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POSTGRADUATE SCHOOL FOR SCIENCES, TECHNOLOGY AND GEOSCIENCES
Laboratory of Mechanics, Materials and Structures

RESIDENCE TIME OF RANDOM ACCELERATION PROCESSES

THESIS
Submitted in Partial Fulfillment of the Requirements for the award of the Degree of Doctorat/Ph.D in Physics

Par : **OUANDJI BOUTCHENG Hermann Joël**
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Nous, Professeur **PELAP François Beceau** et Professeur **WOAFO Paul**, respectivement Examinateur et Président du jury de la Thèse de Doctorat/Ph.D de Monsieur **OUANDJI BOUTCHENG Hermann Joël**, Matricule **02Y248**, préparée sous la direction du Professeur **BOUETOU BOUETOU Thomas** et du Directeur de Recherche **Alberto ROSSO** avec la supervision du Professeur **KOFANE Timoléon Crépin**, intitulée : « **RESIDENCE TIME OF RANDOM ACCELERATION PROCESSES** », soutenue le **Vendredi, 25 Mai 2018**, en vue de l'obtention du grade de Docteur/Ph.D en Physique, Spécialité **Mécanique, Matériaux et Structures**, Option **Mécanique Fondamentale et Systèmes Complexes**, attestons que toutes les corrections demandées par le jury de soutenance ont été effectuées.

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Submitted in Partial Fulfillment of the Requirements for the award of the

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Dedications

This thesis is dedicated

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Abstract

In this thesis, we consider the random acceleration model, which represents possibly one of the simplest non-Markovian stochastic systems and which has been widely studied in connection with applications in Physics and Mathematics. The residence time $T_A(t|x_0, v_0)$ of the random acceleration model, spent within a region A by the particle when observed up to a time t, and their related properties, which are non-trivial and not yet completely understood, has been well characterized. So to speak, we started by the definition of the moment generating function. From the Taylor expression of the generating function, we establish the backward Fokker-Planck equation for the moment and, by using particularly the free propagator or the Green function in absence of the boundaries, we obtain analytically the first two moments of the residence time T_+, and also study the statistics of T_+ with Monte Carlo simulations. Our goal is to ascertain whether the residence time T_+ and the time T_m, at which the maximum of the process is attained, are statistically equivalent. For regular Brownian motion, the distributions of T_+ and T_m coincide and are given by Lévy's arcsine law. We show that, for randomly accelerated motion, the distributions of T_+ and T_m are quite similar but not identical.

Keywords: Random Walk, Normal diffusion, Anomalous diffusion, Continuous Time Random Walk, Diffusion Equation, Fokker-Planck Equation, Time Maximum, Residence Time, Non-Markov Process.

Résumé

Dans cette thèse, nous considérons le modèle d'accélération aléatoire, qui représente probablement un des systèmes stochastiques non-Markoviens les plus simples et qui a été largement étudié en liaison avec des applications en Physique et en Mathématique. Le temps de séjour $T_A(t|x_0, v_0)$ du modèle d'accélération aléatoire, passé dans une région A par la particule lorsqu'elle est observée jusqu'à un instant t, et leurs propriétés relatives, qui sont non triviaux et pas encore comprises, a été bien caractérisé. Tel que parlé, nous débutons par la définition du moment de la fonction génératrice. De l'expression de Taylor, nous établissons l'équation de Fokker-Planck pour les moments et, en utilisant particulièrement le propagateur libre ou la fonction de Green en l'absence des limites, nous obtenons analytiquement les deux premiers moments du temps de séjour T_+, puis par une simulation numérique à partir d'une approche de la méthode Monte Carlo étudions aussi la statistique de T_+. Notre objectif est de s'assurer si le temps de séjour T_+ et le temps T_m ,temps auquel le maximum du processus est atteint, sont statistiquement équivalent. Pour un mouvement Brownien regulier, les distributions de T_+ et T_m coincident et sont données par la loi arcsinus de Lévy. Nous montrons que, pour le mouvement aléatoirement accéléré, les distributions de T_+ et T_m sont qualitativement équivalent mais avec une légère différence sur le plan quantitatif.

Mots clés: Marche aléatoire, Diffusion normale, Diffusion anormale, Temps continue d'une marche alétoire, Equation de dffusion, Equation de Fokker-Planck, Temps maximal, Temps de séjour, Processus non-Markovien

General Introduction

Statistical physics is a branch of physics that uses methods of probability theory and statistics, and particularly the mathematical tools for dealing with large populations and approximations, in solving physical problems. It can describe a wide variety of fields with an inherently stochastic nature [1]. It is a relatively old discipline. Founded in the second half of the nineteenth century(Clausius, Maxwell, Boltzmann and Gibbs), then fertilized by the development of quantum mechanics in the first half of the twentieth century, it is one of the most important physical theoretical frameworks. The objective of statistical physics is to establish the relationships between macroscopic variables, from the equations that govern the behavior of matter at the microscopic scale. It focuses on the study of systems with very large number of degrees of freedom [2]. It is intended to describe the best system properties that the physicist does not control absolutely. This discipline links microscopic physics, which provides access to the detailed description of the physical system and macroscopic physics, where no one of them characterizes the state of the system considered by average properties [3]. The paradigm of the approach from statistical physics is at the foundations of physical chemistry (applied to a macroscopic system), especially of thermodynamics in terms of elementary mechanics. It must also be known that statistical physics aims at describing evolving systems: motion of a particle in a fluid, progress of a chemical reaction, etc [1, 3].

Its development has been accompanied by major advances in mathematics (probabilities, random processes, dynamical systems, ergodic theory), general physics (validation of the atomic hypothesis) and instrumentation. .

One distinguishes equilibrium statistical physics (thermodynamics sense) from nonequilibrium statistical physics. The development of statistical physics describing situations at equilibrium is based on principles of universal significance such as the fundamental postulate of statistical physics, etc. These allow one to develop a clear framework (Ensemble of statistical physics: microcanonical, canonical, etc.), the concrete study of a problem requiring, in principle, only to trigger a proven mechanics, i.e. calculate the appropriate generating function such as entropy, free energy (partition function), etc. The study of the nonequilibrium situation is clearly less well marked, which reflects the greater richness of the dynamic aspects and a relative lack of universality. A wide variety of approaches are

generally proposed (Langevin approach, master equation, Fokker-Planck equation, etc.), whose relations among them are not obvious a priori. These approaches provide tools for analyzing the statistical properties of physical quantities seen as random processes, i.e. their temporal structure.

The physical mechanisms associated with nonequilibrium situations are known as transport phenomena. As in the case of equilibrium systems physics, the laws regulating transport phenomena were first established [3] (often empirically) within a macroscopic framework: an example is the Fick's law which gives the flow of matter, Γ, due to the existence of a concentration gradient, n as illustrated below:

$$\Gamma = -\mathcal{D}\frac{\partial n}{\partial x}, \tag{1}$$

where $\mathcal{D}$ is the transport coefficient.This law can be applied to the diffusion of a gas.

Statistical equilibrium physics gives the probability of observing a given macroscopic state for a system. Here, a question is how a system, initially in a particular state, evolves towards equilibrium. An alternative question is that of equilibrium correlations: which correlation then exists, between the state of the system, at a given time and its state at a later moment [3, 4]?

Answering these questions requires the introduction of a dynamic for the system, i.e a law of evolution. This law must naturally be compatible with the probability distribution at equilibrium. In particular, it can not be deterministic, in which case the probability distribution would always be concentrated on a single state. This dynamics must contain a random or stochastic part. To describe the temporal evolution of a nonequilibrium system obeying a Markovian dynamics, we need to determine the probability laws. Combining temporal evolution and probabilities yield stochastic processes.

Indeed, stochastic processes or random processes are any phenomenon evolving in time whose analysis can be subjected to the calculation of probabilities. From the point of view of observation, a stochastic process is constituted by all its realizations. A realization is obtained by an experiment which consists in recording a sequence of events over time. The randomness of the evolution showing itself by the fact that the repetition of the experiment leads to another temporal sequence.

Stochastic processes are found in daily life and for this reason their quantitative study has constantly attracted interest of scientists from various disciplines. Nowadays, the theoretical study of stochastic processes forms an integral part of the mathematical statistics which can be seen as the frontier of several disciplines. There are many applications of the stochastic processes, particularly in biology (evolution genetics and population genetics) [5–7], in medicine (growth of the tumours, epidemic) [7, 8], in engineering (administration of the networks, Internet, telecommunications) [9, 11–13], in economy (stock exchange) [14], finance [15, 16], and statistical physics (the ferromagnetism, transitions from phase, etc).

The purpose of the theoretical study of stochastic processes is the modeling of the phenomenon starting from experimental observations or numerical results. The first theoretical studies of the evolution laws of distributions had been undertaken starting from

the Fokker-Planck equation [17–22]. In other words, the process can be seen as normal diffusion in presence possibly of external forces [1] [23–26]; but some time, the experimental study of certain stochastic phenomena revealed an anomaly in their density probabilities, which appear especially in the quadratic behavior and which is no longer a linear function of time [27–30]. This anomaly characterizes the anomalous diffusion. Let us note that the anomalous diffusion is a random walk characterized by an average quadratic displacement which grows with time with a larger exponent (superdiffusion) or smaller (subdiffusion) than 1. There are essentially three possible reasons at the origin of this behavior:

(i) The jumps of the walker are strongly correlated [2].

(ii) The walker can make great jumps [3].

(iii) The medium is heterogeneous [4].

In spite of the large number of situations, where anomalous diffusion is observed, there is not a unified description of non-Brownian physics. Often, in front of a concrete question, even if one identifies the relevant stochastic process (fractional Brownian movement for (i), Lévy's flight for (ii), and continuous time random walk(CTRW) for (iii)) [31–33], it is very difficult to make the necessary calculations to answer this question.

A significant example of anomalous diffusion (quadratic displacement grows like $x^2(t) \sim t^3$) is the random acceleration process, which is a non-Markovian stochastic process [5] [34]. This process evolves via the stochastic differential equation

$$\ddot{x}(t) = \eta(t), \tag{2}$$

where we suppose that the terms of dissipation can be considered as stochastic forces; $\eta(t)$ being a Gaussian white noise, with $< \eta(t) >= 0$, and $< \eta(t)\eta(t') >= 2D\delta(t - t')$.

Stochastic differential equation is a generalization of the concept of differential equation taking into account terms of white noise; this evolutionary equation can be obtained in the deterministic case from the dynamic laws (classical or quantum) governing the displacement of a Brownian particle under the effect of its collisions with the particles of the fluid.

Indeed, let a Brownian particle subjected to a succession of molecular impacts from which the force resulting at the time t is noted $\mathcal{F}(t)$. This force does not depend explicitly on time, if the external medium is at equilibrium but implicitly by the co-ordinate and the speed of the large particle and those of small particles of the bath.

[1] the Langevin model

[2] for example the movement of a fluorescent monomer is subdiffusive because of the interaction with the other monomers

[3] for example financial markets

[4] for example propagation of the contaminants in porous environments

[5] the term 'non-Markovian process' covers all random process with the exception of the very small minority that happens to have the Markov property

By simplifying to one dimension, one locates the position of the particle by a $x-$ *coordinate* x. In addition to the resultant force or call it the fluctuating force due to the action of the medium and characterizing the effect of the fluid acting on the particle of mass m, there may exist a well-defined external force noted F_{ext}, which is for example an electric field. In these conditions, the fundamental equation of the dynamics for a particle is written as:

$$m = \frac{d^2x}{dt^2} = F_{ext} + \mathcal{F}(t). \tag{3}$$

The force $\mathcal{F}(t)$ cannot be physically reduced to a single erratic component: the effect of the bath is not only to create disordered movements for the Brownian particle but also to slow it down. The action of the entire bath contained in $F(t)$ must also result in a frictional force.

This analysis suggests thus the replacement of the equation (3) by the following equation:

$$m = \frac{d^2x}{dt^2} = F_{ext} + \mathcal{F}(t) - m\alpha v, \tag{4}$$

where α is the friction's coefficient and $v = dx/dt$ is the velocity of the particle.

If there is no position-dependent applied external force, the Brownian particle is said to be "free" and the equation of motion for the free Brownian particle is given by the Newton's law:

$$m = \frac{d^2x}{dt^2} = -m\alpha v + \mathcal{F}(t), \tag{5}$$

or, equivalently

$$m = \frac{dv}{dt} = -m\alpha v + \mathcal{F}(t), \;\; v = \frac{dx}{dt} \tag{6}$$

The equation under the forms (5), (6) is historically the first example of a stochastic differential equation (called Langevin equation) i.e. which depends on the random variables.

Let us note at the viscous limit ("overdamped") or at the limit of great friction (alternatively at the limit of long times) ($F_{ext} = 0$), $m \to 0$, $\alpha \to \infty$, the degrees of freedom of velocity have been relaxed, and the term of inertia becomes negligible. Then, the Langevin equation of the movement becomes:

$$m\alpha = \frac{dx}{dt} = \mathcal{F}(t). \tag{7}$$

In the Langevin equation for Brownian motion (sometimes called the Ornstein-Uhlenbeck process), there is a damping force in addition to a random force. It is a different, more complicated process, than the random acceleration process.

In the random acceleration process, by definition, there is no damping term. The position $x(t)$ in the random acceleration process corresponds to the integral of $v(t)$, which evolves according to a random walk. Let us consider a point particle; in the random acceleration process, this point particle is subjected to none impacts molecular nor with

any phenomenon of diffusion i.e. which moves freely according to the x axis and is subjected to the random force $F(t) \equiv \eta(t)$, in the form of Gaussian white noise. The Newtonian equation of motion of this point particle is:

$$\frac{d^2x}{dt^2} = \eta(t), \quad or \tag{8}$$

$$\frac{dv}{dt} = \eta(t). \tag{9}$$

which is a differential stochastic equation. According to equation (9), the velocity $v = dx/dt$ performs a random walk.

Thus

$$\frac{dx}{dt} = v, \tag{10}$$

$$\frac{dv}{dt} = \eta(t). \tag{11}$$

is the coupled evolution equations of the randomly accelerated particle.

A variety of systems in physics, in the life and social sciences, and in engineering can be modeled in terms of particles traveling in a host medium, which randomly changes their state (position, direction, energy, etc) in collisions with other particles or with the medium itself. The nature of the randomness may vary widely from one system to another. It may result either from the intrinsic stochastic nature of the underlying process or from uncertainty [35]. Some transport phenomena, while originating in deterministic and reversible events, can in practice only be described by resorting to the laws of probability.

A prominent example of such a stochastic system is the random acceleration model, which has been studied in connection with applications in physics and mathematics. In physics, for example, it appears in the continuum description of the equilibrium Boltzmann weight of a semiflexible polymer chain, with non zero bending energy [36]. It can also describe the steady state profile of a $(1+1)$-dimensional Gaussian interface [37], with dynamical exponent $z = 4$, and the continuum version of the Golubovic-Bruinsma-Das Sarma-Tamborenea model [38]. In addition, the random acceleration process arises in the description of the statistical properties of the Burgers equation with Brownian initial velocity [39]. The random acceleration process is related to the statistics of semiflexible polymers [36] and also plays a role in other physical applications [40,41]. The random acceleration model is a non-trivial, non-Markov model, which is both relevant to real-world applications and simple enough so that it can be studied analytically. The first-passage properties and related properties have been investigated extensively over the last few decades [36, 37, 42]. Recently, the extreme-value statistics of the process was analyzed, with special emphasis on the global maximum in a given time interval [37, 43, 44] and the time at which the global maximum is reached [45]. The residence time in stochastic systems was first considered by mathematicians [46–48] and has more recently been investigated in physical systems with continuous degrees of freedom and in connection with

persistence (see [49, 50]). The residence time, also usually called occupation times,has been extensively studied since the seminal work of Lévy and his arcsine law giving the residence time of a Brownian particle on an infinite line [51]. In the literature, the residence time statistics of the random acceleration model has attracted considerable interest as a tool describing nonequilibrium phenomena [52]. Recently, the study of time at which the maximun of the random acceleration process is reached, has naturally led to a curious observation, where from a numerical evidence made by Rosso et al [45], has shown that unlike in the Brownian case, the two distributions $P(t_m|T)$ and $P(t_{occup}|T)$ (t_{occup} represents the occupation time) are different in the random acceleration process. This curious observation naturally led to calculations of residence time statistic, of the random acceleration model that we will carry out throughout this thesis. By definition, the residence time T_+ denotes time at which the process spends on the positive half axis within the interval $[0, T]$. T_+ can also denote the length of time for which the process is greater than a fixed value α and/or less than a fixed value β. Let us consider a general stochastic process $x(t)$ or $X(t)$; starting from $x(0) = 0$, over a fixed time interval $[0, T]$. Clearly, T_+ is a random variable that fluctuates from one realization of the process to another. The question of determining the residence time arises in many fields:

- In the context of finance, $x(t)$ may be the price of a stock which obeys the stochastic differential equation, and one may be interested in T_+ for which the stock price is a given interval $[\alpha, \beta]$.

- In the context of queueing theory, the stochastic process $x(t)$ may represent the length of a queue at time t, and one would like to know T_+, i.e the time spent by an individual in a queue.

- In the context of biology, $x(t)$ may represent a bacterial population at time t, and one would like to know the time T_+, i.e the time spent by a bacteria in a given bacterial culture medium to multiply or to die.

However, it should also be noted that the residence time and related properties are non trivial and not yet completely understood. In this thesis, we consider a randomly accelerated particle moving in one dimension on the infinite x axis and study the residence time T_+ on the positive x axis. We calculate the first two moments of T_+ analytically and also study the statistics of T_+ with Monte Carlo simulations. One of our aims is to study whether the residence time T_+ of the randomly accelerated particle and the time T_m, at which it attains its maximum displacement, are statistically equivalent. Both our analytical and Monte Carlo results indicate that this is not the case. This is in contrast with regular Brownian motion, where the distributions of T_+ and T_m coincide and are given by Lévy's celebrated arcsine law [46, 53]. Also, we aim by this contribution an essential objective. This objective is to increase the existing literature with this original problem, on the basis of the Fokker-Planck equation and on the average residence time. We find the Green function or the free propagator in the most general case; which is the essential tool to carry out our analytical calculations on the residence time. Taking into account the fact that this Green function was calculated analytically by Burkhardt [36] in the simplest case, we use the Monte Carlo method to check numerically the agreement

with the analytical result.

This thesis is structured as follows:

In Chapter 1 we carry out a literature review on Statistical Physics of the irreversible Processes. The generalities on the irreversible process will be presented in the literature review where we will focus on the concepts of the stochastic processes, Markov processes, Brownian motion and random walks. An interest will be devoted to the anomalous diffusion [54–57], to the polymer translocation and fractional Brownian motion [58,59]; we will be also interested in the random acceleration model more particularly on works by Rosso et al [45], where they calculated time at which the maximum of a random acceleration process is reached. And on the basis of their numerical evidence, they concluded that the distribution of the occupation time does not agree with their result for the distribution of the time maximum from which is born the problem which is the subject of our thesis: the residence time of a random acceleration process.

In Chapter 2, devoted to methodology, we report various methods (analytical and numerical) used to solve our problem, knowing the residence time . As analytical method, we present the fundamental equations allowing us to describe the evolution of the laws of probabilities relating to a Markovian random process starting from the Fokker-Planck equation. As numerical method, we present the Monte Carlo method.

Chapter 3 concentrates on results and discussions, we derive partial differential equations which determine the moment generating function and the moments of the residence time. We calculate explicitly the first two moments of the residence time T_+ and compare with the corresponding moments of the time T_m at which the randomly accelerated particle makes its maximum excursion. Still in this chapter, we study the moments of T_+ and its distribution with Monte Carlo simulations and compare the results with our analytic predictions for the first two moments of T_+ and with exact results for the distribution of T_m. Some technical details about the computation of the ïňĄrst two moments of T_+ are given in the appendix.

Chapter 1

LITERATURE REVIEW ON STATISTICAL PHYSICS OF THE IRREVERSIBLE PROCESSES

Contents

1.1 Introduction

In this chapter, our aim is to introduce the main concepts and fundamental notions on the stochastic processes, normal and anomalous diffusions. One qualifies stochastic process any phenomenon of temporal evolution, whose analysis can be subjected to the theory of probabilities. From the view point of the observation, a stochastic process is considered by the set of its realizations. A realization is obtained by the experiment which consists in recording a continuation of event in the course of time.

The erratic nature and non reproducible of the realizations of the process is owing the fact that their evolution is in general the result of unverifiable agents, or of which the effect is even unknown. The Brownian particle moves under the effect of its collisions with the particle of the fluid: the dynamics laws controlling the latter (classic or quantum) are known. In this case, one could in principle establish the bond between the Brownian motion and subjacent microscopic dynamics but the complexity of the description of these microscopic movements defies the analysis. In the case of the stock exchange fluctuations we realize that it is illusory to make go up the theory with the description of the physico-chemical state of the brains of the operators.

The remarkable fact is that in spite of these multiple random agents, the statistics of the process(mean value, standard deviation,...) obey simple and reproducible laws in the course of time, provided that one analyzes it on scales of suitable times. The theory of the stochastic processes thus endeavours to formulate models of evolution, where the lack of information east compensates by adequate probabilistic assumptions. The situation although much richer in its fields of application, is similar to that of the statistical mechanics of the equilibrium: the assumption of the statistical sets(microcanonical, canonical,...) makes it possible to describe the macroscopic observations of thermodynamics which are, perfectly regular and reproducible [60].

Many good physical phenomena are described by the evolution of one or several sizes in the course of time. At a given moment, these sizes often present a character unforeseeable, random, and it is then natural to represent them by a random variable. The evolution of the phenomenon is then described by the whole. It is described then by the set of the random variables modelling the phenomenon at every moment. This whole of random variables forms a stochastic or random process.

Thus, a stochastic process is a collection of random variables indexed by a parameter.

This can represent time, discrete or continuous or a variable of space. The knowledge of the relations between these random variables, when the parameter varies, makes it possible to obtain interesting properties, which characterize the evolution of the phenomenon.

The applications of the stochastic processes are very numerous. Those are in particular used by the engineers for the construction of the mathematical models of many phenomena. We can quote, for example:

- The economic theory and the econometric whose objectives are to account for the mechanisms which govern the economic facts (often random). The theory of the forecast, which gathers the whole of the methods making it possible to give an estimate (probabilistic) of the evolution of an economic variable, starting from data on its values passed, uses the stochastic processes. One speaks in this case about statistics or stochastic processes.
- Transport and the traffic, which are about transport of people, goods or traffic in the networks (telephone, mobile, Internet).
- The reliability of the systems or a material i.e. evolution in the time of its failures.
- Financial engineering, where the financial models utilize complex concepts of process and stochastic calculations.
- The filtering and information theory.
- Sciences of the environment.

Therefore this chapter is organised as follows. Firstly, the section 1.2 is devoted to the stochastic process. Next section 1.4 is devoted the normal diffusion. Then, the section 1.5 is introduce the anomalous diffusion; after that the section 1.7, is devoted to Continuous Time Random Walk, and finally, section 1.8 presents the random acceleration model.

1.2 Stochastic processes

1.2.1 Absolute and conditional probabilities

The probability of an event is a numerical value which represents the proportion of time, where the event will be carried out, when one repeats the experiment under identical conditions. We can deduce from this definition which a probability must be between 0 and 1 and which probability of one event [1] is the sum of the probabilities of each elementary events which constitutes it. Lastly, the sum of the probabilities of all the elements of Ω is 1.

Definition 1.1 (Probability) A probability (or a measurement of probability) is a function $\mathbb{P}$ of the set of the events $\mathcal{F}$ towards [0, 1] such as:

[1] Let us recall that an event is nothing other than part of Ω.

- $\mathbb{P}(\Omega) = 1$ and $\mathbb{P}(\varnothing) = 0$.
- If $(A_i, i \in I)$ is a finished or countable collection of events $A_i \in \mathcal{F}$ for all $i \in I$ disjoined two to two; then:

$$\mathbb{P}\left(\bigcup_{i\in I} A_i\right) = \sum_{i\in I} \mathbb{P}(A_i). \tag{1.1}$$

This property is called $\sigma - additivity$ (we can talk about additivity if the whole of indices I is finished).

The triplet $(\Omega, \mathcal{F}, \mathbb{P})$ is called probabilized space or space probabilities. It is said that the event A is almost sure (noted a.s) if $\mathbb{P}(A) = 1$. We can also say that the event A is negligible if $\mathbb{P} = 0$.

Let us consider n intervals $I_j = [x_j, x_j + dx_j]$, $j = 1, \ldots, n$, $n = 1, 2, \ldots$. We define the probability distributions joined of the process by:

$$\begin{aligned} W(x_1, t_1; ...; x_n, t_n)dx_1...dx_n &= probability\ \ of\ \ finding\ \ x(t_1) \in I_1, \ldots, x(t_n) \in I_n \\ &= \frac{numbers\ of\ realizations\ which\ pass\ in\ I_1, \ldots, I_n}{total\ \ numbers\ \ of\ \ realizations} \end{aligned} \tag{1.2}$$

with $t_i \neq t_j\ \forall i \neq j$ and $i, j \leq n$, $n = 1, 2, \ldots$

Definition 1.2 (Absolute probabilities) The functions $W(x_1, t_1; ...; x_n, t_n)$, $t_1 \neq t_2 \neq \ldots, \neq t_n$ are called absolute probabilities of the process, [2] and must satisfy the following natural conditions:

(i) $W(x_1, t_1; ...; x_n, t_n) \geq 0$

(ii) $\int_{\mathbb{R}^k} dx_1...dx_n W(x_1, t_1; ...; x_n, t_n) = 1$, $\forall\{x_1, t_1; \ldots; x_n, t_n\}$

(iii) $W(x_1, t_1; ...; x_n, t_n)$ is a symmetric function

(iv) $\int_{\mathbb{R}} dx_n W(x_1, t_1; ...; x_n, t_n) = W(x_1, t_1; ...; x_n - 1, t_n - 1)$

The condition (iii) is owing to the commutative logic of formulation of the joined probability of several events.

