# Chapter 17
# The Random Walk and Diffusion Theory

## 17.1 Introduction

Diffusion is one of the most widely spread processes in science. Its occurrence ranges from random motion of dust particles on fluid surfaces, historically known as Brownian motion, to the motion of particles in numerous physical systems [1, 2], the spreading of malaria by migration of mosquitoes [3], or even to the description of fluctuations in stock markets [4].

For instance, let us regard $N$ neutral, identical, classical particles which solely interact through collisions, for instance an $H_2$-gas in a box, where $N = N_A \approx 6.022 \times 10^{23}$. We are interested in the dynamics of one particle under the influence of all others and under no influence by an external force; we expect that diffusion will be the dominating process. From the microscopic point of view such a situation can be described with the help of $N$ coupled NEWTON's equations of motion. (See Chap. 7.) Anyhow, such a task will not be feasible due to the size of the system – the magnitude of $N$. However, a statistical description can be obtained from BOLTZMANN's equation [5]

$$\frac{\mathrm{d}}{\mathrm{d}t} f(r, \eta, t) = \frac{\partial}{\partial t} f(r, \eta, t)\Big|_{\text{coll.}} , \tag{17.1}$$

where $f(r, \eta, t)$ is the phase space distribution function. Hence, $f(r, \eta, t)\mathrm{d}r\mathrm{d}\eta$ is the number of particles of momentum $\eta$ within the phase-space volume $\mathrm{d}r\mathrm{d}\eta$ which is centered around position $r$ at time $t$. We have, in particular:

$$\frac{\partial}{\partial t} f(r, \eta, t) + \frac{\eta}{m} \cdot \frac{\partial}{\partial r} f(r, \eta, t) + F \cdot \frac{\partial}{\partial \eta} f(r, \eta, t) = C[f](r, \eta, t) . \tag{17.2}$$

Here $C[f](r, \eta, t)$ is the collision integral and $F$ describes an external force. In cases where collisions result solely from two-body interactions between particles that



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are assumed to be uncorrelated prior to the collision,[1] the collision integral can be described by

$$C[f](r,\eta,t) = \int \mathrm{d}\xi_1 \int \mathrm{d}\xi_2 \int \mathrm{d}\xi_3 g(\xi_1,\xi_2,\xi_3,\eta)\,[f(r,\xi_1,t)f(r,\xi_2,t) \\ -f(r,\eta,t)f(r,\xi_3,t)] \ , \tag{17.3}$$

where $g(\xi_1,\xi_2,\xi_3,\eta)$ accounts for the probability that a collision between two particles of initial moments $\xi_1$ and $\xi_2$ and final momenta $\xi_3$ and $\eta$ occurs. This function depends on the particular type of particles under investigation and has, in general, to be determined from a microscopic theory.[2] We now define the particle density $\rho(r,t)$ as a function of space $r$ and time $t$ via

$$\rho(r,t) = \int \mathrm{d}\eta f(r,\eta,t) \ . \tag{17.4}$$

A complicated mathematical analysis of Eq. (17.1) results in a diffusion equation of the well-known form

$$\frac{\partial}{\partial t}\rho(r,t) = D\frac{\partial^2}{\partial r^2}\rho(r,t) \ , \tag{17.5}$$

if collisions dominate the dynamics (*diffusion limit*). Here $D = \text{const}$ is the diffusion coefficient of dimension length$^2\times$ time$^{-1}$. Note that

$$\int \mathrm{d}r\rho(r,t) = N \ , \tag{17.6}$$

is the number of particles within our system.[3] Thus, in our example we can interpret diffusion as the average evolution of the integrated phase space distribution function governed by collisions between particles. Such an interpretation will certainly not hold in the case of fluctuations in stock markets or in the case of the spreading of malaria because typically mosquitoes do not *collide* with humans.

It is the aim of the first part of this chapter to present a purely stochastic approach to diffusion, the so called *random walk* model [7, 8]. This stochastic

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[1] This assumption is known as the approximation of *molecular chaos*. In fact it represents the MARKOV approximation to the dynamics of a many particle system.

[2] For instance, one can employ FERMI's golden rule [6] to obtain this function on a quantum mechanical level. We already came across an expression of the form (17.3) on the right hand side of the master equation, see Sect. 16.3, Eq. (16.42). However, the collision integral of the BOLTZMANN equation is non-linear.

[3] The function $\rho(r,t)$ is referred to as a *physical distribution function* due to the normalization condition (17.6). This is in contrast to distribution functions we encountered so far within this book, which are normalized to unity.

description will prove to have several precious advantages: (i) We will be able to identify criteria for the validity of the diffusion model even for systems lacking a straight-forward physical interpretation. (ii) The stochastic formulation will give us the opportunity to perform diffusion 'experiments' on the computer without much computational effort as the methods employed are based on algorithms discussed in previous chapters. (iii) Within this framework it will be an easy task to generalize the approach to stochastic models of anomalous diffusion [9]: The *fractal time random walk* and LÉVY *flight* models [10]. These models play an increasingly important role in modern statistical physics.

## 17.2 The Random Walk

The random walk is one of the classical examples of MARKOV-chains [11–13]. In this section we discuss some of the basic properties of random walks in one dimension. For convenience, we are going to use the familiar picture of one diffusing particle.

### *Basics*

The random walk [8] is defined as the motion of a single particle which moves at the time instances

$$0, \Delta t, 2\Delta t, \dots, n\Delta t, \dots \ , \tag{17.7}$$

between grid-points

$$\dots, -n\Delta x, \dots, -\Delta x, 0, \Delta x, \dots, n\Delta x, \dots \ . \tag{17.8}$$

For a more transparent notation the lattice point $n\Delta x$, with $n \in \mathbb{Z}$, will be denoted by $x_n$ and the instance $k\Delta t$, with $k \in \mathbb{N}$, will be denoted by $t_k$. This notation follows the conventions of Chap. 2. The initial position is given by

$$\Pr[X(t_0 = 0) = x_i] = \delta_{i0} \ , \tag{17.9}$$

and the transition rates $p_{ij}$ from position $i$ to position $j$ within a single time step $\Delta t$ are defined as

$$\Pr[X(t_{n+1}) = x_i | X(t_n) = x_j] = p\delta_{ji-1} + q\delta_{ji+1} + r\delta_{ij} \ . \tag{17.10}$$

Here $p$ denotes the probability that the particle jumps to the neighboring grid-point on the right-hand side, $q$ stands for the probability that the particle jumps to the neighboring grid-point on the left-hand side, and $r$ denotes the probability of staying at the same-grid point within this time step. Naturally, we have

$$p + q + r = 1 \; . \tag{17.11}$$

Consequently, we have a MARKOV-chain with time instances $t_n$ and a state space spanned by the positions $x_k$. Moreover, we note that the stochastic process is clearly irreducible since all states communicate with each other (see Sect. 16.4). Hence, it follows that either all states are recurrent or all states are transient. Furthermore, in the case that $r \neq 0$ the MARKOV-chain is aperiodic, otherwise the chain is periodic with periodicity $d = 2$ because it takes at least two steps to return to the starting position.

