The discrete solution of the time-fractional diffusion with drift in a potential well

3.1 Introduction

In this chapter, we consider another important generalization of the diffusion equation with drift. Namely, we shall discuss the time-fractional diffusion under various forms of forces (see [28] and [29]). By fractional in time, we mean the replacement of the first-order time derivative by the *Caputo* fractional derivative operator, ${}_{t}D_{*}^{\beta}$, with $\beta \in (0,1]$. The relation between the Caputo fractional derivative and Riemann-Liouville fractional derivative is given in Appendix A. In this case the diffusion equation under the action of the outward external force $F(x)$, with ${}_{t}D_{*}^{\beta} u(x,t) = {}_{t}D^{\beta}(u(x,t) - u(x,0))$, is written as

$$ {}_{t}D_{*}^{\beta}\, u(x,t) \;=\; a\,\frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial}{\partial x}(F(x)u(x,t)) \;,\; 0 < \beta \le 1 \;, \quad (3.1.1) $$

where $u(x,0) = \delta(x - x^*)$, x^* is the origin of the diffusion process. Here $F(x)$ is an odd function of x, where $-F(x) > 0$, and a is a positive constant. If $U(x)$ represents the potential energy, then $F(x) = -\frac{dU}{dx}$.

We remark here that equation (3.1.1) can be written in another form. First we rewrite the R.H.S. of it by using the Fokker-Planck operator L_{FP}, defined in (2.7.13), with $K = a$ [84], then use the Riemann-Liouville fractional derivative operator, ${}_{t}D^{\beta}$, which is defined in Appendix A. We get

$$ {}_{t}D^{\beta}[u(x,t) - u(x,0)] = \; L_{FP}\, u(x,t) \;\; . \quad (3.1.2) $$

This equation can also be written as

$$u(x,t) - u(x,0) = \underset{t}{D}^{-\beta}\ (L_{FP}\, u(x,t))\ ,\ 0 < \beta \leq 1\ , \qquad (3.1.3)$$

where $\underset{t}{D}^{-\beta} = J^{\beta}$ is the Riemann-Liouville fractional integral operator which is defined in Appendix A. This operator and its derivative are important in the theory of continuous time random walk and fractional calculus. Now by differentiating both sides with respect to time, we get

$$\frac{d}{dt}\, u(x,t) = \underset{t}{D}^{1-\beta}\ L_{FP} u(x,t)\ \ , \qquad (3.1.4)$$

where

$$\underset{t}{D}^{1-\beta} = \frac{d}{dt}\ \underset{t}{D}^{-\beta}\ \ .$$

Equation (3.1.4) represents the generalized (fractional in time) Fokker-Planck equation (see for examples: [70], [3], [100] and the references therein). This special form of the Fokker-Planck equation plays an important role in the stochastic processes especially when discussing the continuous time random walk ($CTRW$) of the diffusion under the action of external force. For the special case as $F(x) = -bx$, this equation represents the generalized (fractional in time) Ornstein-Uhlenbeck process or in other words the time-fractional diffusion equation with central linear drift which has a known solution in the case $\beta = 1$ (see Chapter 2).

Now, before going into the details of constructing a solution formula for the more general equation (3.1.1) with $F(x) = -bx$, $u(x,0) = \delta(x-\xi)$, where ξ is the starting point of the diffusing particle, we note that we can calculate the first moment of this process (i. e. $\langle x(t) \rangle$). For this aim we multiply equation (3.1.1) by x and integrate over $x \in \mathbb{R}$. By using the natural properties, namely $u(x,t) \to 0$, $x^2 u(x,t) \to 0$ and $x\frac{\partial u}{\partial x} \to 0$ as $|x| \to \infty$, we get the initial value problem

$$\underset{t\ *}{D}^{\beta}\, \langle x(t) \rangle\ = -b\langle x(t) \rangle\ ,\ \ 0 < \beta < 1\ ,$$

whose solution is obtained by taking the Laplace transformation to its both sides (see [37]). Then by inversion, we get

$$\langle x(t) \rangle = \langle x(0) \rangle E_{\beta}(-bt^{\beta})\, . \qquad (3.1.5)$$

Here

$$E_{\beta}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(1+n\beta)}$$

is the *Mittag-Leffler function.* For $\beta = 1$, the Mittag-Leffler function $E_\beta(-bt^\beta)$ reduces to the exponential function e^{-bt}. The asymptotic expansion of the Mittag-Leffler function will be discussed carefully in Appendix C.

We organize this chapter as follows. First we present a discrete method for solving approximately equation (3.1.1), with several types of $F(x)$, by solving the difference equation for $0 < \beta < 1$. Then, we consider and show the convergence of the model to a stationary state as time t tends to infinity and compare it with the analytic stationary solution of (3.1.1). Finally the difference scheme will be re-interpreted as a random walk model that we use for simulating the particle's paths.

3.2 The discrete solution of the time-fractional diffusion with drift

In this section we consider the approximate solution of equation (3.1.1) with $F(x) = -bx$ obtained by a suitable finite-difference discretization. As in the previous chapter, we define $R = \frac{2a}{bh^2}$, and restrict the index j to the range $(-R, -R+1, -R+2, \ldots, R-2, R-1, R)$. Again, we set $x_j = jh$ and adjust the spatial step h so that $R \in \mathbb{N}$. We set $t_n = n\tau$ where $n \in \mathbb{N}_0$. We complement equation (3.1.1) 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 $|j| > R$. So far, we arrive at the equation

$$\underset{\tau\ *}{D^\beta}\, y_j^{(n+1)} = a\, \frac{y_{j+1}^{(n)} - 2y_j^{(n)} + y_{j-1}^{(n)}}{h^2} + \frac{b}{2h}\left(x_{j+1}y_{j+1}^{(n)} - x_{j-1}y_{j-1}^{(n)}\right) \quad , 0 < \beta \leq 1 \,. \tag{3.2.1}$$