The condition (iv) is obvious because the sum on all the possible events at time t_n reduces the distribution to that of the events at times $t_1, \ldots, t_n - 1$. It is a relation of compatibility between the distributions with n and $n - 1$ arguments.

If $t_n \to t_n - 1$, one poses:

$$\lim_{t_n \to t_{n-1}} W(x_1, t_1; ...; x_n - 1, t_n - 1; x_n, t_n) = W(x_1, t_1; ...; x_n - 1, t_n - 1)\delta(x_n - x_n - 1) \tag{1.3}$$

[2] if that does not lend to confusion, we can qualify W of probability whereas it is about a density of probability if x is a continuous variable.

since then, variables x_n and $x_n - 1$ must be identified.

Definition 1.3 (Conditional probabilities) Let us consider $t_1 \leq t_2 \leq\leq \ldots \leq t_k$. We define then the conditional probability $P(x_1, t_1; \ldots; x_k, t_k \mid x_k{+}1, t_k{+}1; \ldots; x_n, t_n)dx_k{+}1; \ldots; dx_n$ by

$$P(x_1, t_1; \ldots; x_k, t_k \mid x_k + 1, t_k + 1; \ldots; x_n, t_n)dx_k + 1; \ldots; dx_n = \begin{cases} \text{probability of finding} \{x(t_k + 1) \in I_k + 1, \ldots, x(t_n) \in I_n\} \\ \text{knowing that} \{x(t_1) \in I_1, \ldots, x(t_k) \in I_k\} \end{cases} \tag{1.4}$$

and

$$P(x_1, t_1; \ldots; x_k, t_k \mid x_k + 1, t_k + 1; \ldots; x_n, t_n) = \frac{W(x_1, t_1; \ldots; x_n, t_n)}{W(x_1, t_1; \ldots; x_k, t_k)}. \tag{1.5}$$

These distributions enjoy the properties

(a) $P(x_1; t_1; \ldots; x_k; t_k \mid x_k + 1; t_k + 1; \ldots; x_n; t_n) \geq 0.$

(b) $\int_{\mathbb{R}^{n-k}} dx_{k+1} \ldots dx_n P(x_1; t_1; \ldots; x_k; t_k \mid x_k + 1; t_k + 1; \ldots; x_n; t_n) = 1.$

(c) $P(x_1; t_1; \ldots; x_k; t_k \mid x_k + 1; t_k + 1; \ldots; x_n; t_n)$ is symmetrical under the permutations of the arguments $x_1; t_1; \ldots; x_k; t_k$ and $x_k + 1; t_k + 1; \ldots; x_n; t_n$.

(d) $\int_{\mathbb{R}} dx_n P(x_1; t_1; \ldots; x_k; t_k \mid x_k{+}1; t_k{+}1; \ldots; x_n; t_n) = P(x_1; t_1; \ldots; x_k; t_k \mid x_k{+}1; t_k{+}1; \ldots; x_n - 1; t_n - 1.$

which follows immediately from the definition (1.2). It results from this, in particular from Eq.(1.3) that

$$\lim_{t_2 \to t_1} P(x_1; t_1 \mid x_2; t_2) = \delta(x_1 - x_2). \tag{1.6}$$

The data of $P(1, \ldots, k \mid k + 1)$ with $W(1)$ is equivalent to that of W. Indeed, by the definition (1.3) which says that $P(1, \ldots, k \mid k + 1), \ldots, n = \frac{W(1,\ldots,n)}{W(1,\ldots,k)}$, we have

$$W(1, 2){=}W(1)P(1 \mid 2). \tag{1.7}$$

$$W(1, 2, 3){=}W(1, 2)P(1, 2 \mid 3){=}W(1)P(1 \mid 2)P(1, 2 \mid 3). \tag{1.8}$$

$$W(1, 2, 3){=}W(1, 2, 3)P(1, 2, 3 \mid 4){=}W(1)P(1 \mid 2)P(1, 2 \mid 3)P(1, 2, 3 \mid 4). \tag{1.9}$$

$\vdots$

$$W(1, 2, 3, \ldots, k) = W(1)P(1 \mid 2)P(1, 2 \mid 3) \ldots P(1, 2, 3, \ldots, k - 1 \mid k), \tag{1.10}$$

that gives the expression of the absolute probabilities W knowing the conditional probabilities P. A stochastic process, can be well defined by the data of its absolute probabilities as those of its conditional probabilities.

1.2.2 Definition and Terminology of the stochastic process

In intuitive terms, a stochastic process is a probabilistic model for evolution in time of some systems that is regarded as being subject to randomly varying influences [61]; or any process whose temporal evolution can be analyzed in terms of probability is known as stochastic process. We can think that a stochastic process is an overall of waveforms (sample functions or sample paths), a waveform chosen at random. A stochastic process is mathematically speaking, a family of (infinitely many) random random variables defined on the same probability space.

Accordingly, the concept of stochastic process is very general. The process can be vectorial, with discrete or continuous values. It manifests itself by the observation of a variable $x(t)$ size in the course of time t . For example, $x(t)$ can be the co-ordinate of a Brownian particle, the position of a piston subjected to the shock of the molecules of a gas, the concentration of a chemical substance, the number of photons absorptive or emitted by an atom, the stock exchange values. It is often about observable macroscopic subjected to effects of a great number of microscopic variables.

1.2.3 Example

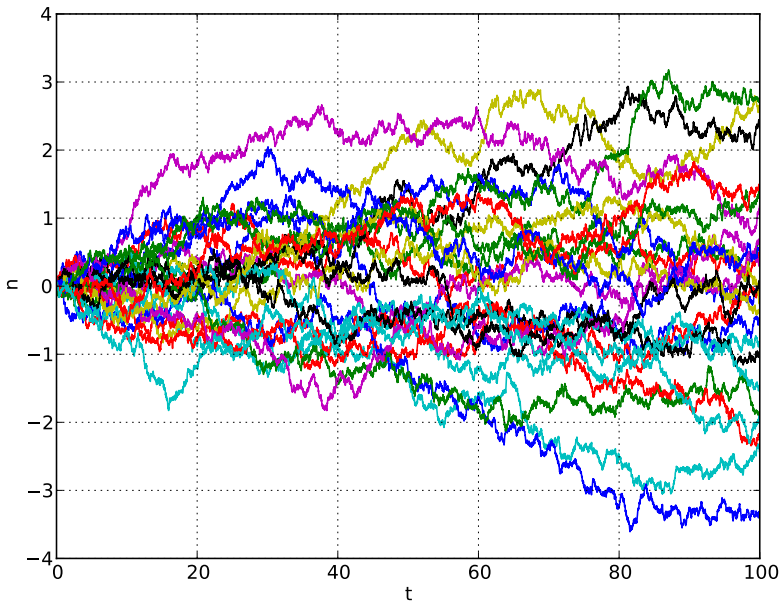

Figure 1.1: (Color online) 25 realizations of the discrete Brownian motion.

Let us lay emphasis on in phenomena where the probability of obtaining a certain result depends on what we have already obtained. Let us take the fundamental example of the Brownian motion at one dimension. Let us suppose that our world is divided into

boxes, which we number using an index n [62]. At each time step, our particle makes a jump to the box immediately to its left or to its right. We now ask ourselves: what is the probability $P(n,t)$ of finding the particle in the number n box at time t?

As such, this question does not have a sense. We must specify where the particle was at the initial moment; the precise question is therefore what is the probability of finding the particle in n at time t knowing what was in the box n_0 at time t_0. We note this probability by $P(n,t;n_0,t_0)$. Figure 1.1 represents 25 realizations of such a process: at the initial moment $t=0$, we pose the particle in box n_0 and we make it evolve from box to box during 100 turns by our probabilistic game: we draw with pile or face; if it is face, we move the particle of a box to the left; if it is pile, we move it of a box to the right.

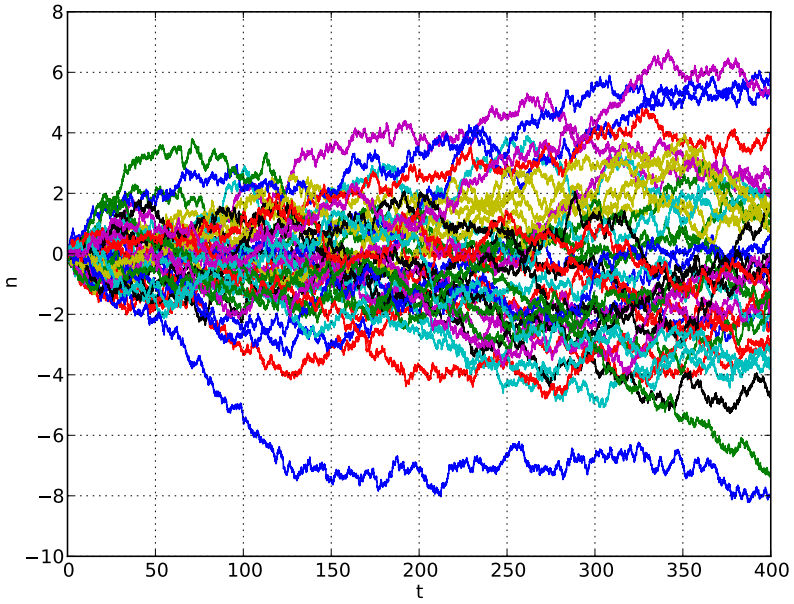

Figure 1.2: (Color online) 40 realizations of the discrete Brownian motion during 400 turns.The proportion of trajectories which lead to $n=4$ at time 400 is the probability $P(4,400;0,0)$.

We repeat this experiment 25 times, each trajectory represents an experiment. Obviously to speak about probability, we need much more than 25 trajectories. We can give a time $t=400$ and ask us the question: how many trajectories arrive in box $n=4$ at that time? This relative number is of course the probability $P(4,400;0,0)$. We can move our measuring device from the relative number of trajectory from box to box and that constitute the distribution law at time $t=400$, $P(n,400;0,0)$ (Figure 1.2).

Definition 1.4 (Stochastic process) A stochastic process is defined by the set of data of the absolute probabilities $\{W(x_1,t_1;...;x_n,t_n)\}_{n\geq 1}$ satisfying the conditions (i)-(iv).

A stochastic process is a family of random variables $X(t)$,

$$\mathbf{X} = \{X(t)|t \in T\},$$

where T is the index set of the process. All random variables $X(t)$ are defined on the same probability space $(\Omega, \mathcal{F}, P)$. Let us set T is $\mathbf{R}$ or a subset of $\mathbf{R}$, e.g., $T = [0, \infty)$ or $T = (-\infty, \infty)$ or $T = [a, b]$, $a < b$, and is not countable. We shall thus talk about stochastic processes in continuous time. [3] There are three ways to view a stochastic process;

(i) For each fixed $t \in T$, X(t) is a random variable $\Omega \mapsto \mathbf{R}$.

(ii) $\mathbf{X}$ is a measurable function from $T \times \Omega$ with value $X(t, \omega)$ at (t, ω).

(iii) For each fixed $\omega \in \Omega$, $T \ni t \mapsto X(t, \omega)$ is a function of t called the sample path (corresponding to ω).

The mathematical theory deals with these questions as follows. Let now $t_1, \ldots, t_n$ be n points in T and $X(t_1), \ldots, X(t_n)$ be the n corresponding random variables in X. Then, for an arbitrary set of real numbers $x_1, x_2, \ldots, x_n$, we have the joint distribution $F_{t_1,t_2,\ldots,t_n}(x_1, x_2, \ldots, x_n) = \mathbf{P}(X(t_1) \leq x_1, X(t_2) \leq x_2, \ldots, X(t_n) \leq x_n)$.

We denote a joint distribution function by

$$F_{t_1,\ldots,t_n}.$$

Definition 1.5 (Stationary process) A stochastic process is known as stationary if $W(x_1, t_1; ...; x_n, t_n) = W(x_1, t_{1+\tau}; ...; x_n, t_{n+\tau}) \quad \forall \tau \in \mathbb{R}, \quad \forall n \geq 1$. In particular

(i) $W(x_1, t_1; x_2, t_2) = W(x_1, 0; x_2, t_2 - t_1)$.

(ii) $W(x_1, t_1) = W(x_1)$ is a independent of time.

1.2.4 Correlations, cumulants and generating functions

Definition 1.6 (Correlation function) The correlation function of order n of the process noted $\mathcal{C}(t_1, \ldots, t_n)$ is defined for $t_1 \neq \ldots \neq t_n$ by

$$\mathcal{C}(t_1, \ldots, t_n) \doteq \langle x(t_1) \ldots x(t_2) \rangle = \int_{\mathbb{R}^n} dx_1 \ldots dx_n x_1 \ldots x_n W(x_1, t_1; \ldots; x_n, t_n). \qquad (1.11)$$

If two times coincide, one uses (1.3), for example

[3] A discrete time stochastic process with $T \subseteq \{0, \pm 1, \pm 2 \ldots\}$ is often called a time series.

$$\begin{aligned}\lim_{t_2\to t_1}\mathcal{C}(t_1,t_2) &= \int_{\mathbb{R}} dx_1 \int_{\mathbb{R}} dx_2 x_1 x_2 \underbrace{\lim_{t_2\to t_1} W(x_1,t_1;x_2,t_2)}_{=W(x_1,t_1)\delta(x_1-x_2)} \\ &= \int_R dx_1 x_1^2 W(x_1,t_1) \\ &= \langle x^2(t_1)\rangle, \end{aligned} \tag{1.12}$$

and so on. The functions of correlations generalize, for the stochastic process, the concept of moment of a probability distribution.

A significant question is to know on which scale of time variables $x(t_1)$ and $x(t_2)$ have nontrivial correlations. This information is given by the behavior of the function of autocorrelation.

Definition 1.7 (Autocorrelation function) The function of autocorrelation of the process $\mathbf{K}(t_1,t_2)$ is defined by [4]

$$\mathbf{K}(t_1,t_2) = \langle (x(t_1)-\langle x(t_2)\rangle)(x(t_2)-\langle x(t_2)\rangle)\rangle = \mathcal{C}(t_1,t_2)-\mathcal{C}(t_1)\mathcal{C}(t_2). \tag{1.13}$$

For a stationary process $\mathbf{K}(t_1,t_2) = \mathbf{K}(\mid t_1 - t_2 \mid)$. If $\mathbf{K}(\mid t_1 - t_2 \mid) \simeq 0$, when $\mid t_1 - t_2 \mid > t_c$, then t_c is called correlation time. Thus, when $\mid t_1 - t_2 \mid > t_c$, we can consider that the random variables $x(t_1)$ and $x(t_2)$ are practically independent.

A significant concept is that of generating function, which makes it possible to obtain the moments of the distribution by derivation for a ordinary random variable.

Definition 1.8 (Generating function of moments) That is to say a variable x of $P(x)$ distribution whose moments are $\langle x^n\rangle = \int_{\mathbb{R}} dx \quad x^n P(x)$, then we can define the generating function of moments $\mathbf{G}(z)$ by:

$$\mathbf{G}(z) = \sum_{n=0}^{\infty} \frac{i^n}{n!}\langle x^n\rangle z^n = \left\langle \sum_{n=0}^{\infty} \frac{(izx)^n}{n!} \right\rangle = \langle e^{izx}\rangle = \int_{\mathbb{R}} dx e^{izx} P(x) \tag{1.14}$$

such as the moments are obtained by derivation.

$$\frac{d^n \mathbf{G}(z)}{dz^n} \mid_{z=0} = i^n \langle x^n\rangle, \tag{1.15}$$

$\mathbf{G}(z)$ is so the Fourier transform of $P(x)$. This last definition shows that the information contained in the set of the moments is equivalent to that of the probability distribution $P(x)$. Indeed, knowing all the moments, it is possible to calculate $P(x)$. This definition is generalized as follows for a stochastic process.

[4] In the literature, we often find the term function of truncated correlation to indicate the function of autocorrelation, while the function of correlation is the moment of order 2. Nevertheless, these denominations are prone to confusion, and certain authors employ the term of function of correlation for to describe the function of truncated correlation.

Definition 1.9 (Generating function of the correlations) Either $f(t)$ a function test, we define the generating function of the $\mathbf{G}(f)$ correlations by:

$$\begin{aligned}\mathbf{G}(f) &= \sum_{n=0}^{\infty} \frac{i^n}{n!} \int_{\mathbb{R}^n} dt_1 \dots dt_n f(t_1) \dots f(t_n) \underbrace{\langle x(t_1) \dots x(t_n)}_{=\mathcal{C}(t_1,\dots,t_n)} \\ &= \sum_{n=0}^{\infty} \frac{i^n}{n!} \left\langle (\int_{\mathbb{R}} dt x(t) f(t))^n \right\rangle \\ &= \langle e^{i \int_{\mathbb{R}} x(t) f(t)} \rangle, \end{aligned} \tag{1.16}$$

such as the correlations, functions are obtained by functional derivation.

$$\frac{\delta^n \mathbf{G}(f)}{\delta f(t_1) \dots \delta f(t_n)} \mid_{f=0} = i^n \langle x(t_1) \dots x(t_n) \rangle, \tag{1.17}$$

The relation (1.17) fact of appearing the operator of functional derivation, whose symbol is $\frac{\delta}{\delta f(t)}$. Its essential formal property is

$$\frac{\delta f(t)}{\delta f(t')} = \delta(t - t'), \tag{1.18}$$

from where we establishe easily (1.17) from (1.16).

Definition 1.10 (Cumulants) The cumulants $\mathbf{K}(\mathbf{t_1}, \dots, \mathbf{t_n})$ are defined by

$$\mathbf{K}(\mathbf{f}) = \ln(\mathbf{G}(\mathbf{f})) = \sum_{n=1}^{\infty} \frac{i^n}{n!} \int_{\mathbb{R}^n} dt_1 \dots dt_n f(t_1) \dots f(t_n) \mathbf{K}(\mathbf{t_1}, \dots, \mathbf{t_n}). \tag{1.19}$$

We can express the correlations in terms of cumulants and screw-poured. For example, one has:

$$\mathcal{C}(t_1) = \mathbf{K}(\mathbf{t_1}), \tag{1.20}$$

$$\mathcal{C}(t_1, t_2) = \mathbf{K}(\mathbf{t_1})\mathbf{K}(\mathbf{t_2}) + \mathbf{K}(\mathbf{t_1}, \mathbf{t_2}), \tag{1.21}$$

$$\begin{aligned}\mathcal{C}(t_1, t_2, t_3) = &\mathbf{K}(\mathbf{t_1})\mathbf{K}(\mathbf{t_2}, \mathbf{t_3}) + \mathbf{K}(\mathbf{t_2})\mathbf{K}(\mathbf{t_1}, \mathbf{t_3}) + \mathbf{K}(\mathbf{t_3})\mathbf{K}(\mathbf{t_1}, \mathbf{t_2}) \\ &+ \mathbf{K}(\mathbf{t_1})\mathbf{K}(\mathbf{t_2})\mathbf{K}(\mathbf{t_3}) + \mathbf{K}(\mathbf{t_1}, \mathbf{t_2}, \mathbf{t_3}) \dots \end{aligned} \tag{1.22}$$

To show Eq.(1.20) to Eq.(1.22), let us pose

$$\mathbf{K_n} = i^n \int_{\mathbb{R}^n} dt_1 \dots dt_n f(t_1) \dots f(t_n), \tag{1.23}$$

so that

$$\mathbf{K}(\mathbf{f}) = \ln(\mathbf{G}(\mathbf{f})) = \sum_{n=1}^{\infty} \frac{\mathbf{K_n}}{n!}. \tag{1.24}$$

To find the correlations, we must establish an expression for $\mathbf{G}(\mathbf{f})$ according to $\mathbf{K_n}$ knowing that of $\ln(\mathbf{G}(\mathbf{f}))$, then to identify this series with that Eq.(1.16) defining the correlations. Thus, while developing until the third order:

$$\begin{aligned}
\mathbf{G}(\mathbf{f}) = e^{\ln(\mathbf{G}(\mathbf{f}))} &\overset{1.23}{=} e^{\mathbf{K_1}+\frac{1}{2!}\mathbf{K_2}+\frac{1}{3!}\mathbf{K_3}+\dots}, \\
&= \mathbf{K_1} + \frac{1}{2!}\mathbf{K_2} + \frac{1}{3!}\mathbf{K_3} + \frac{1}{2!}(\mathbf{K_1} + \frac{1}{2!}\mathbf{K_2})^2 + \frac{1}{3!}(\mathbf{K_1})^3 \dots, \\
&= \mathbf{K_1} + \frac{1}{2!}\mathbf{K_1} + (\mathbf{K_2})^2 + \frac{1}{3!}(\mathbf{K_3} + 3\mathbf{K_1}\mathbf{K_2} + (\mathbf{K_1})^3 + \dots, \\
&\overset{1.22}{=} i\int_{\mathbb{R}} dt_1 f(t_1)\mathbf{K_1} + \frac{i^2}{2!}\int_{\mathbb{R}^2} dt_1 dt_2 f(t_1)f(t_2)(\mathbf{K}(\mathbf{t_1},\mathbf{t_2})) + \mathbf{K}(\mathbf{t_1})\mathbf{K}(\mathbf{t_2}) \\
&\quad + \frac{i^3}{3!}\int_{\mathbb{R}^3} dt_1 dt_2 dt_3 f(t_1)f(t_2)f(t_3)\mathbf{K}(\mathbf{t_1},\mathbf{t_2},\mathbf{t_3}) + 3\mathbf{K}(\mathbf{t_1})\mathbf{K}(\mathbf{t_2},\mathbf{t_3}) \\
&\quad + \mathbf{K}(\mathbf{t_1})\mathbf{K}(\mathbf{t_2})\mathbf{K}(\mathbf{t_3}) + \dots
\end{aligned} \tag{1.25}$$

The result follows identification term in the long term of this series (1.25) with that (1.16) which defines $\mathbf{G}(\mathbf{f})$. One also holds account owing to the fact that the functions $\mathcal{C}(t_1,\dots,t_n)$ and $\mathbf{K}(\mathbf{t_1},\dots,\mathbf{t_n})$ are symmetrical under the exchange of their arguments. We can reverse the relations between correlations and cumulants. For example, it is seen Eq.(1.20) and Eq.(1.21) that $\mathbf{K}(\mathbf{t_1},\mathbf{t_2})$ is nothing other than the function of autocorrelation of the process. Cumulants generalize thus this concept with the correlations of a higher nature. Cumulants are sometimes called functions of correlations truncated.

1.3 Markovian Process

Definition

The class of the stochastic processes defined by the only conditions (i)-(iv) of the definition (1.2) of the absolute probabilities is very vast. So that the concept of process stochastic is useful, it is necessary to specify additional conditions.

Definition 1.11 Process of Markov The process is known as of Markov [5] (or Markovian) if the conditional probabilities have $\forall t_1 < t_2 < \dots < t_n$ the property:

$$P(x_1,t_1;x_2,t_2;\dots;x_n-1,t_n-1 \mid x_n,t_n) = P(x_n-1,t_n-1 \mid x_n,t_n). \tag{1.26}$$

[5] Name of the Russian mathematician Andreï Andreïevitch Markov (1856-1922). It in particular showed the inequalities of Tchebychev, and refined the proof of the theorem limits central. To study the law of large numbers, it introduces chains or Markov processes

Such a definition is equivalent saying that the event $\{x_n, t_n\}$ only depends on preceding $\{x_n - 1, t_n - 1\}$. We say in a full of imagery way that the future is independent of the history of the system, or that the process is without memory. In fact, the character Markovian (or roughly Markovian) of a physical process is a delicate question, as we will see it in the example of the Brownian motion.

Lemma The only data of $W(x,t)$ and the probability of Markov $P(x_1,t_1 \mid x_2,t_2)$ determines entirely the stochastic process of Markov.

Proof Definition (1.3): we knows that the stochastic process is defined by the data of the functions W. Moreover, we showed at the end of the section (1.2.1) that W were entirely determined by the data of $W(x_1,t_1)$ and the conditional probabilities P. By applying the definition of the process of Markov to the equation (1.10), one has:

$$W(x_1,t_1;\ldots;x_n,t_n) = W(x_1,t_1)P(x_1,t_1 \mid x_2,t_2)P(x_2,t_2 \mid x_3,t_3)\ldots P(x_n{-}1,t_n{-}1 \mid x_n,t_n), \tag{1.27}$$

what completes the proof because it is noted that both functions $W(x,t)$ and $P(x_1,t_1 \mid x_2,t_2)$ determine all W. Reciprocally, if W are form (1.27) we see of the definition (1.3) that the property of Markov is checked.

1.4 Brownian motion and Random walks

The observation of the Brownian motion is quite former to Brown himself. Among the precursors, we can quote Dutch Ingenhousz (1785) who observed the erratic movement of coal dust in alcohol. Similar observations made by Buffon and other naturalists show that particles of all organic and inorganic nature, in suspension in a fluid show this movement surprising and disordered which one is unaware of the origin. We talk about particles «irritable» and we advance vitalistic theories which allocate a specific autonomy to these small particles.

The Brownian motion was discovered by the botanist Scott Brown in 1827; it indicates the disordered movement and erratic of a large particle immersed in a fluid (see Fig. 1.3).

