Analysis of classical diffusion in a potential well

2.1 Introduction

In 1827 an English botanist, Robert Brown, 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* [51]. It was not until 1905 that Albert Einstein first advanced a satisfactory theory. Einstein considered the case of the free particle, that is, a particle in which no forces other than those due to the molecules of the surrounding medium are acting. He was able to show that the probability density $u(x,t)$ must satisfy the partial differential equation

$$\frac{\partial u(x,t)}{\partial t} = a\frac{\partial^2 u(x,t)}{\partial x^2}\,, \tag{2.1.1}$$

where $a > 0$ is a certain physical constant depending on the universal gas constant, the absolute temperature, the Avogadro number, and finally the friction coefficient. The range of x is the whole line (i.e. $-\infty < x < \infty$) as $t > 0$. The conditions imposed on u are

$$u(x,t) \geq 0,\ \int_{-\infty}^{\infty} u(x,t)dx = 1\ .$$

The solution $u(x,t)$ of equation (2.1.1) with the initial condition $u(x,0) = \delta(x-x^*)$ is well known as the corresponding *Green function* or the *fundamental solution.* $u(x,t)$ represents at the time instant t the probability density function of a particle being at the point x and takes the form

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

which has variance $\sigma^2(t) = \int\limits_{-\infty}^{\infty} x^2 u(x,t)dx = 2at$. As soon as the theory for the free particle was established, a natural question arose how it should be modified in order to take into account outside forces, for example, gravity which acts in the direction of the $x-$axis. When there is an external force acting towards the origin $x = 0$ and proportional to the particle's distance from it, Smoluchowski [99] has shown that equation (2.1.1) should be replaced by

$$\frac{\partial u(x,t)}{\partial t} = a\frac{\partial^2 u(x,t)}{\partial x^2} + \frac{\partial}{\partial x}(bxu(x,t)) \ , \ a > 0, \ b > 0, \ -\infty < x < \infty, t > 0 \ , \tag{2.1.2}$$

The partial differential equation (2.1.2) which describes the elastic diffusive motion of a bound particle (for example, small pendulum) is a special case of the general *(diffusion-convection equation)* [105], [110] and [99]. However the analytic solution of equation(2.1.2) with the initial conditions $u(x,0) = \delta(x - x^*)$ which has been obtained by many authors, see e.g. [52],[84], [82] and [53], is

$$u(x,t) = p(x_0; x, t) = \frac{1}{\sqrt{2\pi}\,\sigma(t)} \ e^{\frac{-(x - x^* e^{-bt})^2}{2\sigma^2}} \ , \tag{2.1.3}$$

where $\sigma^2 = \frac{a}{b}(1 - e^{-2bt})$. Here $-b$ is called the drift parameter and a is called the diffusion constant. In the limiting case $b = 0$, we have the classical diffusion equation. In what follows we find the first moment of equation (2.1.2). For this aim we multiply equation (2.1.2) by x and integrate over $x \in \mathbb{R}$. By using the natural properties, namely $u(x,t) \to 0$ and $x^n u(x,t) \to 0$ for all $n \geq 1$ as $|x| \to \infty$, we get the initial value problem

$$\frac{d\langle x(t)\rangle}{dt} = -b\langle x(t)\rangle \ ,$$

whose solution is

$$m(t) = \langle x(t)\rangle = \langle x(0)\rangle e^{-bt} \ .$$

At this point it must be strongly emphasized that the theories based on equation (2.1.1) and on equation (2.1.2) are only approximate. They are only valid for relatively large t and in the case of an elastically bound particle (i.e. only in the over-damped case). This means that, the theories are valid only if the friction coefficient is sufficiently large. These limitations of the theory were already recognized by Einstein and Smoluchowski but are often disregarded by writers who stress in the Brownian motion the velocity of the particle to be infinite. An improved theory (known as exact) was advanced by Uhlenbeck and Ornstein and by Kramers where equation (2.1.2) is named as the Ornstein-Uhlenbeck equation. The stochastic process described by this equation is a *Markov process*.

In what follows we are concerned with the discrete approach to the Einstein-Smoluchowski (approximate) theory. This means that we give a full discussion for the diffusion equation with central linear drift and give examples for other drifts (see [28] and [29]). Therefore we organize this chapter as follows.

In Section 2, we discuss Marc Kac's discretization of the classical diffusion in a potential well and its relation to the classical Ehrenfest urn model.

In Section 3, we give the discretization of equation (2.1.2) and use the explicit difference scheme to approximate its discrete solution. We also give the relation between equation (2.1.2) and the Ehrenfest urn model (see [15] and [16]).

In Section 4, we devise the implicit difference scheme.

In Section 5, we discuss the convergence of the approximate solution of equation (2.1.2) for time tending to infinity.

In Section 6, we discuss the random walk of this model.

In Section 7, we give examples of other possible forces and the discretization of their corresponding partial differential equations.

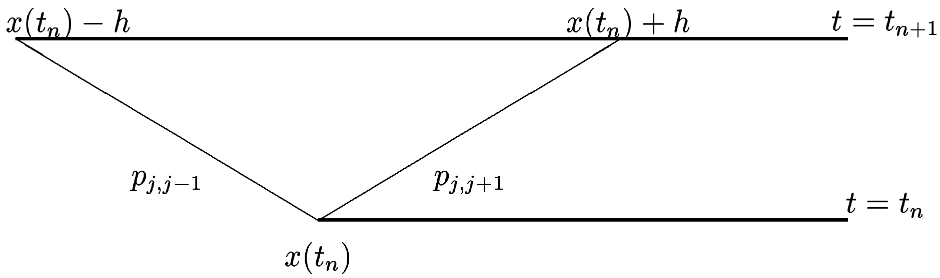
In Section 8, the numerical results of the cases of study are displayed.