Here the difference operator $\underset{\tau\ *}{D^\beta}$ is the discretization of the Caputo time derivative (see Appendix A). For $\beta = 1$, equation(3.2.1) is reduced to the classical diffusion with drift which has been studied with full details in Chapter 2. For discretizing the Caputo time derivative, we utilize a backward Grünwald- Letnikov scheme in time (starting at level $t = t_{n+1}$) which reads

$$\underset{\tau\ *}{D^\beta}\, y_j^{(n+1)} = \sum_{k=0}^{n+1} (-1)^k \binom{\beta}{k} \frac{y_j^{(n+1-k)} - y_j^{(0)}}{\tau^\beta} \quad , 0 < \beta \leq 1 \,. \tag{3.2.2}$$

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(3.2.1) has order of accuracy $O(h^2 + \tau)$. For simplicity and without loosing generality, we let

$$b = a = 1 ,$$

and introduce the scaling parameter

$$\mu = \frac{\tau^\beta}{h^2} \, , \; 0 < \mu \le \frac{\beta}{2} . \tag{3.2.3}$$

Now, solving for $y_j^{(n+1)}$, we get

$$\begin{aligned} y_j^{(n+1)} &= \sum_{k=0}^{n} (-1)^k \binom{\beta}{k} y_j^{(0)} + \sum_{k=1}^{n} (-1)^{k+1} \binom{\beta}{k} y_j^{(n+1-k)} \\ &+ y_{j+1}^{(n)} [\mu + \frac{\mu h^2}{2}(j+1)] - 2\mu y_j^{(n)} + y_{j-1}^{(n)} [\mu - \frac{\mu h^2}{2}(j-1)] . \end{aligned} \tag{3.2.4}$$

Again $y_j^{(n+1)}$ represents the probability vector for where to find the particle at the time 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 can be interpreted as a random walk with memory. For convenience, we introduce the following coefficients

$$b_n = \sum_{k=n+1}^{\infty} (-1)^k \binom{\beta}{k} \, , n = 0, 1, 2, \ldots \; , \tag{3.2.5}$$

and

$$c_k = (-1)^{k+1} \binom{\beta}{k} \, , k = 1, 2, \ldots \; . \tag{3.2.6}$$

Then $b_0 = c_1 = \beta$, and all $c_k \ge 0$, $b_n \ge 0$, $\sum_{k=1}^{\infty} c_k = 1$. In the case $0 < \beta < 1$ (see [39], [40]) we have $c_1 = \beta > c_2 > c_3 > \cdots \to 0$, and finally the relation

$$b_n + \sum_{k=1}^{n} c_k = 1 . \tag{3.2.7}$$

With the aid of the coefficients b_n and c_k in equation (3.2.4) 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

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

represents the diffusion part, by one step to the right, one step to the left or by staying at the same position. For $\beta = 1$, all these coefficients will vanish and we have the natural discretization of the generalized Ehrenfest model discussed in the previous chapter.

In equation (3.2.4) $y_j^{(n+1)}$ represents the probability of finding the position of the particle at the point x_j at the time instant t_{n+1}. Therefore $y_j^{(n+1)}$ must be non-negative and the summation of y over all $j \in [-R, R]$ at any time t_n must give 1. This means that

$$s_{n+1} = \sum_{j=-R}^{R} y_j^{(n+1)} = s_n = \sum_{j=-R}^{R} y_j^{(n)} = 1 \ \ \forall n \in \mathbb{N}_0 \ .$$

We prove this by the induction.

First for $n = 0$, we use the initial condition for $y^{(0)}$ which satisfies $s_0 = 1$ and get

$$y_j^{(1)} = (1-2\mu) y_j^{(0)} + \mu \left(1 + \frac{j+1}{R}\right) y_{j+1}^{(0)} + \mu \left(1 - \frac{j-1}{R}\right) y_{j-1}^{(0)} \ . \tag{3.2.8}$$

Now, summing over both sides of equation(3.2.8), we get

$$s_1 = \sum_{j=-R}^{R} y_j^{(1)} = s_0 \ .$$

Second for $n \geq 1$, we rewrite equation(3.2.4) in the form

$$\begin{aligned} y_j^{(n+1)} \ &= \ b_n y_j^{(0)} \ + \sum_{k=1}^{n} c_k y_j^{(n+1-k)} \ - \ 2\mu y_j^{(n)} + \\ & + \ \mu \left(1 + \frac{j+1}{R}\right) y_{j+1}^{(n)} \ + \ \mu \left(1 - \frac{j-1}{R}\right) y_{j-1}^{(n)} \ . \end{aligned} \tag{3.2.9}$$

Summing over all j at both sides and using the relation (3.2.7), 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. Equation (3.2.9) is consistent the time-fractional diffusion equation with the following sense. For $h \to 0$ which is equivalent to $R \to \infty$, equation (3.2.9) goes over into equation (3.1.1), for $x \in \mathbb{R}$ and $t > 0$.

3.3 The explicit solution of the diffusion equation with drift

The explicit scheme of the time-fractional diffusion equation with central linear drift, equation (3.2.4), is completely different from the explicit scheme of the diffusion with drift as $\beta = 1$, studied in Chapter 2. The dependence on the past appears in this model for $n \geq 1$. Therefore, the solution is obtained separately at $n = 0$ and at $n \geq 1$.

