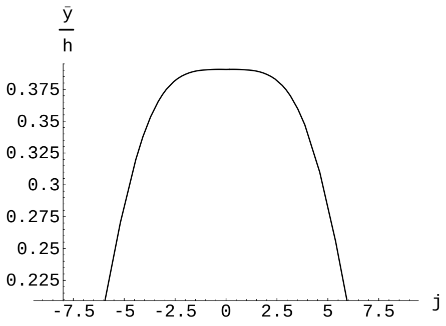

Figure 25:

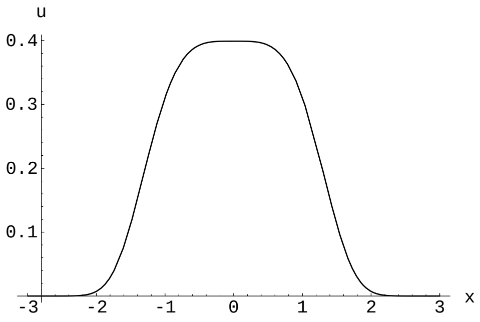

Figure 26:

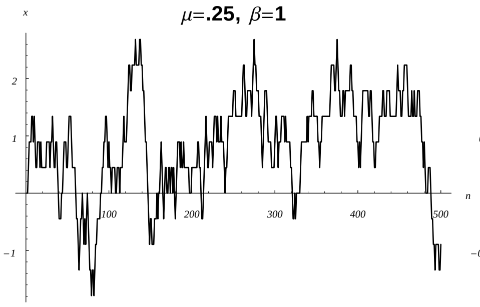

Figure 27:

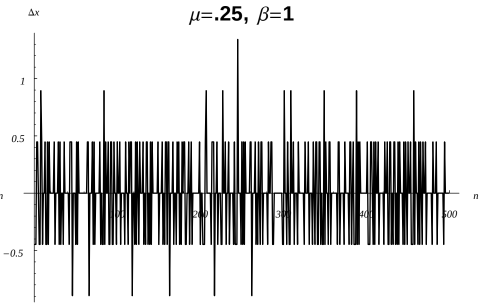

Figure 28:

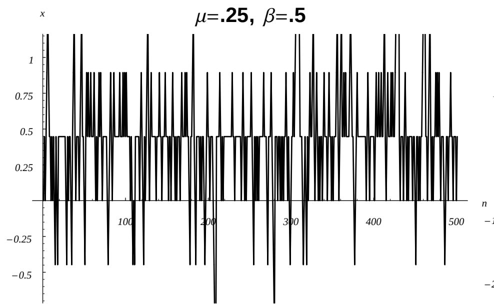

Figure 29:

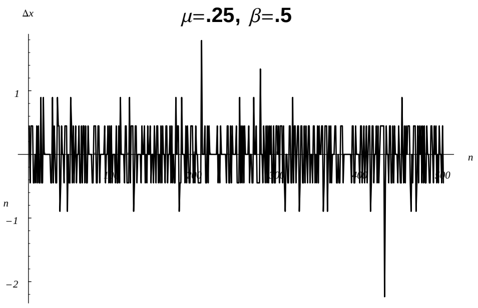

Figure 30:

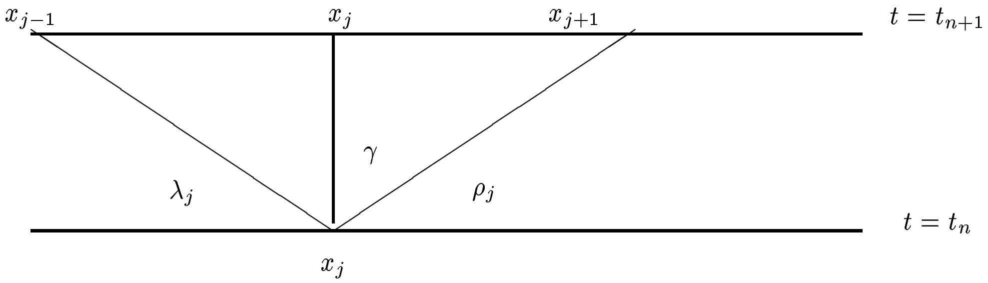

Figure 31 **: The transition diagram of the possible jumps for** $\beta = 1$

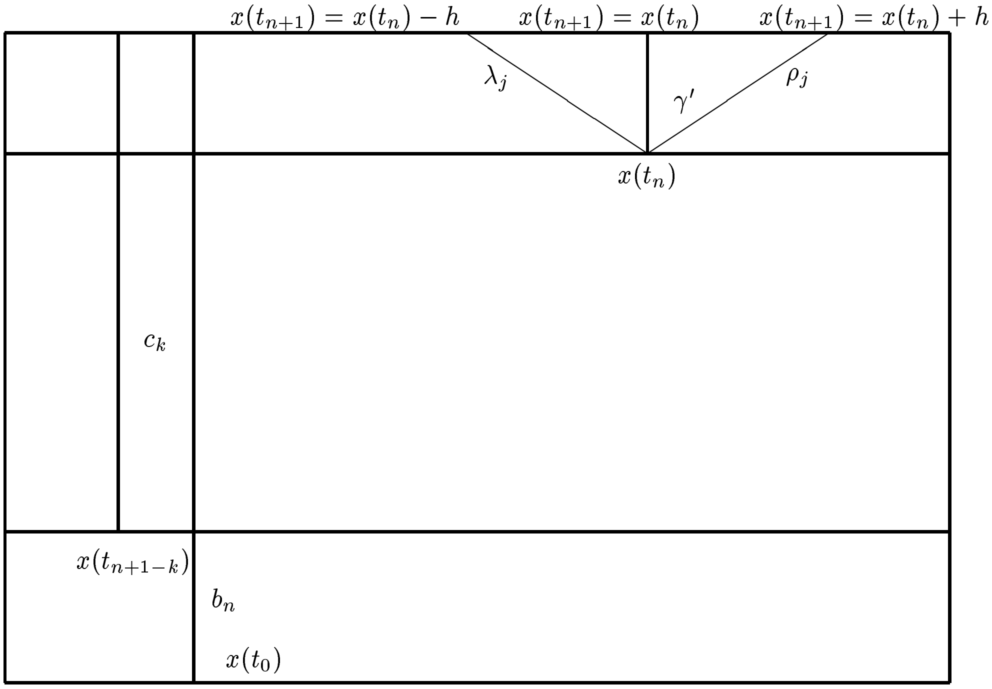

Figure 32 **: The transition diagram of the possible jumps for** $0 < \beta < 1$

A Important definitions

For the purpose of this paper,we use the Riemann-Liouville fractional derivative of order $\beta > 0$ with $0 < \beta \le 1$ for a function $f(t)$ given in the interval $[0, b]$, $b < \infty$, defined for $t > 0$ by the expressions (see [22], [11], [18] and [19]).

$$(D^\beta f)(t) = \begin{cases} \frac{1}{\Gamma(1-\beta)} \frac{d}{dt} \int_0^t \frac{f(\tau)}{(t-\tau)^\beta} d\tau \ , & 0 < \beta < 1 \\ \frac{df(t)}{dt} \ , & \beta = 1 \end{cases} . \tag{A.1}$$

We refer the readers to the books [18], [19] and [22] for the general theory of fractional derivatives and integrals. The Riemann-Liouville fractional integral of order $\beta > 0$ is defined as

$$J^\beta f(t) = \frac{1}{\Gamma(\beta)} \int_0^t (t-\tau)^{(\beta-1)} f(\tau) d\tau \ , t > 0, \ \beta \in \mathbb{R}^+ \ . \tag{A.2}$$

The alternative fractional derivative operator(see [11]) is the Caputo fractional derivative of order $0 < \beta < 1$.

$$(\underset{*}{D^\beta} f)(t) = \begin{cases} \frac{1}{\Gamma(1-\beta)} \int_0^t \frac{\dot{f}(\tau)}{(t-\tau)^\beta} d\tau \ , & 0 < \beta < 1 \\ \frac{df(t)}{dt} \ , & \beta = 1 \end{cases} . \tag{A.3}$$

This definition is more restrictive than (A.1), and it is instructive to mention the relation between the Riemann-Liouville fractional derivative and integral operators and the Caputo fractional derivative $\underset{*}{D}^{\beta} f(t) = J^{1-\beta} D^1 f(t)$, $0 < \beta < 1$. Whereas, the Riemann-Liouville fractional derivative and integral operators satisfy the equation $D^{\beta} f(t) = D^1 J^{1-\beta} f(t)$, $0 < \beta \leq 1$ with $D^1 = \frac{d}{dt}$, we have, if $0 < \beta < 1$,

$$(\underset{*}{D}^{\beta} f)(t) = D^{\beta}[f(t) - f(0^+)] = D^{\beta} f(t) - \frac{f(0)t^{-\beta}}{\Gamma(1-\beta)} \, . \tag{A.4}$$

In Eq. (1.5) we have written $\frac{\partial^{\beta}}{\partial t^{\beta}}$ in place of $\underset{*}{D}^{\beta}$ for reasons of notational analogy to $\frac{\partial}{\partial t}$. Eq.(A.4) represents the relation between the Riemann-Liouville and Caputo fractional derivative and the dependence on the initial value $f(0)$. It is important for solving fractional differential equations with prescribed initial values. Finally, since $D^{\beta} t^{\mu} = \frac{\Gamma(\mu+1)}{\Gamma(\mu+1-\beta)} t^{\mu-\beta}$, $\beta \geq 0$, $\mu \geq 0$, the Riemann-Liouville fractional derivative of a constant is not zero, but the Caputo fractional derivative of a constant is zero.

Let us now give some information on the Grünwald-Letnikov approximation of fractional derivatives. For more details, see [22], [18], [19] and [32]. For a sufficiently smooth function, defined and bounded on the whole real line, we have

$$f^{(\beta)}(x) = \lim_{h \to 0^+} \frac{(\Delta_h^{\beta} f)(x)}{h^{\beta}} \quad , \beta > 0 \ , \tag{A.5}$$

where $(\Delta_h^{\beta} f)(x) = \sum_{k=0}^{\infty} \binom{\beta}{k} f(x - kh)$. With the binomial coefficients $\binom{\beta}{k}$ this series converges absolutely and uniformally for each $\beta > 0$ and for every sufficiently smooth bounded function. Eq.(A.5) is called the Grünwald-Letnikov fractional derivative of order $\beta > 0$ on the whole line. Grünwald-Letnikov defined also the fractional difference of order $\beta > 0$ on a finite interval as

$$(\Delta_h^{\beta} f)(x) = \sum_{k=0}^{\frac{x-a}{h}} (-1)^k \binom{\beta}{k} f(x - kh) \, , h = \frac{x-a}{n} \, , n \in \mathbb{N} \ . \tag{A.6}$$

Here $a \leq x \leq b$, and $f(x)$ is defined only in the interval $[a, b]$, $b > a$. Then, $f^{(\beta)}(x) = \lim_{h \to 0^+} \frac{1}{h^{\beta}} (\Delta_h^{\beta} f)(x)$ is used as reason for our discretization.

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