2.2 The discretization of the diffusion-convection equation

The classical diffusion in a potential well can be discretely modeled by the random walk of an elastically bound particle equation (2.1.1). Marc Kac [51] considered the case of the particle which can move one step to the right or one step to the left. If the duration of the step is τ and its length is h, then the probability of moving in either direction depends on the position of the particle [51]. More precisely, if the particle is at $x_j = jh, j \in \mathbb{Z}$, the probabilities of moving to the right or to the left are

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

where $\lambda_{-R} = 0$ and $\rho_R = 0$, respectively. Here, R is a certain integer and the possible positions of the particle are limited by the condition $-R \leq j \leq R$, where $R \in \mathbb{N}$. If $t_n = n\tau$, $n \in \mathbb{N}$, then the sketch of the movement of the particle from the point x_j at the time instant t_n to the point x_{j-1} or x_{j+1} at the time instant t_{n+1} is as follows

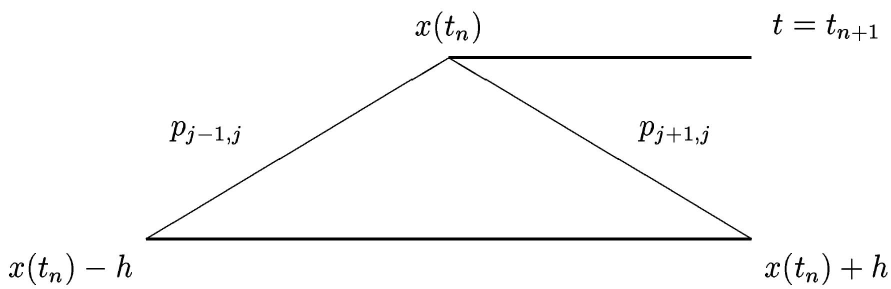


Here $\rho_j = p_{j,j+1}$ and $\lambda_j = p_{j,j-1}$. These transition probabilities satisfy the conservation relation (with integer indices j)

$$\rho_j + \lambda_j = 1\,,\ -R \leq j \leq R\,.$$

Random walk models, discrete in space and time, for the standard diffusion equation and its generalization (e.g. the presence of the drift term) play an important rule in the theory of stochastic processes. Such models are not only valuable for illuminating the meaning of the diffusion but also for the numerical calculations, either as *Monte Carlo Simulation* of the path of the particle in the diffusion process or as *discrete imitation* of the process in form of redistribution of clumps of an extensive quantity (e.g. charge or mass).

Now, we are interested in the probability of finding the particle at the point x_j at the instant t_{n+1}. To this aim, we use Kac's transition probabilities λ_j and ρ_j to calculate this probability. The sketch of the movement of the particle from the point x_{j-1} or x_{j+1} at the time instant t_n to the point x_j at the time instant t_{n+1} is as follows



Here

$$\rho_{j-1} = p_{j-1,j} = \frac{1}{2}(1-\frac{j-1}{R}),\ \lambda_{j+1} = p_{j+1,j} = \frac{1}{2}(1+\frac{j+1}{R}),\ -R \leq j \leq R\,.$$

Then the probability $y_j^{(n+1)}$ of finding the particle at the point x_j at the time instant t_{n+1} satisfies the difference equation [51]

$$y_j^{(n+1)} = \lambda_{j+1} y_{j+1}^{(n)} + \rho_{j-1} y_{j-1}^{(n)} . \qquad (2.2.1)$$

In the interest of formal completeness, we set $\lambda_{-R} = \rho_R = 0$. This means that $y_j^{(n)} = 0$, for $R+1 \le j \le -R-1$. Equation (2.2.1) in which the particle can move one step to the left or one step to the right, is equivalent to the classical Ehrenfest urn model (see for example [15] and [16]).

The relation between the Brownian motion of an elastically bound particle with $h > 0$ and $\tau > 0$ and the classical Ehrenfest urn model has first been pointed out by Schrödinger, Kohlrausch [97].

2.3 The discrete scheme and its relation to the Ehrenfest model

The common numerical approach for the standard diffusion equation is known to be based on the finite-difference method where the first time derivative and the second space derivative are approximated by difference quotients. For this purpose we discretize the space variable x by the grid points

$$x_j = jh \ , \quad h > 0 \ , \quad j \in \mathbb{Z} \ , \qquad (2.3.1)$$

and the time variable t by

$$t_n = n\tau \ , \quad \tau > 0 \ , \ n \in \mathbb{N}_0 \ . \qquad (2.3.2)$$

The dependent variable is then discretized by introducing $y_j(t_n)$ as approximation to the integral of the density $u(x,t)$ over a small interval of width h

$$y_j(t_n) \approx \int_{x_j - h/2}^{x_j + h/2} u(x, t_n) dx \approx h u(x_j, t_n) \ , \qquad (2.3.3)$$

where $u(x,t)$ satisfies the differential equation (2.1.2) and is interpreted as a probability density function. Then according to equation (2.3.3), we introduce a vector

$$y^{(n)} = \{ y_{-R}^{(n)}, y_{-R+1}^{(n)}, \ldots, y_{R-1}^{(n)}, y_R^{(n)} \}^T \ .$$

Here $y^{(n)} = y(t_n)$ is a probability column vector. We suitably choose the initial value $y^{(0)}$ such that $\sum_{j=-R}^{R} y_j^{(0)} = 1$. Therefore we must have $\sum_{j=-R}^{R} y_j^{(n)} = 1 \, \forall n \in \mathbb{N}_0$.

Discretizing by symmetric differences in space and forward in time, we obtain an explicit difference scheme for generating a discrete approximate solution to our model (i.e. to the diffusion with central linear drift $-bx$ described by equation (2.1.2),

$$\frac{y_j^{(n+1)} - y_j^{(n)}}{\tau} = a\frac{y_{j+1}^{(n)} - 2y_j^{(n)} + y_{j-1}^{(n)}}{h^2} + \frac{b}{2h}\left(x_{j+1}y_{j+1}^{(n)} - x_{j-1}y_{j-1}^{(n)}\right) . \tag{2.3.4}$$

As always, $a > 0$ and $b > 0$. For the grid points $x_j = jh$, the index j is restricted to the range $\{-R, -R+1, \ldots, R-1, R\}$ where $R \in \mathbb{N}$. We adjust the spatial step h such that $R = \frac{2a}{bh^2}$ is an integer and define the scaling parameter

$$\mu = \frac{\tau}{h^2} . \tag{2.3.5}$$

We complement equation (2.3.4) by prescribing the non-negative initial value $y^{(0)}$ obeying $\sum_{j=-R}^{R} y_j^{(0)} = 1$, and for convenience $y_j^{(0)} = 0 \, \forall |j| \geq R+1$. It is worth now to say that equation (2.2.1) with $\frac{\tau}{h^2} = \frac{1}{2}$, $R = \frac{2a}{bh^2}$ can be rewritten in the form of equation (2.3.4). With symmetric difference quotients in space, we have consistency of this approximation scheme of order $(\tau + h^2)$ for ($h \to 0$ and $\tau \to 0$) to the partial differential equation (2.1.2), where $R = \frac{2a}{bh^2} \to \infty$, so that in the limit the whole real axis is covered for the variable x.