For $n = 0$, we have with $y^{(1)}$ the first state after the initial state. By returning back to equation (3.2.8), we find that $y_j^{(1)}$ represents the probability of finding the particle at the point x_j at the time instant t_1, while being at the points x_{j-1}, x_j, or x_{j+1} at the time instant $t_0 = 0$. This transition is as in a Markov chain because we have only one past level. Equation(3.2.8) is equivalent to the equation

$$y_j^{(1)} = \gamma y_j^{(0)} + \lambda_{j+1} y_{j+1}^{(0)} + \rho_{j-1} y_{j-1}^{(0)} \ , \tag{3.3.1}$$

where the transition probabilities from the time instant t_0 to t_1 are respectively

$$\lambda_j = \mu(1 + \frac{j}{R}) \ , \gamma = (1 - 2\mu) \ , \rho_j = \mu(1 - \frac{j}{R}) \ ,$$

Our intention is that equation (3.3.1) should describe a random walk with sojourn probability $y_j^{(0)}$ of a particle at the point x_j at the instant t_0. The particle then jumps to one of the points x_{j-1}, x_j, x_{j+1} at the time instant t_1. The transition probabilities in equation (3.3.1) should satisfy the essential condition

$$\lambda_j + \gamma + \rho_j = 1 \ , \ \lambda_j \geq 0 \, , \gamma \geq 0 \, , \ \rho_j \geq 0 \ , \ \forall j \in [-R, R] \ .$$

As in Chapter 2, we have for the column vectors, $y^{(1)}$ and $y^{(0)}$, the relation

$$y^{(1)} = P^T . y^{(0)} \ , \tag{3.3.2}$$

where the matrix P is a stochastic matrix and is defined in (2.3.13). By using row vectors, we define

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

then we have

$$z^{(1)} = z^{(0)} . P \ . \tag{3.3.3}$$

It is convenient to write the stochastic matrix P, in the form

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

where I is a $(2R+1) \times (2R+1)$ unit matrix and H, defined in (2.3.17), is a $(2R+1) \times (2R+1)$ matrix having the property that its rows sum to zero.

Now for $n \geq 1$, we have the same transition probabilities ρ_{j-1} and λ_{j+1}, as in Chapter 2, from the points x_{j-1} and x_{j+1} respectively to the point x_j as the time proceeds from t_n to t_{n+1} but the transition probability $\acute{\gamma}$ from the point x_j to the same position depends on β, i. e.,

$$\acute{\gamma} = (\beta - 2\mu) \ ,$$

giving

$$\lambda_{j+1} + \acute{\gamma} + \rho_{j-1} = \beta \ .$$

This means that the transition from t_n to t_{n+1} is not Markov-like. Therefore, recalling $c_1 = \beta$, it is convenient to define the matrix

$$Q = \beta I + \mu H = (q_{i,j}) \ ,$$

which has the form

$$Q = \begin{pmatrix} (\beta-2\mu) & 2\mu & 0 & \dots & \dots & \dots & 0 \\ \frac{\mu}{R} & (\beta-2\mu) & \mu(2-\frac{1}{R}) & 0 & \dots & \dots & 0 \\ 0 & \frac{2\mu}{R} & (\beta-2\mu) & \mu(2-\frac{2}{R}) & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & 0 & \mu(2-\frac{2}{R}) & (\beta-2\mu) & \frac{2\mu}{R} & 0 \\ \dots & \dots & \dots & 0 & \mu(2-\frac{1}{R}) & (\beta-2\mu) & \frac{\mu}{R} \\ \dots & \dots & \dots & 0 & 0 & 2\mu & (\beta-2\mu) \end{pmatrix} \tag{3.3.4}$$

By taking into account the memory part, we rewrite equation (3.2.9) as

$$z^{(n+1)} = b_n z^{(0)} + \sum_{k=2}^{n} c_k z^{(n+1-k)} + z^{(n)}.Q \ . \tag{3.3.5}$$

Observe that Q is a stochastic matrix if and only if $c_1 = \beta = 1$

3.4 The implicit scheme for solving the time-fractional diffusion equation with central linear drift(Θ-method)

The idea of the θ- method is discussed in Chapter 2. The relation between μ and the order of the fractional derivative is governed by the the scaling relation given by (3.2.3). We use the θ- method to predict the future so fast in order to save the computing time. Again, we solve our model differently, at $n = 0$, and at $n \geq 1$.

For $n = 0$, we rewrite equation (3.3.3) in the form

$$z^{(1)}.(I - \mu\theta H) = z^{(0)}.(I + \mu\bar{\theta}H) \quad , \tag{3.4.1}$$

where $\bar{\theta} = (1 - \theta)\,, \theta \in [0, 1]$. Solving equation (3.4.1) for the row vector $z^{(1)}$ gives

$$z^{(1)} = z^{(0)}.(I + \mu\bar{\theta}H).(I - \mu\theta H)^{-1} \quad . \tag{3.4.2}$$

As we have discussed in Chapter 2 the matrix

$$(I + \mu\bar{\theta}H).(I - \mu\theta H)^{-1} = P_\theta \quad ,$$

is a stochastic matrix only for special values of μ related to θ. But here μ is also related to β

$$0 < \mu \leq \beta/2 \qquad \text{if} \qquad \theta = 0 \ ,$$

$$0 < \mu \leq \frac{\beta}{2(1-\theta)} \qquad \text{if} \qquad 0 < \theta < 1 \ ,$$

$$0 < \mu < \infty \qquad \text{if} \qquad \theta = 1 \ .$$

For $n \geq 1$, we rewrite equation (3.3.5) in the form

$$z^{(n+1)} = b_n z^{(0)} + \sum_{k=1}^{n} c_k z^{(n+1-k)} + \mu\, z^{(n)}.H \quad . \tag{3.4.3}$$

Then, we apply the θ-method to it , and solve for $z^{(n+1)}$. We get

$$z^{(n+1)} = \left[b_n z^{(0)} + \sum_{k=1}^{n} c_k z^{(n+1-k)} + \mu\,\bar{\theta}\, z^{(n)}.H \right] [I - \mu\theta H]^{-1} \ . \tag{3.4.4}$$

Here $(I - \mu\theta H)^{-1}$ is a non negative matrix and all b_n and c_k are non-negative numbers, moreover the relation between b_n and c_k is governed by (3.2.7). Finally by using the last conditions governing μ, θ and β, we get all $z^{(n)} \geq 0$.

To prove that the row vector $z^{(n)}$ is a probability row vector, we must also prove that $\sum_j z_j^{(n)} = 1 \ \forall n \in \mathbb{N}$. We prove this by induction.