Brown devotes himself to systematic observations of this movement and its conclusions, confirmed by other careful experiments at the end of the nineteenth century are as follows:

1. The movement is very irregular and unforeseeable, it is not possible to assign tangents with the trajectory.

2. The movement is independent of the nature of the particle.

3. The movement is all the more erratic as the particle is small, the temperature is high, low viscosity.

4. The movement never ceases.

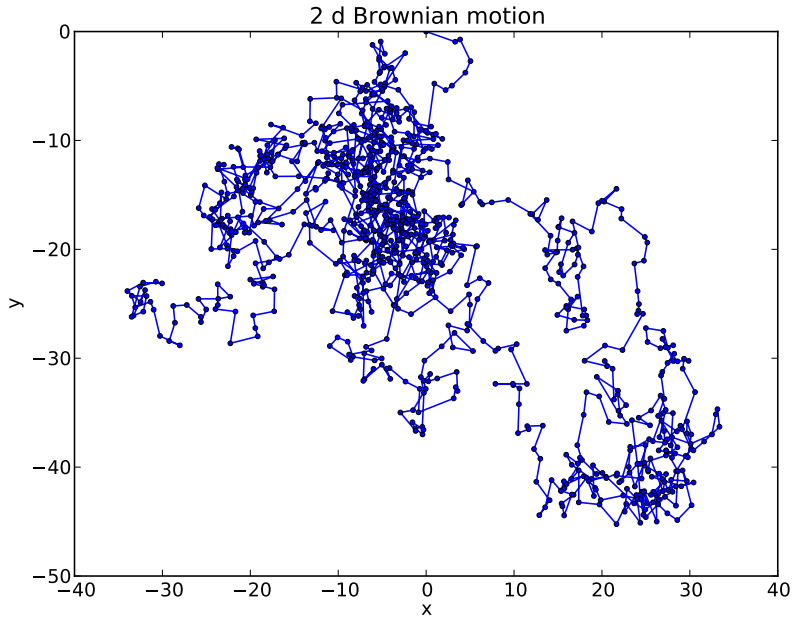

Figure 1.3: (Color online): A path of a Brownian Movement Particle.

It is allowed that the movement is not «vitalistic» origin, but quite mechanical.

During the same time, the question of the validation of the atomic assumption and its experimental confirmation arises; it is this question which justifies the work of Einstein.

To do it, Einstein adopts a view point purely probabilistic for the description of the Brownian trajectories, giving up at any concept utilizing velocity and mechanics. It is there the key of its success. Initially, introducing the density of probability $P(x,t)$ of finding the Brownian particle in x at time t, it shows that this probability obeys the diffusion equation:

$$\frac{\partial}{\partial t}P(x,t) = \mathbf{D}\frac{\partial^2}{\partial x^2}P(x,t), \tag{1.28}$$

then, it connects the constant of diffusion $\mathbf{D}$ to the physical sizes for the famous formula

$$\mathbf{D} = \frac{k_B T}{m\gamma}, \tag{1.29}$$

where $k_B = R/\mathcal{N}$ (R being the constant of perfect gas and $\mathcal{N}$ the number of Avogadro), the desired bond is established. A measurement of $\mathbf{D}$ allows a determination of $\mathcal{N}$ and a confrontation of this value that obtained by chemical stoichiometry. The measurement, taken by Perrin in 1910 gives an agreement of twenty percent, however sufficient at the period to confirm the atomic assumption. As $\mathbf{D}$ is connected to the average standard deviation of Brownian displacement, Einstein inaugurates and shows the importance of a new science, the theory of the fluctuations.

1.4.1 Models for Normal diffusion: Langevin's equation

Let us consider a particle with mass m performing a random walk inside a fluid due to the bombardment by the fluid molecules, which obey an equilibrium distribution [33]. Pierre Langevin described this motion with a simple but very interesting stochastic differential equation

$$m\ddot{x} = -\alpha\dot{x} + F(t), \tag{1.30}$$

where the term $\alpha\dot{x}$ represents the friction force, $\dot{x}$ is the particle velocity, α is the damping rate and depends on the radius of the particle and the viscosity of the fluid, and $F(t)$ is a random fluctuating force due to the random bombardment of the particle by the fluid molecules. If the random fluctuating force were absent, the particle starting with an initial velocity v_0 would gradually slow down due to the friction term. Multiplying (1.30) with x, then we have

$$mx\dot{x} \;\; = m[\tfrac{d(x\dot{x})}{dt} - \dot{x}^2] \;\; = -\alpha x\dot{x} + xF(t), \tag{1.31}$$

and after taking averages over a large number of particles we find,

$$m\frac{d\langle x\dot{x}\rangle}{dt} = m\langle\dot{x}^2\rangle - \alpha\langle x\dot{x}\rangle, \tag{1.32}$$

since $\langle xF(t)\rangle = 0$ due to the irregular nature of the force $F(t)$.

Since the background gas is in equilibrium, the kinetic energy of the particle is proportional to the gas temperature, $m\langle\dot{x}^2\rangle/2 = kT/2$, where k is the Boltzmann constant and T the temperature of the gas. Equation (1.32) takes the form

$$(\frac{d}{dt} + \gamma)\langle x\dot{x}\rangle = \frac{kT}{m}, \tag{1.33}$$

where $\gamma = \alpha/m$, which has the solution

$$\langle x\dot{x}\rangle \;\; = \tfrac{1}{2}\tfrac{d\langle x^2\rangle}{dt} \;\; = Ce^{-\gamma t} + \frac{kT}{\alpha}. \tag{1.34}$$

At $t = 0$, the mean square displacement is zero, so that $C + kT/\alpha = 0$ and Eq.(1.34) becomes

$$\frac{1}{2}\frac{d\langle x^2\rangle}{dt} = \frac{kT}{\alpha}(1 - e^{-\gamma t}). \tag{1.35}$$

On integrating the above equation we find the solution

$$\langle x^2\rangle = \frac{2kT}{\alpha}\Big[t - \frac{1}{\gamma}(1 - e^{-\gamma t})\Big]. \tag{1.36}$$

In the limit $t << \frac{1}{\gamma}$(time much shorter than the collision time), the solution of Eq.(1.36) is of the form $\langle x^2 \rangle \sim t^2$, which is called "ballistic" diffusion and mean that at small times particles are not hindered by collisions yet and diffuse very fast. In the other limit, $t >> 1/\gamma$, the solution has the form

$$\langle x^2 \rangle \sim \frac{2kT}{\alpha} t. \tag{1.37}$$

or, for the 3-dimensional case, if again the gas is in equilibrium and isotropic so that $\langle r^2 \rangle / 3 = \langle x^2 \rangle$,

$$\langle r^2 \rangle \ = \frac{6kT}{\alpha} t \ = \mathbf{D} t. \tag{1.38}$$

where $\mathbf{D} = 6kT/\alpha$ is an expression for the diffusion constant in terms of particles and fluid characteristics.

1.4.2 Einstein relation for the constant of diffusion

Let us suppose that we have N independent Brownian particles (or in interaction sufficiently weak to be able to be neglected) of which density $n(x,t)$ is given by $n(x,t) = N$, with normalization $\int_{\mathbb{R}} dx n(x,t) = N$. As $P(x,t)$ satisfies the diffusion equation $\frac{\partial}{\partial t} P(x,t) = \mathbf{D} \frac{\partial^2}{\partial x^2} P(x,t)$, then it is the same for $n(x,t)$. The current of particles due to the diffusive effects is defined by the Fick law's

$$j_D(x,t) = -\mathbf{D} \frac{\partial}{\partial x} n(x,t), \tag{1.39}$$

in such way that the continuity equation is checked

$$\frac{\partial}{\partial} n(x,t) + \frac{\partial}{\partial} j_D(x,t) = 0. \tag{1.40}$$

Now, let us suppose that the particles are in a constant field, for example a gravific field and that these particles are in a viscous fluid thus undergo a friction proportional at their velocity v. Let γ the damping constant of the velocity, $m\gamma$ the coefficient of friction, then the Newton's equation gives:

$$m \frac{d}{dt} v(t) = -mg - m\gamma v(t). \tag{1.41}$$

The field of force produces a current of particles $j_g(x,t)$ defined by:

$$j_g(x,t) = n(x,t) v(t). \tag{1.42}$$

Let us notice that the recourse to the Newton's equation consists of a macroscopic description, deterministic and nonrandom of the phenomenon. On the other hand, the

Fick's law translates a diffusive phenomenon, therefore in nondeterministic and random character.

Let us consider now the stationary regime, characterized by the thermal equilibrium , in which $\frac{d}{dt}v = 0$. Consequently, the Newton's (1.41) equation allows to obtain the expression $v = -\frac{g}{\gamma}$ for the velocity in the stationary state. In substituting this last expression in the definition (1.42) of $j_g(x,t)$, we obtain

$$j_g = -\frac{gn(x)}{\gamma}. \tag{1.43}$$

In addition, to thermal equilibrium in the external field, the statistical physics of Gibbs applies. Consequently, $n(x)$ is given by the barometric formula

$$n(x) = n(x_0)e^{-\frac{v(x-x_0)}{k_BT}} = n(x_0)e^{-\frac{mg(x-x_0}{k_BT}}, \tag{1.44}$$

with k_B the Boltzmann's constant and $v(x) = mgx$ the gravific potential. While inserting (1.44) in the definition (1.39) of the diffusion current $j_D(x,t)$, we obtain

$$j_D(x) = \mathbf{D}\frac{mgn(x)}{k_BT}. \tag{1.45}$$

The total current

$$j(x,t) = j_g(x,t) + j_D(x,t) \tag{1.46}$$

has two components, one due with the field of force g and the other due to the gradient of density. However, the equilibrium corresponds to a total current nil. Thus, while inserting (1.43) and (1.45) in (1.46), we obtain

$$j(x) = -\frac{gn(x)}{\gamma} + \mathbf{D}\frac{mgn(x)}{k_BT}, \tag{1.47}$$

what leads finally to the relation of Einstein for the diffusion constant $\mathbf{D}$

$$\mathbf{D} = \frac{k_BT}{m\gamma}. \tag{1.48}$$

Remarks

(i) The constant of diffusion is independent of the field of gravitation g and more generally, as one will check it on several occasions, of the nature of the field of force acting on the Brownian particle. Equation (1.48) is an example of a fundamental relation which exists between the fluctuations (represented by coefficient $\mathbf{D}$) and dissipation (represented by coefficient γ. It is the germ of what is called a relation of fluctuation - dissipation.

(ii) As $k_B = \frac{R}{\mathcal{N}}$, with $\mathcal{N}$ the number of Avogadro and R the constant of perfect gases, then $\mathcal{N}$ can be measured starting from the Brownian motion.

1.5 Anomalous diffusion

Many physical and biological systems can be described in terms of a particle undergoing random displacements. When the spread of these particles at long times asymptotically scales as $x^2(t) \sim t^{2H}$, with $H \neq 1/2$, the walker diffusion is said to be anomalous, as opposed to regular diffusion, which corresponds to plain Brownian motion. Examples of anomalous diffusion emerge for instance when considering the motion of polymers through nanopores, or the percolation of tracer particles in heterogeneous soils. Here, we will review some relevant examples of anomalous diffusion and show by which mathematical and numerical tools the corresponding first-passage properties can be assessed.

Beyond Brownian motion: anomalous diffusion

Brownian motion plays a key role in modern theoretical physics and it has proved very successful in explaining several key features of physical and biological systems. Actually, it is currently used in various fields of science so as to interpret, for instance, the dynamics of complex molecules within the cell, animal food-searching strategies, or tracer dispersion in soils, only to name a few [54, 55]. In all such cases, the system can be conveniently represented as a fluctuating particle, whose position has a stochastic evolution in time. The signature of Brownian motion is that the mean square displacement of the particle grows linearly as a function of time. However, fluctuations of real-world systems are often observed to grow in a nonlinear fashion, which demands to go beyond the Brownian motion paradigm. This situation is referred to as *anomalous diffusion*, where by opposition *normal diffusion* corresponds to regular Brownian motion; more precisely, *subdiffusion* if the mean square displacement grows slower than linearly in time, and *superdiffusion* if it grows faster

Consider for example the random walker depicted in Fig. 1.4. The walker starts at the origin at time $t = 0$ and holds its position until a random time τ_1, whereupon it makes a random jump to the position $x_1 = \xi_1$. The walker then waits at x_1 up to a random time $\tau_1 + \tau_2$, whereupon it jumps to the new random position $x_2 = \xi_1 + \xi_2$, and the process is renewed. The times $\tau_1, \tau_2, \ldots \tau_n$ are named *waiting times* and the jumps $\xi_1, \xi_2, \ldots, \xi_n$ are named *increments*. Both waiting times and increments are random variables. For the sake of simplicity, we assume that the waiting times are independent and identically distributed, and that the increments are symmetric (i.e., the set $\xi_1, \xi_2, \ldots, \xi_n$ is generated with the same probability as $-\xi_1, -\xi_2, \ldots, -\xi_n$).

Let $x(t)$ be the position held by the walker at time t. At large times, the fluctuations of $x(t)$ typically become independent of (most of) the microscopic details of the waiting times and increment distributions [54, 55]. In particular, if the increments are independent and identically distributed, and if both $\langle \tau_i \rangle = \tau$ and $\langle \xi_i^2 \rangle = \sigma^2$ are finite [6], the process exhibits a

[6] Here $\langle \ldots \rangle$ stays for the average over all realizations and $\langle \xi_i \rangle = 0$ because by assumption the process is symmetric.

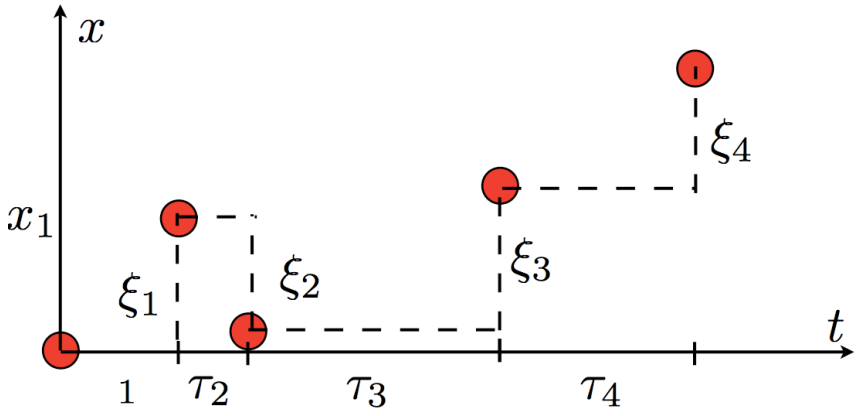

Figure 1.4: (Color online) Sketch of a generic random walk in one dimension. The positions of the walker after the jumps are marked with a red dot.

diffusive behavior, i.e., $x(t)$ asymptotically obeys a Gaussian [7] probability density function as $t \to \infty$, and the memory of the waiting times and increment distributions are kept only in σ^2 and τ:

$$\langle x^2(t) \rangle = 2\frac{\sigma^2}{2\tau}t = 2\,D\,t, \tag{1.49}$$

where D is the diffusion coefficient [54, 55]. Brownian motion corresponds to the continuum limit [8] of this family of random walks and it is self affine with a characteristic exponent $H = 1/2$. Self-affinity with a characteristic (Hurst) exponent $H > 0$ means that $x(bt)$ and $b^H x(t)$ have the same probability density for $b > 0$.

Anomalous diffusion occurs whenever the process $x(t)$ is self-affine (at least at large times) with $H \neq 1/2$, so that the mean square displacement grows with time as t^{2H} [56]. This is achieved whenever the random walk $x(t)$ falls out of the basin of attraction of the Central Limit Theorem for one of the following reasons:

1. The increments are not independent and the process is non-Markovian: for instance, the motion of a fluorescent monomer in a polymer is subdiffusive because of the interactions with the other monomers;

2. The increments can be very large and $\langle \xi_i^2 \rangle = \infty$ (e.g., wild fluctuations in the stock market prices), and/or the waiting times can be very long $\langle \tau_i \rangle = \infty$ (e.g., high retention rates of colloids in porous media);

3. The increments are not identically distributed: for instance, a small particle in a non-viscous fluid is subjected to a random force which induces increments growing with $\sqrt{t}$.

[7] Because of the Central Limit Theorem.

[8] The continuum limit is obtained by taking both τ and σ^2 vanishing small, and keeping $x(t)$ and t fixed. This implies for standard diffusion that the ratio $D = \sigma^2/2\tau$ remains finite.

Anomalous diffusion has been reported to occur in a huge number of physical and biological systems [56,57]. Knowledge of the walker spread $\langle x^2 \rangle$ in unbounded domains typically allows inferring the exponent H. However, real-world systems often involve confined geometries, where the microscopic behavior of the walker (hence the spread) is not directly observable. When the process itself is not accessible, one can try to measure the time taken for the walker to reach some detector, e.g., the outer surface of the domain where particles evolve. Given the stochastic nature of the underlying process, such *first-passage times* are also random variables, whose exact distribution would provide invaluable information on the precise nature of the anomalous dynamics [63]. Unfortunately, determining the distribution of first-passage times for an anomalous diffusion process is generally a prohibitively difficult task, and a unified description of non-Brownian behavior is still missing. Possibly, one of the reasons is that very different systems can exhibit anomalous diffusion with the same exponent H, which makes the interpretation of the physical origins of such behavior tougher than in the case of (somehow universal) Brownian motion.

In the following, we review the first-passage properties of some physically relevant examples of anomalous walkers, namely, fractional Brownian motion (having non-independent increments, as in case (1)), Lévy flights and Continuous Time Random Walks (having very large increments and waiting times, respectively, as in case (2)), and random acceleration processes (having non identically distributed increments, as in case (3)). Our aim is twofold: on one hand, to illustrate the rather intriguing features of anomalous walkers, and on the other hand to show by which mathematical and numerical tools the properties of the resulting first-passage distributions can be singled out.

1.6 Polymer translocation and fractional Brownian motion

A prominent goal of biophysics is to set up efficient DNA sequencers. A fundamental prerequisite is the comprehension of the transfer mechanism of a molecular fragment through a nanopore, the so-called *translocation*. The translocation of a single polymer through a pore in a hard wall is the most schematic modelization of this sequencer; yet, the mechanics of this process is still poorly understood [64]. Direct simulations of the dynamics of the entire polymer are cumbersome, because of the large number of degrees of freedom involved [65]. The translocation coordinate $s(t)$, namely the label of the monomer crossing the pore at time t, has been shown to be key in understanding the translocation process [58, 59], which begins when $s = 1$ and ends when $s = N$, i.e., when the first and the last monomer of the chain, respectively, enter the pore (see Fig. 1.5 left).

Various dynamical regimes of $s(t)$ have been identified: in the absence of driving forces and hydrodynamic effects (free polymer), fluctuations dominate, and $s(t)$ can be regarded as a stochastic process, whose features vary with the polymer length N [58, 59]. Understanding the full dynamics of $s(t)$ represents a challenging problem. A free polymer is characterized by two natural time scales (see Fig. 1.5 right). First, the intrinsic

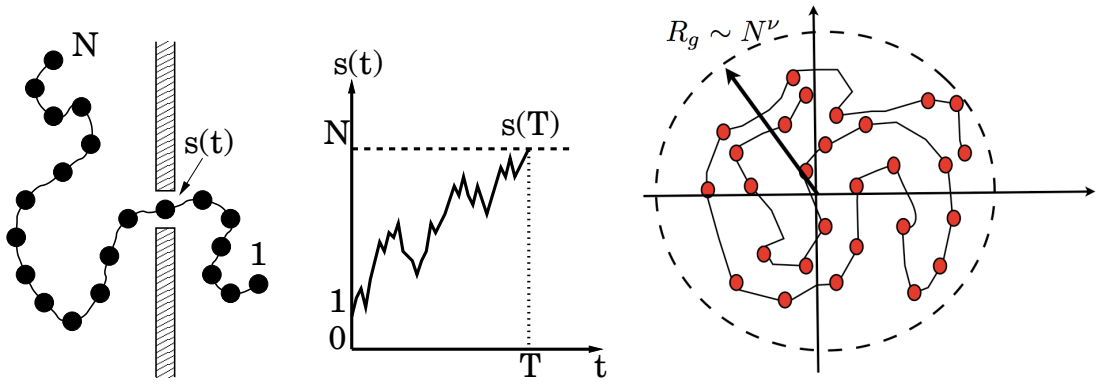

Figure 1.5: (Color online) Left: Translocation of a polymer chain through a pore. Middle: The translocation coordinate $s(t)$ denotes the number of the monomer that is crossing the pore at time t. Right: Sketch of a free self-avoiding polymer.

equilibration time t_{eq} required by the center of mass of the polymer R_{cm} to travel a distance of the order of the typical size of the chain. This size is given by the radius of gyration R_g, which scales as $R_g \sim N^\nu$ in the large N limit. In a good solvent, $\nu = 3/4$ in $2d$ and $\nu \simeq 0.59$ in $3d$ when excluded-volume effects for the monomers are considered; moreover, $\nu = 1/2$ for an ideal ('phantom') polymer. The center of mass diffuses with a diffusion coefficient $\sim 1/N$. Then, $R_{cm} \sim \sqrt{t/N}$. Hence, $\sqrt{t_{eq}/N} \sim R_g$ and $t_{eq} \sim N^{2\nu+1}$ for large N. On the other hand, the translocation time T (much longer than t_{eq}) is the time required by the polymer to go through the pore, so that $s(T) = N$ (Fig. 1.5 middle). Under the hypothesis that the translocation is a self-affine process, i.e., $s(t) \sim t^H$, with Hurst exponent H, it follows that $T \sim N^{1/H}$.

For short polymers, excluded-volume effects are negligible, $s(t)$ undergoes diffusion, and $T \sim N^2$. However, as N increases, the excluded-volume interactions become relevant and $s(t)$ undergoes subdiffusion, $0 < H < 1/2$ [58]. Numerical simulations (mostly $2d$) support the following conclusions:

i) T and t_{eq} have the same scaling, up to a large prefactor, i.e., $T \sim t_{eq}$. Hence, $H = 1/(1+2\nu)$ [58]; (Note that for 'phantom' polymers $s(t)$ always diffuses, even for large N.)

ii) The probability $P(s,t)$ of finding the monomer s in the pore at time t for an infinite chain (i.e., in the absence of boundaries) is Gaussian [65].

Upon gathering these hints from simulations, a natural candidate for $s(t)$ appears to be the fractional Brownian motion [66], whose properties are briefly recalled in the following.

1.6.1 Fractional Brownian motion

Fractional Brownian motion (fBm) is a self-affine Gaussian process with $0 < H < 1$ [67, 68]. A Gaussian process is completely defined by its autocorrelation function, which for

fBm writes

$$\langle x(t_1)x(t_2)\rangle = D\left(t_1^{2H} + t_2^{2H} - |t_1 - t_2|^{2H}\right) . \tag{1.50}$$

As a particular case, for $H = 1/2$ the fBm corresponds precisely to regular Brownian motion, namely,

$$\langle x(t_1)x(t_2)\rangle = 2D\min(t_1, t_2) . \tag{1.51}$$

Note that the process $x(t)$ is Markovian only for $H = 1/2$, whereas for $H \neq 1/2$ the process is non-Markovian. The peculiarity of the fBm is that the process is *homogeneous*, i.e., its increments are identically distributed. To check this property, it is useful to sample a fBm process $x(t)$ at discrete times $t_1 = 1, t_2 = 2, \ldots$, as proposed in Fig. 1.4 (with $\tau_1 = \tau_2 = \ldots = 1$).

Using Eq.(1.50), we can compute the autocorrelation function of the Gaussian increments $\xi_t = x(t) - x(t-1)$,

$$\langle \xi_{t_0}\xi_{t_0+t}\rangle = C(t) = D\left[|t-1|^{2H} + (t+1)^{2H} - 2\,t^{2H}\right] . \tag{1.52}$$

We note that this function is independent on the initial time t_0 and thus the increments are identical Gaussian numbers with variance $2D$, displaying power-law correlations. By taking the limit $t \to \infty$, the power-law decay of these correlations can be easily singled out. For superdiffusive fBm (i.e., $H > 1/2$), $C(t)$ is positively correlated with a decay $t^{-2(1-H)}$. Positive correlations mean that there is a high probability to observe a long sequence of increments with the same sign. For subdiffusive fBm (i.e., $H < 1/2$), $C(t)$ is negatively correlated and decays as $-t^{-2(1-H)}$. Negative correlations mean that there is a high probability to observe a long sequence of increments of alternating signs.

Discrete fBm can be easily implemented numerically by observing that the autocorrelation matrix C is symmetric and has positive eigenvalues; it is thus possible to find a positive and symmetric matrix A such that $C = A^2$. The matrix A is called the square root of C. The paths of fBm are simulated by using the standard procedure for Gaussian correlated processes:

(i) determine A, the square root of C;

(ii) a set of increments $\vec{\xi} = \{\xi_1, \xi_2 \ldots\}$ is given by the matrix multiplication $\vec{\xi} = A\vec{\eta}$, where the vector $\vec{\eta} = \{\eta_1, \eta_2, \ldots\}$ is a set of independent Gaussian numbers with variance equal to $2D$ and zero mean.

It is easy to verify that these paths are characterized by the exact autocorrelation function as in Eq.(1.50) [9]. The outcome is shown in Fig. 1.6, where we compare an example of

[9] Unfortunately, this procedure is exact but time-consuming, since for step (i) it demands the full diagonalization of C. Better results are obtained by observing that fBm is homogeneous, so that C is a Toeplitz matrix. Efficient numerical methods for Toeplitz matrices allow avoiding the full diagonalization of C. For instance, one can resort to the Levinson algorithm (for a practical implementation see [69] and [70]).