Now solving equation (2.3.4) for $y_j^{(n+1)}$, we get

$$y_j^{(n+1)} = (1-2a\mu)y_j^{(n)} + a\mu\left(1 + \frac{j+1}{R}\right)y_{j+1}^{(n)} + a\mu\left(1 - \frac{j-1}{R}\right)y_{j-1}^{(n)} . \tag{2.3.6}$$

Equation(2.3.6) is equivalent to

$$y_j^{(n+1)} = \gamma y_j^{(n)} + \lambda_{j+1}y_{j+1}^{(n)} + \rho_{j-1}y_{j-1}^{(n)} \, , -R \leq j \leq R \, , \tag{2.3.7}$$

with

$$\rho_j = p_{j,j+1} = a\mu\left(1 - \frac{j}{R}\right), \quad \gamma = p_{j,j} = (1 - 2a\mu),$$
$$\lambda_j = p_{j,j-1} = a\mu\left(1 + \frac{j}{R}\right) , \tag{2.3.8}$$

These transition probabilities satisfy the essential condition

$$\rho_j + \lambda_j + \gamma = 1 \,\forall j \in [-R, R] \ . \tag{2.3.9}$$

and

$$\rho_R = \lambda_{-R} = 0 \ . \tag{2.3.10}$$

We interpret $y_j^{(n+1)}$ at equation (2.3.7) as the probability of finding the particle at the point x_j, $j \in [-R, R]$, at the time instant t_{n+1}, $n \in \mathbb{N}_0$. In order to have transition probabilities from the time instant t_n to t_{n+1}, it is required that $\gamma \geq 0$, which yields to the *scaling relation*

$$0 < \mu \leq \frac{1}{2a} \ ,$$

and all the occurring $\lambda_j \geq 0$ and $\rho_j \geq 0$. Besides the interpretation of equation (2.3.7) as a random walk, it can also be considered as a generalized Ehrenfest urn model. As $\gamma = 0$, it converts into the classical Ehrenfest urn model represented by equation(2.2.1). We give in this section a brief review about the generalized Ehrenfest urn model in order to show the connection between it and the Brownian motion of an elastically bound particle.

With these conditions, the transition probabilities λ_j, γ and ρ_j constitute a tridiagonal matrix $P = (p_{i,j})$, where $p_{i,j} = 0 \,\forall |i-j| \geq 2$. For ease of writing, we henceforth take

$$a = 1, \ \ b = 1 \tag{2.3.11}$$

This simplification is allowed because the change of variables

$$x = \alpha\grave{x}, \ , \ t = \beta\grave{t}\,, \ u(x,t) = v(\grave{x},\grave{t}) \ ,$$

transforms equation (2.1.2) into

$$\frac{\partial v}{\partial \grave{t}} = \frac{a\beta}{\alpha^2}\frac{\partial^2 v}{\partial \grave{x}^2} + b\beta\frac{\partial}{\partial x}(\grave{x}v) \ , \tag{2.3.12}$$

and with $\beta = 1/b$, $\alpha = \sqrt{a/b}$, we get $\frac{a\beta}{\alpha^2} = 1$, $b\beta = 1$. Then the matrix P takes the form

$$P = \begin{pmatrix} (1-2\mu) & 2\mu & 0 & 0 & 0 & \dots & 0 \\ \frac{\mu}{R} & (1-2\mu) & \mu(2-\frac{1}{R}) & 0 & 0 & \dots & 0 \\ 0 & \frac{2\mu}{R} & (1-2\mu) & \mu(2-\frac{2}{R}) & 0 & \dots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \dots & 0 & \mu(2-\frac{2}{R}) & (1-2\mu) & \frac{2\mu}{R} & 0 \\ 0 & \dots & 0 & 0 & \mu(2-\frac{1}{R}) & (1-2\mu) & \frac{\mu}{R} \\ 0 & \dots & 0 & 0 & 0 & 2\mu & (1-2\mu) \end{pmatrix} \tag{2.3.13}$$

Since

$$p_{i,j} \geq 0, \text{ and } \sum_{j=-R}^{R} p_{i,j} = 1 \; \forall i \; ,$$

the matrix P is a stochastic matrix and represents the transition matrix of a *Markov chain.* For the interpretation of $y^{(n)}$ as a vector of probabilities, we need the condition of preservation of non-negativity which requires that

$$0 < \mu \leq 1/2 \text{ and } -R \leq j \leq R \; .$$

By using the stochastic matrix P, we can rewrite equation (2.3.4) in the form

$$y^{(n+1)} = P^T . y^{(n)} \; . \tag{2.3.14}$$

Actually, the evolution of $y^{(n)}$ is that of a Markov chain [19] with possible states $x_{-R}, x_{-R+1}, \dots, x_{R-1}, x_R$. In order to find the explicit discrete solution of equation (2.3.4), we take the transpose of each side of the matrix equation (2.3.14) and let

$$(y^{(n)})^T = z^{(n)}, \; \forall n \in \mathbb{N}_0 \, , \; z^{(n)} = \{z_{-R}^{(n)}, z_{-R+1}^{(n)}, \dots, z_{R-1}^{(n)}, z_R^{(n)}\} \; .$$

Therefore, equation (2.3.14) is rewritten as

$$z^{(n+1)} = z^{(n)}.P \quad , \tag{2.3.15}$$

and for the numerical calculations, it is convenient to write the matrix P in the form

$$P = (I + \mu H) \; , \tag{2.3.16}$$

where I is a unit matrix and H is a square matrix whose rows sum to zero and is defined as

$$H = \begin{pmatrix} -2 & 2 & 0 & 0 & \dots & \dots & \dots & 0 \\ \frac{1}{R} & -2 & (2-\frac{1}{R}) & 0 & \dots & \dots & \dots & 0 \\ 0 & \frac{2}{R} & -2 & (2-\frac{2}{R}) & 0 & \dots & \dots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \dots & \dots & 0 & (2-\frac{2}{R}) & -2 & \frac{2}{R} & 0 \\ 0 & \dots & \dots & 0 & 0 & (2-\frac{1}{R}) & -2 & \frac{1}{R} \\ 0 & \dots & \dots & 0 & 0 & 0 & 2 & -2 \end{pmatrix} \tag{2.3.17}$$

By using equation (2.3.16), we rewrite equation(2.3.15) as:

$$z^{(n+1)} = z^{(n)}.(I + \mu H) . \tag{2.3.18}$$

Before describing the implicit analogue of equation (2.3.15), we compare this model with the discrete generalized Ehrenfest model described by Vincze [107]. 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 papers ($s \geq 0$) 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. If ($s=0$), we have the classical Ehrenfest model described by many authors see [92], [51],[6], [24], [4], and [7].