First for $n = 0$, as in Chapter 2, the matrix P_θ is a stochastic matrix and $\eta = \{1, \ldots, 1\}^T$ is one of its eigenvectors satisfying

$$[(I + \mu\bar{\theta}H).(I - \mu\theta H)^{-1}].\eta = \eta$$

Generally for any probability column vector w, we have $w \geq 0$ and $w^T.\eta = 1$. Now, we know that $(I - \mu\theta H)^{-1}$ is an M matrix and P_θ is a stochastic matrix. Hence by a suitable choice of the initial row vector $z^{(0)}$ such that $z_j^{(0)} \geq 0$, for all $j \in [-R, R]$, and $z^{(0)}.\eta = 1$, equation (3.4.2) implies $z^{(1)}.\eta = z^{(0)}.(P_\theta.\eta) = z^{(0)}.\eta = 1$.

Second, assuming the relation to be true for $n \geq 1$ (i.e. we assume $\sum_j z_j^{(n)} = 1$), we must prove that it is true for $n+1$. Multiplying each side of equation(3.4.4) by η, and using the auxiliary equation (3.2.7), we get $\sum_j z_j^{(n+1)} = 1$. So the relation is true for all values $n \geq 0$. As a matter of fact, the implicit scheme allows us to predict the future faster than the explicit scheme, because μ and τ depend on each other by the scaling relation given in (3.2.3) and μ can be taken larger and larger as θ is increased from 0 to 1. This property will be useful in the numerical calculations of the following section.

3.5 Convergence to the stationary discrete solution for time tending to infinity

For $\beta = 1$, equation (3.2.9) reduces to the modified Ehrenfest model (see for example [107], [19], [22], and [92]) which describes the motion of a particle moving one step to the left, or one step to the right, or remaining in its position. The matrix representation of this model is a stochastic matrix with the special property that the limit of the power matrix P^n for $n \to \infty$, exists and the elements of the matrix converge to the binomial distribution. In this case we have a Markov chain.

For $0 < \beta < 1$, i.e. for the non-Markov chain, we apply the more general method for calculating the discrete stationary solution of equation (3.2.9). This is done by omitting the dependence on time t. To this purpose, we replace all the indices $n+1, 0$ and $n+1-k$ by simply n in equation (3.4.3). Then for $n \to \infty$, equation (3.4.3) converges to $z.H = 0$ which is equivalent to $H^T.y = 0$, and we accept the column vector $y = z^T$ as the discrete stationary solution. This equation is valid for $0 < \beta \leq 1$ and H^T has an eigenvector y^* of eigenvalue zero. Now the vector $\bar{y} = cy^*$ with $c = 1/\sum_{j=-R}^{R} y_j^*$ is a vector whose elements sum to 1. We form a sequence of numbers $d = \{d(t_1), d(t_2), \cdots\}$, where $t_1 < t_2 < \cdots \to \infty$. The number $d(t_i)$

is defined as

$$d(t_i) = \sum_{j=-R}^{R} |y_j(t_i) - \bar{y}_j| \ , i = 1, 2, \dots \ . \qquad (3.5.1)$$

The simulation for $0 < \beta < 1$ shows that the row vector d approximates a power function

$$d(t) \approx c\,t^{-\gamma} \ ,$$

where c and γ are constants and γ is called the rate of convergence. The implicit scheme allows us to calculate the vector d so fast because the number of steps are less than those of the explicit scheme.

By analogy, we can estimate the convergence, the explicit and the implicit solution of the model under the action of the other types of forces defined in Chapter 2. It will be by the same procedure, the only difference lies in the elements of the matrix H which depend directly on the structure of the force. This is so because 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 equation (3.2.4) 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.

3.6 Random walk simulation

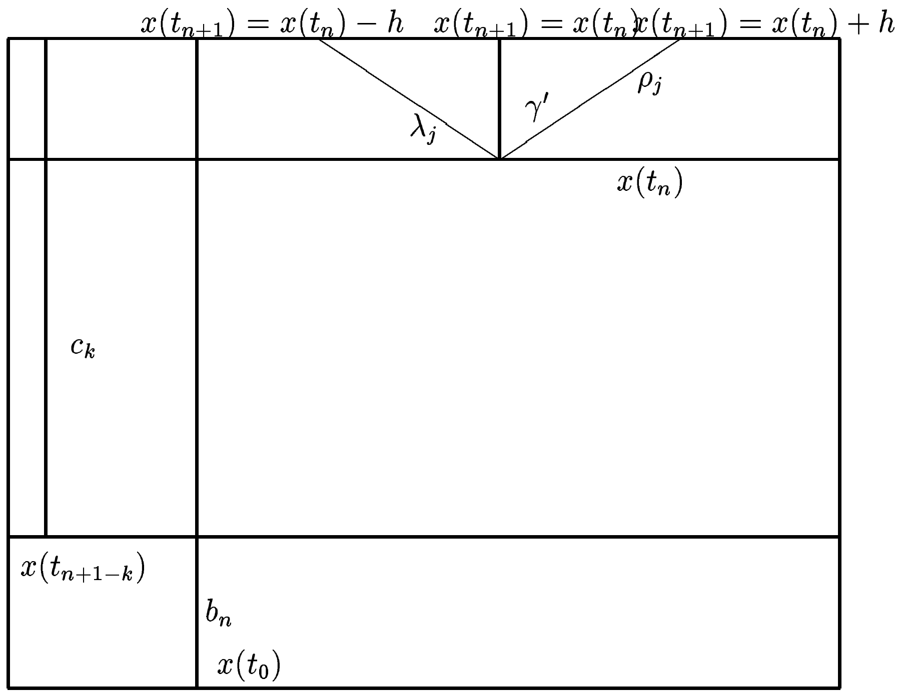
We discuss in this section the random walk of the elastically bound particle (diffusion under the action of the force bx, $b > 0$), after replacing the time derivative by the fractional time derivative, to see the effect of the memory part. To do this, we generate random numbers $\in (0, 1]$ and keep in mind the whole past history of the wandering particle. Its history consists of its positions at the times $t_0 = 0, t_1, \cdots$ and up to t_n. This means, the path of the particle is $x(t_o), x(t_1), \dots, x(t_n)$. The initial position of the particle $x(0) = x_0$ may be any grid point mh inside the interval $[-Rh, Rh]$ and $m \in [-R, R]$. As we have done in the previous sections, we distinguish the cases corresponding to $n = 0$ and $n \geq 1$ in the simulation. For $n = 0$, the random walk of this case is typically Markov-like. For $n \geq 1$ and as the time proceeds from $t = t_n$ to $t = t_{n+1}$, the sojourn-probabilities are redistributed according to equation (3.2.9) which we rewrite as

$$y_j^{(n+1)} = \left(1 - \sum_{k=1}^{n} c_k\right) y_j^{(0)} + c_n y_j^{(1)} + c_{n-1} y_j^{(2)} + \cdots + c_2 y_j^{n-1} + (c_1 - 2\mu) y_j^{(n)} + \mu \left(1 + \frac{j+1}{R}\right) y_{j+1}^{(n)} + \mu \left(1 - \frac{j-1}{R}\right) y_{j-1}^{(n)} \tag{3.6.1}$$