We concentrate first on the *classical random walk* that is a one-dimensional random walk with $\Delta t = \Delta x = 1$, $r = 0$, and $p + q = 1$. This ensures that the probability of remaining in the actual position within one time step is equal to zero. If, furthermore, $p = q = 1/2$ the random walk is referred to as *unbiased* and for $p \neq q$ we call it *biased*. We write the position $X(t_n) = x_n$ at time $t_n = n$ as

$$x_n = \sum_{i=1}^{n} \xi_i \; , \tag{17.12}$$

where $\xi_i \in \{-1, 1\}$ and $\Pr(\xi_i = +1) = p$, $\Pr(\xi_i = -1) = q$. Let us assume that within these $n$ steps the particle moved $m$ times to the right and, consequently, $n-m$ times to the left. The actual position $x_n$ after $n$ steps can then be determined from

$$x_n = m - (n - m) = 2m - n \equiv k \; , \tag{17.13}$$

where we used that $x_0 = 0$. It is interesting to calculate the probability $\Pr(x_n = k)$ to find the particle after $n$ time steps at some particular position $k$. This is simply the sum over all paths along which the particle moved $m = (n + k)/2$ times to the right and $n - m = (n - k)/2$ times to the left multiplied by the probability for $m$ steps to the right and $n - m$ steps to the left. In total, this yields $\binom{n}{m} = \binom{n}{(n+k)/2}$ different contributions and we have

$$\begin{aligned} \Pr(x_n = k) &= \binom{n}{m} p^m q^{n-m} \\ &= \binom{n}{(n+k)/2} p^{\frac{n+k}{2}} q^{\frac{n-k}{2}} \; . \end{aligned} \tag{17.14}$$

In particular, we find for the unbiased random walk:

$$\Pr(x_n = k) = \binom{n}{(n+k)/2} \left(\frac{1}{2}\right)^n \; . \tag{17.15}$$

Due to the aperiodicity of the classical random walk, $k$ can only take on the values $k = -n, -n+2, \dots, n-2, n$. Consequently $n \pm k$ has to be even. For all other values of $k$ we have $\Pr(x_n = k) = 0$. Furthermore,

$$\begin{aligned}\sum_{\substack{k=-n\\ n\pm k\,\text{even}}}^{n} \Pr(x_n = k) &= \sum_{m=0}^{n} \binom{n}{m} p^m q^{n-m} \\ &= (p+q)^n \\ &= 1 \ ,\end{aligned} \tag{17.16}$$

and the probability of finding the particle at time $n$ within $[-n, n]$ is equal to one. A simple algorithm to simulate the one-dimensional biased random walk consists of the following steps:

1. Define values $x_0$, $p$, and $q = 1 - p$ .
2. Draw a uniformly distributed random number $r \in [0, 1]$ .
3. If $r < p$ set $x_{n+1} = x_n + 1$ , otherwise set $x_{n+1} = x_n - 1$ .
4. Return to step 2.

In Fig. 17.1 we present three different realizations of an unbiased one-dimensional random walk for (a) $N = 50$, (b) $N = 100$, and (c) $N = 1000$ consecutive steps.

Comparison between Figs. 17.1 and 16.2 already suggests a connection between the random walk and the WIENER process and we shall come back to this point in the course of this chapter.

## *Moments*

Let us briefly elaborate on the moments of the random walk (see Appendix, Sect. E.2). The first moment or expectation value $\langle x_n \rangle$ is given by

$$\begin{aligned}\langle x_n \rangle &= \sum_{\substack{k=-n\\ n\pm k\ \text{even}}}^{n} k \binom{n}{(n+k)/2} p^{(n+k)/2} q^{(n-k)/2} \\ &= \sum_{m=0}^{n} (2m - n) \binom{n}{m} p^m q^{n-m} \\ &= (2\langle m \rangle - n) \\ &= n(2p - 1) \ .\end{aligned} \tag{17.17}$$

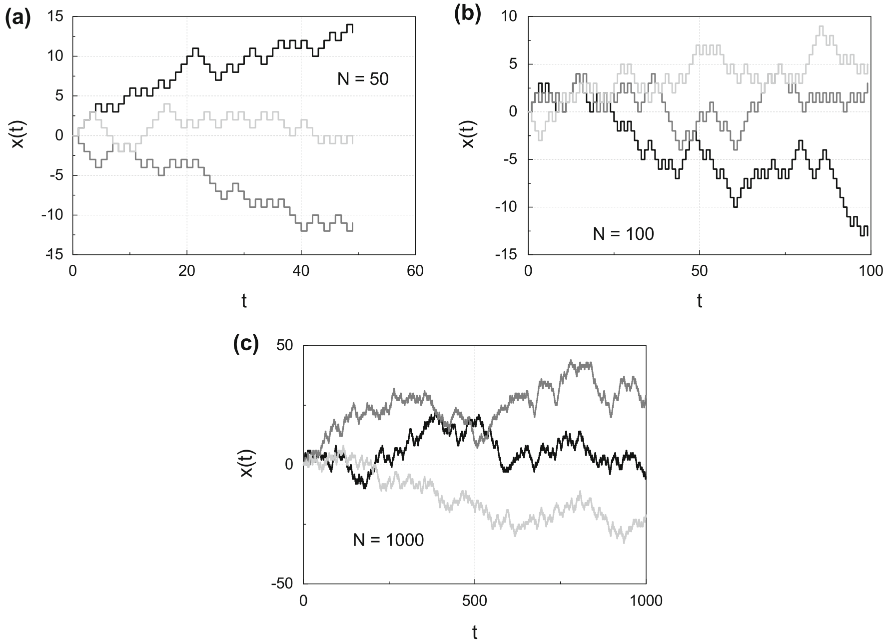


**Fig. 17.1** Three different realizations of an unbiased one-dimensional random walk for **(a)** $N = 50$, **(b)** $N = 100$, and **(c)** $N = 1000$ time steps and different seeds

We now introduce a *bias* $v$ such that

$$p = \frac{1}{2}(1 + v) \quad \text{and} \quad q = \frac{1}{2}(1 - v) \ , \tag{17.18}$$

and obtain

$$\langle x_n \rangle = nv \ . \tag{17.19}$$

We calculate the second moment $\langle x_n^2 \rangle$ using the above method and get:

$$\langle x_n^2 \rangle = n(1 - v^2) + n^2 v^2 \ . \tag{17.20}$$

The variance $\text{var}(x_n)$ follows immediately:

$$\text{var}(x_n) = \langle x_n^2 \rangle - \langle x_n \rangle^2 = n(1 - v^2) \ . \tag{17.21}$$

We note the following: The expectation value $\langle x_n \rangle$ moves according to Eq. (17.19) with a uniform velocity defined by the bias $v = p - q$. In particular, for the unbiased random walk $v = 0$ and, thus, $\langle x_n \rangle = 0$ for all $n$. Furthermore, we observe that $\text{var}(x_n)$ increases linearly with time $n$ – a property we already noted for the WIENER process in Sect. 16.3 – and it is maximal for $v = 0$. For $v = \pm 1$, which describes a pure drift motion in the positive or negative $x$ direction, the variance is equal to zero.