In other words, if $x_n^{(s)}$ is the number of balls in urn U_1 after n-steps, then the transition probabilities are

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

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

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

and we have

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

This model is also called the modified Ehrenfest model, and if $s = 0$, the only possible changes of states are from k to $k-1$ or from k to $k+1$ with probabilities k/N or $(N-k)/N$ respectively. The stochastic matrix representing the generalized Ehrenfest model is

$$P_s =$$
$$\begin{pmatrix} \frac{s}{s+N} & 1-\frac{s}{s+N} & 0 & \dots & \dots & \dots & \dots & 0 \\ \frac{1}{s+N} & \frac{s}{s+N} & 1-\frac{s+1}{s+N} & 0 & \dots & \dots & \dots & 0 \\ 0 & \frac{2}{s+N} & \frac{s}{s+N} & 1-\frac{s+2}{s+N} & 0 & \dots & \dots & 0 \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\ 0 & \dots & \dots & 0 & \frac{N-2}{s+N} & \frac{s}{s+N} & 1-\frac{s+N-2}{s+N} & 0 \\ 0 & \dots & \dots & \dots & 0 & \frac{N-1}{s+N} & \frac{s}{s+N} & 1-\frac{s+N-1}{s+N} \\ 0 & \dots & \dots & \dots & 0 & 0 & \frac{N}{s+N} & \frac{s}{s+N} \end{pmatrix} \tag{2.3.19}$$

This matrix is the same as the matrix P defined at (2.3.13), if N is an even number ($N \in 2\mathbb{N}$), $R = \frac{N}{2}$, and $\mu = \frac{N}{2a(s+N)}$. The position $x = 0$ corresponds to $N/2$ balls in U_1, the position $x = Rh$ corresponds to N balls in urn U_1, and the position $x = -Rh$ corresponds to 0 balls in urn U_1. The absolute probability of finding k balls in urn U_1 after $n+1$ steps is written as

$$P_k^{(n+1)} = P(x_{n+1}^{(s)}) = p_{k-1}^{(n)} \frac{N-k+1}{s+N} + p_k^{(n)} \frac{s}{s+N} + p_{k+1}^{(n)} \frac{k+1}{s+N} \ , \tag{2.3.20}$$

where $k = 0, 1, \dots, N-1$. This equation can be interpreted as the discrete diffusion with central linear force. In the limit, this equation tends also to the partial differential equation(2.1.2).

2.4 The implicit scheme ($\Theta - Method$)

The θ- method is also known as the weighted method. The idea of the θ- method is to replace $y_k^{(n)}$ in the R. H. S. of equation (2.3.4) by $(\theta y_k^{(n+1)} + (1-\theta) y_k^{(n)})$ for $k = j-1, j, j+1$. Let

$$1 - \theta = \bar{\theta} \ ,$$

where $\theta \in [0, 1]$. With $\theta = 0$, we have the explicit difference scheme, with $\theta = 1/2$, the *Crank-Nicholson* implicit scheme, finally with ($\theta = 1$), the fully implicit scheme. Now applying this method on our model, we get the equation.

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

where H is defined in (2.3.17). Solving for $z^{(n+1)}$, we get

$$z^{(n+1)} = z^{(n)}. \left((I + \mu\bar{\theta}H).(I - \mu\theta H)^{-1}\right) \ . \tag{2.4.1}$$

Now let

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

where we want P_θ to represent a stochastic matrix whose rows sum to one. This wish leads us to various conditions regarding the relations between μ and θ. It is sufficient that $(I - \mu\theta H)$ is a *diagonally dominant M-matrix* and the matrix $(I + \mu\bar{\theta}H)$ is a *non-negative matrix* (see [33] and [106]). Obviously, $I - \mu\theta H$ is a strictly diagonally dominant M-matrix,and hence its inverse is non-negative because it has the property of $\{(-), (+)\}$: (-) all off-diagonal elements are ≤ 0, $(+)$ all rows sums are > 0. $I + \mu\bar{\theta}H$ is non-negative iff $1 - 2\mu\bar{\theta} \geq 0$. So we arrive at the conditions

$$0 < \mu \leq 1/2 \qquad \text{if} \qquad \theta = 0 \ ,$$

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

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

Now we introduce the column vector

$$\eta = \{1, 1, , \ldots, 1\}^T \ .$$

The rows of P_θ must sum to 1 which is equivalent to

$$P_\theta.\, \eta = \eta \ .$$

To show that this is true is an easy exercise. Since the sum of the rows of H are all zero, we have $H.\eta = 0$. This leads to $(I - \mu\theta H).\eta = \eta$, and $(I + \mu\bar{\theta}H).\eta = \eta$. Therefore $\eta = (I + \mu\bar{\theta}H).\eta = (I + \mu\bar{\theta}H).(I - \mu\theta H).\eta$.

Now, we prove $\sum\limits_j y_j^{(n)} = 1\,\forall n$ which is equivalent to prove that $\sum\limits_j z_j^{(n)} = 1\,\forall n$. To this purpose, we use the simple rule: a column vector $w = (w_1, w_2, \cdots)^T$ is a probability column vector iff $w_i \geq 0, \quad i = 1, 2, \cdots$, and $w^T.\eta = 1$. Till now, it is proved that $(I - \mu\theta H)^{-1}$ and P_θ are stochastic matrices. Then to complete the proof, we choose the initial value $y^{(0)}$ such that $\sum\limits_{j=-R}^{R} y_j^{(0)} = 1$, hence $z^{(0)}.\eta = 1$. So the desired relation is true for $n = 0$ and by induction for all $n > 0$.

It is known that the implicit scheme allows to predict the future faster than the explicit scheme. This property is considered as the most important advantage of the implicit scheme. Therefore, we shall use the implicit scheme to predict the convergence of the model as $t \to \infty$ because the number of steps, calculated according to the relation $n = \frac{t}{\tau}$, is less than the corresponding number of steps of the explicit scheme.

2.5 Convergence to the stationary solution of the model for time tending to infinity

Vincze, Fritz et al. and Kac (see [107], [22] and [51]) showed that the elements of the iterated stochastic matrix P_s defined in (2.3.19) of the generalized discrete Ehrenfest model (Urn model) converge to the binomial distribution for $n \to \infty$. This means

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

with

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

N being the total number of balls. As $N \to \infty$. The vector $p = (p_0, \ldots, p_N)$ satisfies $\sum_{k=0}^{N} p_k = 1$, and is interpreted as the stationary distribution of the Markov chain whose matrix is P_s.

Both the probability of finding k balls in the urn U_1 after $n+1$ steps, see equation (2.3.20), and the probability of finding the particle at the point x_j at the time instant t_{n+1}, see equation (2.3.7), are interpreted as discrete approximation to a diffusion with central linear force. In other words, by taking the limit as $Rh \to \infty$ they could be modeled by equation (2.1.2) (see [99]).

Since the stochastic matrix P defined in (2.3.13) representing the random walk approach for equation (2.3.7) and the stochastic matrix P_s representing the random walk approach for equation (2.3.20) are related to each other (see Section 3), the matrix P^n has an analogous limit as $n \to \infty$ and the elements of each row converge to the binomial distribution. So far, to show the behaviour of the model as $n \to \infty$, 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

$$d(t_i) = \sum_i |z_j^{(n)} - \bar{y}_j| \;, \tag{2.5.1}$$

where $-R \leq j \leq R$, and

$$\bar{y}_j = 2^{-2R} \binom{2R}{j+R} . \qquad (2.5.2)$$

The iteration index n is calculated from the relation $n\tau = t_i$, $i = 1, 2, \cdots \to \infty$, while τ is calculated from the scaling parameter (2.3.5).