Clearly all the coefficients $c_1, c_2, \ldots, c_n, (1 - \sum_{k=1}^{n} c_k)$, defined in 3.2.6, are non-negative. The idea of simulation is analogous to that of [40]. 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

$$s_k = \sum_{i=1}^{k} c_i \ , \ k = 1, 2, \ldots, n \tag{3.6.2}$$

and generate a uniformly in $[0, 1]$ distributed random number u. Then we test successively into which one of the intervals $[0, s_1)$, $[s_1, s_2)$, $[s_2, s_3)$, . . . , $[s_n, 1)$, 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 sketch of the movements is as follows.



The sketch of the possible jumps as $0 < \beta < 1$

3.7 Numerical results

We display some figures to show the evolution of the diffusion process as the time proceeds from $t = 1$ to $t = 10$ for different values of β including $\beta = 1$ and for different initial conditions.

First: some figures representing the fractional in time diffusion process under the action of a linear force (i.e. $F(x) = -x$):

Figures [1-4] correspond to the explicit scheme where $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$.

Figures [5-8] correspond to the explicit scheme where $y^{(0)} = \{\frac{1}{2R+1}, \cdots, \frac{1}{2R+1}, \cdots, \frac{1}{2R+1}\}$.

Figures [9-12] correspond to the fully implicit scheme where $y^{(0)} = \{0, \cdots, 0, 1\}$.

Figures [13-16] illustrate the convergence of the model where $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$. In these figures we have plotted *log d* against time t and *log t* against *log d*.

Figures [17,18] show the approximate stationary solution and the approximate solution of the model with central linear force $F(x) = -x$.

Second: some figures representing the fractional in time diffusion process under the action of a cubic force (i.e. $F(x) = -x^3$):

Figures [19-24] correspond to the implicit scheme where $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$.

Figures [25-28] correspond to the implicit scheme where $y^{(0)} = \{0, \cdots, 0, \cdots, 1\}$.

Figures [29-30] 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 and *log t* against *log d*.

Figures [31,32] show the approximate stationary solution and the stationary analytic solution of the model for the cubic force $F(x) = -x^3$.

Finally, figures [33-36] 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 $R = 10$.