## *Recurrence*

Let us briefly investigate the recurrence behavior of the random walk. We are interested in the probability $f_{00}^{(2\ell)}$ of a first return to the origin $x_0 = 0$ after $2\ell$ steps. We already know that $f_{00}^{(2\ell)} \propto p^\ell q^\ell$ from our previous analysis. In the very first time step the particle moves either to $x_1 = 1$ or to $x_1 = -1$ and, consequently, within the following $2\ell - 2$ steps it must not cross or touch the line $x_k = 0$ and the particle has to terminate at position $x_{2\ell-1} = x_1$. Therefore, the walker performs $\ell - 1$ steps to the left and $\ell - 1$ steps to the right within these $2\ell - 2$ steps. The total number of possible paths $N$ from $x_1$ to $x_{2\ell-1} = x_1$ is, thus, given by

$$N = \binom{2\ell - 2}{\ell - 1} . \tag{17.22}$$

Moreover, $N$ may also be written as the sum of $N_c$ paths which cross or touch the line $x_k = 0$ and $N_{nc}$ paths which do not cross or touch the line $x_k = 0$, i.e.

$$N = N_c + N_{nc} . \tag{17.23}$$

Obviously, we are only interested in the paths which do not cross or touch the line $x_k = 0$. We employ the reflection principle to solve this problem. In general, the number of paths which go from $x_1 = i > 0$ to $x_{k+1} = j > 0$ within $k$-steps and cross the line $x_\ell = 0$ is equal to the total number of paths which go from $x_1 = -i$ to $x_{k+1} = j$, as is schematically illustrated in Fig. 17.2.

Let us regard the case $x_1 = 1$: The walker moved in the first step to the right. Hence, from the reflection principle we obtain that the number of paths from $x_1$ to $x_{2\ell-2} = x_1$ in $2\ell - 2$ steps which cross or touch the line $x_k = 0$ is given by the total

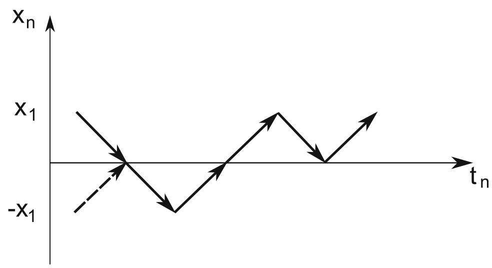


**Fig. 17.2** Illustration of the reflection principle

number of paths from $-x_1$ to $x_{2\ell-2} = x_1$. Thus, $N_c$ is determined by:

$$N_c = \binom{2\ell-2}{\ell} . \tag{17.24}$$

We note that in this picture, the walker moves $\ell$ steps to the right and $\ell - 2$ steps to the left. Hence, we obtain that the number of paths which do not cross or touch the line $x_k = 0$ is given by

$$2N_{nc} = 2(N - N_c) = \frac{1}{2\ell - 1}\binom{2\ell}{\ell} . \tag{17.25}$$

The prefactor 2 accounts for the fact that the walker can move in its first step either to $x_1 = -1$ or to $x_1 = 1$. Thus, the probability for the first return of the particle after $2\ell$ steps is described by:

$$f_{00}^{(2\ell)} = \frac{1}{2\ell - 1}\binom{2\ell}{\ell} p^\ell q^\ell . \tag{17.26}$$

We calculate the recurrence probability according to Eq. (16.66) and this results in

$$\sum_{\ell=0}^{\infty} f_{00}^{(2\ell)} = \begin{cases} 1 & \text{for } p = q = \frac{1}{2} , \\ 2p & \text{for } p < q , \\ 2q & \text{for } p > q , \end{cases} \tag{17.27}$$

with the consequence that the one-dimensional random walk is only recurrent in the unbiased case $v = 0$.

Another possibility to demonstrate the recurrence of the unbiased one-dimensional random walk is provided by Eq. (16.69). The probability that a walker returns to $x_0 = 0$ after $2n$ steps is given by

$$P^{(2n)}(x_0) = \binom{2n}{n} p^n q^n = \frac{(2n)!}{n!n!}(pq)^n . \tag{17.28}$$

In this case we are not interested in the question whether or not it is the particle's first return. By STIRLING's approximation [Appendix, Eq. (E.20)]

$$n! \propto n^{n+\frac{1}{2}} e^{-n} \sqrt{2\pi} , \tag{17.29}$$

and we obtain for $P^{(2n)}(x_0)$:

$$P^{(2n)}(x_0) \propto \frac{(4pq)^n}{\sqrt{n\pi}} . \tag{17.30}$$

We assume $p \leq 1/2$ and since $pq = p(1-p) \leq 1/4$ one gets

$$\sum_{n=0}^{\infty} P^{(2n)}(x_0) \to \infty \quad \text{only for} \quad p = q = \frac{1}{2} . \tag{17.31}$$

The same argument holds for $p > 1/2$ since we can write $pq = (1-q)q \leq 1/4$. According to Eq. (16.69) this means that the process is recurrent only for $p = q$, in accordance with our previous result (17.27), and transient otherwise. We note that this agrees also with the more physical picture of an external force inducing a bias or *drift* velocity $v \neq 0$.

It should be noted that the unbiased random walk in two dimensions is also recurrent while it can be proved to be transient in higher dimensions. For instance, the recurrence probability is approximately 0.34[4] in 3D.

## 17.3 The WIENER Process and Brownian Motion

It is the purpose of this section to demonstrate that the WIENER process is the scaling limit of the random walk. Moreover, we discuss briefly the LANGEVIN equation and derive the diffusion equation.

As a starting point we consider the one-dimensional unbiased random walk on an equally spaced grid according to Eq. (17.8) and time instances given by Eq. (17.7). We denote the stochastic process by $X_n = X(t_n)$ and it is described by

$$X_n = \sum_{i=1}^{n} \xi_i \Delta x , \tag{17.32}$$

where $\xi \in \{-1, 1\}$ together with $X_0 = 0$. Since we regard the unbiased case $\Pr(\xi_i = \pm 1) = 1/2$, $\langle \xi_i \rangle = 0$, and $\mathrm{var}(\xi_i) = 1$. This is equivalent to

$$\langle X_n \rangle = 0 \quad \text{and} \quad \mathrm{var}(X_n) = n\Delta x^2 , \tag{17.33}$$

[4] This is one of PÓLYA's random walk constants [14–16].

as we already demonstrated in the previous section, Eq. (17.21). The variance var $(X_n)$ can be reformulated as

$$\operatorname{var}(X_n) = t_n \frac{\Delta x^2}{\Delta t} , \tag{17.34}$$

using the definition $t_n \equiv n\Delta t$. The simultaneous limit $\Delta t$, $\Delta x \to 0$ is now performed in such a way that

$$\lim_{\substack{\Delta t \to 0 \\ \Delta x \to 0}} \frac{\Delta x^2}{\Delta t} = D = \text{const} , \tag{17.35}$$

with $D$ the diffusion coefficient. This limit is known as the *continuous limit* and it will be denoted by the operator $\mathscr{L}$. Hence, in the continuous limit Eq. (17.34) results in

$$\mathscr{L}\left[\operatorname{var}(X_n)\right] = Dt , \tag{17.36}$$

where we renamed $t_n \equiv t$. We also note that the limit $\Delta t \to 0$ for constant $t$ is equivalent to $n \to \infty$ and we obtain in accordance with the central limit theorem (see Appendix, Sect. E.8):

$$\mathscr{L}(X_n) \to W_t \sim \mathscr{N}(0, Dt) . \tag{17.37}$$

Here $\mathscr{N}(0, Dt)$ denotes the normal distribution of mean zero and variance $Dt$, Appendix Eq. (E.43). Furthermore, the symbol $W_t$ was introduced to represent the WIENER process and the symbol '$\sim$' stands, within this context, for the notion *follows the distribution*. If $W_t$ describes a WIENER process it is necessary to prove that $W_t$ has independent increments $W_{t_2} - W_{t_1}$ which follow, according to Sect. 16.3, a normal distribution with mean zero and a variance proportional to $t_2 - t_1$. This is demonstrated quite easily: We learn from our discussion of the random walk that