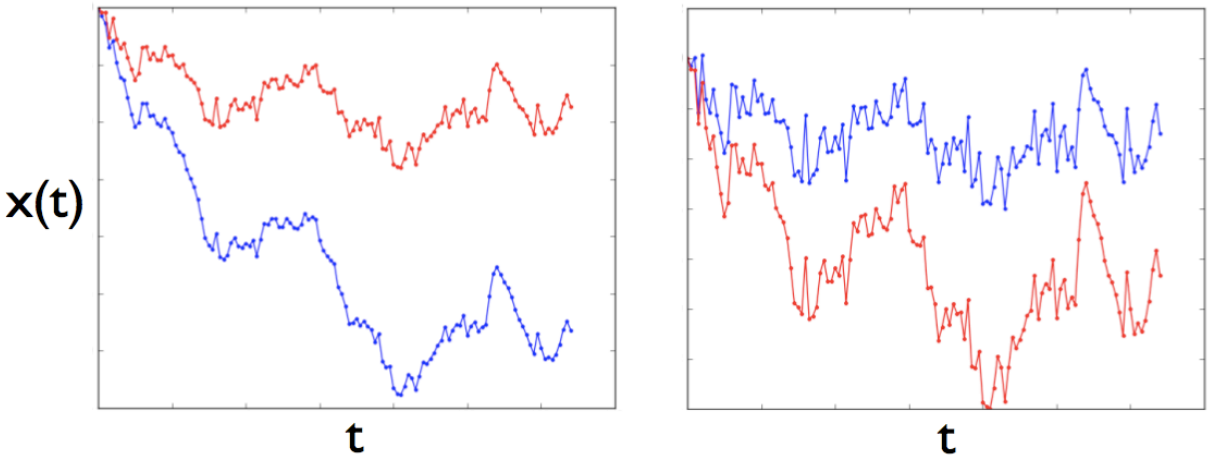

Figure 1.6: (Color online) Fractional Brownian motion (blue) generated with the correlated increments $\xi_1, \xi_2, \ldots$ versus Brownian motion (red) generated with the uncorrelated increments $\eta_1, \eta_2, \ldots$. Left: $H = 1/4$, subdiffusive case. Right: $H = 3/4$, superdiffusive case.

fBm generated with the correlated increments $\xi_1, \xi_2, \ldots$ with the Brownian motion generated with the uncorrelated increments $\eta_1, \eta_2, \ldots$. In the subdiffusive case, the negative correlations prevent the occurrence of a long sequence of consecutive positive (or negative) increments, whereas in the superdiffusive case, the positive correlations enhance the occurrence of such events.

1.6.2 First-passage properties: the hitting probability

On the basis of the considerations exposed above, fBm satisfies conditions *i*) and *ii*) upon taking $H = 1/(1 + 2\nu)$, which relates the Hurst exponent to the scaling parameter ν. Identification of the underlying stochastic process governing the motion of $s(t)$ allows extracting information about translocation without having to deal with the cumbersome study of the full polymer dynamics. In particular, it is possible to answer some relevant questions connected to the first-passage properties of the anomalous diffusing polymer. A natural question is whether a finite polymer chain will ultimately succeed in translocating through a pore, which corresponds to characterizing the *hitting probability* of the process [71].

Moreover, numerical simulations for a finite chain yet to have completed translocation show that the distribution of $s(t)$ converges to a non-Gaussian form at long times [65]. In particular, this distribution vanishes *nonlinearly* as s^ϕ and $(N-s)^\phi$ at the two boundaries $s = 0$ and $s = N$ respectively, with $\phi \simeq 1.44$ in $2d$ [65]. In the next section, we will show that it is actually possible to precisely compute the exponent ϕ [71, 72]. Here, we begin our analysis by first addressing the hitting probability.

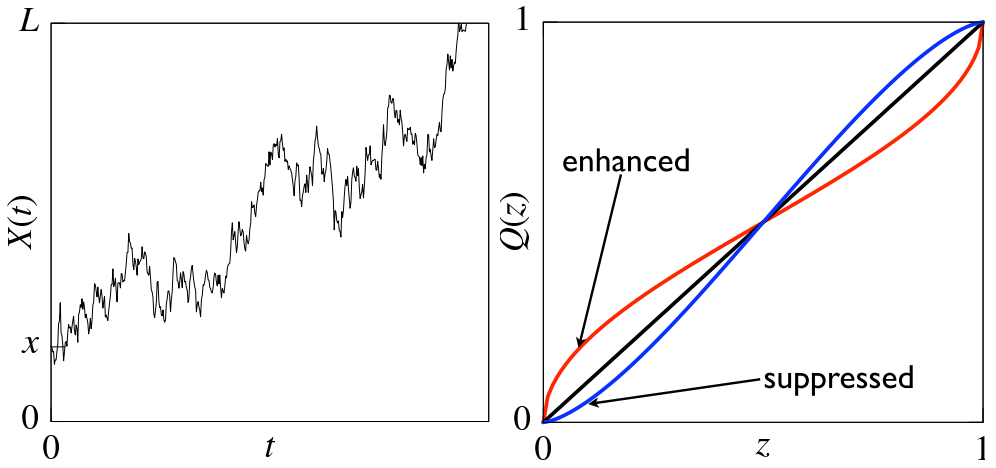

Figure 1.7: (Color online) Left. The evolution of a stochastic process initiated at $X(0) = x$ and terminated upon exiting from the box of size L. Right: The hitting probability $Q(z)$ of a self-affine walker. The solid black line corresponds to the solution for standard diffusion. When $z \to 0$, the hitting probability in presence of anomalous diffusion can be enhanced (red curve) or depressed (blue curve).

The translocation coordinate $s(t)$ can be seen as a random walker evolving in a finite box of size L (L being the polymer length), starting from some initial value $X(0) = x$, $0 < x < L$, and terminated upon touching either boundary for the first time (Fig. 1.7 left). We define the hitting probability $Q(x, L)$ as the probability of exiting the domain through the boundary at L, which corresponds to the polymer completing the translocation. If the stochastic process associated with $s(t)$ is self-affine, the only length scale in the problem is L; thus, $Q(x, L)$ is a function only of the scaled variable x/L: $Q(x, L) = Q(x/L = z)$. For a Brownian motion, $Q(z) = z$, a simple linear function [63]. For a generic stochastic process, $Q(z)$ is non trivial (see for example Fig. 1.7 right) [71].

Observe that the hitting probability is precisely equal to the probability that the global maximum of the process $S(t)$ stays below L until the first time at which it crosses the origin (see Fig. 1.8). This time is actually the so-called first passage time, during which the process does not change sign, and is therefore related to the persistence of the process. The cumulative distribution of the first-passage time for this problem is the survival probability $S(x, t)$ on the half-axis, i.e., the probability that the walker has not left the positive half-axis up to time t. For self affine processes, $S(t)$ is known to have a power law decay at long times, namely,

$$S(x, t \to \infty) \to \frac{1}{t^\theta}, \tag{1.53}$$

where $\theta > 0$ is the so called *persistence exponent* [73]. This non trivial exponent can be computed for a few processes: for instance, the Sparre-Andersen theorem shows that for Brownian motion $\theta = 1/2$ [74]. The value of θ for homogeneous and continuous processes, like fBm, is known explicitly, and reads $\theta = 1 - H$ [68]. The relation between persistence

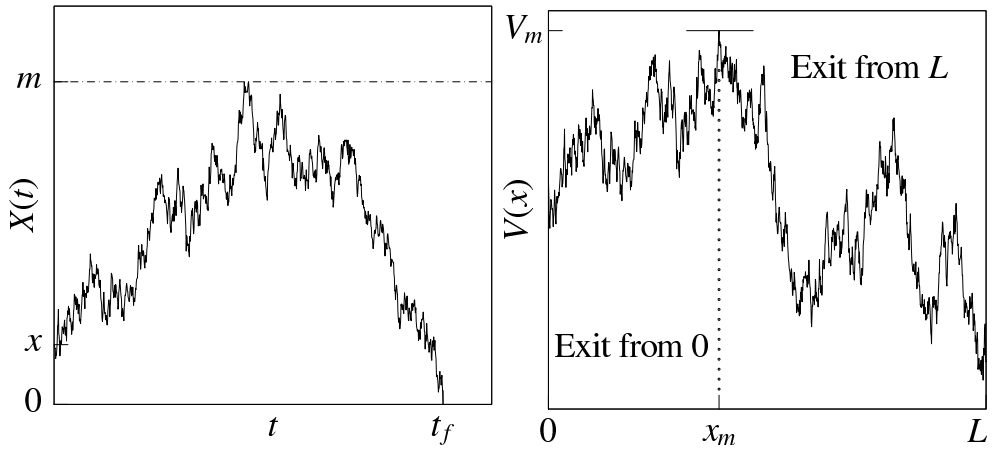

Figure 1.8: Hitting probability. Left: A stochastic process starting at x leaves the positive half-axis for the first time at t_f; m denotes its maximum till t_f (see Sec. 1.6.2). Right: A self-affine disordered potential with maximum at x_m: when L is large, the diffusing particle, starting at $0 < x < L$, exits the box through 0 for $x < x_m$ and through L for $x > x_m$ (see Sec. 1.9).

properties and hitting probability can be then used to infer the properties of the hitting probability close to the origin: it has been shown in [71] that for a self-affine symmetric process, the hitting probability vanishes as

$$Q(z \to 0) \sim z^{\theta/H}. \tag{1.54}$$

In particular, for fBm one gets $Q(z \to 0) \sim z^{(1-H)/H}$, a result which is also supported by direct numerical simulations of fBm paths [71].

For long polymers, the excluded volume effects make the translocation process subdiffusive ($H < 1/2$), which implies that $Q(z)$ vanishes faster than linearly with an exponent $(1-H)/H$ smaller than 1. This means that the translocation of a real self-avoiding polymer is not only longer (because of subdiffusion), but also less likely with respect to the phantom-polymer ideal case.

1.6.3 Effects of the boundaries: the exponent ϕ

We now address a somewhat complementary first-passage problem: we are interested in computing the probability $P(s,t)$ to find a portion s of the polymer translocated at time t, for a finite chain yet to have completed translocation. Up to a normalization constant, $P(s,t)$ coincides with the *propagator* [10] of the process $s(t)$ in the presence of two absorbing boundaries at $s = 0$ and $s = N$. When the method of images holds, the propagator in the

[10] The only difference between the distribution $P(s,t)$ and the propagator is that the latter is not normalized to 1. For a fixed time t, the integral over s of the propagator gives the probability that the process has not been absorbed, i.e., the survival probability in presence of absorbing boundaries.

presence of a boundary can be expressed as a linear combination of free propagators, i.e., propagators of the same process in the absence of boundaries. For a standard Brownian motion, for instance, the free propagator is the Gaussian distribution, and in the presence of two absorbing boundaries the method of the images gives $P(s, t \to \infty) \propto \sin(\pi s/N)$. By construction, this method predicts that $P(s, t)$ vanishes linearly close to an absorbing boundary.

Numerical simulations of the polymer translocation show in contrast that the distribution of $s(t)$ has a non-Gaussian shape [65]. In particular, $P(s, t)$ vanishes *nonlinearly* as s^ϕ and $(N - s)^\phi$ at the two boundaries $s = 0$ and $s = N$, respectively, with $\phi \simeq 1.44$ in $2d$ [65]. This is a rather general feature: actually, it turns out that the method of images systematically fails when the stochastic process displays anomalous diffusion [11]. The simplest geometry for studying the behavior of anomalous walkers close to an absorbing boundary is that of a particle moving on the positive half-axis and killed upon crossing the origin. In this case, the probability density $P_+(s, t)$ of the particle position on the positive half-axis has the scaling form

$$P_+(s, t) \sim t^{-H} R_+(s/t^H), \tag{1.55}$$

where the function $R_+(y)$ vanishes as $\sim y^\phi$. Based on scaling arguments, it has been shown that for homogeneous processes, the exponent ϕ is related to θ by

$$\phi = \frac{\theta}{H}, \tag{1.56}$$

close to the absorbing boundary $y = 0$ [66]. In particular, for fBm one has $\phi = (1-H)/H$. For $2d$ polymers with excluded-volume effects, using $\nu = 3/4$ one gets $H = 2/5$ and $\phi = 3/2$, which is coherent with the value observed in numerical simulations, namely, $\phi \simeq 1.44$ [65]. In $3d$, using $\nu \simeq 0.59$, one predicts $H \simeq 0.46$ and $\phi \simeq 1.18$. More generally, for all homogeneous processes with Hurst exponent H the exponent ϕ is related to the persistence exponent θ of the process via $\phi = \theta/H$. These results are well supported by direct numerical simulations of fBm paths [66].

1.6.4 Perturbation methods

The exact form of $R_+(y)$ is known for Brownian motion, and reads $R_+(y) = y \exp(-y^2/2)$ (setting the diffusion constant $D = 1$). To gain some analytical intuition of non-Markovian processes and to go beyond the scaling arguments or the numerical simulations, one can develop perturbation schemes around the known Brownian solution [72].

Our starting point will be the propagator $P(x, x_0, t)$ of a standard Brownian motion, defined as the probability to find the particle in the interval $[x, x + dx]$ at time t, knowing that the particle was in x_0 at time 0 and is confined by a region of the space. Using the

[11] With the remarkable exception of subdiffusive CTRW, which we will discuss later.

Gaussianity of Brownian motion, we can write the propagator by resorting to the path integral formalism [75], namely,

$$P(x, x_0, t) = \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}[x]\, e^{-\mathcal{S}[x]}\, \Theta[x] \ . \tag{1.57}$$

Note that we use the field-theoretic notation: $f(x)$ is a function of the variable x, and $\mathcal{S}[x]$ is a functional (the action), depending on the function $x(t')$, with $0 < t' < t$. Here, $\Theta[x]$ is an indicator function that is 1 if the path $x(t')$ stays inside the allowed region over the interval $[0, t]$, and 0 otherwise. For regular Brownian motion, the action writes as

$$\mathcal{S}[x] = \frac{1}{4D} \int_0^t dt' \left(\partial_{t'} x\right)^2 , \tag{1.58}$$

and the path integral can be computed.

The first step consists in writing the action for a fractional Brownian motion. To this aim, recall that for any Gaussian process, the statistical weight of a path $x(t')$ without any boundary is proportional to $\exp(-\mathcal{S}[x])$, where the action $\mathcal{S}[x]$, quadratic in x, is given by

$$\mathcal{S}[x] = \int_0^t dt_1 \int_0^t dt_2\, \frac{1}{2} x(t_1) G(t_1, t_2) x(t_2). \tag{1.59}$$

The kernel $G(t_1, t_2)$ of the action is related to the auto-correlation function of the process via $G^{-1}(t_1, t_2) = \langle x(t_1) x(t_2) \rangle$. Then, for a generic fBm we need to invert Eq. 1.50. While it is possible to find the exact action for a generic H, it will be very hard to compute the path integral in Eq. 1.58 in a confined geometry. For this reason, it is preferable to expand the action around the well-known Brownian solution. For $H = 1/2 + \epsilon$, one can write

$$\mathcal{S}[x] = \mathcal{S}^{(0)}[x] + \epsilon\, \mathcal{S}^{(1)}[x] + \ldots , \tag{1.60}$$

where $\mathcal{S}^{(0)}[x]$ is the action in Eq.(1.58) and $\mathcal{S}^{(1)}[x]$ reads

$$\mathcal{S}^{(1)}[x] \ = \ -\frac{1}{2} \int_0^t dt_1 \int_{t_1}^t dt_2\, \frac{\partial_{t_1} x(t_1) \partial_{t_2} x(t_2)}{|t_1 - t_2|} - 2\mathcal{S}^{(0)}[x](1 + \log \tau) \ . \tag{1.61}$$

Note that a regularization for coinciding times $t_1 = t_2 \to \log|t_1 - t_2| = \log \tau$ has been introduced, where $\tau > 0$ is the so-called Ultra Violet cutoff. By using the expansion $e^{-\mathcal{S}[x]} \sim e^{-\mathcal{S}^{(0)}[x]} \left(1 + \epsilon\, \mathcal{S}^{(1)}[x]\right)$ in Eq.(1.57), one realizes that the expression of the first correction $P^{(1)}(x, x_0, t)$ is

$$P^{(1)}(x, x_0, t) = \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}[x] \mathcal{S}^{(1)}[x]\, e^{-\mathcal{S}^{(0)}[x]}\, \Theta[x] \ . \tag{1.62}$$

Here, the path integral is performed over the standard Brownian motion, which is the cornerstone of the proposed perturbation approach.

Setting $H = 1/2 + \epsilon$, $P^{(1)}$ and the scaling function $R_+(y)$ can be computed explicitly to the first order in ϵ [72]. The asymptotic expansions of $R_+(y)$ read

$$\begin{aligned} R_+(y) &\xrightarrow{y\to 0} y\,[1 - 4\epsilon \log y - 2\epsilon(\gamma_{\rm E} + \log 2) + \dots]\,, \\ R_+(y) &\xrightarrow{y\to\infty} y e^{-y^2/2}\,[1 - 2\epsilon \log y + \epsilon(1 - \log 2 - \gamma_{\rm E})]\,, \end{aligned} \tag{1.63}$$

and can be recast to

$$\begin{aligned} R_+(y) &\sim y^{\phi}, \quad y \to 0 \\ R_+(y) &\sim y^{\gamma} e^{-\frac{y^2}{2}}, \quad y \to \infty\ , \end{aligned} \tag{1.64}$$

where the two exponents ϕ and γ are given by

$$\phi = 1 - 4\epsilon + O(\epsilon^2)\ , \quad \gamma = 1 - 2\epsilon + O(\epsilon^2)\ . \tag{1.65}$$

at the first order in ϵ. Using $H = 1/2 + \epsilon$, from Eq.(1.56) one expects $\phi = (1 - H)/H = 1 - 4\epsilon + O(\epsilon^2)$ for fBm. This is in agreement with the results in Eq.(1.65), which sets the scaling arguments on a firmer footing.

Remark that the scaling function $R_+(y)$ given in Eq.(1.63) displays the same leading large-y behavior $\sim e^{-y^2/2}$ as in absence of boundary, at least to $O(\epsilon)$. This behavior can be understood by a simple heuristic argument: the process is not yet aware of the boundary, when being located far from it. This calculation reveals that the process nevertheless knows about the boundary, and $R_+(y)$ correspondingly shows a subleading power-law prefactor y^{γ}, where γ is a new (independent) exponent, whose expression to the order ϵ is given in Eq.(1.65).

1.6.5 Tagged monomer

So far, we have considered the first-passage properties of fBm in connection with the problem of polymer translocation. Fractional Brownian motion is actually the key to the description of several physical and biological systems [76–79]. Among non-Markovian processes, fBm is rather unique, due to its continuous and homogeneous nature: this entails, in particular, the persistence exponent $\theta = 1 - H$. In order to better understand the relevance of these properties, we conclude by discussing in detail an example where fBm plays an important role: the dynamics of a tagged monomer in a standard Rouse chain. This model describes the conformational dynamics of an ideal polymer. Excluded volume interactions are neglected, and each monomer is subjected to a random thermal force and an elastic force induced by the interactions with the neighbours. The Langevin equation for the polymer reads

$$\partial_t U(x,t) = \partial_x^2 U(x,t) + \eta(x,t), \tag{1.66}$$

where U is the position of monomer x at time t, and η is a Gaussian white noise, namely, $\langle \eta(x,t)\eta(x',t')\rangle = 2T\delta(x-x')\delta(t-t')$; here, we will take the temperature $T = 1$. Eq.(1.66)

is linear with respect to U: this means that the process $X(t) = U(x = 0, t) - U(x = 0, 0)$ associated to the tagged monomer is Gaussian and entirely characterized by its autocorrelation function $\langle X(t_1)X(t_2)\rangle$. It is possible to integrate Eq.(1.66) by resorting to the Fourier transform $U_p(t) = \int dx \exp(-ipx)U(x,t)$. Then, Eq.(1.66) becomes

$$\partial_t U_p(t) = -p^2 U_p(t) + \eta_p(t), \tag{1.67}$$

where $\langle \eta_p(t)\eta_{p'}(t')\rangle = 4\pi\,\delta(p+p')\delta(t-t')$, and we get

$$U_p(t) = U_p(0)e^{-p^2 t} + \tilde{U}_p(t) \quad \text{with} \quad \tilde{U}_p(t) = \int_0^t ds e^{-p^2(t-s)}\eta_p(s). \tag{1.68}$$

The autocorrelation function in Fourier space can be computed, and yields

$$\langle \tilde{U}_p(t_1)\tilde{U}_{p'}(t_2)\rangle = 2\pi\,\delta(p+p')\frac{e^{-p^2|t_1-t_2|} - e^{-p^2(t_1+t_2)}}{p^2}. \tag{1.69}$$

Let us recall that $X(t) = \int dp \left[\tilde{U}_p(t) + (e^{-p^2 t} - 1)U_p(0)\right]/(2\pi)$. Now, two relevant cases can be considered: *i*) an equilibrated initial condition, corresponding to $\langle U_{p'}(0)U_p(0)\rangle = 2\pi\,\delta(p+p')/p^2$, and *ii*) a flat initial condition, corresponding to $U_p(0) = 0$. In the former case,

$$\langle X(t_1)X(t_2)\rangle = \frac{1}{\sqrt{\pi}}\left[(t_1)^{1/2} + (t_2)^{1/2} - |t_1 - t_2|^{1/2}\right], \tag{1.70}$$

and the tagged monomer is precisely a fBm with $H = 1/4$, whereas in the second case

$$\langle X(t_1)X(t_2)\rangle = \frac{1}{\sqrt{\pi}}\left[(t_1 + t_2)^{1/2} - |t_1 - t_2|^{1/2}\right], \tag{1.71}$$

a Gaussian process with $H = 1/4$ that is not a fBm. In case *i*), the dynamics is equilibrated and the tagged monomer displacements are identically distributed. In case *ii*), the system evolves from a far-from-equilibrium condition (the flat initial condition) and the jumps are not identically distributed. This provides an example of ageing system: with time, the polymer equilibrates on larger and larger scales. Even in the Gaussian case, very little is known about the first-passage properties of such a process.

1.7 Continuous Time Random Walks and Lévy Flights

The continuous time random walk (CTRW) was initially introduced in [80], and is defined as the process sketched in Fig. 1.4. In its simplest version, one can assume that increments are independent and identically distributed. While in principle CTRW allows for spatially and/or temporally correlated displacements, a fully decoupled version of the model is often considered, which considerably lightens the treatment. Under such assumption, assuming waiting times to have a finite mean and increments to have a finite variance would asymptotically lead to regular Brownian motion, as recalled above. To mimic

the trapping effects often encountered by walkers when traversing complex and/or sticky media, it is common to assume that waiting times have a power-law decay of the kind $\tau^{-1-\alpha}$ with $0 < \alpha < 1$, so that the first moment $\langle\tau\rangle$ is divergent (this implies that very long trapping times become rather frequent). Power-law waiting times coupled with finite-variance spatial increments lead to a subdiffusive behavior, with $H = \alpha/2$. In the limit of a large number of increments, the probability of finding the particle in x at time t converges to

$$P(x,t) = \frac{1}{t^{\alpha/2}} R\left(\frac{x}{t^{\alpha/2}}\right) , \tag{1.72}$$

where $R(y)$ is the Mittag-Leffler function (thus the process is non-Gaussian). CTRW is a well-known model for anomalous diffusion, for which a large number of exact results are available; for instance, the persistence exponent reads $\theta = 2/\alpha$ [56, 57].

Conversely, one can conceive a walker with finite-mean waiting times and (independent and identically distributed) increments having a broad distribution $\varphi(\xi)$, with a diverging second moment, i.e.,

$$\varphi(\xi) \sim \frac{c}{|\xi|^{1+\alpha}} , \ |\xi| \gg 1 , \tag{1.73}$$

with $0 < \alpha < 2$. For the sake of simplicity, we will assume that the process is discrete in time ($\tau_1 = \tau_2 = \ldots = 1$). In this case, the random walk is *Markovian*, *homogeneous* and exhibits a superdiffusive behavior, namely, $x^2(t) \sim t^{2/\alpha}$, i.e., $H = 1/\alpha$. Power-law distributions such as in Eq.(1.73) have been initially studied in the early sixties in economics [81] and in financial theory [82]. Later on, these processes have become very common in Physics, where they have found many applications, encompassing laser-cooling of cold atoms [83], random matrices [84], disordered systems [30], photons in hot atomic vapours [85], and many others. One striking feature of such processes is that their statistical behavior is dominated by a few rare and very large events, whose occurrence is thus governed by the *tail* of the distribution. Moreover, this simple hopping model immediately shows that jumps between far apart sites occur with a finite probability [86].

Analogously as for Brownian motion, after a large number of steps, we expect the statistical properties of $x(t)$ to become independent of the details of $\varphi(\xi)$, except for the index α and the constant c. In this limit, the process is named Lévy flight. In particular, the probability density of finding the particle in x, at a time t, converges to

$$P(x,t) = \frac{1}{t^{1/\alpha}} R\left(\frac{x}{t^{1/\alpha}}\right) , \tag{1.74}$$

where the function $R(y)$ is a Lévy stable distribution (thus the process is non-Gaussian). Although the Fourier transform of $R(y)$ (the characteristic function) has a very simple expression. In general there is no closed-form expression for $R(y)$. An asymptotic expansion shows that

$$R(y) \sim \frac{c}{y^{1+\alpha}} + \mathcal{O}(y^{-1-2\alpha}) . \tag{1.75}$$

The amplitude c plays the same role as σ^2 for the Brownian motion.

First-passage properties of Lévy Flights

By taking the continuous time limit of the hopping process described above, one can derive the so-called Fractional Fokker-Planck equation for a Lévy flight propagator [56], namely,

$$\frac{\partial}{\partial t}P(x,t) = \frac{\pi\, c}{\sin\left(\frac{\alpha\pi}{2}\right)\Gamma(\alpha+1)}\frac{\partial^\alpha}{\partial|x|^\alpha}P(x,t)\ ,\quad P(x,t=0)=\delta(x)\ , \tag{1.76}$$

where $\frac{\partial^\alpha}{\partial|x|^\alpha}$ is the Riesz-Feller derivative of fractional order $\alpha > 0$ [86]. In the Fourier space, $\frac{\partial^\alpha}{\partial|x|^\alpha}$ has the simple form $-|k|^\alpha$, whereas in the real space it takes an integral representation involving a singular kernel of power-law form, which intuitively stems from the long-range increments distribution.

The first-passage properties of Lévy flights, which typically involve eigenvalue problems for the operator $\mathcal{H} = \frac{\pi\, c}{\sin\left(\frac{\alpha\pi}{2}\right)\Gamma(\alpha+1)}\frac{\partial^\alpha}{\partial|x|^\alpha}$, are particularly difficult to solve, precisely due to the non-local nature of the spatial increments (infinite variance implies that walkers can jump across a boundary without touching it, which is not the case of regular Brownian motion; as a consequence, the method of images does not apply). The solution is known in the absence of boundaries, where the Fourier representation is diagonal and the eigenfunctions are simple plane waves. On the contrary, only a very limited number of results are known for Lévy flights on bounded and semi-bounded domains, even for the very simplest geometries; for a survey, see, e.g., [86–89]. The Sparre-Andersen theorem shows that symmetric Lévy flights share the same persistence exponent as the Brownian motion, namely, $\theta = 1/2$ [74]. As a particular case, for $\alpha = 2$, one recovers the standard Laplacian, for which exact results are often known even in confined geometries.