For the Ehrenfest model, the row vector d approximates an exponential function

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

where ω and c are constants and ω is called the rate of convergence. Such exponential convergence is a general property of an ergodic Markov chain. The numerical estimation of ω, shows that it seems to tend to 1 as t tends to infinity.

For calculating the sequence of numbers d, we used the The implicit scheme because the number of steps in this case is less than needed with the explicit scheme. At the numerical simulation of the convergence of this model, we plot $log\, d$ against $log\, t$ because the numbers $d(t_i)$ are so small.

We deduce from the relation (2.3.3) that the binomial vector $\bar{y}/h$ approximates the normalized exact solution $u(x)$ of the stationary equation of the Ehrenfest model equation (2.1.2). By stationary solution we mean, the solution of the system as $t \to \infty$. In other words

$$\lim_{t \to \infty} u(x,t) = u(x) .$$

Then equation(2.1.2) with $a = b = 1$ takes, after replacing $\frac{\partial u}{\partial t}$ by 0, the form

$$0 = \frac{\partial^2 u(x)}{\partial x^2} + \frac{\partial\,(xu)}{\partial x} . \qquad (2.5.3)$$

The solution of this equation is

$$u(x) = \frac{c_1}{x} + c_2\, e^{-x^2/2} .$$

The requirement that $u(x)$ should be a probability density function and hence $u(x) \geq 0$ leads to $c_1 = 0$. To calculate the second constant, we use the normalization condition

$$\int_{-\infty}^{\infty} u(x) dx = 1 .$$

So we get the stationary solution of the diffusion equation (2.1.2) with $a = b = 1$

$$u(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} = \frac{1}{\sqrt{2\pi}} e^{-U(x)} \ .$$

In our numerical imitation of the stationary solution we plot the vector $\bar{y}/h$ and $u(x)$ to make visible that they approximate each others.

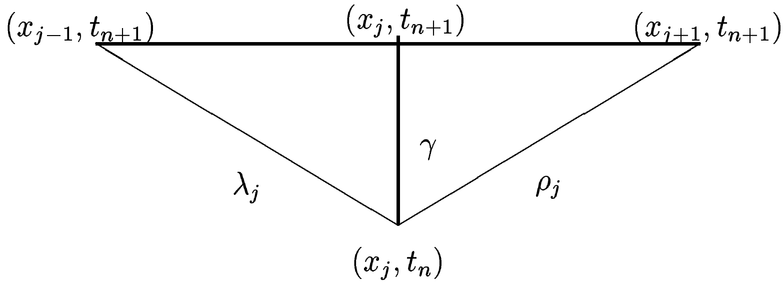
2.6 Random walk simulation

We discuss in this section the random walk of the elastically bound particle (diffusion under the action of the force bx, $b > 0$), which is also known as the generalized Ehrenfest model. We deduce from the previous sections that for a particle making a random walk on the spatial grid x_j in discrete instants t_n, $y_j^{(n)}$ in equation (2.3.7) represents the sojourn probability. In addition we proved that it has the properties of conservation of total probability and preservation of non-negativity. We proved also that the discrete redistribution process is related to a Markov chain in which if time proceeds from t_n to t_{n+1}, the sojourn-probabilities are redistributed according to the transition law

$$y_j^{(n+1)} = \sum_{k=-\infty}^{\infty} p_{j,j-k} y_{j-k}^{(n)} \ , \quad n \in \mathbb{N}, \ j \in [-R, R] \ , \ k = \pm 1 \ . \tag{2.6.1}$$

Here $p_{j,j-k}$ denote the suitable transfer coefficients, which represent the probability of transition from $x_{j\pm h}$ to x_j. The transfer coefficients are to be found consistently with the finite-difference equation (2.3.4) equipped with the given proper initial condition. Thus the summation in equation (2.6.1) is over all indices k for which $p_{j-k,j} \neq 0$. The transfer coefficients must be non-negative and their sum must be one. In our case $p_{j,j} = \gamma$, $p_{j,j+1} = \rho_j$, $p_{j,j-1} = \lambda_j$ and $p_{j,j+k} = 0 \ \forall \, |k| \geq 2$ (see Section 3).

The interpretation of the motion is as follows: Suppose the particle is sitting at the point x_j at the time instant t_n. Then for the next time instant t_{n+1} the particle has the opportunity to jump to the point x_{j-1} with transition probability λ_j, or to the point x_{j+1} with transition probability ρ_j, or to stay at its position x_j with transition probability γ. So far we can imagine the sketch of the motion of the particle as follows



To simulate this process, we generate a uniform random numbers $u \in [0, 1)$ and then use the *Monte Carlo method*. Suppose the particle is sitting at the point x_j at the time instant t_n. Then the particle will, as time proceeds from t_n to t_{n+1}, jump to the point x_{j-1}, x_j, or x_{j+1} depending on whether $u \in [0, \lambda_j)$, $u \in [\lambda_j, \lambda_j + \gamma)$, or $u \in [\lambda_j + \gamma, 1)$, respectively. The results of this simulation is considered in the special case $a = b = 1$.

We found from the simulation of this model that although the presence of the drift, the particle can freely jump far away from its initial positions. It can reach every grid-point in the interval $[-Rh, Rh]$, but always returns back to the origin. In strict mathematical words, it always return to the origin with probability 1.

2.7 The diffusion under the action of a general drift

After Smulochowski had extended the theory of Einstein, Fokker and Planck discussed the effect of the presence of a general external field $F(x)$ on the diffusion process. The most essential restrictions are that $F(x)$ must be an odd and non-negative function for $x > 0$. We assume $U(x)$ to be defined as a symmetric differentiable potential (i. e. $U(x) = U(-x)$) and increasing for $x > 0$, and define $F(x)$ as $F(x) = -\frac{d}{dx}U(x)$. Now we rewrite equation (2.1.2) as

$$\frac{\partial u(x,t)}{\partial t} = a\frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial}{\partial x}\left(F(x)\,u(x,t)\right) \, . \tag{2.7.1}$$

In this general situation of a *potential well*, the drift is directed towards the origin. Many forms of $U(x)$ can affect the particle to be attracted by the origin so they can also be studied. In this section we consider three types of over-damped non-linear oscillators driven by Lévy noise. The three Lévy oscillators are characterized by the potentials (with $b > 0$) (see [10]):-

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

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

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

Therefore, equation(2.1.2) can be interpreted as the diffusion of a particle under the action of the external linear force $F(x) = -bx, b > 0$, which is derived from the quadratic potential $U(x) = \frac{bx^2}{2}$.