$$X_n - X_m = \sum_{i=1}^{n} \xi_i - \sum_{i=1}^{m} \xi_i = \sum_{i=m+1}^{n} \xi_i , \tag{17.38}$$

and, therefore, $X_n - X_m$ and $X_m - X_k$ are clearly independent for $n > m > k$ and it follows that also $W_t - W_s$ and $W_s - W_u$ are independent. Furthermore, we have

$$X_n - X_m \stackrel{d}{=} X_{n-m} , \tag{17.39}$$

where the symbol '$\stackrel{d}{=}$' stands for the notion *to follow the same distribution* or *to be distributionally equivalent*. Therefore, in the limit $\mathscr{L}$ for $t > s$

$$W_t - W_s \stackrel{d}{=} W_{t-s} \sim \mathscr{N}\left[0, D(t-s)\right] \ , \tag{17.40}$$

which completes the proof. We note that the particular case $D = 1$ is commonly referred to as the *standard* WIENER *process*. We remark that in many cases the terms WIENER process and Brownian motion are used as synonyms for a stochastic process satisfying the above properties. However, strictly speaking, the stochastic process is the WIENER process while Brownian motion is the physical phenomenon which can be described by the WIENER process.

If we suppose that $p \neq q$ then

$$\mathscr{L}\left(\langle X_n \rangle\right) = \nu t \ , \tag{17.41}$$

with the drift constant $\nu$, describes a WIENER process with a drift term

$$\mathscr{L}(X_n) \to \tilde{W}_t = \nu t + W_t \ . \tag{17.42}$$

This process behaves like $W_t$ with the only difference that it fluctuates around mean $\nu t$ instead of mean zero. Note that for $\nu > 0$ the mean $\langle \tilde{W}_t \rangle$ increases, while for $\nu < 0$ it decreases with time $t$.

Another interesting property of the WIENER process is its *self-similarity*. In particular, we have the property that for $\alpha > 0$

$$W_t \stackrel{d}{=} \alpha^{-\frac{1}{2}} W_{\alpha t} \ , \tag{17.43}$$

with the consequence that it is completely sufficient to study the properties of the WIENER process for $t \in [0, 1]$ to know its properties for arbitrary time intervals. Relation (17.43) follows from the fact that $W_t \sim \mathscr{N}(0, Dt)$.

Furthermore, *white noise*, $\eta(t)$, is defined as the formal derivative of the WIENER process $W_t$ with respect to time. We give its most important properties without going into details[5]:

$$\langle \eta(t) \rangle = 0, \quad \text{and} \quad \langle \eta(t)\eta(s) \rangle = \delta(t-s) \ . \tag{17.44}$$

[5]In fact, it can be shown that $W_t$ is non-differentiable with probability one. This is the reason why it is defined as the *formal* derivative of $W_t$. Let $\varphi(t)$ be a test function and $f(t)$ an arbitrary function which does not need to be differentiable with respect to $t$. Then the formal derivative $\dot{f}(t)$ is defined by

$$\int_0^\infty \mathrm{d}t \dot{f}(t)\varphi(t) = -\int_0^\infty \mathrm{d}t f(t)\dot{\varphi}(t) \ .$$

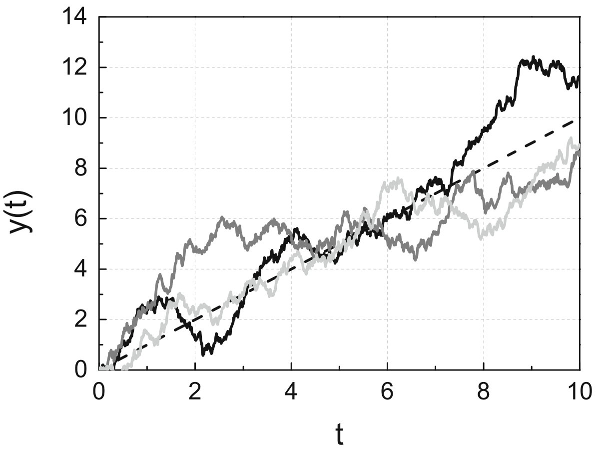


**Fig. 17.3** Three different realizations of the standard WIENER process with drift $\nu = 1$ according to Eq. (17.42). The expectation value $\langle x \rangle = \nu t$ of the process is presented as a *dashed line*

White noise is referred to as *Gaussian white noise* if $\eta(t)$ follows a normal distribution.

Figure 17.3 presents three different realizations of the standard WIENER process with drift according to Eq. (17.42). The curves in this figure were generated using the procedure outlined in Sect. 16.3 in connection with Fig. 16.2.

Let us derive the diffusion equation from the random walk model. The probability $\Pr(x,t)$ of finding the particle at time $t$ at position $x$ is expressed by

$$\begin{aligned}\Pr(x,t) &= \Pr(x,t-\Delta t)r + \Pr(x-\Delta x, t-\Delta t)p \\ &\quad + \Pr(x+\Delta x, t-\Delta t)q \\ &= \Pr(x,t-\Delta t)(1-p-q) + \Pr(x-\Delta x, t-\Delta t)p \\ &\quad + \Pr(x+\Delta x, t-\Delta t)q \ ,\end{aligned} \tag{17.45}$$

where we made use of relation (17.11). The interpretation of this equation is straight-forward: The probability to find the particle at the position-time point $(x,t)$ is the sum of three terms. The first term describes the probability that the particle arrived already at position $x$ in the previous time step $t-\Delta t$ and that it will stay there during the next time step. The remaining two terms describe the probability that the particle arrived at position $x-\Delta x$ $(x+\Delta x)$ in the previous time step and that it will move one step to the right (left) in the next time step. Each particular term is now expanded into a TAYLOR series up to order $\mathcal{O}(\Delta x^2)$ and $\mathcal{O}(\Delta t)$, respectively. This requires the transition from a discrete to a continuous state space and, consequently, the probabilities $\Pr(\cdot)$ are replaced by pdfs $p(\cdot)$. We get

$$\begin{aligned}p(x,t) &= (1-p-q)\Big[p(x,t) - \Delta t\frac{\partial p(x,t)}{\partial t}\Big] \\ &\quad + p\Big[p(x,t) - \Delta t\frac{\partial p(x,t)}{\partial t} - \Delta x\frac{\partial p(x,t)}{\partial x}\end{aligned}$$

$$+\frac{1}{2}\Delta x^2 \frac{\partial^2 p(x,t)}{\partial x^2}\Big]$$
$$+q\Big[p(x,t) - \Delta t \frac{\partial p(x,t)}{\partial t} + \Delta x \frac{\partial p(x,t)}{\partial x}$$
$$+\frac{1}{2}\Delta x^2 \frac{\partial^2 p(x,t)}{\partial x^2}\Big] , \tag{17.46}$$

and furthermore:

$$\frac{\partial p(x,t)}{\partial t} = -\frac{(p-q)\Delta x}{\Delta t}\frac{\partial p(x,t)}{\partial x} + \frac{(p+q)\Delta x^2}{2\Delta t}\frac{\partial^2 p(x,t)}{\partial x^2} . \tag{17.47}$$