A possible strategy to gain some insight on the behavior of a Lévy flight in the presence of boundaries is to use a perturbation scheme around the $\alpha = 2$ case [90], not dissimilarly as done for fBm. Our starting point will be again the regular Brownian motion. Using the Markovian property of Brownian motion, we can write the Fokker-Planck equation for the propagator P in the familiar Schrödinger form

$$\partial_t P(x,x_0,t) = \mathcal{H}P(x,x_0,t)\ , \tag{1.77}$$

$$P(x,x_0,t=0) = \delta(x-x_0)\ , \tag{1.78}$$

where the operator $\mathcal{H}$ is the standard Laplacian. In Quantum Mechanics, Eq.(1.77) corresponds to the Schrödinger equation of the element (x,x_0) of the density matrix P at the temperature $1/t$, whose general solution reads

$$P(x,x_0,t) = \int dq\, \psi_q^*(x_0)\psi_q(x)e^{E(q)t}\ , \tag{1.79}$$

where $E(q)$ are the eigenvalues and $\psi_q(x)$ the associated eigenfunctions of the operator $\mathcal{H}$. These are the solutions of the eigenvalue problem $\mathcal{H}\psi_q(x) = E(q)\psi_q(x)$, *with the appropriate boundary conditions*, and satisfy the ortho-normality $\int \psi_q(x)\psi_{q'}^*(x)dx = \delta(q-$

q') and closure $\int \psi_q(x)\psi_q^*(x')dq = \delta(x-x')$ relations. Here, the domain of integration over x depends on the boundary conditions and the integration over q is meant over the entire spectrum. If the spectrum is discrete, the integral is replaced by a discrete sum.

Then, we write the Fokker-Planck equation associated to the Lévy flight propagator. For $\alpha = 2-\epsilon$, the operator $\mathcal{H}$ and the propagator can be expanded in powers of ϵ, namely,

$$\begin{aligned} &P(x,x_0,t) = P^{(0)}(x,x_0,t) - \epsilon P^{(1)}(x,x_0,t) + \mathcal{O}(\epsilon^2), \\ &\mathcal{H} = \mathcal{H}_0 - \epsilon\mathcal{H}_1 + O(\epsilon^2)\ , \end{aligned} \tag{1.80}$$

where $P^{(0)}(x,x_0,t)$ is the propagator associated to $\mathcal{H}_0 = \partial_x^2$, with the prescribed boundary conditions. The expression of the first correction $P^{(1)}(x,x_0,t)$ in Eq.(1.80) is known from Quantum Mechanics, and reads

$$P^{(1)}(x,x_0,t) = \int_q \int_{q'} \psi_q(x)\psi_{q'}^*(x_0)\frac{e^{E(q)t} - e^{E(q')t}}{E(q') - E(q)}\langle q|\mathcal{H}_1|q'\rangle, \tag{1.81}$$

where we use the notation $\int_q \equiv \int dq$ and it is understood that $\psi_q(x)$ are the eigenvectors and $E(q)$, the corresponding eigenvalues of $\mathcal{H}_0$. For the matrix elements $\langle q|\mathcal{H}_1|q'\rangle$, we use the bra-ket notation, borrowed from Quantum Mechanics, with $\langle x|q\rangle = \psi_q(x)$. The formula in Eq.(1.81) is the cornerstone of the subsequent perturbation approach.

Setting $\alpha = 2-\epsilon$, one can compute $P^{(1)}$ and $R_+(y)$ at the first order in ϵ. Close to the origin, one gets [90]

$$R_+(y) \sim y - \frac{\epsilon}{2} y\log(y) \sim y^{\alpha/2}\ , \tag{1.82}$$

in agreement with the results $\phi = \theta/H = \alpha/2$. The (non-normalized) propagator in presence of a single boundary has been studied for generic α [87]: it has been shown that $R_+(y)$ vanishes as $\sim y^{\alpha/2}$ when $y \to 0$. This perturbative approach allows conjecturing the exact behavior of the tail of $R_+(y)$, which governs the statistics of rare events:

$$R_+(y) = \frac{c_+}{y^{1+\alpha}} + \begin{cases} \frac{d_+}{y^{2+\alpha}} + o(y^{-2-\alpha})\ ,\ 2 > \alpha > 1\ , \\ \\ \frac{d_+}{y^{1+2\alpha}} + o(y^{-1-2\alpha})\ ,\ 1 > \alpha > 0\ , \end{cases} \tag{1.83}$$

where d_+ is a constant. The leading term $R_+(y) \propto y^{-1-\alpha}$ is coherent with previous investigations [87]. The perturbative approach allows also the amplitude c_+ to be explicitly computed [90], namely, $c_+ = 2c$, where c is the amplitude of the tail of the jump distribution in Eq.(1.73). Observe that the first sub-leading corrections in Eq.(1.83) are also affected by the absorbing wall, as seen by comparison with the free case of Eq.(1.75). These results are supported by numerical simulations.

1.8 Random acceleration model

The random acceleration model is a stochastic process defined by

$$\ddot{x}(t) = \eta(t), \tag{1.84}$$

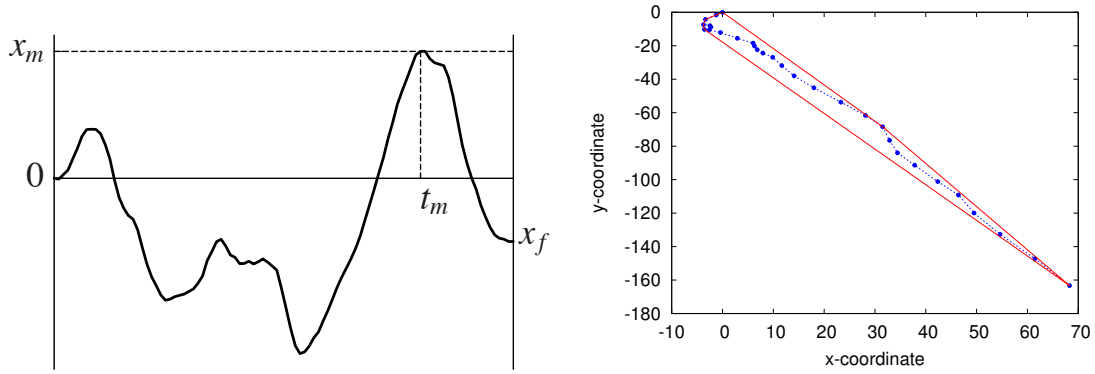

Figure 1.9: (Color online) Left: A realization of a random acceleration process reaching its maximum x_m at t_m. Right: Convex hull of 30 points generated using the discrete random acceleration process. The convex hull is constructed using the Graham span algorithm [91].

where $\eta(t)$ is a Gaussian white noise with $\langle \eta(t) \rangle = 0$ and $\langle \eta(t)\eta(t') \rangle = 2D\delta(t-t')$l [36,92]. The process starts at $x(0) = 0$, with the initial velocity $v(0) = 0$, and it is superdiffusive, with $x^2(t) \sim t^3$, i.e., $H = 3/2$. The random acceleration process in the single variable $x(t)$ is non-Markovian, whereas the position-velocity process is Markovian and does not depend on the past history. The increments $\xi_t = x(t) - x(t-1) = \sum_0^t \eta(t)$ are Gaussian numbers growing as $\sqrt{t}$, so that ξ_t are random numbers not identically distributed. The random acceleration process appears for instance in the continuum description of the equilibrium Boltzmann weight of a semiflexible polymer chain with non-zero bending energy [36]. It can also describe the steady state profile of a $(1+1)$-dimensional Gaussian interface [125] with dynamical exponent $z = 4$, and the continuum version of the Golubovic-Bruinsma-Das Sarma-Tamborenea model [38]. As we will see in the following, in addition to being relevant in many applications, the random acceleration model represents a simple, yet nontrivial, non-Markov process, where some observables of physical interest can be explicitly computed.

1.8.1 Extreme statistics

Recently, the exact distribution of the time t_m, at which a random acceleration process attains its maximum, has been computed [45] (see Fig. 2.3 left). This result represents for the random acceleration process the equivalent of the arcsine law emerging when considering the first-passage properties of Brownian motion and Lévy flights. Further on, we will show that the fluctuations of t_m appear when computing the hitting probability of a particle moving in a random self-affine potential [71], and also in connection with the properties of the convex hull of a two dimensional random walk [93] (see Fig. 2.3 right).

Consider a process $x(t)$, starting from $x(0) = 0$ and observed over a fixed time interval $[0, T]$. Let t_m denote the time at which the process achieves its maximum value x_m during

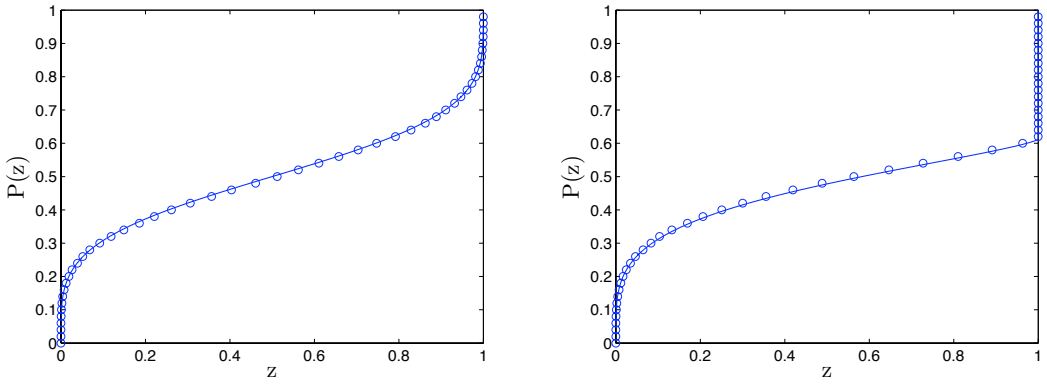

Figure 1.10: (Color online) Simulation results for the cumulative distribution $P(z)$ compared to the analytical results. Left: Integral of a Brownian bridge, the solid line corresponds to Eq.(1.87). Right: Integral of a free Brownian motion, the solid line corresponds to Eq.(1.89).

the interval $[0, T]$ (see Fig. 2.3 left). Since the only time scale in the problem is T, the probability density $p(t_m|T)$ must have the scaling form

$$p(t_m|T) = \frac{1}{T}\, p\left(\frac{t_m}{T}\right), \tag{1.85}$$

where the scaling function $p(z)$, is defined over $0 \leq z \leq 1$. For a random acceleration process, it is possible to compute $p(z)$ with two different boundary conditions [45]: the integral of a Brownian bridge and the integral of a free Brownian motion.

Integral of a Brownian bridge

When the final velocity of the random acceleration process vanishes, $v_f = 0$, the process formally corresponds to the integral of a Brownian bridge. In this case, it has been shown that

$$p(z) = \frac{\Gamma(1/2)}{\Gamma^2(1/4)} \frac{1}{[z(1-z)]^{3/4}}, \tag{1.86}$$

which is evidently *symmetric* around the mid-point $z = 1/2$ and diverges at the two end-points as $z^{-3/4}$ and $(1-z)^{-3/4}$, respectively [45]. It is also useful to consider the cumulative distribution $P(z) = \int_0^z p(z')\, dz'$, which reads

$$P(z) = \frac{\Gamma(1/2)}{\Gamma^2(1/4)}\, B_z\left(\frac{1}{4}, \frac{1}{4}\right). \tag{1.87}$$

Here $B_z(p, q) = \int_0^z x^{p-1}\,(1-x)^{q-1}\, dx$ is the incomplete Beta function.

Integral of a free Brownian motion

When v_f is arbitrary, the random acceleration process formally coincides with the integral of a free Brownian motion. In this case, it is possible to show that

$$p(z) = C\,\delta(z-1) + \frac{(1-C)}{\pi\sqrt{2}} z^{-3/4}\,(1-z)^{-1/4}, \tag{1.88}$$

where $C = 1 - \sqrt{\frac{3}{8}}$ [45]. The density is thus *asymmetric* around the mid-point $t_m = T/2$ (i.e., $z = 1/2$), and the maximum may either occur at some time *strictly* shorter than T, namely $t_m < T$ (i.e., $z < 1$), or with a finite non-vanishing probability $C = 0.387628..$ at the end point of the interval $t_m = T$ (or equivalently $z = 1$). In other words, roughly 38.67% of all trajectories, starting at $x(0) = 0$ and $v(0) = 0$, achieve their maximum only at the end of the interval $[0, T]$. The corresponding cumulative distribution $P(z) = \int_0^z p(z')\,dz'$ is given by

$$P(z) = C\,\Theta(z-1) + \frac{(1-C)}{\pi\sqrt{2}}\, B_z\left(\frac{1}{4}, \frac{3}{4}\right), \tag{1.89}$$

where $\Theta(z-1)$ vanishes for $z < 1$ and is equal to 1 for $z = 1$, i.e, $P(z)$ exhibits a discontinuous jump at $z = 1$ from $1 - C = \sqrt{3/8}$ to 1.

A plot of $P(z)$ for both boundary conditions is provided in Fig. 1.10, where it is also compared to direct simulation results: an excellent agreement between analytical and numerical results is found.

1.8.2 Convex hull of a random acceleration process

It has been recently shown that the problem of computing the mean perimeter and area of the convex hull of *any two dimensional* stochastic process can be mapped, using Cauchy's formulae [94], to the problem of computing the moments of the maximum and the time at which the maximum occurs for the associated one dimensional component stochastic process [95, 96]. Following this general mapping, the average perimeter and area of the convex hull are given by

$$\langle L(t)\rangle = 2\pi\langle x_m(t)\rangle \tag{1.90}$$

$$\langle A(t)\rangle = \pi\left[\langle x_m^2(t)\rangle - \langle y^2(t_m)\rangle\right], \tag{1.91}$$

where $y(t_m)$ is the ordinate of the process at t_m, i.e., when the displacement along the x direction is maximal. Using the results obtained for the extreme statistics of the one dimensional random acceleration process it is possible to show that the mean perimeter and area of the convex hull associated to a two-dimensional random acceleration process of duration T, starting from the initial zero velocity conditions $v_x(0) = v_y(0) = 0$, are

given by the following exact expressions

$$\langle L(T)\rangle = \sqrt{\frac{3\pi}{2}}\, T^{3/2} = (2.1708\ldots)\, T^{3/2} \tag{1.92}$$

$$\langle A(T)\rangle = \frac{5\pi}{192}\sqrt{\frac{3}{2}}\, T^{3} = (0.100199\ldots)\, T^{3}. \tag{1.93}$$

1.9 Digression on the hitting probability

We have previously discussed the fundamental role played by the hitting probability in the context of polymer translocation. More generally, the hitting probability $Q(x, L)$ of a particle undergoing anomalous diffusion is key to understanding phenomena as diverse as the classical gambler's ruin problem in finance and risk management [63] or the transport of charge carriers in conductors with disordered impurities [30]. In this latter case, it is important to discuss the behavior of a particle in a correlated disordered potential $V(x)$. To provide an example, we consider the case of a strongly correlated self-affine disordered potential $V(x) \sim x^{H_V}$ with $H_V > 0$. For $H_V = 1/2$, the potential $V(x)$ is a trajectory of a Brownian motion in space and one recovers the Sinai model. In this class of models, the maximal barrier that the particle has to overcome grows with the size of the system as L^{H_V}. By the Arrhenius law for the activated dynamics, the time required for a particle diffusing in $V(x)$ to overcome an energy barrier scales as $t \sim e^{V(x)}$. We deduce that

$$x(t) \sim [\log(t)]^{1/H_V}\,, \tag{1.94}$$

where for $H_V = 1/2$, one recovers the well known $x(t) \sim \log^2(t)$. Thus, the particle motion is a self-affine process as a function of the variable $\log(t)$, with a Hurst exponent $H = 1/H_V$. It is actually possible to show that for this problem the hitting probability is related to the statistics of the *maximum location* x_m of the process $V(x)$ (see Fig. 5 right). The location of the extreme value of a process plays an important role in many situations. In the context of finance, for example, a trader is interested in knowing the time at which the stock price is at its highest. For symmetric Lévy flights and Brownian motion, the distribution of such maxima is the celebrated Lévy arcsine law [97], namely,

$$p(x_m) = \frac{1}{\pi}\frac{1}{\sqrt{x_m(L - x_m)}}. \tag{1.95}$$

Computing this quantity for a generic process is a formidable task (we have actually shown that $p(x_m)$ can be computed for the random acceleration process). Using the relation between the hitting probability and the maximum location it is possible to prove that the survival probability of a particle in a correlated disorder potential $V(x)$ behaves as

$$S(x, t \to \infty) \to \frac{1}{[\log(t)]^{\theta_V/H_V}}, \tag{1.96}$$

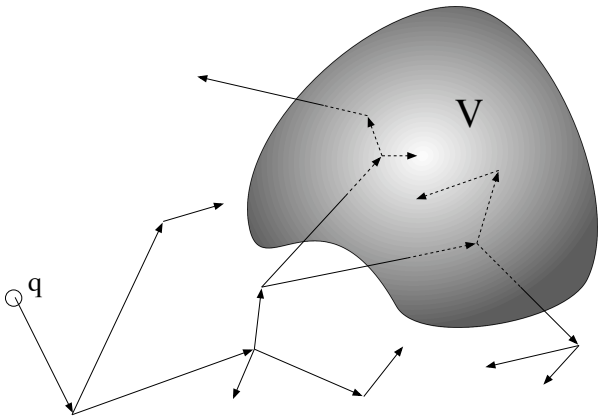

Figure 1.11: A random walk with branching and death, starting from a source q and traversing a volume V.

where θ_V is the persistence exponent of the process $V(x)$. For instance, in the Sinai model, using $\theta_V = 1/2$, $H_V = 1/2$, we get $S(t) \sim 1/\log(t)$, in agreement with the exact result [98,99]. A random acceleration process potential would be self-affine with $H_V = 3/2$ and persistence exponent $\theta_V = 1/4$ [36]. Thus, for this potential the survival probability up to time t would decay as $\sim (\log t)^{-1/6}$, with $\theta = 1/6$.

1.10 Problems: Residence Time for the random acceleration processes

After having to study the random acceleration model which is a non- Markov stochastic processes Rosso *et al* [45] have analyzed the distribution $p(t_m|T)$ of the time t_m at which the particle reaches its maximum displacement if it begins at the origin with velocity zero and is randomly accelerated for a time T. They obtain simple analytic expressions both for integrals of Brownian bridges (trajectories constrained to return to $v = 0$ in a time T) and integrals of free Brownian motion (no restrictions on the trajectory at T). For ordinary unrestricted Brownian motion beginning at the origin, both distributions $p(t_m|T)$ and $p(t_{occup}|T)$, where t_{occup} is the time the process spends on the positive half axis within the interval [0,T], are given by [46, 53] Lévy's arcsine law $p(t|T) = \pi^{-1}[t(T-t)]^{-1/2}$. For random acceleration, on the basis of their numerical evidence, Rosso *et al* [45] conclude that $p(t_{occup}|T)$ does not coincide with either of their results for $p(t_m|T)$. Therefore, computing the occupation time distribution $p(t_{occup}|T)$ for random acceleration model remains a challenging, currently unsolved problem.

1.11 Conclusion

In this chapter, we have presented some basic concepts necessary to understand irreversible processes. We have analyzed some of the first-passage properties of a few relevant anomalous diffusion processes, namely, fractional Brownian motion, Lévy flights and Continuous Time Random Walks, and the random acceleration model. To this aim, different and often complementary approaches have been adopted: scaling arguments, numerical simulations, perturbation schemes and mapping to extreme value statistics. Several extensions of the results recalled here are possible: for instance, the analytical and numerical tools described above are invaluable also in the analysis of the first-passage properties of branching random walks with death, which emerge in relation with, e.g., the spread of epidemics, the migration of reproducing bacteria and the multiplication of neutrons in nuclear reactors [100, 101]. In this context, some results have been recently obtained concerning the statistical fluctuations of the convex hull of a branching Brownian motion (via the mapping based on Cauchy's formulae) [102], and the residence time spent by branching processes within a given volume (by resorting to a path-integral formulation) [103,104]. The tools to model these phenomena, continuous time random walk, stochastic processes, and fractional diffusion equations, are still active research topics. The residence time mentioned in this chapter will be on interest in the next chapter, where we will study with numerical and analytical tools, the statistics of the residence time, for the non markovian process.

Chapter 2

METHODOLOGY

Contents

2.1 Introduction

Over the past decades, it has turned out that the Fokker-Planck equation provides a powerfull tool with which the eïňĂects of fluctuations close to transition points can be adequately treated and that the approached based on the Fokker-Planck equation are superior to other approaches, e.g, based on the Langevin equations. Quite generally, the Fokker-Planck equation plays an important role in problems which involve noise. Fluctuations are a very common feature in a large number of fields. Nearly, every system is subjected to complicated external or internal influences that are not fully known and that are often termed noise or fluctuations. The Fokker-Planck equation was first applied to the Brownian motion problem. Here the system is a small, but macroscopic particle [17], immersed in fluid. The molecules of the fluid kick around the particle in an unpredictable way so the position of the particle fluctuates. Because of these fluctuations, we do not know its position exactly, but instead we have a certain probability to find the particle in a given region. With the Fokker-Planck equation, such a probability density can be determined. This equation is now used in a number of different fields in natural science, for instance in statistical physics, chemical physics, and theoretical biology.

In this chapter, we will present numerical and analytical tools used like framework of our thesis to study the statistics of the residence time for the non-Markovian process. To undertake the analytical studies, we will call upon the Fokker-Planck equation, and as for the numerical aspect, we will employ Monte Carlo methods.

2.2 Random variable and probability density

We assume that there is a certain prescription how to obtain a number ξ. This prescription may consist for instance [17] in the following experiments:

(i) tossing a coin and writing 0 for head and 1 for tail;

(ii) casting a die and counting the number of spots;

(iii) measuring the length of a rod.

We call ξ a random variable if the number ξ can not be predicted. By repeating the experiment N times(N realizations), we obtain N numbers

$$\xi_1, \xi_2, \ldots, \xi_N. \tag{2.1}$$

These numbers ξ_N may take only integer (case (i),(ii)) or continuous (case(iii)) values.

2.2.1 Average

Whereas the numbers ξ_1,ξ_2 ... can not be predicted, some averages for $N \to \infty$ may be predicted and should give the same value for identical systems. The simplest average value is the mean value:

$$\langle \xi \rangle = \lim_{N\to\infty} \frac{1}{N}(\xi_1 + \xi_2 + \ldots \xi_N). \tag{2.2}$$

A general average value is

$$\langle f(\xi) \rangle = \lim_{N\to\infty} \frac{1}{N}[f(\xi_1) + \ldots f(\xi_N)], \tag{2.3}$$

where $f(\xi)$ is some arbitrary function.

The set of states and the probability distribution together fully define the stochastic variable, but a number of additional concepts are often used. The average or expectation value of any function $f(\xi)$ defined on the same state space is

$$\langle f(\xi) \rangle = \int f(x)p(x)dx. \tag{2.4}$$

In particular $\langle f(\xi) \rangle = \mu_m$ is called the $m - th$moments of ξ and μ_1 the average of mean. Also

$$\sigma^2 = \left\langle (\xi - (\langle \xi \rangle)^2) \right\rangle = \mu_2 - \mu_1^2, \tag{2.5}$$

is called the variance or dispersion, which is square of the standard deviation σ.

2.2.2 Characteristic Function and Cumulants

The characteristic function $\mathcal{C}_\xi(u)$ of the stochastic variable u, whose range I is the set of real numbers or a subset, thereof is the average

$$\mathcal{C}_\xi(u) = \langle e^{iu\xi} \rangle = \int_I e^{iux}\, W_\xi(x)\, dx. \tag{2.6}$$

It exists for real ξ and has the properties

$$\mathcal{C}_\xi(0) = 1, \mid \mathcal{C}_\xi(u) \mid \leq 1. \tag{2.7}$$

From this characteristic function we obtain the nth moment M_n

$$M_n = \langle \xi^n \rangle = \frac{1}{i^n} \frac{d^n C_\xi(u)}{du^n} \mid_{u=0} . \tag{2.8}$$

The characteristic function Eq.(2.6) is also the moment generating function in the sense that the coefficients of its Taylor expansion in u are the moments:

$$\mathcal{C}_\xi(u) = \sum_{m=0}^{\infty} \frac{(iu)^m}{m!} M_m. \tag{2.9}$$

This implies that the derivatives of $\mathcal{C}_\xi(u)$ at $u = 0$ exist up to the same m as the moments. If we know all the moments, we thus have the characteristic function. The same function also serves to generates the cumulants $\mathcal{K}_m$ which are defined by:

$$\ln \mathcal{C}_\xi(u) = \ln \sum_{m=0}^{\infty} \frac{(iu)^m}{m!} M_m = \sum_{m=1}^{\infty} \frac{(iu)^m}{m!} \mathcal{K}_m. \tag{2.10}$$

It follows from these relations that the first n cumulants can be expressed by the first n moments, e.g, [1]

$$\begin{aligned} \mathcal{K}_1 &= M_1, \\ \mathcal{K}_2 &= M_2 - M_1^2, \\ \mathcal{K}_3 &= M_3 - 3M_1M_2 + 2M_1^3, \\ \mathcal{K}_4 &= M_4 - 3M_2^2 - 4M_1M_3 + 12M_1^2M_2 - 6M_1^4. \end{aligned} \tag{2.11}$$

2.2.3 Gaussian Distribution

Let us consider only those probability densities where all cumulants [17],

$$\mathcal{K}_{m_1,\ldots,m_r} = \left(\frac{\partial}{\partial i u_1}\right)^{n_1} \ldots \left(\frac{\partial}{\partial i u_r}\right)^{n_r} \ln \mathcal{C}_r(u_1, \ldots, u_r) \mid_{u_1=\ldots=u_r=0},$$

except those with $n_1 + n_2 + \ldots + n_r \leq 2$ vanish. We then must have:

$$\mathcal{C}_r(u_1, \ldots, u_r) = exp\Big(\sum_{j=1}^{r} a_j i u_j + \frac{1}{2} \sum_{j,k=1}^{r} \sigma_{jk} i u_j i u_k \Big). \tag{2.12}$$

It follows that the first two moments are given by:

$$\begin{aligned} \langle \xi_j \rangle &= a_j, \\ \langle \xi_j \xi_k \rangle &= \sigma_{jk} + a_j a_k. \end{aligned} \tag{2.13}$$

Equations (2.13) imply that the variance ($j = k$) and the covariance ($j \neq k$) read

$$\langle (\xi_j - \langle \xi_j \rangle)(\xi_k - \langle \xi_k \rangle) \rangle = \sigma_{jk}. \tag{2.14}$$

[1] The general formula is given by H. Risken p. 18. also Yu. V. Prohorov and Yu. A. Rozanov, Probability Theory(Springer, Berlin 1969)p. 165.