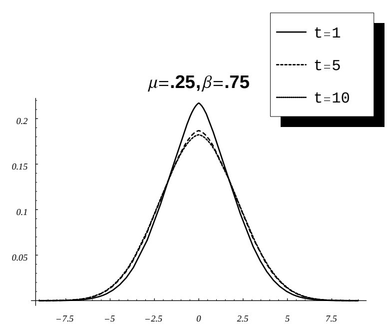


Figure 3.1: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

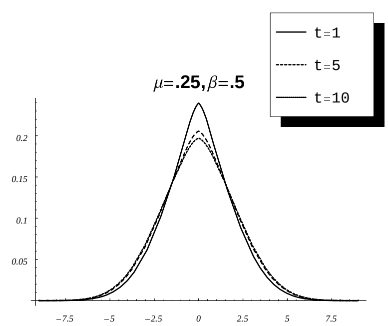


Figure 3.2: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

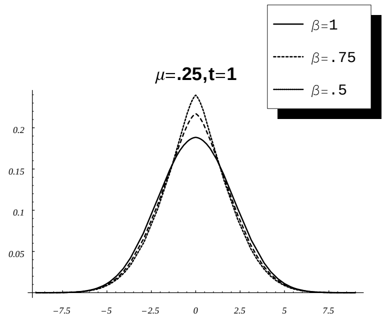


Figure 3.3: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

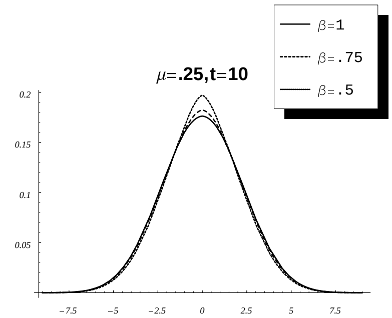


Figure 3.4: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

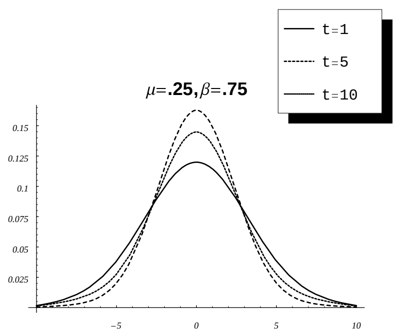


Figure 3.5: $y^{(0)} = \{\frac{1}{2R+1}, \cdots, \frac{1}{2R+1}\}$

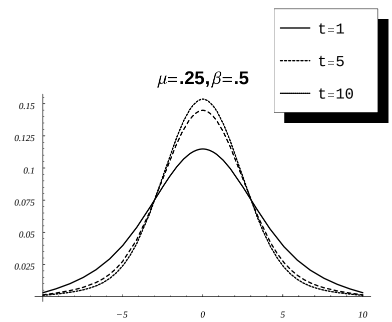


Figure 3.6: $y^{(0)} = \{\frac{1}{2R+1}, \cdots, \frac{1}{2R+1}\}$

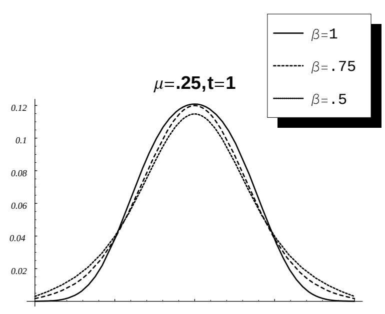


Figure 3.7: $y^{(0)} = \{\frac{1}{2R+1}, \cdots, \frac{1}{2R+1}\}$

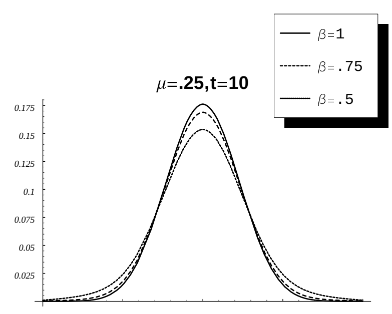


Figure 3.8: $y^{(0)} = \{\frac{1}{2R+1}, \cdots, \frac{1}{2R+1}\}$

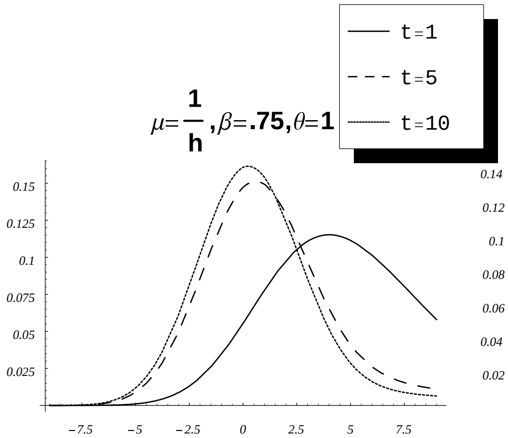


Figure 3.9: $y^{(0)} = \{0, \cdots, 0, 1\}$

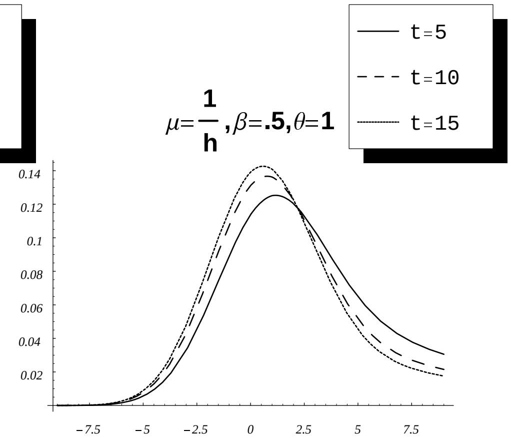


Figure 3.10: $y^{(0)} = \{0, \cdots, 0, 1\}$

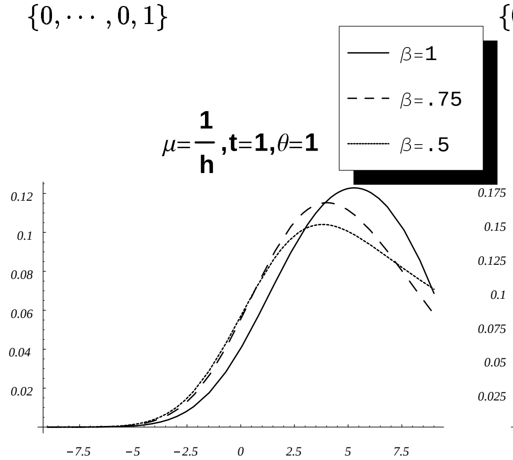