We draw the continuous limit and define the drift constant

$$\nu = \mathscr{L}\left[(p-q)\frac{\Delta x}{\Delta t}\right] = \lim_{\substack{\Delta t \to 0 \\ \Delta x \to 0}} \frac{(q-p)}{\Delta t}\Delta x , \tag{17.48}$$

the diffusion constant

$$D = \mathscr{L}\left[(p+q)\frac{\Delta x^2}{2\Delta t}\right] = \lim_{\substack{\Delta t \to 0 \\ \Delta x \to 0}} \frac{(p+q)}{2\Delta t}\Delta x^2 , \tag{17.49}$$

and arrive at the one-dimensional diffusion equation with drift term:

$$\frac{\partial p(x,t)}{\partial t} = \nu \frac{\partial p(x,t)}{\partial x} + D\frac{\partial^2 p(x,t)}{\partial x^2} . \tag{17.50}$$

This equation is referred to as a FOKKER-PLANCK equation [17]. In the specific case $p = q$ the drift term disappears and we obtain, as expected, the classical diffusion equation

$$\frac{\partial}{\partial t}p(x,t) = D\frac{\partial^2}{\partial x^2}p(x,t) , \tag{17.51}$$

which we solved already numerically in Chaps. 9 and 11. It follows from this discussion that the position of a diffusing particle can be described as a stochastic process where, in the continuous limit, the jump-lengths follow a normal distribution. In addition, we know from our discussion of continuous-time MARKOV-chains in Sect. 16.5, that the waiting times between two successive jumps will certainly follow an exponential distribution. These insights will serve as a starting point in the discussion of general diffusion models in Sect. 17.4. Moreover, we note that the anisotropy of the jump-length distribution is a model for the presence of an external field which manifests itself in a drift term.

An alternative approach to the formal description of Brownian motion goes back to LANGEVIN. He considered the classical equation of motion of a particle in a fluid which reads

$$\dot{v} = -\beta v \ , \tag{17.52}$$

where $\beta$ denotes the friction coefficient and we set the particle's mass $m$ equal to one. LANGEVIN argued that this equation may only be valid for the average motion of the particle which corresponds to the long time behavior of the motion of massive particles. However, if the particle is not heavy at all its trajectory can be highly affected by collisions with solvent's molecules. He supposed that a reasonable generalization of Eq. (17.52) should be of the form [18]

$$\dot{v} = -\beta v + F(t) \ , \tag{17.53}$$

where $F(t)$ is a *random force*. In particular, $F(t)$ is a stochastic process which satisfies

$$\langle F(t)\rangle = 0 \quad \text{and} \quad \langle F(t)F(s)\rangle = A\delta(t-t') \ , \tag{17.54}$$

where $A$ is a constant and we obtain

$$F(t) \overset{d}{=} \sqrt{A}\eta(t) \ . \tag{17.55}$$

Equation (17.53) is referred to as the LANGEVIN equation and it is *the* prototype *stochastic differential equation*. Based on the definition of white noise $\eta(t)$ the LANGEVIN equation can be rewritten:

$$\mathrm{d}v = -\beta v \mathrm{d}t + \sqrt{A}\mathrm{d}W_t \ . \tag{17.56}$$

The solution of the LANGEVIN equation describes a stochastic process referred to as the ORNSTEIN-UHLENBECK *process* [19]. This process is essentially the only stochastic process which is stationary, Gaussian and Markovian. Its master equation is a FOKKER-PLANCK equation of the form [17]

$$\frac{\partial}{\partial t}p(v,t) = \beta\frac{\partial}{\partial v}vp(v,t) + \frac{A}{2}\frac{\partial^2}{\partial v^2}p(v,t) \ , \tag{17.57}$$

where $p(v,t)$ is the pdf of the ORNSTEIN-UHLENBECK process. If the initial velocity $v_0$ is given then the pdf $p(v,t)$ can be proved to be

$$p(v,t) = \frac{\sqrt{\beta}}{\sqrt{\pi A\left(1-e^{-2\beta t}\right)}}\exp\left[-\frac{\beta\left(v-v_0e^{-\beta t}\right)^2}{A\left(1-e^{-2\beta t}\right)}\right] \ . \tag{17.58}$$

It is possible to solve the LANGEVIN equation (17.53) analytically with the result:

$$v(t) = v_0 \exp(-\beta t) + \sqrt{A} \int_0^t \mathrm{d}t' \eta(t') \exp\left[-\beta(t - t')\right] . \tag{17.59}$$

We write in particular

$$v(t_{n+1}) = v(t_n) \exp(-\beta \Delta t) + Z_n , \tag{17.60}$$

with $Z_n$ defined as:

$$Z_n = \sqrt{A} \int_0^{\Delta t} \mathrm{d}t' \eta(t_n + t') \exp\left[-\beta(\Delta t - t')\right] . \tag{17.61}$$

Since $\eta(t)$ was assumed to be Gaussian white noise, $Z_n$ can be proved to be described by

$$Z_n \sim \mathcal{N} \left\{0, \frac{A}{2\beta} \left[1 - \exp(-2\beta \Delta t)\right]\right\} , \tag{17.62}$$

which offers a very convenient way to simulate the ORNSTEIN-UHLENBECK process. This particular formulation of Brownian motion allows to model this process by sampling changes in the velocity $Z_n$ from the normal distribution with mean zero and the variance given in Eq. (17.62). The walker's position $x(t)$ can then be obtained by approximating the velocity $v = \dot{x}$ with the help of finite difference derivatives, as described in Chap. 2. In conclusion we remark that although the LANGEVIN equation was introduced in a heuristic manner, it represents a very useful tool due to its rather simple interpretation.

Figure 17.4 presents three different realizations of the ORNSTEIN-UHLENBECK process based on three different initial velocities $v_0$. The corresponding random trajectories $x(t)$ of the Brownian particle are illustrated in Fig. 17.5.

## 17.4 Generalized Diffusion Models

We formulate now a very general approach to diffusive behavior which is based on continuous random variables. We start with the introduction of the pdf $\Lambda(x, t)$. Its purpose is to describe the event that a particle arrives at time $t$ at position $x$. It can be expressed as [20, 21]

$$\Lambda(x, t) = \int \mathrm{d}x \int_0^t \mathrm{d}t' \psi(x, t; x', t') \Lambda(x', t') , \tag{17.63}$$

where $\psi(x, t; x', t')$ is the *jump pdf*. We offer the following interpretation: $\psi(x, t; x', t')$ describes the probability for an event that a particle which arrived

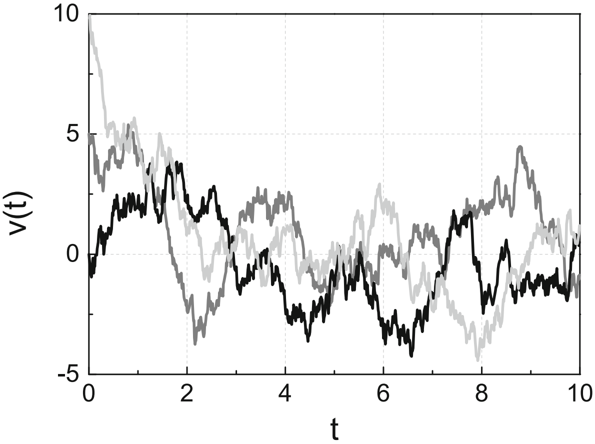


**Fig. 17.4** Three different realizations of the ORNSTEIN-UHLENBECK process $v(t)$ vs $t$. For this simulation we chose $\beta = 1$, $A = 5$, $\mathrm{d}t = 10^{-2}$ and $N = 10^3$ time steps. Furthermore, we chose three different initial velocities, i.e. $v_0 = 0$ (*black*), $v_0 = 5$ (*gray*) and $v_0 = 10$ (*light gray*)