First, we deal with the quartic Lévy oscillator. This means the diffusion is under the effect of the central cubic force $F(x) = -bx^3$. In this case equation (2.7.1) is rewritten as

$$\frac{\partial u(x,t)}{\partial t} = a\frac{\partial^2 u(x,t)}{\partial x^2} \; + \; b\frac{\partial}{\partial x}\left(bx^3\, u(x,t)\right) \;, \tag{2.7.2}$$

where $a > 0$. As we have done before for ease of writing we put $a = b = 1$. Then by discretizing equation (2.7.2) and solving for $y_j^{(n+1)}$, we get

$$\frac{y_j^{(n+1)} - y_j^{(n)}}{\tau} = \frac{y_{j+1}^{(n)} - 2y_j^{(n)} + y_{j-1}^{(n)}}{h^2} + \frac{1}{2h}\left(x_{j+1}^3 y_{j+1}^{(n)} - x_{j-1}^3 y_{j-1}^{(n)}\right) \;.$$

Setting $\mu = \tau/h^2$, and solving for $y_j^{(n+1)}$, we get

$$y_j^{(n+1)} = (1-2\mu)y_j^{(n)} + \mu\left(1 + \frac{h^4}{2}(j+1)^3\right)y_{j+1}^{(n)} + \mu\left(1 - \frac{h^4}{2}(j-1)^3\right)y_{j-1}^{(n)} \;. \tag{2.7.3}$$

In analogy to the diffusion with central linear drift, $y_j^{(n)}$, $n \in \mathbb{N}_0$ in equation(2.7.3), represents the probability of finding the particle at the point x_j, at the time instant t_{n+1}. We define $R = (\frac{2}{h^4})^{1/3}$ and require $R \in \mathbb{N}$, and the interval of computation as $[-Rh, Rh]$. The transition probabilities from the time instant t_n to the time instant t_{n+1} are

$$\gamma = (1 - 2\mu) = p_{j,j+1} \;, \tag{2.7.4}$$

$$\acute{\rho}_j = \mu(1 - \frac{j^3}{R^3}) = p_{j,j+1} \;, \tag{2.7.5}$$

$$\acute{\lambda}_j = \mu(1 + \frac{j^3}{R^3}) = p_{j,j-1} \;. \tag{2.7.6}$$

The condition of non-negativity for these transition probabilities limits the range of j, to be $-R \leq j \leq R$, $R \in \mathbb{N}$. With these conditions, we see that the condition of conservation is fulfilled

$$\gamma + \acute{\rho}_j + \acute{\lambda}_j = 1 \; \forall j \in \{-R, -R+1, \cdots, R-1, R\} \;.$$

The solution of equation(2.7.2) by using the explicit scheme is

$$y^{(n+1)} = y^{(n)}.(I - \mu \acute{H}) ,$$

where $y^{(n)}$ is a row vector, and the matrix $\acute{H}$ is a tridiagonal matrix whose rows sum to zero. By using the transition probabilities $\gamma, \acute{\rho}_j$ and $\acute{\lambda}_j$, we find that each j/R in the matrix H defined at (2.3.17) is replaced by j^3/R^3 in the matrix $\acute{H}$, and the matrix $(I - \mu\acute{H})$ is also a stochastic matrix (i.e. its rows sum to 1).

The partial differential equation which represents the diffusion under the effect of an anharmonic Lévy oscillator.

$$\frac{\partial u(x,t)}{\partial t} = a\frac{\partial^2 u(x,t)}{\partial x^2} + \frac{\partial}{\partial x}\left((cx + dx^3)\, u(x,t)\right) . \qquad (2.7.7)$$

Here $a > 0$, $c > 0$ and $d > 0$. Putting $a = d = c = 1$ and Discretizing this equation and solving for the sojourn probability y_j^{n+1}, we get

$$y_j^{(n+1)} = (1-2\mu)y_j^{(n)} + \mu\left(1 + \frac{h^2}{2}(j+1) + \frac{h^4}{2}(j+1)^3\right) y_{j+1}^{(n)} + \mu\left(1 - \frac{h^2}{2}(j-1) - \frac{h^4}{2}(j-1)^3\right) y_{j-1}^{(n)} . \qquad (2.7.8)$$

The transition probabilities to jump from the point x_j at the time instant t_n to the point x_{j-1}, or to x_j, or finally to x_{j+1} at the time instant t_{n+1}, respectively are

$$\acute{\lambda}_j = \mu((1 + \frac{jh^2}{2} + \frac{j^3h^4}{2}) = p_{j,j-1} , \qquad (2.7.9)$$

$$\gamma = (1-2\mu) = p_{j,j} , \qquad (2.7.10)$$

$$\acute{\rho}_j = \mu(1 - \frac{jh^2}{2} - \frac{j^3h^4}{2}) = p_{j,j+1} . \qquad (2.7.11)$$

The condition of conservation is also fulfilled:

$$\gamma + \acute{\rho}_j + \acute{\lambda}_j = 1 \; \forall j .$$

Therefore the transition probabilities form a stochastic matrix if the following conditions are satisfied

$$0 < \mu \leq 1/2 \, , -R \leq j \leq R \, ,$$

where in this case

$$R = \frac{-1}{\left[3h^2(9 + \sqrt{3}\sqrt{27 + h^2})\right]^{1/3}} + \frac{(9 + \sqrt{3}\sqrt{27 + h^2})}{(9h^4)^{1/3}} .$$

The explicit scheme and the implicit scheme of this model take the same form as for the previous drifts. The only difference is in the elements of the matrix H defined at (2.3.17). The stationary solution of equation (2.7.1) is

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

where C is a constant to be determined from the normalization condition.

In the following section, we give the numerical simulation of the diffusion under the effect of some of these types of forces as well as the comparison between the convergent numerical solutions as $n \to \infty$ and the stationary solutions of the differential equation.

It is worth to say that equation (2.7.1) is a special form of the so called *Fokker-Planck* equation. Usually the abbreviation *FPE* is used in mentioning this equation. The FPE describes normal diffusion problems involving external fields and often modelled as

$$\frac{\partial}{\partial t} u(x,t) = L_{FP}\, u(x,t)\ . \tag{2.7.12}$$

Here L_{FP} is a linear operator often defined by its action on a function

$$L_{FP} u(x,t) = K \frac{\partial^2}{\partial x^2}\, u(x,t) + \frac{1}{m\mu_1} \frac{\partial}{\partial x}\, \left(\frac{dU(x)}{dx} u(x,t)\right)\ . \tag{2.7.13}$$

Here $\frac{dU(x)}{dx} = -F(x)$, represents the external field, m is the mass of the diffusing particle, μ_1 is the friction coefficient, and K is the generalized diffusion constant. This equation has many applications in the stochastic processes and physics and has been widely studied by many authors (see for example [86], [84], [82] and [53]).