Figure 3.11: $y^{(0)} = \{0, \cdots, 0, 1\}$

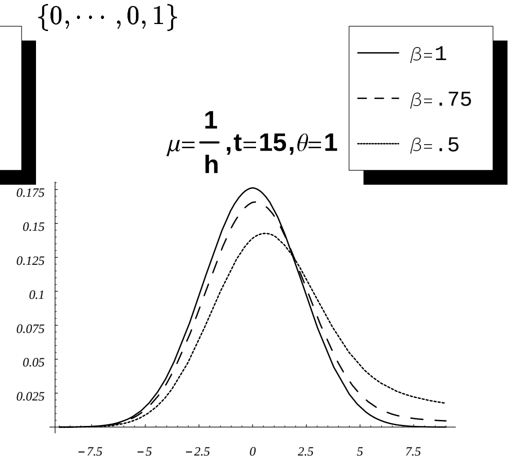


Figure 3.12: $y^{(0)} = \{0, \cdots, 0, 1\}$

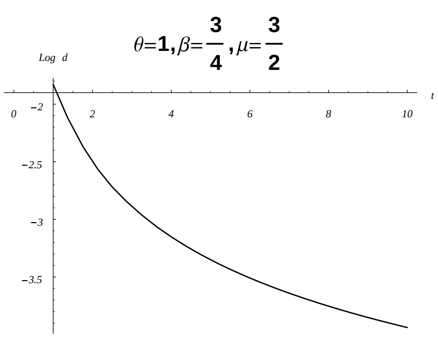


Figure 3.13: convergence for $F(x) = -x$

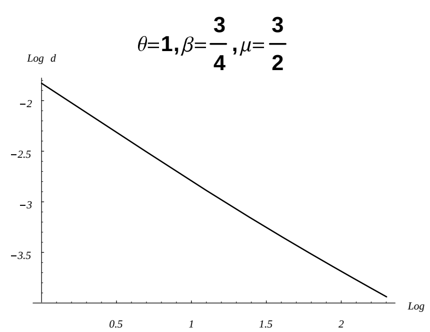


Figure 3.14: convergence for $F(x) = -x$

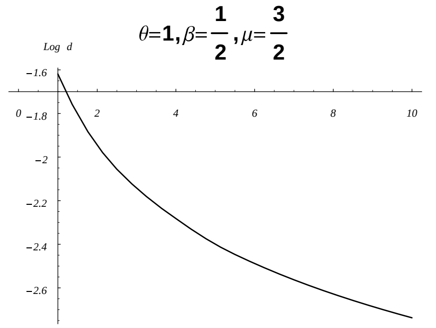


Figure 3.15: convergence for $F(x) = -x$

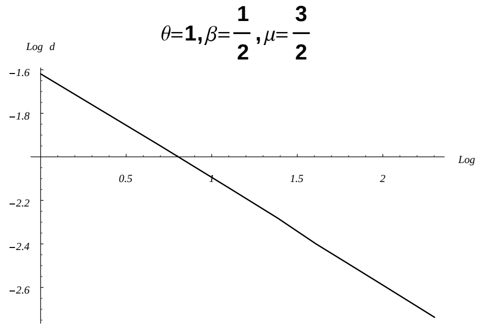


Figure 3.16: convergence for $F(x) = -x$

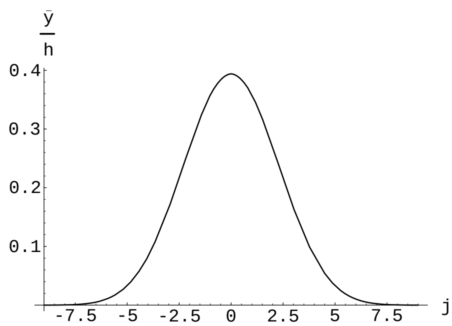


Figure 3.17: approximate solution

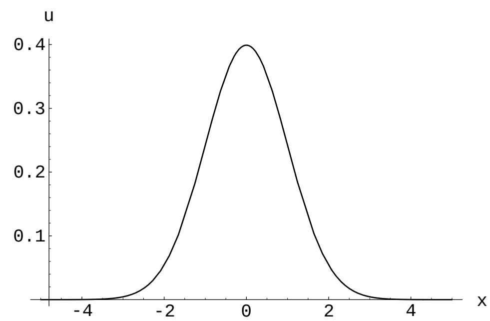


Figure 3.18: stationary solution

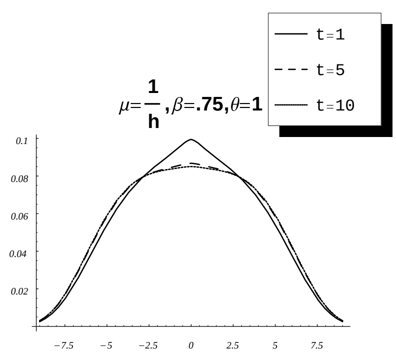


Figure 3.19: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

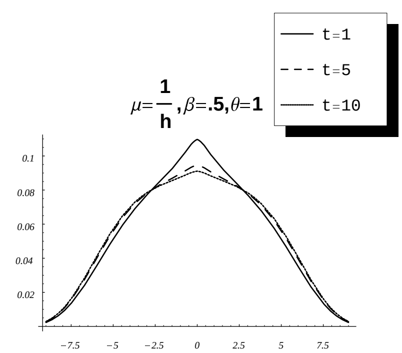


Figure 3.20: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

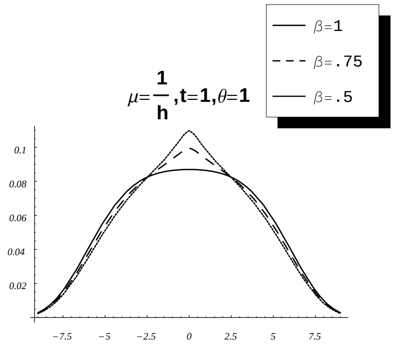


Figure 3.21: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

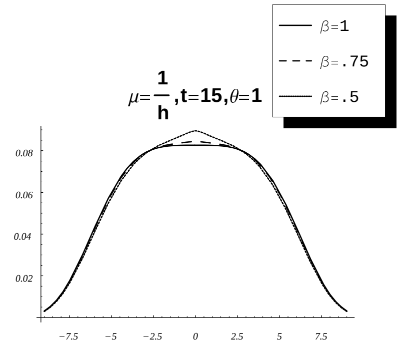


Figure 3.22: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

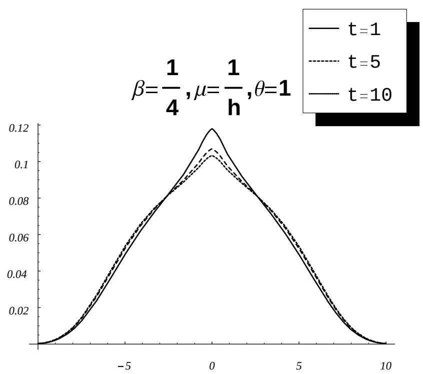