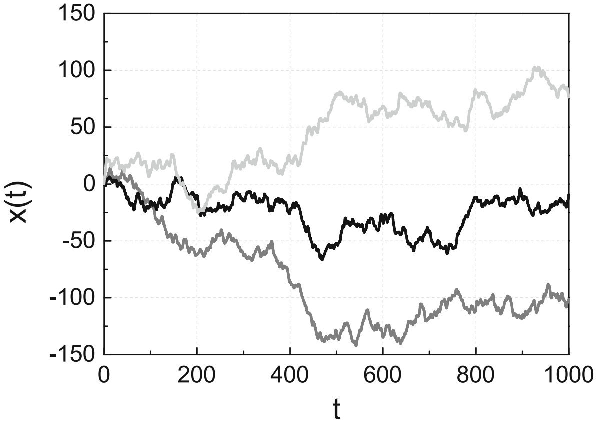


**Fig. 17.5** Random trajectories $x(t)$ vs $t$ of the Brownian particle which correspond to the velocities $v(t)$ illustrated in Fig. 17.4 with initial position $x_0 = 0$. Note that we used for this figure $N = 10^5$ time steps

at time $t'$ at position $x'$ – with pdf $\Lambda(x', t')$ – waited at position $x'$ until the time $t$ was reached and then jumped within an infinitesimal time interval from position $x'$ to $x$. If we regard a space and time homogeneous process then $\psi(x, t; x', t')$ is replaced by $\psi(x - x', t - t')$. This allows the introduction of a jump length pdf $p(x)$ and of a waiting time pdf $q(t)$. They are related to the jump pdf by

$$p(x) = \int_0^\infty \mathrm{d}t' \psi(x, t') \quad \text{and} \quad q(t) = \int_{-\infty}^\infty \mathrm{d}x' \psi(x', t) \ . \tag{17.64}$$

If the jump length pdf and the waiting time pdf are conditionally independent one can simply write $\psi(x,t) = p(x)q(t)$. The probability $\varphi(x,t)$ of finding a particle at position $x$ at time $t$ is, furthermore, given by

$$\varphi(x,t) = \int_0^t \mathrm{d}t' \Lambda(x,t')\Psi(t-t') \;, \tag{17.65}$$

where $\Psi(t)$ is the probability, that a particle stayed at least for a time interval $t$ at the same position, i.e.

$$\Psi(t) = 1 - \int_0^t \mathrm{d}t' q(t-t') \;. \tag{17.66}$$

Finally, the jump length variance $\sigma^2$ and the characteristic waiting time $\tau$ are given by

$$\sigma^2 = \int_{-\infty}^{\infty} \mathrm{d}x' x'^2 p(x') \quad \text{and} \quad \tau = \int_0^{\infty} \mathrm{d}t' t' q(t') \;. \tag{17.67}$$

We conclude from our discussion of the WIENER process that for Brownian motion the jump length pdf is a Gaussian and the waiting time pdf is an exponential distribution:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right) \quad \text{and} \quad q(t) = \frac{1}{\tau}\exp\left(-\frac{t}{\tau}\right) \;. \tag{17.68}$$

The characteristic function [Appendix Eq. (E.54)] of the waiting time pdf $q(t)$ is given by

$$\hat{q}(s) = \int_0^{\infty} \mathrm{d}t\, q(t) e^{-st} = \frac{1}{s\tau + 1} \;, \tag{17.69}$$

and we find for the jump length pdf $p(x)$:

$$\hat{p}(k) = \int \mathrm{d}x e^{-ikx} p(x) = \exp\left(-\sigma^2 k^2/2\right) \;. \tag{17.70}$$

For $x, t \to \infty$, i.e. $k, s \to 0$, the characteristic functions $\hat{q}(s)$ and $\hat{p}(k)$ develop the asymptotic behavior

$$\lim_{s\to 0} \frac{1}{1+s\tau} \approx 1 - s\tau + \mathscr{O}(s^2) \;, \tag{17.71}$$

and

$$\lim_{k \to 0} \exp\left(-\sigma^2 k^2/2\right) \approx 1 - \sigma^2 k^2/2 + \mathscr{O}(k^4) \; . \tag{17.72}$$

In fact, it can be shown that any pair of jump length and waiting time pdfs lead in first order to the same asymptotic behavior, namely $\mathscr{O}(\tau)$ and $\mathscr{O}(\sigma^2)$, as long as the moments $\tau$ and $\sigma^2$ exist.

However, there is a variety of processes which cannot be accounted for within the basic framework of Brownian motion. Such processes are described within the concept of anomalous diffusion [9, 20]. Examples are, for instance, the foraging behavior of spider monkeys, particle trajectories in a rotating flow, diffusion of proteins across cell membranes, diffusion of tracers in polymer-like breakable micelles, the traveling behavior of humans, charge carrier transport in disordered organic molecules, etc.

We concentrate now on two particular models of anomalous diffusion. The first model can, from a qualitative point of view, be characterized as a diffusion process which consists of small clustering jumps which are intersected by very long *flights*. Such behavior is, for instance, encountered in the context of human travel behavior, Fig. 17.6 [22], charge carrier transport in disordered solids, etc. The incorporation of these long jumps on a stochastic level is referred to as LÉVY *flight* [10]. The second model, which is referred to as the *fractal time random walk* incorporates

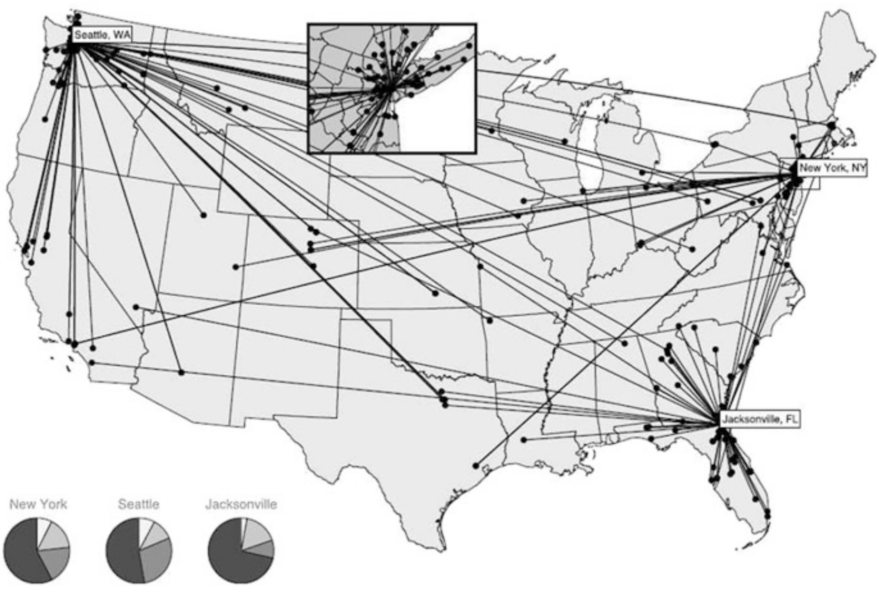


**Fig. 17.6** Traveling behavior of humans (Adapted from [22]. Copyright © 2006, Rights Managed by Nature Publishing Group)

anomalously long waiting times between two successive jumps. In particular, these long waiting times account for non-Markovian effects which could be due to, for instance, trapping processes of charge carriers in disordered solids. It has to be emphasized at this point that the resulting diffusion models are still linear in the pdf $\varphi(x, t)$. The inclusion of non-linear effects will not be discussed here, however, can be achieved within the framework of *non-extensive thermodynamics* [23].