2.8 Numerical results

Figures[1-8] correspond to the motion under the action of the linear force (i.e. $F(x) = -x$):
Figure [1] corresponds to the explicit scheme where $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$.
Figure [2] corresponds to the explicit scheme where $y^{(0)} = \{\frac{1}{2R+1}, \cdots, \frac{1}{2R+1}, \cdots, \frac{1}{2R+1}\}$.
Figure[3] corresponds to the implicit scheme with $\theta = 1/2$ where $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$.
Figure[4] corresponds to the implicit scheme with $\theta = 1$ where $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$.
Figure[5] describes the convergence of the model, in which we plot

t against $log\ d$.
Figure[6] describes the convergence of the model, in which we plot $log\ t$ against $log\ d$.
Figures [7,8] show the approximate stationary numerical solution and the stationary solution of the model.

Figures [9-16] describing the motion under the action of the cubic force (i.e. $F(x) = -x^3$):
Figure[9] corresponds to the explicit scheme where $y^{(0)} = \{0, \cdots, 0, \cdots, 1\}$.
Figure[10] corresponds to the fully implicit scheme where $y_j^{(0)} = \delta_{j0}, j \in [-R, R]$.
Figure[11] correspond to the fully implicit scheme where all $y_j^{(0)} = \frac{1}{2R+1}, j \in [-R, R]$.
Figure[12] corresponds to the fully implicit scheme where $y^{(0)} = \{0.5, \cdots, 0, \cdots, 0.5\}$.
Figure[13] illustrates the convergence of the model, in which we plot t against $log\ d$.
Figure[14] illustrates the convergent of the model, in which we plot $log\ t$ against $log\ d$.
Figures [15,16] show the approximate stationary solution and the approximate solution of the model.

Figures [17-20] correspond to the simulation of the random walk of a particle moving under the action of a linear force. Finally, we note that all these figures are plotted for $R = 10$.