The probability density is the inverse Fourier transform of the characteristic function (2.12), i.e

$$W_r(x_1,\ldots,x_r) = (2\pi)^{-r}\int\ldots\int exp\Big[\sum_{j=1}^{r}(a_j-x_j)iu_j - \frac{1}{2}\sum_{j,k=1}^{r}\sigma_{jk}u_ju_k\Big]du_1\ldots du_r. \quad (2.15)$$

The matrix $\sigma_{jk}=\sigma_{kj}$ is assumed to be positive definite. The inverse matrix $(\sigma^{-1})_{jk} = (\sigma^{-1})_{kj}$ and its square root $(\sigma^{1/2})_{jk} = (\sigma^{1/2})_{kj}$, as well as its inverse square root $(\sigma^{-1/2})_{jk} = (\sigma^{-1/2})_{kj}$, exist. [2]

To calculate the integral, we introduce as integration variables

$$\beta_j = \sum_k[(\sigma^{1/2})_{jk}u_k + i(\sigma^{-1/2})_{jk}(x_k-a_k)], \quad (2.16)$$

then, we may write the exponential in equation (2.14) as

$$[\,] = -\frac{1}{2}\sum_j\beta_j\beta_j - \frac{1}{2}\sum_{j,k}(\sigma^{-1})_{jk}(x_j-a_j)(x_k-a_k). \quad (2.17)$$

Because of the jacobian

$$\begin{aligned}\frac{du_1\ldots du_r}{d\beta_1\ldots d\beta_r} = (\frac{d\beta_1\ldots d\beta_r}{du_1\ldots du_r})^{-1} &= [Det(\sigma^{1/2})_{jk}]^{-1},\\ &= (Det\sigma_{jk})^{-1/2},\end{aligned}$$

and because of

$$\begin{aligned}\int\ldots\int exp\Big(-\frac{1}{2}\sum_{j=1}^{r}\beta_j\beta_j\Big)d\beta_1\ldots d\beta_r &= \Big(\int_{-\infty}^{\infty}e^{-\beta^2/2}d\beta\Big)^r,\\ &= (2\pi)^{r/2}.\end{aligned}$$

The final result for the probability density is the general Gaussian distribution

$$W_r(x_1,\ldots,x_r) = (2\pi)^{-r/2}(Det\sigma_{jk})^{-1/2}\times exp\Big[-\frac{1}{2}\sum_{j,k}(\sigma^{-1})_{jk}(x_j-a_j)(x_k-a_k)\Big]. \quad (2.18)$$

2.3 Fokker-Planck equation

Fokker-Planck equation is an partial derivative linear equation which should satisfy the transition probability density from a Markov process. At the origin, a simplified form

[2] The square root of σ may be uniquely defined in such a way that it has positive eigenvalues.

of this equation made it possible to study the Brownian motion. As the majority of the partial derivative equations, it gives explicit solutions only in quite particular cases relating to the same time to the form of the equation, on the form of the field where it is studied. This section is devoted to the presentation of the fundamental equation making it possible to describe the evolution of the laws of probabilities relating to a random Markovian process. We will present specializations of the Chapman-Kolmogorov equation for homogeneous Markovian processes which are very useful to describe various physical situations. In what follows, we consider the Markov continuous processes. They are saying diffusive in the sense where the developed theory makes it possible to generalize the concept of Brownian diffusion to a large class of systems. It ends in applications to the Brownian motion, concerning the distribution of velocity in the general case, and that of the position in the limit of friction.

The characteristic evolution equation of a Markov process, in continuous form, is written

$$p(x, t + \Delta t) = \int_{x \in X} dx' w(x, t + \Delta t \mid x', t) p(x', t). \tag{2.19}$$

The quantity w is the transition probability, probability of passing from value x' at the moment t at the value x at the neighbour later moment $t + \Delta t$.

Let us pose $\Delta x = x - x'$. Equation (2.19) takes now the form [3]

$$p(x, t + \Delta t) = \int d\Delta x W(x, t + \Delta t \mid x - \Delta x, t) p(x - \Delta x, t). \tag{2.20}$$

Let us center the Taylor's development of the integrand on the point $x + \Delta x$. Thus:

$$\begin{aligned} W(x, t + \Delta t \mid x - \Delta x, t) p(x - \Delta x, t) = W(x + \Delta x, t + \Delta t \mid x, t) p(x, t) + \\ \sum_{m=1}^{+\infty} \frac{1}{m!} (-\Delta x)^m \frac{\partial^m}{\partial x^m} W(x + \Delta x, t + \Delta t \mid x, t) p(x, t). \end{aligned} \tag{2.21}$$

Let us defer equation (2.21) in equation (2.20). The first term of the second member, once integrated on Δx, gives simply $p(x, t)$; making pass $p(x, t)$ to the first member, then dividing per Δt and making tend Δt towards zero, one finds:

$$\frac{\partial}{\partial t} p(x, t) = \sum_{m=1}^{+\infty} (-1)^m \frac{\partial^m}{\partial x^m} \left\{ \left[\lim_{\Delta t \to 0} \frac{1}{m!} \frac{1}{\Delta t} \int d\Delta x (\Delta x)^m W(x + \Delta x, t + \Delta t \mid x, t) \right] p(x, t) \right\}. \tag{2.22}$$

While posing:

$$M_m(x) = D^m(x) = \lim_{\Delta t \to 0} \frac{1}{m!} \frac{1}{\Delta t} \int d\Delta x (\Delta x)^m W(x + \Delta x, t + \Delta t \mid x, t) \equiv \lim_{\Delta t \to 0} \frac{1}{m!} \frac{1}{\Delta t} \langle (\Delta x)^m \rangle, \tag{2.23}$$

[3] From now on, the boundary on the variable Δx are not mentioned any more, but it is clear that the integrals are defined.

where the average $\langle \ldots \rangle$ is taken with the distribution $W(x, t \mid x', t')$, the evolution equation (2.20) gives [4]:

$$\frac{\partial}{\partial t}p(x,t) = \sum_{m=1}^{N}(-1)^m \frac{\partial^m}{\partial x^m}\Big[(D)^{(m)}(x)p(x,t)\Big], \tag{2.24}$$

where $N \to +\infty$. Equation (2.24) is what is called the Kramers-Moyal expansion and $(D)^m(x) = M_m(x)$ are the Kramers-Moyal coefficients or the moments of the distribution of $(x-x')$ relatively at the transition probability $W(x, \Delta t \mid x', 0)$. For an ordinary diffusion, with drift, the average deviation $\langle \Delta x \rangle$ grows with time, as well as the standard deviation Δx^2, so that these two quantities are both proportional to the increase Δt: it results from it that at least the first two moments M_1 and M_2 are surely different from zero. However, there is a theorem due to Pawula [105], which states that for a positive transition probability $p(x,t)$, the expansion (2.24) may stop either after the first term or after the second term. If on the other hand, it does not stop after the second term it must contain an infinite numbers of terms. In these conditions, the Kramers-Moyal expansion stops with order 2 included and produced the so called Fokker-Planck equation [5]:

$$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial x}\Big[D^{(1)}(x)p(x,t)\Big] + \frac{\partial}{\partial x^2}\Big[D^{(2)}(x)p(x,t)\Big] \equiv -\widehat{L}_{FP}p(x,t). \tag{2.25}$$

Then, the Fokker-Planck equation can be written as:

$$\frac{\partial p(x,t)}{\partial t} = -\widehat{L}_{FP}p(x,t), \tag{2.26}$$

where $\widehat{L}_{FP}p(x,t)$ is the differential operator.

$$\widehat{L}_{FP}p(x,t) = \frac{\partial}{\partial x}D^{(1)}(x,t) - \frac{\partial^2}{\partial x^2}D^{(2)}(x,t). \tag{2.27}$$

The Fokker-Planck equation (2.25) is well also an assessment equation. By introducing the current J:

$$J(x,t) = \Big[D^{(1)}(x)p(x,t)\Big] + \frac{\partial}{\partial x}\Big[D^{(2)}(x)p(x,t)\Big], \tag{2.28}$$

then, equation (2.25) takes the form:

$$\frac{\partial}{\partial t}p(x,t) + divJ(x,t) = 0. \tag{2.29}$$

The first term with the second member of (2.28) gives the drift [6](and contain the mobolity); the second term is the diffusion current, always present even in the absence of an external force; if $D^{(2)}$ is constant, we find the ordinary Fick's law.

[4] the M_m or D^m do not depend on time by assumption of stationarity

[5] in its simplest form, it is the Einstein equation for the Brownian motion

[6] this term is also called the convection current

Equation (2.29) is in the form of a continuity equation for the probability density $p(x,t)$ where $J(x,t)$ is the probability current. Indeed if we integrate equation (2.29) for $x \in [a,b]$ we get:

$$\frac{\partial}{\partial t}\int_a^b p(x,t)dx = -\int_a^b \frac{\partial}{\partial x}J(x,t)dx = J(a,t) - J(b,t), \tag{2.30}$$

i.e a change in probability density in the interval $[a,b]$, is compensated by a change of flux in that region.

As for the 1-dimensional case, the local form of the continuity equation has an integral counterpart that can be obtained in the following way. Let Ω be the domain of integration (where the stochastic process lives), whose boundary is given by $\partial\Omega$. The n dimensional version of equation (2.29) is then

$$\frac{\partial}{\partial t}\int_\Omega p(\vec{z},t)d\vec{z}) = -\int_{\partial\Omega} \hat{n}.\vec{J}(\vec{z},t)dS. \tag{2.31}$$

where $\hat{n}$ is the unit normal to the boundary $\partial\Omega$ (pointing out). If the probability current vanishes on the $\partial\Omega$, the continuity equation implies that the total probability remains constant (in time) inside the boundary. If $p(\vec{z},t)$ is then normalized at time $t = t_0$, it will remain so far any later times, i.e,

$$\int_\Omega p(\vec{z},t)d\vec{z} = 1 \qquad \forall t > t_0. \tag{2.32}$$

In order to illustrate what precedes, let us take the case where x is a co-ordinate of space, unlimited, noted y,($y \in \mathbb{R}$) and suppose that the moments $D^{(1)}$ and $D^{(2)}$ are constant. p indicates then a density of probability of presence at the point of X-coordinate y on the real line: remultiplied by the numbers of particles, this probability gives the density of particles to the point y. The Fokker-Planck equation (2.25) takes the simple form:

$$\frac{\partial}{\partial t}p(x,t) = -D^{(1)}\frac{\partial}{\partial x}p(x,t) + D^{(2)}\frac{\partial}{\partial x^2}p(x,t). \tag{2.33}$$

Equation (2.33) is nothing other than a skewed ordinary equation. The solution is easily on the basis of the initial condition [7]

$$p(x,t=0) = \delta(x), \tag{2.34}$$

we obtain:

$$p(x,t) = \frac{1}{\sqrt{4\pi D^{(2)}t}}e^{-(x-D^{(1)}t)^2/(4D^{(2)}t)}. \tag{2.35}$$

[7] Any other initial condition is treated by superposition of the solution (2.35), under the terms of the linearity of the Fokker-Planck equation (2.33).

who is a Gaussian package whose center $\langle x\rangle(t)$ varies like $D^{(1)}t$ and whose standard deviation $\langle(x-\langle x\rangle)^2\rangle \equiv \Delta x^2$ varies like $2D^{(2)}t$. It is thus natural to pose:

$$D^{(1)} \equiv v,\ D^{(2)} \equiv D. \tag{2.36}$$

and then:

$$\langle x\rangle(t) = vt,\ \Delta x^2(t) \equiv \langle x^2\rangle(t) - \langle x\rangle^2(t) = 2Dt. \tag{2.37}$$

Remarks

1. The Fokker-Planck equation is defined by the drift term $D^{(1)}(x)$ that characterizes a ballistic motion, and by the diffusion term $D^{(2)}(x)$ characterizing a diffusive motion.

2. The Fokker-Planck equation is said to be linear if the drift and diffusion term do not depend explicitly on time and if

$$D^{(1)}(x) = D^{(1)}(x,t) = D^{(1)} + D^{(1)},\ D^{(2)}(x) = D^{(2)}(x,t) = D^{(2)} \tag{2.38}$$

If on the other hand $D^{(2)}(x) = D_2$, but $D^{(1)}(x)$ is non linear, one has a almost-linear Fokker-Planck equation.

3. Equation (2.35) obtained above starting from the initial condition $\delta(x)$ is actually the transition probability (or conditional probability), noted W before. This assertion is justifiable by the following argument. First of all, let us notice that, by a change of origin of space and time, the solution of the equation of diffusion resulting from $\delta(x-x_0)$ to $t=t_0$ is given by:

$$p(x,t=t_0) = \delta(x-x_0) \quad \Longrightarrow \quad p(x,t) = \frac{1}{\sqrt{4\pi D(t-t_0)}} e^{-[x-x_0-v(t-t_0)]^2/[4D(t-t_0)]}. \tag{2.39}$$

It is thus legitimate to identify this new solution with $W(x,t \mid x_0,t_0)$ and to thus write, for the Fokker-Planck equation with its first two constant moments:

$$W(x,t \mid x_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}} e^{-[x-x_0-v(t-t_0)]^2/[4D(t-t_0)]}. \tag{2.40}$$

This observation makes it possible to find the law of distribution $p(x,t)$ for an unspecified initial condition.

$$p(x,t) \equiv p_1(x,t) = \int_{\mathbb{R}} dx_0 \quad p_2(c,t,x_0,t_0),\ p_2(x,t,x_0,t_0) = W(x,t \mid x_0,t_0)p_1(x_0,t_0), \tag{2.41}$$

by definition of the laws of distribution to one and two values. We deduce from it that the solution at the moment t exits of the unspecified distribution at the initial moment is the convolution of space:

$$p(x,t) = \int_{\mathbb{R}} dx' \, \frac{1}{\sqrt{4\pi D(t-t_0)}} e^{-[x-x_0-v(t-t_0)]^2/[4D(t-t_0)]} p_0(x'), \tag{2.42}$$

where $p_0(x')$ is not other than $p(x', t_0)$. On such an expression, we check the following points easily:

- if $t \to t_0$, the core W tends towards $\delta(x - x_0)$, so that $p(x,t)$ tends well towards $p_0(x)$
- if $p_0(x)$ is related again a Dirac function, $\delta(x - x_0)$, the solution [8] (2.39) well is found.
- if $p_0(x)$ is Gaussian, (2.42) revealed the convolution of two Gaussian, whose result is still Gaussian.

2.3.1 Boundary conditions for the Fokker-Planck equation

The continuity equation in its integral form (Eq.(2.30) and Eq.(2.31)) suggests that, in order to have a well defined problem, boundary conditions (BC) for the Fokker-Planck equation have to be specified. Let's consider first the 1-dimensional case. Different BC can be taken into account

a. Natural boundary conditions In this case, the process is defined on $\mathbb{R}$ and the condition is the one in which the probability current vanishes at the boundaries $s = x_{min} = -\infty$ and $x_{max} = +\infty$. This would imply the conservation of the normalization for $p(x,t)$ since

$$\int_{-\infty}^{+\infty} p(x,t)dx = const. \tag{2.43}$$

Clearly the decay must be sufficiently rapid to ensure the normalization of the integral above.

b. Reflecting boundary conditions For a reflecting boundary condition at $x = a$ the flux at a must be zero

$$J(a,t) = 0 \ \ \forall t. \tag{2.44}$$

This gives:

$$D^{(1)}(a,t)p(a,t) - \frac{\partial}{\partial x} D^{(2)}(x,t)p(x,t)|_{x=a} = 0 \ \ \forall t. \tag{2.45}$$

Let us note that the natural boundary conditions can be seen as a particular case of reflecting BC. A physical example is the case of a Brownian particle near an impenetrable wall at $x = a$.

c. Absorbing boundary conditions An absorbing wall at $x = a$ means that particles are removed from the interval $(-\infty, a]$ as soon as they first hit $x = a$. This can occur for example when a chemical reaction at the wall causes molecule to be absorbed or changed to a different chemical species. Another more mathematical reason of using

[8] this is why it is also said that (2.40) is the Green's function of Fokker-Planck equation (2.33)

absorbing boundary conditions is when one is interested in looking at the first passage time of a process as we will see later. The appropriate boundary conditions for an absorbing wall at $x = a$ is

$$p(a,t) = 0 \ \ \forall t, \tag{2.46}$$

i.e there is a zero probability of finding particles at the wall, since they are immediately absorbed.

The above classification can be easily generalized to the multidimensional case of Eq. (2.31). For example, for natural boundary conditions, $\vec{J}$ vanishing at infinity giving

$$\int_{\mathbb{R}^n} p(\vec{z},t)d\vec{z} = 1 \ \ \forall t > t_0. \tag{2.47}$$

2.3.2 Multidimensional case

Definition Chapman-Kolmogorov equation Given a stochastic process of Markov, then the probability of transition $p(x_1;t_1 \mid x_2;t_2)$ and the distribution $W(x;t)$ satisfy:

$$P(x_1;t_1 \mid x_3;t_3) = \int dx_2 p(x_1;t_1 \mid x_2;t_2)p(x_2;t_2 \mid x_3;t_3), \tag{2.48}$$

$$W(x_2;t_2) = \int dx_1 W(x_1;t_1)p(x_1;t_1 \mid x_2;t_2). \tag{2.49}$$

Equation (2.48) is called Chapman-Kolmogorov equation.

In the case of multidimensional Markov processes, in which the random variable ξ is a vector, $\vec{\xi}$, the variable x becomes a vector that we denote as

$$\vec{r}(t) = \{r_1(t), \ldots, r_M(t)\}, \tag{2.50}$$

and the Chapman-Kolmogorov equations becomes:

$$\begin{aligned}\frac{\partial}{\partial t}p(\vec{r},t \mid \vec{r_0},t) = \\ -\sum_i \frac{\partial}{\partial r_i}\Big[D_i^{(1)}(\vec{r},t)p(\vec{r},t \mid \vec{r_0},t)\Big] + \sum_{i,j}\frac{\partial^2}{\partial r_i \partial r_j}\Big[D_i^{(2)}(\vec{r},t)p(\vec{r},t \mid \vec{r_0},t)\Big] \\ + \int_{PV} d\vec{r}\Big[w(\vec{r},t \mid \vec{r'},t)p(\vec{r},t \mid \vec{r_0},t_0) - w(\vec{r'},t \mid \vec{r},t)p(\vec{r'},t \mid \vec{r_0},t_0)\Big].\end{aligned} \tag{2.51}$$

For continuous paths $\vec{r}(t)$, $w(\vec{r},t \mid \vec{r'},t) = w(\vec{r'},t \mid \vec{r},t) = 0$, and we end up with the multidimensional Fokker-Planck equation:

$$\frac{\partial}{\partial t}p(\vec{r},t \mid \vec{r_0},t) = -\sum_i \frac{\partial}{\partial r_i}\Big[D_i^{(1)}(\vec{r},t)p(\vec{r},t \mid \vec{r_0},t)\Big] + \sum_{i,j}\frac{\partial^2}{\partial r_i \partial r_j}\Big[D_i^{(2)}(\vec{r},t)p(\vec{r},t \mid \vec{r_0},t)\Big].$$

where the drift term $D^{(1)}(\vec{r},t)$ is now a vector and the diffusive term $D^{(2)}(\vec{r},t)$ is a semidefinite positive and symmetric matrix.

2.3.3 Fokker-Planck for the 2D(x,v) process

If the stochastic Markov diffusive process considered is a n-component vector $\vec{r}(t) = (r_1(t), r_2(t), \ldots, r_n(t))$ process, we have seen that the one dimensional Fokker-Planck equation generalizes to:

$$\frac{\partial}{\partial t}p(\vec{r},t \mid \vec{r_0},t_0) = -\sum_i \frac{\partial}{\partial r_i}\Big[D^{(1)}(\vec{r},t)p(\vec{r},t \mid \vec{r_0},t_0)\Big] + \sum_{i,j}\frac{\partial^2}{\partial r_i \partial r_j}\Big[D^{(2)}(\vec{r},t)p(\vec{r},t \mid \vec{r_0},t_0)\Big], \tag{2.52}$$

where $D^{(1)}(\vec{r},t)$ is a vector and $D^{(2)}(\vec{r},t)$ a semidefinite positive and symmetric matrix. Perhaps the simplest vectorial stochastic process is related to the one dimensional motion of a mesoscopic particle in a fluid. The motion is described by the position x and by the velocity v of mesoscopic particle. Since x and v are obviously coupled and they are both stochastic, we can see the whole process as a bidimensional stochastic process $\vec{r} = (x(t), v(t))$, whose Langevin equation is given by:

$$\begin{aligned} \Delta x(t) &= v(t)\Delta t, \\ \Delta v(t) &= [-\gamma v(t) + F(x(t))/m]\Delta t + \frac{\sigma}{m}\Delta t^{1/2}\Delta\hat{W}(t). \end{aligned} \tag{2.53}$$

In order to establish the corresponding Fokker-Planck equation we have to determine the vector:

$$D^{(1)}(\vec{r},t) = \begin{pmatrix} D_x^{(1)}(x,v,t) \\ D_v^{(1)}(x,v,t), \end{pmatrix} \tag{2.54}$$

and the matrix:

$$D^{(2)}(\vec{r},t) = \begin{pmatrix} D_{xx}^{(2)}(x,v,t) & D_{xv}^{(2)}(x,v,t) \\ D_{vx}^{(2)}(x,v,t) & D_{vv}^{(2)}(x,v,t), \end{pmatrix} \tag{2.55}$$

with $D_{vx}^{(2)}(x,v,t) = D_{xv}^{(2)}(x,v,t)$. By following the method presented above, we can say that, as $t \to t_0$

$$\mathbb{E}\{\Delta x(t) \mid x(t) = x', v(t) = v'\} = v'\Delta t, \tag{2.56}$$

$$\mathbb{E}\{\Delta v(t) \mid x(t) = x', v(t) = v'\} = \Big(-\gamma v' + \frac{F(x')}{m}\Big)\Delta t + \mathcal{O}((\Delta t)^2), \tag{2.57}$$

$$\mathbb{E}\{(\Delta x(t))^2 \mid x(t) = x', v(t) = v'\} = (v'\Delta t)^2 = \mathcal{O}((\Delta t)^2), \tag{2.58}$$

$$\mathbb{E}\{\Delta x(t)\Delta v(t) \mid x(t) = x', v(t) = v'\} = v'\Big(-\gamma v' + \frac{F(x')}{m}\Big)(\Delta t)^2, \tag{2.59}$$

$$\mathbb{E}\{(\Delta v(t))^2 \mid x(t) = x', v(t) = v'\} = \frac{\sigma^2}{m^2}\Delta t + \mathcal{O}((\Delta t)^2). \tag{2.60}$$

Dividing by Δt and letting $\Delta t \to 0$, we get:

$$\begin{aligned} D_x^{(1)}(x,v,t) &= v, \\ D_v^{(1)}(x,v,t) &= -\gamma v + \frac{F(x)}{m}, \\ D_{xx}^{(2)}(x,v,t) &= 0, \\ D_{vv}^{(2)}(x,v,t) &= \frac{\sigma^2}{2m^2}, \\ D_{xv}^{(2)}(x,v,t) &= 0. \end{aligned} \tag{2.61}$$

The $2D$ Fokker-Planck equation is then

$$\begin{aligned} \frac{\partial}{\partial t}[p(x,v,t \mid x_0,v_0,t_0)] = & \\ & - \frac{\partial}{\partial x}[vp(x,v,t \mid x_0,v_0,t_0)] - \frac{\partial}{\partial v}\Big[\frac{F-\gamma v}{m} p(x,v,t \mid x_0,v_0,t_0)\Big] \\ & + \frac{\sigma^2}{2m^2}\frac{\partial^2}{\partial v^2}[p(x,v,t \mid x_0,v_0,t_0)]. \end{aligned} \tag{2.62}$$

In general $F(x) = -\frac{\partial u}{\partial x}$.

Remark. If we rewrite the above equation as:

$$\begin{aligned} \frac{\partial}{\partial t}[p(x,v,t \mid x_0,v_0,t_0)] + v\frac{\partial}{\partial x}[p(x,v,t \mid x_0,v_0,t_0)] + \frac{F(x)}{m}\frac{\partial}{\partial v}[p(x,v,t \mid x_0,v_0,t_0)] & \\ = \gamma\Big(\frac{\partial}{\partial x}[vp(x,v,t \mid x_0,v_0,t_0)] + \frac{\sigma^2}{2\gamma m^2}\frac{\partial^2}{\partial v^2}[p(x,v,t \mid x_0,v_0,t_0)]\Big), & \end{aligned} \tag{2.63}$$

we can notice that it has a structure typical of a kinetic equation, i.e. of the form

$$\frac{\partial}{\partial t}[p(x,v,t \mid x_0,v_0,t_0)] + v\frac{\partial}{\partial x}[p(x,v,t \mid x_0,v_0,t_0)] + \frac{F(x)}{m}\frac{\partial}{\partial v}[p(x,v,t \mid x_0,v_0,t_0)] = I_p(x,v,t), \tag{2.64}$$

where the linear operator $I_p(x,v,t)$ is a collision operator that represents the effects of the collisions of the mesoscopic particle with its environment.