Let us start with LÉVY flights. In this case one modifies the asymptotic behavior of the characteristic function of the jump length pdf according to

$$\hat{p}(k) \propto 1 - (\sigma |k|)^{\alpha} , \tag{17.73}$$

where $\alpha \in (0, 2]$. We recognize that this is the asymptotic behavior $|k| \to 0$ of the characteristic function of a symmetric LÉVY $\alpha$-stable distribution [19] following Appendix Eq. (E.69). In the limit $\alpha \to 2$ normal, Gaussian behavior is recovered. According to Appendix Eq. (E.70) the characteristic function (17.73) corresponds to a jump length pdf:

$$p(x) \propto |x|^{-\alpha-1} \qquad \text{for} \qquad |x| \to \infty . \tag{17.74}$$

It is commonly referred to as a *fat-tailed jump length pdf* because of its asymptotic behavior.

A LÉVY flight is, in principle, a random walk where the length of the jumps at discrete time instances $t_n$ follow the pdf (17.74). In the continuous time limit, the waiting times are distributed exponentially as was illustrated in Sect. 16.5. It has to be noted that in such a case the jump length variance diverges, i.e. $\Sigma^2 \to \infty$. Consequently, LÉVY $\alpha$-stable distributions are *not* subject to the central limit theorem (see Appendix, Sect. E.8). In particular, the distance from the origin after some finite time $t$ follows a LÉVY $\alpha$-stable distribution. Moreover, we note that if $0 < \alpha < 1$ even the mean jump length $\langle x \rangle$ diverges. A detailed mathematical analysis proves, that Lévy flights result in a diffusion equation of the form

$$\frac{\partial}{\partial t} p(x, t) = D_{\alpha} \mathscr{D}^{\alpha}_{|x|} p(x, t) , \tag{17.75}$$

where $D_\alpha$ is the fractional diffusion coefficient of dimension length$^\alpha \times$ time$^{-1}$ and $\mathscr{D}^{\alpha}_{|x|}$ is the symmetric RIESZ fractional derivative operator of order $\alpha \in (1, 2)$[6]:

$$\mathscr{D}^{\alpha}_{|x|} f(x) = \frac{1}{2\Gamma(2-\alpha)\cos\left(\frac{\alpha\pi}{2}\right)} \int \mathrm{d}x' \frac{f''(x')}{|x - x'|^{\alpha-1}} , \tag{17.76}$$

where $f''(x)$ is the second spatial derivative of $f$.

[6] A short introduction to fractional derivatives and integrals can be found in Appendix G.

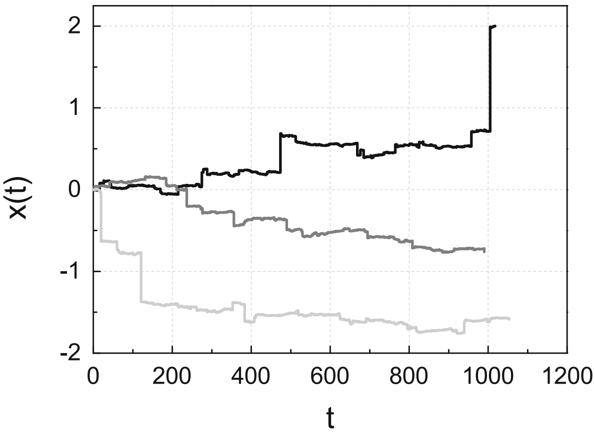


**Fig. 17.7** Three different realizations of the one dimensional Lévy flight. The parameters are $\ell = 0.001$, $\alpha = 1.3$ and we performed $N = 1000$ time steps

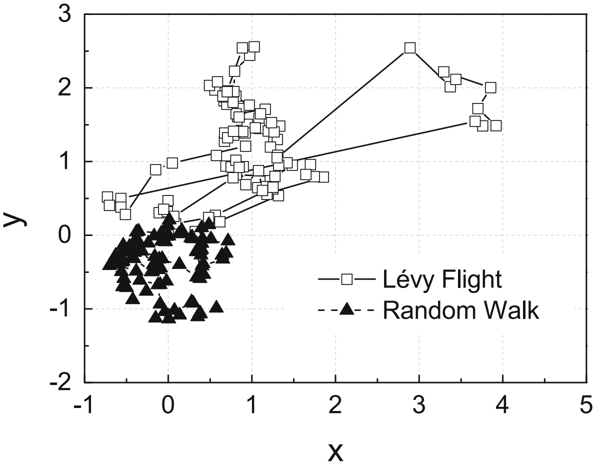


**Fig. 17.8** Comparison between the two-dimensional WIENER process (*solid up-triangles*) and the two-dimensional LÉVY flight (*open squares*) for $\alpha = 1.3$. The minimal flight length of the LÉVY flight as well as the jump length variance of the WIENER process were set $\ell = \Sigma^2 = 0.1$ and we performed $N = 100$ time steps

Figure 17.7 illustrates a one-dimensional LÉVY flight and Fig. 17.8 presents a comparison between a two-dimensional LÉVY flight and a two-dimensional WIENER process. These figures were generated by sampling an exponential distribution with mean $\langle t \rangle = 1$ for the waiting times. On the other hand a jump length pdf

$$p(x) = \alpha \ell^{\alpha} \frac{\Theta(x - \ell)}{x^{\alpha+1}} , \quad x > 0 . \tag{17.77}$$

was sampled for the jump length of the LÉVY flight. Here $\alpha$ is referred to as the LÉVY index, $\Theta(\cdot)$ denotes the HEAVISIDE $\Theta$ function and $\ell > 0$ is the *minimal flight length*. We introduced this particular form of the pdf because it can rather easily be sampled with the help of the inverse transformation method – Sect. 13.2 – and it obeys the asymptotic behavior, Eq. (17.74). Moreover, it can be proved that it gives the correct behavior in the limit $\ell \to 0$. Finally, the direction of the jump has to be sampled in an additional step. Figure 17.8 is particularly instructive because the different physics described by these two models becomes immediately apparent.

Let us turn our attention to the second scenario, the fractal time random walk. In this case the asymptotic behavior of the waiting time pdf is modified according to

$$\hat{q}(s) \propto 1 - (Ts)^\beta \ , \tag{17.78}$$

where $\beta \in (0, 1]$ and for $\beta \to 1$ regular behavior, an exponentially distributed waiting time, is recovered. A pdf of such a form is commonly referred to as a *fat-tailed waiting time pdf*. After an inverse LAPLACE transform we obtain

$$q(t) \propto t^{-\beta-1} \quad \text{for} \quad t \to \infty \ . \tag{17.79}$$

We note that in this case the mean waiting time $T = \langle t \rangle$ diverges for $\beta < 1$. This clearly indicates a non-Markovian time evolution since we demonstrated in Sect. 16.5 that every Markovian discrete time process converges in the continuous time limit to a process with exponentially distributed waiting times. Again, the ansatz

$$q(t) = \beta \tau^\beta \frac{\Theta(t-\tau)}{t^{\beta+1}} \ , \tag{17.80}$$

is employed, where $\tau > 0$ is the *minimal waiting time*. The process is essentially a random walk with waiting times distributed according to Eq. (17.80), i.e. the jump length $\Delta x$ is constant. In the continuous space limit $\Delta x \to 0$ the jump lengths follow a Gaussian, as in the case of a regular random walk. A detailed analysis proves that in the limit $\tau \to 0$ the corresponding diffusion equation is given by

$$^C D_t^\beta p(x,t) = D_\beta \frac{\partial^2}{\partial x^2} p(x,t) \ , \tag{17.81}$$

where the diffusion constant $D_\beta$ is of dimension length$^2\times$ time$^{-\beta}$. Here, $^C D_t^\beta$ is the CAPUTO fractional time derivative of order $\beta \in (0, 1)$ (see Appendix G). It is of the form

$$^C D_t^\beta f(t) = \frac{1}{\Gamma(1-\beta)} \int_0^t \mathrm{d}t' \frac{\dot{f}(t')}{(t-t')^\beta} \ . \tag{17.82}$$