Figure 3.23: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

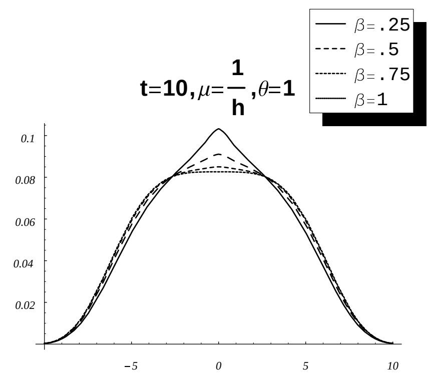


Figure 3.24: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

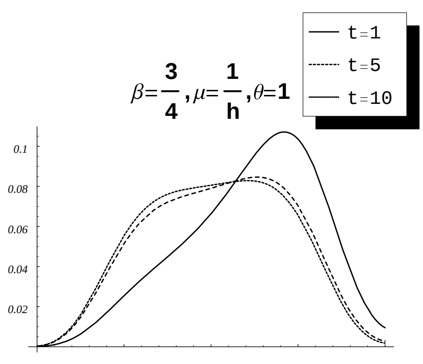


Figure 3.25: $y^{(0)} = \{0, \cdots, 0, \cdots, 1\}$

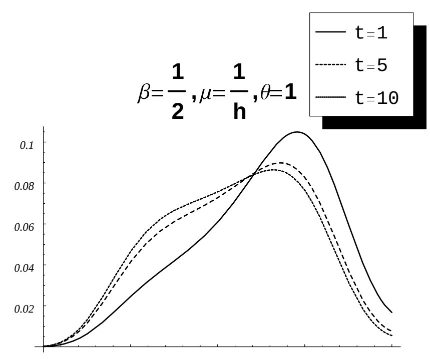


Figure 3.26: $y^{(0)} = \{0, \cdots, 0, \cdots, 1\}$

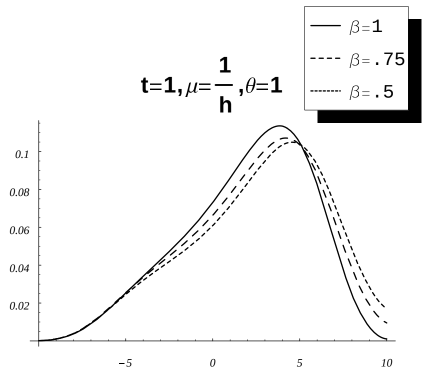


Figure 3.27: $y^{(0)} = \{0, \cdots, 0, \cdots, 1\}$

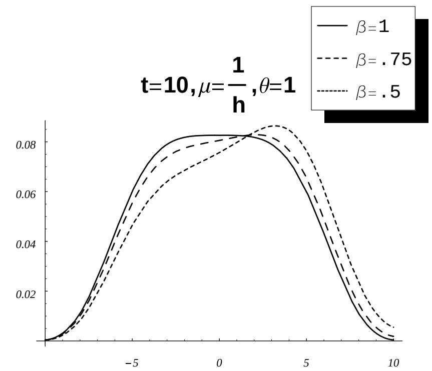


Figure 3.28: $y^{(0)} = \{0, \cdots, 0, \cdots, 1\}$

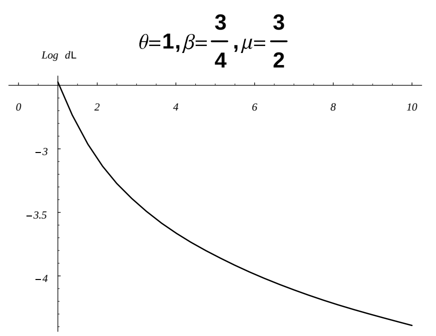


Figure 3.29: convergence

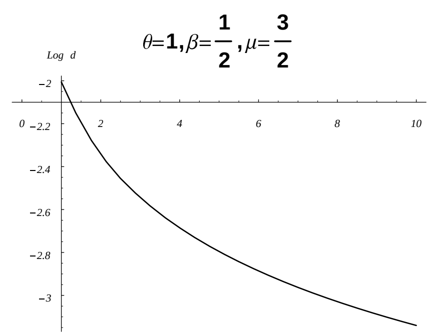


Figure 3.30: convergence

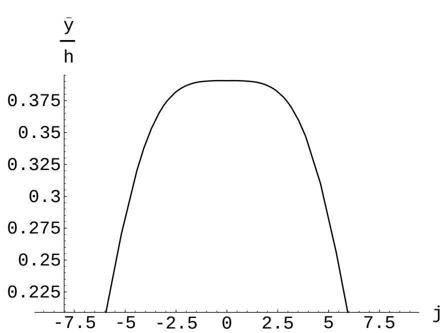


Figure 3.31: approximate solution

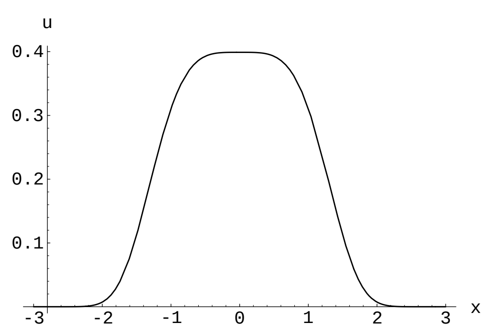


Figure 3.32: stationary solution

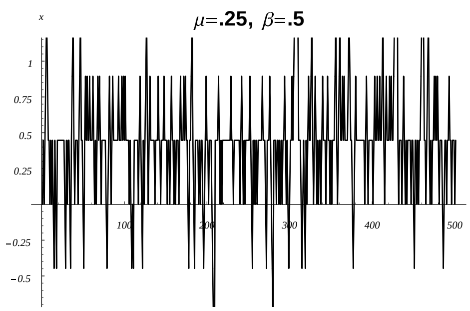


Figure 3.33: discrete random walk

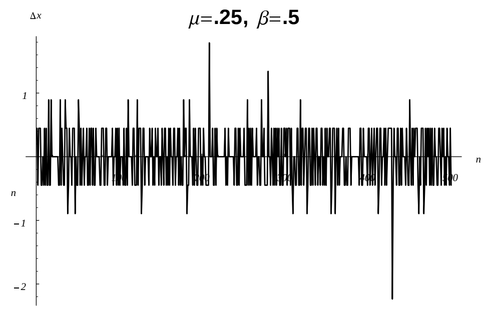


Figure 3.34: increments

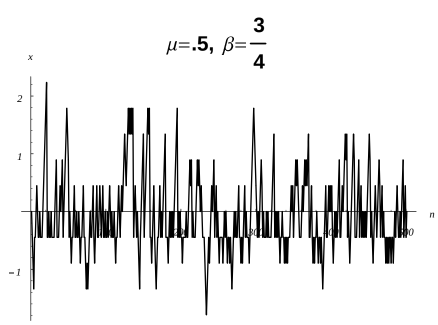


Figure 3.35: discrete random walk

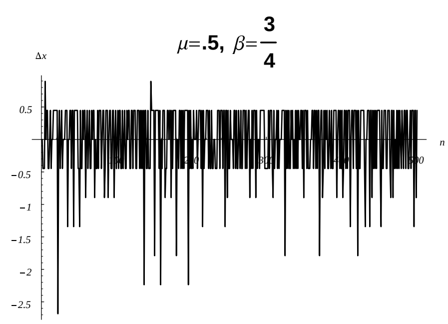


Figure 3.36: increments