2.3.4 Fokker-Planck equation for the co-ordinate

Given a particle subjected to a force of recall and which, drawn aside from its position of balance, returns there "slowly" (with the direction where all the potential energy is consumed almost exclusively by friction, kinetic energy remainder negligible). Under

these conditions, where inertia is negligible, the equation of Langevin in the presence of an external force $F_0(x)$(not-random) is simplified in:

$$\alpha\frac{dx}{dt} = F_0(x) + F(t) \ \ (\alpha = m\gamma). \tag{2.65}$$

It is possible to write a Fokker-Planck equation, but, now, it will be associated to the only process $x(t)$ and will describe the law of distribution of the position and either velocity.

It is necessary to calculate the moments $D^{(m)}$ corresponding to the increases $\Delta x = x(t+\Delta t) - x(t)$, $x(t)$ playing the role of some initial condition. The integration of the equation in times of (2.65) provides:

$$\Delta x \equiv x(t+\Delta t) - x(t) = \frac{1}{m\gamma}\int_t^{t+\Delta t} dt'[F_0(x(t')) + F(t')]. \tag{2.66}$$

By taking the average and while dividing by Δt:

$$D^{(1)}(x) \equiv \frac{1}{\Delta t}\langle\Delta x\rangle = \frac{1}{m\gamma}\lim_{\Delta t\to 0}\frac{1}{\Delta t}\int_t^{t+\Delta t} dt'[F_0(x(t')) + \langle F(t')\rangle] = \frac{1}{m\gamma}F_0(x). \tag{2.67}$$

In the same way:

$$\begin{aligned} D^{(2)}(x) \equiv \frac{1}{2}\frac{1}{\Delta t}\langle(\Delta x)^2\rangle &= \frac{1}{(m\gamma)^2}\int_t^{t+\Delta t} dt'\int_t^{t+\Delta t} dt''\langle[F_0(x(t')) + F(t')][F_0(x(t'')) + F(t'')]\rangle \\ &= \frac{1}{(m\gamma)^2}\Big[[F_0(x(t))\Delta t]^2 + g\Delta t\Big]. \end{aligned} \tag{2.68}$$

Within the limit $\Delta t = 0$, only the second term contributes to $D^{(2)}$ which is worth:

$$D^{(2)} = \frac{g}{(m\gamma)^2}. \tag{2.69}$$

Thus, the Fokker-Planck equation for the Langevin equation within the viscous limit is written taking into account the fact that the first two moments are the only ones to be not-null:

$$\frac{\partial}{\partial t}p(x,t) = -\frac{1}{(m\gamma)}[F_0(x)p(x,t)] + \frac{g}{2(m\gamma)^2}\frac{\partial^2}{\partial x^2}p(x,t). \tag{2.70}$$

The first term is the drift current induced by the external force, the second is the diffusion current

Subsequently, we suppose to simplify that the force F_0 is constant in space. The ratio $F_0/(m\gamma)$, homogeneous at a velocity [9], is constant and is obviously the drift velocity, v, of

[9] According to (2.65) there are now $\langle v\rangle = F_0/(m\gamma)$:$1/(m\gamma)$ is not other than the mobility μ, connected to the constant of diffusion $\mathbf{D}$ by the relation of Einstein $\mathbf{D}/\mu = k_B T$.

the particle under the effect of external force F_0. As for the factor $g/[2(m\gamma)^2]$, we know that it is precisely the coefficient of diffusion of the position D. We have then:

$$\frac{\partial}{\partial t}p(x,t) = -v\frac{\partial}{\partial x}p(x,t) + D\frac{\partial^2}{\partial x^2}p(x,t). \tag{2.71}$$

For the initial condition $p(x, t = 0) = \delta(x)$, the solution of (2.50) is:

$$p(x,t) = \frac{1}{\sqrt{4\pi Dt}}exp\Big[-\frac{(x-vt)^2}{4Dt}\Big]. \tag{2.72}$$

which gives:

$$\langle x\rangle(t) = vt, \;\; \langle (x - \langle x\rangle)^2\rangle = 2Dt. \tag{2.73}$$

Let us make tend towards zero the constant of diffusion D. Equation (2.71) becomes:

$$\frac{\partial}{\partial t}p(x,t) = -v\frac{\partial}{\partial x}p(x,t), \tag{2.74}$$

equation sometimes called [106] equation of Liouville, where space and times appear symmetrically by first order derivative. Its solution which we can find besides while looking at (2.74) is for the same initial condition $p(x, t = 0) = \delta(x)$ as previously, the limit [10] of (2.72).

2.4 Ornstein-Uhlenbeck process

2.4.1 On Langevin Equations

In 1908, the French physicist Paul Langevin (1872-1946) published [107], a description of the Brownian movement different from Einstein′s. Langevin′s approach is based on the Newtonian equations of motion. In fact, we talk in physics more generally about Langevin dynamics as a technique for mathematical modelling of the dynamics of molecular systems. The Langevin approach applies for simplified models accounting for omitted degrees of freedom by the use of stochastic differential equations.

Both Einstein and Langevin obtained by their respective mathematical methods the same physical statement, namely:

$$\sigma_X = \sqrt{E[X(t)^2]} = \sqrt{2Dt}. \tag{2.76}$$

Then, the root-mean-squared displacement of a Brownian particle increases with the square root of time for large times. We derive(2.76) by the Langevin theory. Langevin

[10] For an unspecified initial condition,$p(x, t = 0) = \delta(x)$, the solution within the limit $D = 0$ is:

$$p(x,t) = p(x - vt, 0) \tag{2.75}$$

introduced a stochastic force that pushes the Brownian particle in the velocity space, while Einstein worked in the configuration space. Langevin described the Brownian particle′ s velocity as an Ornstein-Uhlenbeck process (to be defined below) and its position as the time integral of its velocity, whereas Einstein described it as a Wiener process. Thus, $X(t)$ is the position of the large suspended particle at time $t > 0$ and is given by:

$$X(t) = X(0) + \int_0^t U(s)ds, \tag{2.77}$$

where $U(s)$ is the velocity of the particle. The Newtonian second law of motion gives

$$\frac{d}{dt}U(t) = -aU(t) + \sigma F(t) \tag{2.78}$$

where $a > 0$ is a coefficient that reflects the drag force that opposes the particle′ s motion through the solution and $F(t)$ is a random force representing the random collisions of the particle and the surrounding molecules.

We can also write these equations, in very formal fashion, as

$$\frac{d^2}{dt^2}X(t) = -a\frac{d}{dt}X(t) + \sigma F(t). \tag{2.79}$$

The expression (2.78) is called the Langevin equation (for the velocity of the Brownian motion). In physical terms the parameters are $a = \frac{\gamma}{m}$, $\sigma = \frac{\sqrt{g}}{m}$, where γ is the friction coefficient, and is by Stokes law given as $\gamma = 6\pi\eta r$, $r = radius \quad of \quad the \quad diffusing \quad particle$, $\eta = viscosity \quad of \quad the \quad fluid$, m is the mass of the particle, g is measure of the strength of the force F(t).

2.4.2 Wiener process

The process considered is a particular case of the Fokker-Planck equation for a vanishing drift coefficient $D^{(1)} = 0$ and constant diffusion coefficient $D^{(2)}(x) = D = (\beta m\gamma)$. $D^{(1)}$ and $D^{(2)}(x)$ in (2.25) gives the diffusion equation:

$$\frac{\partial}{\partial t}p(x_1, t_1 \mid x_2, t_2) = \frac{\partial^2}{\partial x^2}p(x_1, t_1 \mid x_2, t_2).$$

The Markovien process [11] corresponding is defined as follows:

$$p(x_1; t_1 \mid x_2; t_2) = \frac{1}{\sqrt{4\pi D(t_2 - t_1)}}e^{-\frac{(x_2-x_1)^2}{4D(t_2-t_1)}} \quad t_2 > t_1. \tag{2.80}$$

The general solution for the probability density with the initial distribution $W(x_2, t_2)$ is:

$$W(x, t) = \frac{1}{\sqrt{4\pi Dt}}e^{-\frac{x^2}{4Dt}} \quad t > 0. \tag{2.81}$$

[11] this process is known as Wiener process . It is homogeneous (but non-stationary), Gaussian and of null average.

We need an auxiliary notation:

$$p(t,y,x) = \frac{1}{\sqrt{2\pi t}} e^{-\frac{(y-x)^2}{2t}}, t > 0, -\infty < x < \infty, -\infty < y < \infty. \tag{2.82}$$

Clearly $p(t,x,y)$ is the p.d.f.(probability density function) of a random variable with the distribution $N(x,t)$. This $p(t,x,y)$ is in fact the transition p.d.f. of a Wiener process , as will be made clear below.

Remark. If we with $\sigma > 0$ set

$$p(t,y,x;\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2 t}} e^{-\frac{(y-x)^2}{2\sigma^2 t}}, t > 0, -\infty < x < \infty, -\infty < y < \infty. \tag{2.83}$$

We shall get a process that is also called the Wiener process. In fact, scaling of time, i.e., the definition in (2.70), which has $\sigma = 1$, is known as the standard Wiener process, but we shall not add the qualifier to our statements.

Definition The Wiener process or Brownian motion is a stochastic process $W = W(t)|t \geq 0$ such that:

(i) $W(0) = 0$ almost surely.

(ii) For any n and any finite suite of times $0 < t_1 < t_2 < \ldots < t_n$ and any $x_1, x_2, \ldots, x_n$ the joint p.d.f. of $W(t_1), W(t_2), \ldots, W(t_n)$ is

$$f_W(t_1), W(t_2), \ldots, W(t_n)(x_1, x_2, \ldots, x_n) = p(t_1, x_1, 0)p(t_2 - t_1, x_2, x_1) \ldots p(t_n - t_n - 1, x_n, x_n - 1). \tag{2.84}$$

A sample path of the one-dimensional Wiener process is given in Fig. 2.1.

2.4.3 Fokker-Planck equation for the distribution of the velocity

This process is defined by $D^{(1)}(v) = -\gamma v$ and $D^{(2)}(v) = 2\gamma\mathbf{D} = \frac{2\gamma}{(\beta m\gamma)}$ and described the thermalization of a particle in a fluid at the thermal equilibrium. Then, the Fokker-Planck equation for the distribution of the velocity, $p(v,t)$ is:

$$\frac{\partial}{\partial t}p(v,t) = -\frac{\partial}{\partial v}[(-\gamma v)p(v,t)] + \frac{\partial^2}{\partial v^2}[D^{(2)}p(v,t)], \tag{2.85}$$

$$\frac{\partial}{\partial t}p(v,t) = +\gamma\left[p + v\frac{\partial}{\partial v}\right] + \gamma^2 D\frac{\partial^2}{\partial v^2}. \tag{2.86}$$

For the initial condition $p(v,t \mid v_0,t_0)$ at $t = 0$, it is known that $p(v,t)$ is nothing other that $W(v,t \mid v_0,0)$.

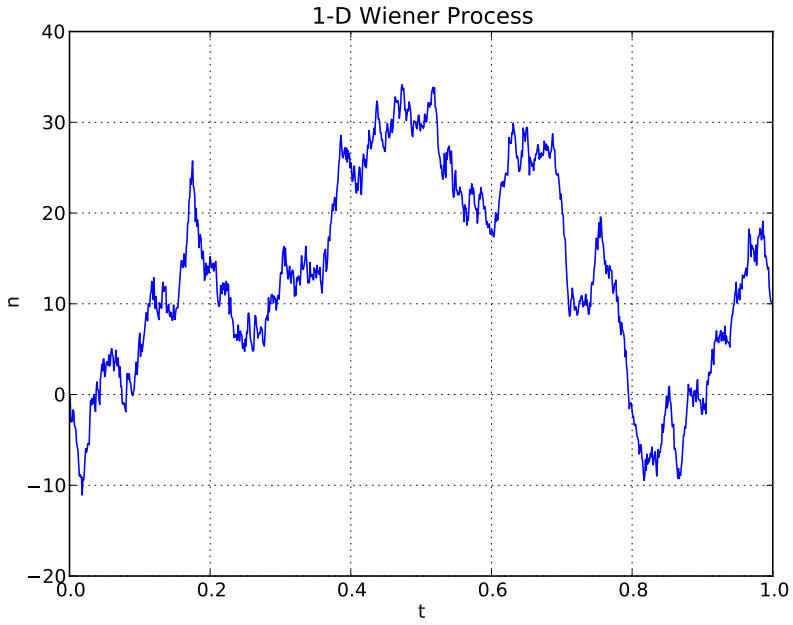

Figure 2.1: (Color online): A sample path of a Wiener Process.

The solution of (2.86) can be found by various methods; simplest being to undoubtedly pass in Fourier transform, which produces the characteristic function of $W(v,t \mid v_0,0)$ and makes it possible to obtain all moments [12]. While thus posing:

$$w_1(s,t) = \int_{-\infty}^{+\infty} dv\, e^{ivs} W(v,t \mid v_0,0). \tag{2.87}$$

We find easily starting from (2.71) that

$$w_1(s,t) = exp\Big[-\frac{D^{(2)}s^2}{2\gamma}(1-e^{-2\gamma t}) + isv_0 e^{-\gamma t}\Big] \tag{2.88}$$

By inverse Fourier transformation, we obtain:

$$W(v,t \mid v_0,0) = \frac{1}{\sqrt{2\pi \mathcal{D}_v(t)t}} exp\Big[-\frac{(v-\langle v(t)\rangle)^2}{2\mathcal{D}_v(t)}\Big] \tag{2.89}$$

with:

$$\langle v(t)\rangle = v_0 e^{-\gamma t}, \;\; \mathcal{D}_v(t) = \frac{D}{\gamma}(1-e^{-2\gamma t}). \tag{2.90}$$

[12] One can also use the method known as of the characteristics ([106], P. 75), which is classical for the partial derivative equations of this type

Finally, we get:

$$p(v,t) = \sqrt{\frac{\gamma}{2\pi D(1-e^{-2\gamma t})}} exp\Big[-\frac{\gamma(v-\langle v(t)\rangle)^2}{2D(1-e^{-2\gamma t})}\Big]. \tag{2.91}$$

The distribution $p(v,t)$, resulting from the Dirac distribution $\delta(v-v_0)$ is thus Gaussian. $\langle v\rangle(t)$ is the average speed at the moment, t when this one is worth surely v_0 at the initial moment; one can thus return the certain factor v_0 in the average and thus deduce the autocorrelation function velocity noted $\mathcal{C}_{vv}(v_0 \equiv v(t=0))$:

$$\langle v(0)v(t)\rangle = v_0^2 e^{-\gamma t}, \tag{2.92}$$

γ^{-1} is the relaxation time associated with an initial fluctuation velocity.

2.4.4 Fokker-Planck equation to several variables

For the Ornstein-Uhlenbeck process, the drift coefficient is linear and the diffusion coefficient constant, i.e.,

$$D^1 = D_i = -\gamma_{ij}x_j; \;\; \gamma_{ij}, D_{ij} = D_{ji}. \tag{2.93}$$

The Fokker-Planck equation can also be solved exactly for an Ornstein-Uhlenbeck process. Given

$$\frac{\partial}{\partial t}W = -\frac{\partial}{\partial x_i}D_i(\{x\}) + \frac{\partial^2}{\partial x_i \partial x_j}D_{ij}(\{x\}). \tag{2.94}$$

We now want to solve this equation. For the transition probability, $p(\{x\},t \mid \{x'\},t')$ equation (2.94) reads:

$$\frac{\partial}{\partial t}p = \gamma_{ij}\frac{\partial}{\partial x_i}(x_j p) + D_{ij}\frac{\partial^2}{\partial x_i \partial x_j}. \tag{2.95}$$

Where p must satisfy the initial condition

$$p(\{x\},t \mid \{x'\},t') = \delta(\{x\}-\{x'\}) \tag{2.96}$$

If we express p by Fourier transform with respect to the variable $\{x\}$, i.e; by

$$p(\{x\},t \mid \{x'\},t') = (2\pi)^{-N}\int e^{i(k_1x_1+\ldots+k_Nx_N)}\tilde{p}(\{k\},t \mid \{x'\},t')d^Nk, \tag{2.97}$$

while replacing $\partial/\partial x_j$ by ik_j and x_j by $i\partial/\partial k_j$, we obtain, for the Fourier transform, the first-order differential equation:

$$\frac{\partial \tilde{p}}{\partial t} = -\gamma_{ij}k_i\frac{\partial \tilde{p}}{\partial k_j} - D_{ij}k_ik_j\tilde{p}. \tag{2.98}$$

Initial condition (2.96) is transformed to:

$$\tilde{p}(\{k\}, t \mid \{x'\}, t') = exp(-ik_j x'_j). \tag{2.99}$$

Because we already know that p and therefore $\tilde{p}$ must be Gaussian functions, we make the 'ansatz' ($\sigma_{ij} = \sigma_{ji}$)

$$\tilde{p}(\{k\}, t \mid \{x'\}, t') = exp[-ik_i M_i(t-t') - \frac{1}{2}k_i k_j \sigma_{ij}(t-t')]. \tag{2.100}$$

Inserting this 'ansatz' into (2.98) leads to

$$\begin{aligned} &\dot{\tilde{p}} + \gamma_{ij}k_i \frac{\partial \tilde{p}}{\partial k_j} + D_{ij}k_i k_j \tilde{p}, \\ &= (-ik_i \dot{M}_i - \frac{1}{2}k_i k_j \dot{\sigma}_{ij} - \gamma_{ij}k_i i M_j - \gamma_{ij}k_i \gamma_{il}k_l + D_{ij}k_i k_j)\tilde{p}, \\ &= 0. \end{aligned} \tag{2.101}$$

This equation requires that M_i and σ_{ij} must obey the differential equations

$$\dot{M}_i = -\gamma_{ij} M_j, \tag{2.102}$$

$$\dot{\sigma}_{il} = -\gamma_{lj}\sigma_{lj} - \gamma_{jl}\sigma_{li} + 2D_{ij}. \tag{2.103}$$

The initial conditions (2.96) requires the following initial conditions for M_i and σ_{ij}:

$$M_i(0) = x'_i;\ \sigma_{ij}(0) = 0 \tag{2.104}$$

The solution of (2.102) with (2.104) can be written as:

$$M_i(t-t') = G_{ij}(t-t')x'_j, \tag{2.105}$$

where $G_{ij}(t)$ is the Green's function of the homogeneous Langevin equation.

Transition Probability Density

Let us insert (2.100) into (2.97), we arrive at:

$$\begin{aligned} p(\{x\}, t \mid \{x'\}, t') \;=\; & (2\pi)^{-N/2}[Det\sigma(t-t')]^{-1/2} \\ & \times exp\{-\frac{1}{2}[\sigma^{-1}(t-t')]_{ij}[x_i - G_{ik}(t-t')x'_k] \\ & \times [x_j - G_{jl}(t-t')x'_l]\}. \end{aligned} \tag{2.106}$$

2.5 Feynman-Kac formula

Solutions of many partial differential equations can be represented as expectation functionals of stochastic processes known as Feynman-Kac formulas; see [108], [109] and [110] for pioneering work of these representations.

Feynman-Kac formulas are useful to investigate properties of partial differential equations in terms of appropriate stochastic models, as well as to study probabilistic properties of Markov processes by means of related partial differential equations. Feynman-Kac formulas naturally arise in the potential theory for Schrödinger equations [111], in systems of relativistic interacting particles with an electromagnetic field [112], and in mathematical finance [113], where they provide a bridge between the probabilistic and the partial differential equation representations of pricing formulae.

Richard Feynman discovered that the Schrödinger equation (the differential equation governing the time evolution of quantum states in quantum mechanics) could be solved by (a kind of) averaging over paths, an observation which led him to a far-reaching reformulation of the quantum theory in terms of "path integrals". [13] Upon learning of Feynman's ideas, Mark Kac realized that a similar representation could be given for solutions of the heat equation (and other related diffusion equations) with external cooling terms. This representation is now known as the Feynman-Kac formula. Later it became evident that the expectation occurring in this representation is of the same type that occurs in derivative security pricing.

The simplest heat equation with a cooling term is:

$$\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2 u}{\partial x^2} - K(x)u, \tag{2.107}$$

where $K(x)$ is a function of the space variable x representing the amount of external cooling at location x.

Theorem: (Feynman-Kac Formula) Let $K(x)$ be a nonnegative, continuous function, and let $f(x)$ be bounded and continuous. Suppose that $u(t;x)$ is a bounded function that satisfies the partial differential equation (2.107) and the initial condition

$$u(0;x) = \lim_{(t;y)\to(0;x)} u(t;y) = f(x) \tag{2.108}$$

Then,

$$u(t;x) = E^x exp\Big\{ -\int_0^t K(W_s)ds \Big\} f(W_t); \tag{2.109}$$

where, under the probability measure P^x, the process $\{F(W_t)\}_{t\geq 0}$ is Brownian motion started at x.

[13] The theory is spelled out in considerable detail in the book Quantum Mechanics and Path Integrals by Feynman and Hibbs. For a nontechnical explanation, read Feynman's later book QED, surely one of the finest popular expositions of a scientific theory ever written.

The hypotheses given are not the most general under which the theorem remains valid, but suffice for many important applications. Occasionally we encounter functions $K(x)$ and $f(x)$ that are not continuous everywhere, but have only isolated discontinuities; the Feynman-Kac formula remains valid for such functions, but the initial condition (2.109) holds only at points x where f is continuous.

An obvious consequence of the formula is uniqueness of solutions to the Cauchy problem (the partial differential equation (2.107) together with the initial condition (2.109).

corollary. Under the hypotheses of Theorem, there is at most one solution of the heat equation (2.107) with initial condition (2.109), specifically, the function u defined by the expectation.

Generalizations of the Feynman-Kac Formula

Two types of generalizations are of particular usefulness in financial applications: (1) those in which the Brownian motion W_t is replaced by another diffusion process, and (2) those where the Brownian motion (or more generally diffusion process) is restricted to stay within a certain region of space.

2.5.1 Feynman-Kac for other diffusion process.

Let P^x be a family of probability measures on some probability space, one for each possible initial point x, under which the stochastic process X_t is a diffusion process started at x with local drift $\mu(x)$ and local volatility $\sigma(x)$.

Theorem in one Dimension

Suppose that under each P^x the process X_t obeys the stochastic differential equation

$$dX_t = \mu(X_t, t)dt + \sigma(X_t, t)dW_t^{\mathbb{Q}}, \tag{2.110}$$

where $W_t^{\mathbb{Q}}$ is Brownian motion under the measure $\mathbb{Q}$. Let $V(x_t, t)$ be a differentiable function of x_t and t; and suppose that $V(x_t, t)$ follows the partial differential equation (PDE) given by:

$$\frac{\partial V}{\partial t} + \mu(x_t, t)\frac{\partial V}{\partial x} + \frac{1}{2}\sigma(x_t, t)\frac{\partial^2 V}{\partial x^2} - r(x_t, t)V(x_t, t) = 0, \tag{2.111}$$

and with boundary condition $V(X_T; T)$. The theorem asserts that $V(x_t; t)$ has the solution

$$V(x_t, t) = E^{\mathbb{Q}}\Big[exp\Big\{-\int_t^T r(x_u, u)du\Big\}V(X_T, T)|\mathcal{F}_t\Big]. \tag{2.112}$$

Note that the expectation is taken under the measure $\mathbb{Q}$ that makes the stochastic term in Equation (2.110) Brownian motion. The generator of the process in (2.110) is defined as the operator:

$$\mathcal{A} = \frac{1}{2}\sigma(x_t, t)^2\frac{\partial^2}{\partial x^2} + \mu(x_t, t)\frac{\partial}{\partial x}. \tag{2.113}$$

So the PDE in $V(x_t, t)$ is sometimes written:

$$\frac{\partial V}{\partial t} + \mathcal{A}V(x_t, t) - r(x_t, t)V(x_t, t) = 0. \tag{2.114}$$

The Feynman-Kac theorem can be used in both directions. That is,

1. If we know that x_t follows the process in Equation(2.110) and we are given a function $V(x_t; t)$ with boundary condition $V(X_T; T)$, then we can always obtain the solution for $V(x_t; t)$ as Equation(2.112).

2. If we know that the solution to $V(x_t; t)$ is given by Equation (2.112) and that x_t follows the process in (2.110), then we are assured that $V(x_t; t)$ satisfies the PDE in Equation(2.114).

2.6 Numerical simulations: a Monte-Carlo approach

Monte carlo methods(by reference to the games of chance of the casinos) are methods of numerical integrations which use random hard copies to realize the calculation of a deterministic quantity. They allows to solve many differently insoluble problem such as for example the evaluation of integrals on complex and/or large-sized fields; the calculation of functional stochastic process or exploration of complex probability distributions. The use of these methods of numerical approximations requires to know to obtain realizations of random variables; to know to control the error of approximation and to study the asymptotic behavior of the methods of simulations; to check in particular which one has a law of the large numbers or a central limit theorem.

Such methods are in particular used in finances by the valorization of options for which there does not exist the closed formula but only numerical approximations. These methods converge slowly and they have like interest to be insensitive at the dimension to studied problems and with the regularity of the function g which we seek to calculate the integral

$$\int_{[0,1]^d} g(x_1, ..., x_d dx_1 ... dx_d = \mathbf{E}[g(u_1, ..., u_d)], \tag{2.115}$$

when the random variables $(u_i, 1 \leq i \leq d)$ are independent and identically distributed from uniform law $\mathfrak{u}([0, 1])$.