It follows from the properties of fractional derivatives that an alternative form of Eq. (17.81) can be found, namely

$$\frac{\partial}{\partial t} p(x,t) = D_\beta \frac{\partial^2}{\partial x^2} D_t^\beta p(x,t) \ , \tag{17.83}$$

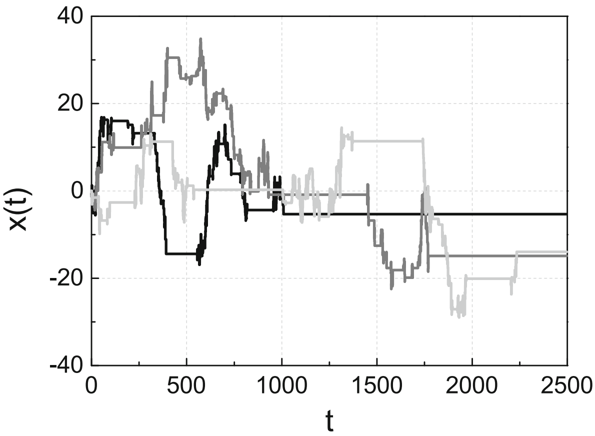


**Fig. 17.9** Three different realizations of the fractal time random walk in one dimension for $\beta = 0.8$ and $\tau = 0.1$

where $D_t^\beta$ is the RIEMANN-LIOUVILLE fractional derivative of order $\beta$ (see Appendix G).

Figure 17.9 presents three different realizations of the fractal time random walk. The waiting times were sampled from the pdf (17.80) with the help of the inverse transformation method – Sect. 13.2 – and the jump lengths were sampled from a normal distribution with jump length variance $\Sigma^2 = 1$.

It is a straight-forward task to combine fractal time random walks and LÉVY flights to so called *fractal time* LÉVY *flights*. The resulting diffusion equation can be written as

$$ {}^C D_t^\beta p(x,t) = D_{\alpha\beta} \mathscr{D}_{|x|}^\alpha p(x,t) \;, \tag{17.84} $$

where the diffusion constant $D_{\alpha\beta}$ has units length$^\alpha \times$ time$^{-\beta}$ and ${}^C D_t^\beta$ and $\mathscr{D}_{|x|}^\alpha$ are the fractional CAPUTO and RIESZ derivatives, respectively.

Figure 17.10 illustrates three different realizations of such a diffusion process. The waiting times were sampled from the pdf (17.80) where we set $\tau = 0.1$ and $\beta = 0.8$. The jump lengths were sampled from the pdf (17.77) with $\alpha = 1.3$ and $\ell = 0.01$. Finally, the direction of the jump was sampled in an additional step.

We close this chapter with a short discussion: The description of diffusion processes with the help of stochastics proofed to be one of the most powerful methods in modern theoretical physics. Within this chapter we discussed several different paths toward a description of Brownian motion, namely the random walk, the WIENER process, and the LANGEVIN equation, as well as models which describe phenomena beyond Brownian motion. It has to be emphasized that the field of anomalous diffusion in general is still developing rapidly, however, its importance for the description of various phenomena in science is already impressive. We refer the interested reader to the excellent review articles by R. METZLER and J. KLAFTER on anomalous diffusion [20, 21].

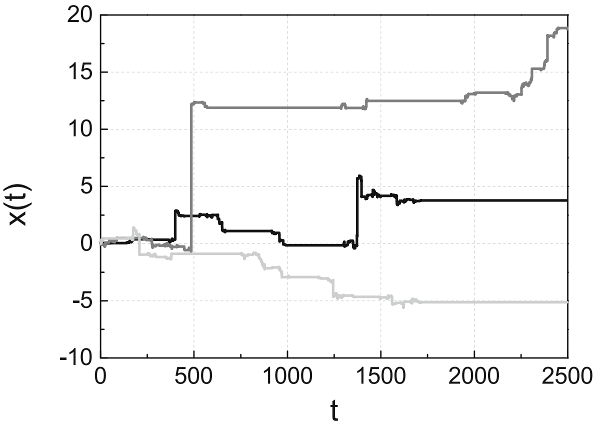


**Fig. 17.10** Three possible realizations of the fractal time LÉVY flight in one dimension. The parameters are $\tau = 0.1$, $\beta = 0.8$, $\ell = 0.01$ and $\alpha = 1.3$

## Summary

The random walk, a classical example of MARKOV-chains, was used to open the door to the realm of diffusion theory. Random walks have been used for a long time to simulate Brownian motion and related problems. From a theoretical point of view random walks were described by the scaling limit of the WIENER process. The biased WIENER process was then used to demonstrate that the FOKKER-PLANCK equation followed in the limit of a continuous state space, as the classical diffusion equation followed from the unbiased WIENER process in the same limit. Brownian motion was also the basis for the rather heuristic introduction of the stochastic differential equation by LANGEVIN. A direct consequence of this equation was the ORNSTEIN-UHLENBECK process with its master equation, the FOKKER-PLANCK equation. It was the only stationary, Gaussian, and Markovian process in this class of stochastic diffusion processes. An extension of these processes was then possible by the introduction of a jump pdf which in turn allowed to define a jump length pdf and a waiting time pdf. These two pdfs resulted in a more general description of diffusion processes in a space and time homogeneous environment. Furthermore, the observation that many diffusive processes (not only in physics) cannot be understood within the framework of 'classical' Brownian motion resulted in the introduction of LÉVY flights. This was particularly motivated by the need for a process whose jump-length variance diverges which enabled, for instance the simulation of human travel behavior. In the very last step the fractal time random walk was introduced. It was characterized by a specific form of the waiting time pdf which made it possible to describe on a stochastic level anomalously long waiting times between two consecutive jumps. Such behavior can, for instance, be observed by trapping phenomena in solids. The combination of both extensions resulted in the fractal time LÉVY flight.

## Problems

1. Write a program which simulates different realizations of the following stochastic processes in one spatial dimension:
   a. A random walk.
   b. A standard WIENER process and a WIENER process with drift.
   c. An OHRNSTEIN-UHLENBECK process.
   d. A LÉVY flight.
   e. A fractal time random walk.
   f. A fractal time LÉVY flight.

   Illustrate three different sample paths graphically for each process. Furthermore, perform the following tests:
   a. Calculate the expectation value $\langle x_n \rangle$ and the variance $\text{var}(x_n)$ of the random walk numerically by restarting the process several times with different seeds.
   b. In a similar fashion, calculate numerically $\langle W_t \rangle$ and $\text{var}(W_t)$.
   c. Try different parameters $\alpha, \beta$ for LÉVY flights and fractal time random walks.
2. Write a program which simulates the WIENER process in two dimensions. This can be achieved by drawing the jump length from a normal distribution and sampling the *jump angle*, i.e. the direction, in an additional step. Augment this program with LÉVY flight jump lengths pdfs.

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