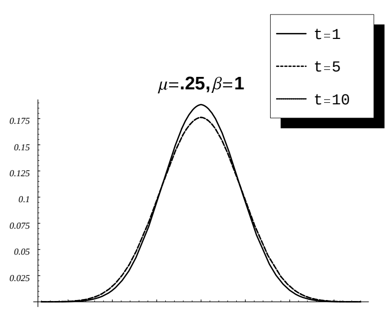


Figure 2.1: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

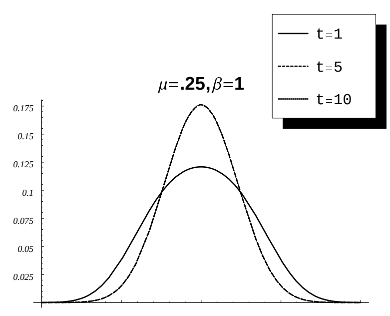


Figure 2.2: $y^{(0)} = \{\frac{1}{2R+1}, \cdots, \frac{1}{2R+1}\}$

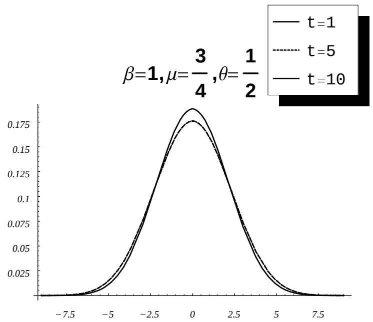


Figure 2.3: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

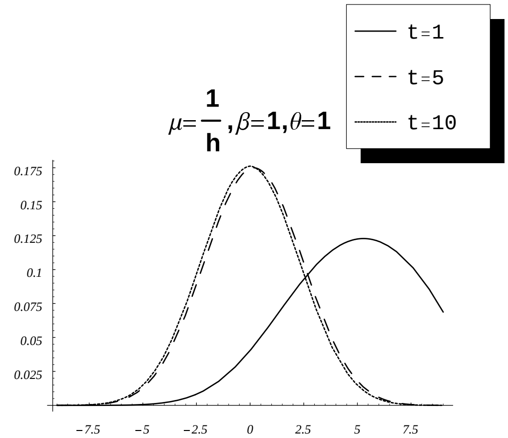


Figure 2.4: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

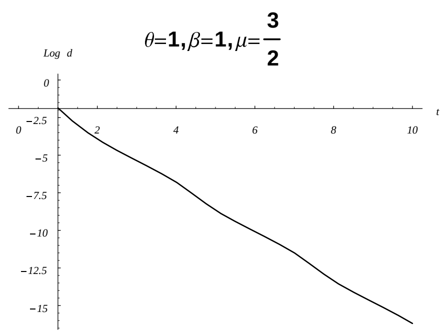


Figure 2.5: convergent

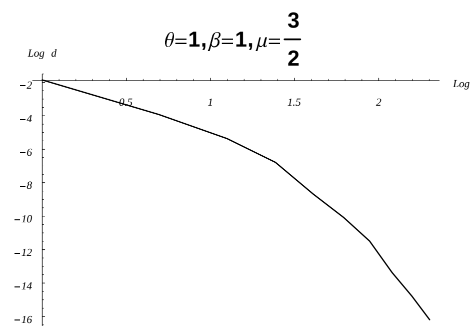


Figure 2.6: convergent

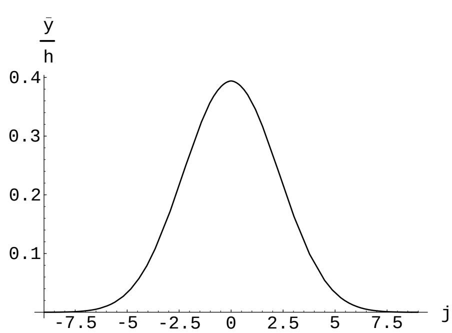


Figure 2.7: approximate solution

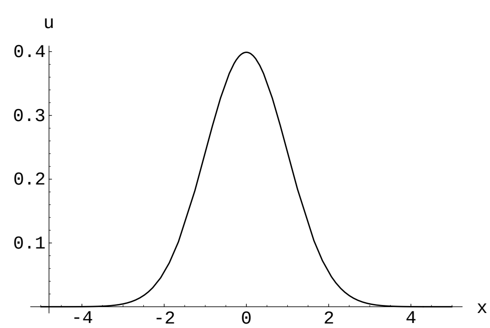


Figure 2.8: stationary solution

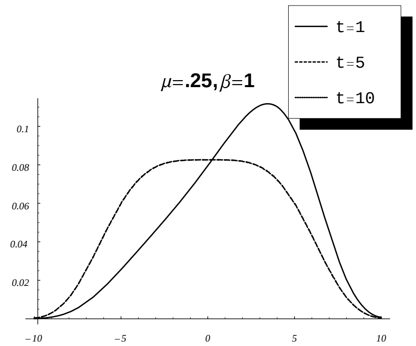


Figure 2.9: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

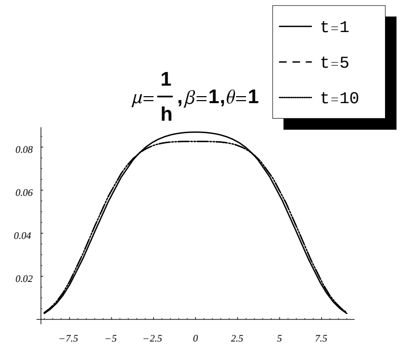


Figure 2.10: $y^{(0)} = \{0, \cdots, 1, \cdots, 0\}$

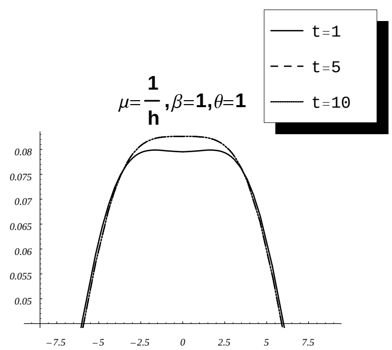


Figure 2.11: $y^{(0)} = \{\frac{1}{2R+1}, \cdots, \frac{1}{2R+1}\}$

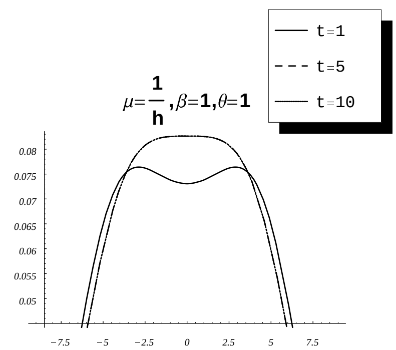


Figure 2.12: $y^{(0)} = \{0.5, \cdots, 0, 0 \cdots, 0.5\}$

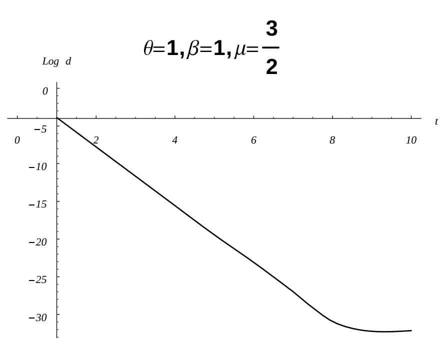


Figure 2.13: convergent

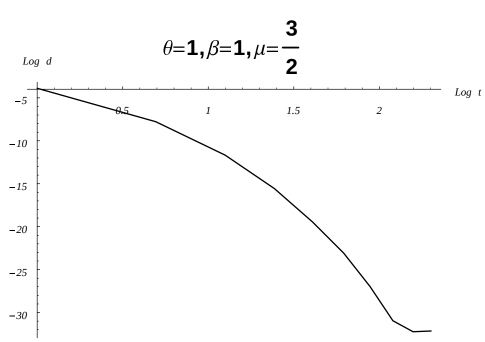


Figure 2.14: convergent

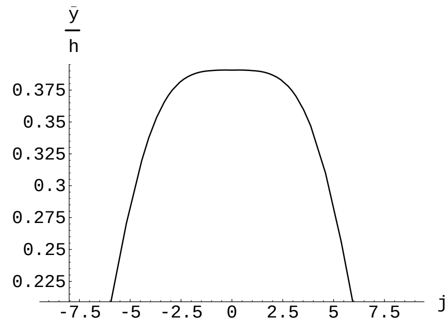


Figure 2.15: approximate solution

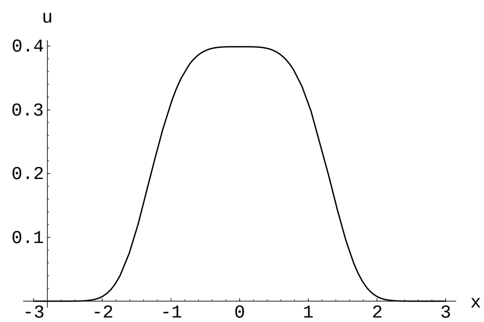


Figure 2.16: stationary solution

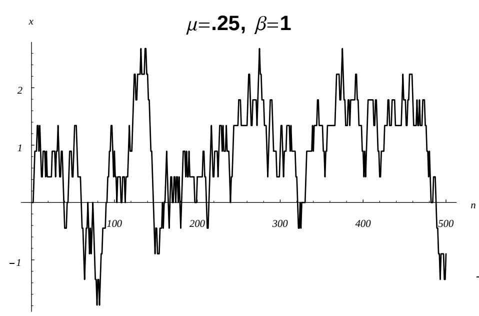


Figure 2.17: discrete random walk

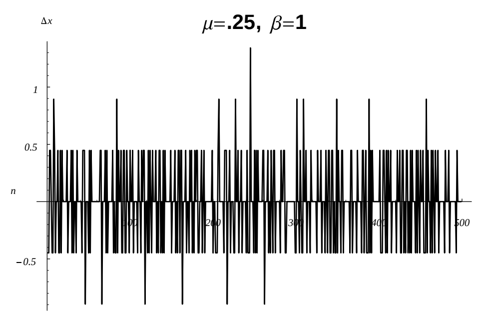


Figure 2.18: increment

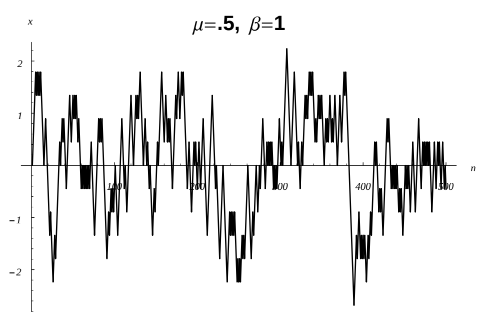


Figure 2.19: discrete random walk

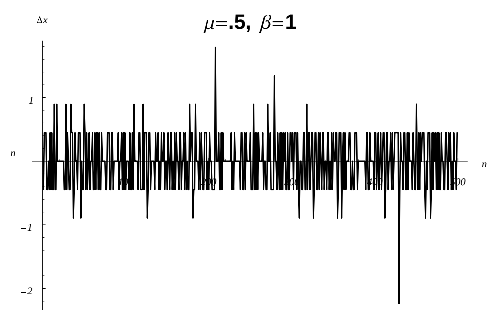


Figure 2.20: increment