The theoretical justification of the method is the strong law of the large numbers which makes it possible to call only upon one realization of a sample; that is at the series $X(w)$ for w. In this section, we present an approach of this method in two non-Markov stochastic processes: (i) the integral of a Brownian bridge up to time T and (ii)the integral of a free Brownian motion up to time T to determine the occupation time distribution $P(t_{occup}|T)$ of the stochastic time t_{occup}; time at which the process spends on the positive half axis within the interval $[0, T]$ of the random acceleration motion.

Our numerical experiments use a Monte Carlo approach, random variables independent identically distributed are simulated with a random number generator and expected

values are approximated by computed averages. For both processes we simulated 10^5 realizations with $T = 1$ and an integration step 1..

→ **Description of the Monte-Carlo method**

To use this method, of Monte-Carlo, one must initially put in the form of an average quantity which we seek to calculate. It is often simple (calculation of integral for example) but can be more complicated (partial derivative equations for example).

At the end of this step, it remains to calculate a quantity of the form $\mathbb{E}(X)$, i.e. the average of the random variable X. To calculate $\mathbb{E}$, it is necessary to know how to sample uncorrelated numbers X_i according to the probability distribution of X. We then have a serie $(X_i)_{1\leq i\leq N}$ of N realizations of the random variable X. We approximate then $\mathbb{E}$ by:

$$\mathbb{E}(X) \simeq \frac{1}{N}(X_1 + \dots X_N). \tag{2.116}$$

2.6.1 Integral of a free Brownian motion

A free Brownian motion is a real random process $x(t)$ coming from zero ($x(0) = 0$) which after T steps is at a random or arbitrary position $x(T)$; and satisfying Langevin's equation

$$\frac{dx}{dt} = \eta(t) \tag{2.117}$$

where $\eta(t)$ is a Gaussian white noise.

Still called Wiener process, over $[0, T]$ it's a random variables $X(t)$ that depends continuously on $t \in [0, T]$ and satisfies the following three conditions [124]:

1. $X(0) = 0$.
2. For $0 < t' < t \leq T$, the random variables given by the increments $X(t) - X(t')$ is normally distributed with mean zero and variance $\delta(t - t')$.
3. For $0 \leq t' < t < t'' < t''' \leq T$, the increments $X(t) - X(t')$ and $X(t''') - X(t'')$ are independent.

But, in this subsection, we are still talking about Brownian motion. For that, We first perform a simulation of 100.000 discretized a random acceleration processes evolving up to time $T = 500$ with a discrete time step δt. Each path is constructed using $T/\delta t$ gaussian random numbers of zero mean and variance $2\delta t$. The python function cumsum() computes first a free Brownian path. A second iteration of cumsum() generates a sample of random acceleration process. Finally, we count the total fraction, of time that each process remains positive and obtain the blue curve of the figure 2.2 which is that of the cumulative distribution of the occupation time.

In this case, by observing the corresponding Figure(see Figure 2.2), we note that for $z = [0, 0.3[$, the numerical curve of the occupation time distribution $P(t_{occup}|T)$ is below the numerical curve of the probability density $P(tm|T)$ of the time maximum tm and for z = [0.3, 0.4[, both curves become confused; and ïňĄnally, the curve of the occupation time

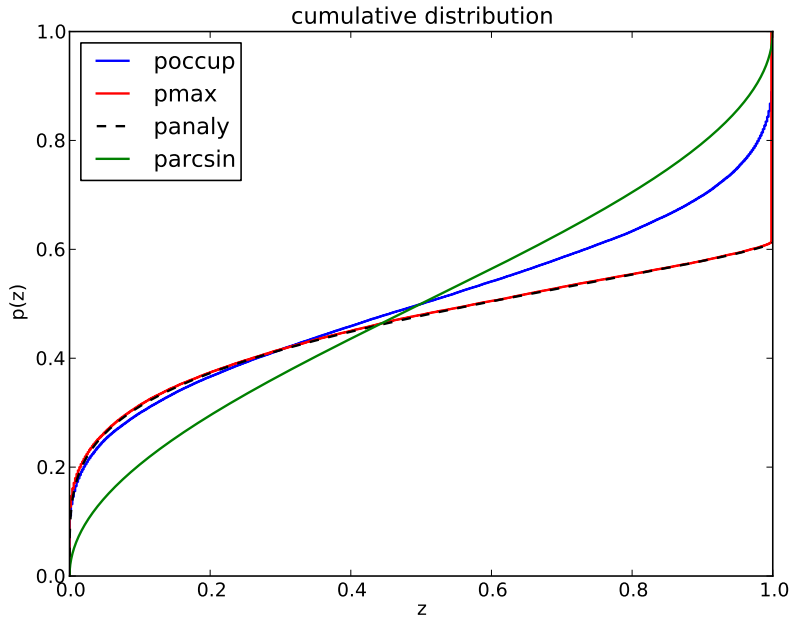

Figure 2.2: Simulation results for the cumulative distribution $p(t_{occup}|T)$(p_{occup}: solid line in blue) as compared to the simulation results for the cumulative distribution (p_{max} or $p(t_m|T)$) $p(z) = \int_0^z p(z')dz'$ (indents line in black) with $0 \leq z \leq 1$, and analytical formula in equation (9) (solid line in red) [45], for the integral of a free Brownian motion. Here parcsin is the arcsine law.

distribution $P(t_{occup}|T)$ increases until $z = 1$, whereas the probability density $P(t_m|T)$ of the time maximum tm exhibits a discontinuous jump at $z = 1$.

2.6.2 Integral of a Brownian bridge

A Brownian bridge is a conditioned Brownian motion to return to its starting point at the end of the fixed time interval T. If one designate by x_l a free Brownian motion coming from 0 on $[0, T]$, we can obtain from x_l a Brownian bridge x_p on $[0, T]$ of the following manner:

$$x_p(t) = x_l(t) - \frac{t}{T}x_l(T). \tag{2.118}$$

We first perform a simulation of 100.000 discretized a random acceleration processes evolving up to time $T = 500$ with a discrete time step δt. Each path is constructed using $T/\delta t$ gaussian random numbers of zero mean and variance $2\delta t$. The python function cumsum() computes first a free Brownian path. A second iteration of cumsum() generates a sample of random acceleration process. Finally, we count the total fraction of time that each process remains positive and obtain the blue curve of the figure 2.3 which is that

of the cumulative distribution of the occupation time. In the case of the integral of a Brownian bridge, we compare our numerical curve of the occupation time distribution t_{occup}, which is a new result with the numerical curve and analytical curve of probability density of time maximum tm obtained in Ref. [45].

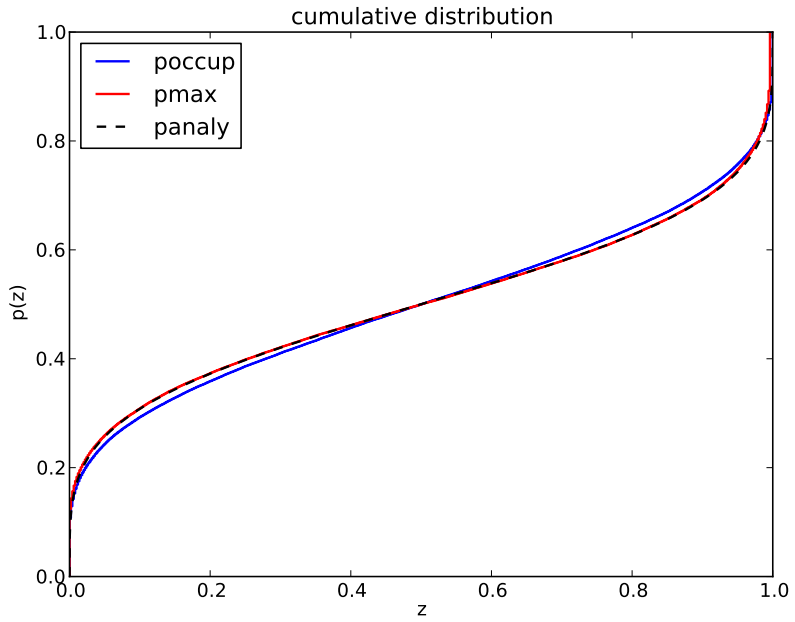

Figure 2.3: Simulation results for the cumulative distribution $p(t_{occup}|T)(p_{occup}$: solid line in blue) as compared to the simulation results for the cumulative distribution (p_{max} or $p(t_m|T)$) $p(z) = \int_0^z p(z')dz'$ with $0 \leq z \leq 1$, (indents line in black) and analytical formula in equation (6) (solid line in red) [45], for the integral of a Brownian bridge.

In this case, by observing the corresponding Figure(see Figure 2.3), we notice that for $z = [0, 0.4[$, the curve of probability density $P(t_m|T)$ of the time maximum is above the numerical curve of the occupation time distribution $P(t_{occup}|T)$. For $z = [0.4, 0.6]$, both curves become confused and for $z =]0.6, 1]$, the numerical curve of the occupation time t_{occup} is above the numerical and analytical curves of the probability density $P(t_m|T)$ of the time maximum.

2.7 Conclusion

In this chapter, we presented the tools as well as the mathematical techniques, and the numerical methods such as Fokker-Planck equations used for the determination of the Green's function or the transition probability density which is the tool necessary to study analytically the statistics of the residence time; and the Monte-Carlo method to find this residence time. The next chapter deals with the results and discussions.

Chapter 3

RESULTS AND DISCUSSION

Contents

3.1 Introduction

Recently, the extreme-value statistics of the process was analyzed, with special emphasis on the global maximum in a given time interval [36,43,44] and the time at which the global maximum is reached [45]. However, the residence time statistics of random acceleration is still not understood in detail. In this chapter we consider a randomly accelerated particle moving in one dimension on the infinite x axis and study the residence time T_+ on the positive x axis. We calculate the first two moments of T_+ analytically and also study the statistics of T_+ with Monte Carlo simulations. Our aims was to learn whether the residence time T_+ of the randomly accelerated particle and the time T_m at which it attains its maximum displacement are statistically equivalent. Both our analytical and Monte Carlo results indicate that this is not the case. This is in contrast to regular Brownian motion, where the distributions of T_+ and T_m coincide and are given by Lévy's celebrated arcsine law [46, 53].

This chapter present the results of our work carried out on the process of acceleration random: the residence time of the random acceleration following by some discussions. In the first section we present the analytical results emerging to the derivation of partial differential equations which determine the moment generating function and the moments

of residence time where the first two moments of the residence time T_+ are calculated and compared with the corresponding moments of the time T_m at which the randomly accelerated particle makes its maximum excursion; in the second section we present the study of the moments T_+ and its distribution with Monte Carlo simulations and compare the results with our analytic predictions for the first two moments of T_+ and with exact results [45] for the distribution of T_m; the third section present the applications and we will finish by a conclusion.

3.2 Analytical Results of the residence time

Consider a randomly accelerated particle moving in one dimension, with coupled evolution equations

$$\frac{dx}{dt} = v, \tag{3.1}$$
$$\frac{dv}{dt} = \eta(t). \tag{3.2}$$

Where $x(t)$ is the particle position, $v(t)$ is the particle velocity, and η is an uncorrelated random white noise [1], with $\langle \eta(t) \rangle = 0$ and $\langle \eta(t)\eta(t') \rangle = 2\gamma\delta(t-t')$, $\gamma > 0$. The process is completed by the initial conditions $x(0) = x_0$ and $v(0) = v_0$ at the time $t = 0$. For the sake of simplicity, we will consider here a one-dimensional setup. The direction of the velocity will be represented by its sign, namely $v_0 > 0$ means that the particle is pointing towards positive x, and vice-versa.

We want to characterize the residence time $T_V(t|x_0, v_0)$ spent within a region A by a particle subject to a random acceleration process starting from x_0 with velocity v_0 when observed up to a time t. The residence time is defined by the path integral

$$T_A(t|x_0, v_0) = \int_0^t V(x(t'))dt', \tag{3.3}$$

where the function $V(x(t))$ is equal to one if $x(t) \in A$ and zero otherwise. In other terms, $V(x(t))$ is the marker function of the region A. By construction, $T_A(t = 0|x_0, v_0) = 0$. Since the underlying process is stochastic, the functional $T_A(t|x_0, v_0)$ defined on the random trajectories of the process is also intrinsically stochastic, and we are interested in determining its distribution.

To this aim, let us define the moment generating function

$$Q_t(s|x_0, v_0) = \langle e^{-sT_A(t|x_0,v_0)} \rangle, \tag{3.4}$$

where s is the variable conjugate to the variable T_A and carries the dimensions of the inverse of a time. Then, it can be verified that the moments of the residence time can

[1] A white noise is a complete process associated a random force $\eta(t)$ definite like Gaussian with singular covariance $\langle \eta(t)\eta(t') \rangle = 2\gamma\delta(t-t')$, $\gamma > 0$; $\langle \eta(t) \rangle = 0$. This terminological origin comes owing to the fact that the Fourier transform of $\langle \eta(t)\eta(t') \rangle$ is constant, i.e. independent of the frequencies, therefore gives even weight to all the frequencies of the spectrum from where the terminological association of this noise with the white color.

be obtained by derivation of the generating function with respect to the variable s. In particular, for the average residence time we have

$$\langle T_A \rangle_t(x_0, v_0) = -\frac{\partial}{\partial s} Q_t(s|x_0, v_0)|_{s=0}. \tag{3.5}$$

For the second moment we have

$$\langle T_A^2 \rangle_t(x_0, v_0) = \frac{\partial^2}{\partial s^2} Q_t(s|x_0, v_0)|_{s=0}. \tag{3.6}$$

By recurrence, we get the m-th moment

$$\langle T_A^m \rangle_t(x_0, v_0) = (-1)^m \frac{\partial^m}{\partial s^m} Q_t(s|x_0, v_0)|_{s=0}, \tag{3.7}$$

for $m \geq 1$. Observe moreover that we have

$$\langle T_A^0 \rangle_t(x_0, v_0) = Q_t(s|x_0, v_0)|_{s=0} = 1. \tag{3.8}$$

It is possible to write down an equation for the evolution of the generating function $Q_t(s|x_0, v_0)$. Let us start with a single particle in x_0 with velocity v_0 at time $t = 0$. Let us consider a total observation time $t + dt$, with dt arbitrary small. Since the process is Markovian with respect the extended phase space (x, v), we can decompose the total observation time $[0, t + dt]$in a first interval between $t = 0$ and $t = dt$, and then a second interval between dt and the final time $t + dt$.

$$Q_{t+dt}(s|x_0, v_0) = \langle e^{-sT_A(t+dt|x_0,v_0)} \rangle = \langle e^{-s\int_0^{dt} V(x(t'))dt'} e^{-s\int_{dt}^{t+dt} V(x(t'))dt'} \rangle. \tag{3.9}$$

By supposing that dt is small, the first term between the expectation time can be evaluated to be

$$e^{-s\int_0^{dt} V(x(t'))dt'} \simeq e^{-sV(x(dt))dt} = e^{-sV(x_0)dt}, \tag{3.10}$$

where we have used the initial condition $V(x(0)) = V(x_0)$. We realize that this term is actually completely deterministic and can be then singled out from the brackets signs:

$$Q_{t+dt}(s|x_0, v_0) = e^{-sV(x_0)dt} \langle e^{-s\int_{dt}^{t+dt} V(x(t'))dt'} \rangle. \tag{3.11}$$

We can then rearrange the integral by translating back by dt the time interval:

$$Q_{t+dt}(s|x_0, v_0) = e^{-sV(x_0)dt} \langle e^{-s\int_0^{t} V(x(t'))dt'} \rangle. \tag{3.12}$$

Concerning the exponential term in the brackets, we observe that is contains two sources of randomness: the fact that the underlying trajectories are stochastic, and the fact that the starting conditions of each realization have now evolved during a time dt. Indeed, since the initial condition of the process is now evaluated at time dt after the initial condition, the behaviour of $x(dt)$ and $v(dt)$ is not known in advance and must be

determined. Observe that the term in the brackets by definition is precisely the generating function of the residence time with an observation time t and random initial conditions:

$$Q_{t+dt}(s|x_0,v_0) = e^{-sV(x_0)dt}\langle e^{-s\int_0^t V(x(t'))dt'}\rangle = e^{-sV(x_0)dt}\langle Q_t(s|x_0+\Delta x, v_0+\Delta v)\rangle, \quad (3.13)$$

where Δx is the amount of displacement of the coordinate x from the initial condition x_0 during the time interval dt, and similarly Δv is the amount of displacement of the coordinate v from the initial condition v_0 during the same time interval dt.

We can now use the Taylor expansion of the function $Q_t(s|x_0+\Delta x, v_0+\Delta v)$ for small Δx and Δv: we have

$$Q_t(s|x_0+\Delta x, v_0+\Delta v) = Q_t(s|x_0,v_0) + \Delta x\frac{\partial}{\partial x_0}Q_t(s|x_0,v_0) + \Delta v\frac{\partial}{\partial v_0}Q_t(s|x_0,v_0) +$$

$$\frac{1}{2}(\Delta x)^2\frac{\partial^2}{\partial x_0^2}Q_t(s|x_0,v_0) + \frac{1}{2}(\Delta v)^2\frac{\partial^2}{\partial v_0^2}Q_t(s|x_0,v_0) + \frac{1}{2}(\Delta x)(\Delta v)\frac{\partial^2}{\partial x_0\partial v_0}Q_t(s|x_0,v_0) + \cdots \quad (3.14)$$

These terms should be now put under the brackets that denote ensemble average with respect to the random realizations. Now, by construction of the process, we have the following

$$\langle \Delta x\rangle = v_0 dt, \quad (3.15)$$

$$\langle \Delta v\rangle = 0, \quad (3.16)$$

$$\langle (\Delta x)^2\rangle = 0, \quad (3.17)$$

$$\langle (\Delta v)^2\rangle = \gamma dt. \quad (3.18)$$

Then, the terms in the previous equation can be reorganized as follows

$$Q_{t+dt}(s|x_0,v_0) = e^{-sV(x_0)dt}\left[Q_t(s|x_0,v_0) + v_0 dt\frac{\partial}{\partial x_0}Q_t(s|x_0,v_0) + \gamma dt\frac{\partial^2}{\partial v_0^2}Q_t(s|x_0,v_0)\right], \quad (3.19)$$

Finally, for small dt we can expand the exponential term as

$$e^{-sV(x_0)dt} = 1 - sV(x_0)dt, \quad (3.20)$$

We can then take the limit for $dt \to 0$ and retain the terms of the order of dt at most:

$$Q_{t+dt}(s|x_0,v_0) = Q_t(s|x_0,v_0) + v_0 dt\frac{\partial}{\partial x_0}Q_t(s|x_0,v_0) + \gamma dt\frac{\partial^2}{\partial v_0^2}Q_t(s|x_0,v_0) - sV(x_0)dtQ_t(s|x_0,v_0). \quad (3.21)$$

By diving by dt we finally get

$$\frac{\partial}{\partial t}Q_t(s|x_0,v_0) = v_0\frac{\partial}{\partial x_0}Q_t(s|x_0,v_0) + \gamma\frac{\partial^2}{\partial v_0^2}Q_t(s|x_0,v_0) - sV(x_0)Q_t(s|x_0,v_0). \quad (3.22)$$

This is precisely the evolution equation for the generating function. We recognize that this equation is formally a backward equation, because derivatives are acting on the initial coordinates x_0 and v_0 of the process.

If we want to derive the equations for the moments, we have to take the derivatives with respect to the variable s. For the average residence time by taking the derivative once we get the equation

$$\frac{\partial}{\partial t}\langle T_A\rangle_t(x_0,v_0) = v_0\frac{\partial}{\partial x_0}\langle T_A\rangle_t(x_0,v_0) + \gamma\frac{\partial^2}{\partial v_0^2}\langle T_A\rangle_t(x_0,v_0) + V(x_0). \quad (3.23)$$

For the second moment, by taking the derivative twice we get

$$\frac{\partial}{\partial t}\langle T_A^2\rangle_t(x_0,v_0) = v_0\frac{\partial}{\partial x_0}\langle T_A^2\rangle_t(x_0,v_0) + \gamma\frac{\partial^2}{\partial v_0^2}\langle T_A^2\rangle_t(x_0,v_0) + V(x_0)\langle T_A^1\rangle_t(x_0,v_0). \quad (3.24)$$

Let us calculate these moments. Using the evolution equations (1) and (2), the position $x(t)$ and the velocity $v(t)$ is obtain from initial values x_0 and v_0 at $t = 0$ following equations:

$$\begin{aligned}\frac{dv}{dt} = \eta(t) &\Longrightarrow v(t) = \int \eta(t')dt' + c \\ &\Longrightarrow v(t) = v_0 + \int_0^t \eta(t')dt'\end{aligned}$$

and

$$\begin{aligned}\frac{dx}{dt} = v(t) &\Longrightarrow x(t) = \int v(t)dt + c \\ &\Longrightarrow x(t) = x_0 + \int_0^t v(t')dt' \\ &\Longrightarrow x(t) = x_0 + v_0t + \int_0^t dt'(\int_0^{t'} \eta(t_1)dt_1) \\ &\Longrightarrow x(t) = x_0 + v_0t + \int_0^t (t-t')\eta(t')dt'\end{aligned}$$

Thus, $v(t)$ corresponds to a Brownian curve or random walk, and $x(t)$ to the integral of a Brownian curve.

We will be particularly interested in the Green function or the propagator or probability density $G_t(\{x\}|\{x\})$ for propagation from the initial position and velocity x_0, v_0 to

the values x, v in a time t to calculate the residence time; thus the equation (3.23) can reads as follow:

$$\begin{aligned} G_t(\{x\}|\{x'\}) &= \sum_{i=1}^{N}\gamma_{ij}\frac{\partial}{\partial x_i}\Big(x_jG_t\Big) + \frac{1}{2}\sum_{i,j=1}^{n}\frac{\partial^2}{\partial x_i\partial x_j}(b_{ij})G_t \\ &= \sum_{i=1}^{N}\gamma_{ij}\frac{\partial}{\partial x_i}\Big(x_jG_t\Big) + D_ij\frac{\partial^2}{\partial x_i\partial x_j}G_t \end{aligned} \tag{3.25}$$

with γ_{ij} and D_{ij} the drift and diffusion matrix.

G_t should satisfy the initial condition

$$G(\{x\}|\{x'\},t') = \delta(\{x\}-\{x'\}). \tag{3.26}$$

Let us express G_t by its Fourier transform with respect to the variables x

$$G_t(\{x\},t|\{x'\},t') = (2\pi)^{-N}\int e^{-i(k_1x_1+.....+k_Nx_N)}\widetilde{G_t}(\{k\},t|\{x'\},t')d^Nk \tag{3.27}$$

and by replacing $\frac{\partial}{\partial x_j}$ by ik_j and x_j by $i\frac{\partial}{\partial k_j}$, we obtain for the Fourier transform the differential equation following:

$$\frac{\partial}{\partial t}\widetilde{G_t} = -\gamma_{ij}k_i\frac{\partial}{\partial k_j}\widetilde{G_t} - D_{ij}\widetilde{G_t}. \tag{3.28}$$

and the initial condition yields:

$$\widetilde{G_t}(\{k\},t|\{x\},t') = exp(-ik_jx'_j). \tag{3.29}$$

since we know that G_t and $\widetilde{G_t}$ must be Gaussian functions, let's apply the ansatz following:

$$\widetilde{G_t}(\{k\},t|\{x'\},t') = exp\Big[\sum_{j=1}^{N}ik_jM_j(t-t') + \frac{1}{2}\sum_{j,k=1}^{N}ik_jik_k\sigma_{jk}(t-t')\Big]. \tag{3.30}$$

Inserting (3.30) into (3.27) $G_t(\{x\},t|\{x'\},t')$ becomes:

$$\begin{aligned} G_t(x,t|x',t') &= (2\pi)^{-N}\int e^{-i(k_1x_1+...+k_Nx_N)}\Big(exp\Big[\sum_{j=1}^{N}ik_jM_j(t-t') + \frac{1}{2}\sum_{j,k=1}^{N}ik_jik_k\sigma_{jk}(t-t')\Big]\Big)d^Nk \\ &= (2\pi)^{-N}\Big(\int e^{-i(k_1x_1+...+k_Nx_N)}\int exp\Big[\sum_{j=1}^{N}ik_jM_j(t-t') - \frac{1}{2}\sum_{j,k=1}^{N}k_jk_k\sigma_{jk}(t-t')\Big]\Big)dk_1\,. \end{aligned} \tag{3.}$$

Let us introduce like variables of integration:

$$\alpha_j = \sum_k \Big[(\sigma^{1/2})_{jk} k_k i (\sigma^{-1/2})_{jk}(x_k - M_k)\Big] \Longrightarrow \sum_k (\sigma^{1/2})_{jk} k_k = \alpha_j - \sum_k i(\sigma^{-1/2})_{jk}(x_k - M_k)$$
$$\Longrightarrow k_k = \frac{\alpha_j}{\sum_k(\sigma)_{jk}} + \frac{\sum_k(\sigma^{-1/2})_{jk} i (M_k - x_k)}{\sum_k(\sigma^{1/2})_{jk}}$$
$$\Longrightarrow dk_k = \frac{d\alpha_j}{\sum_k(\sigma^{1/2})_{jk}}.$$

We arrive at:

$$\begin{aligned}
G_t(\{x\},t|x',t') &= (2\pi)^{-N}\int\ldots\int exp\Big[\sum_{j=1}^{N}(M_j - x_j)ik_j - \frac{1}{2}\sum_{j,k=1}^{N} k_j k_k \sigma_{jk}(t-t')\Big]dk_1\ldots dk_N \\
&= (2\pi)^{-N}\int\ldots\int exp\Bigg[\sum_{j=1}^{N}(M_j - x_j)i\Bigg(\frac{\alpha_j}{\sum_k(\sigma)_{jk}} + \frac{\sum_k(\sigma^{-1/2})_{jk} i(M_j - x_j)}{\sum_k(\sigma^{1/2})_{jk}}\Bigg) \\
&\quad - \frac{1}{2}\sum_{j,k=1}^{N}(\sigma)_{jk}\Bigg(\frac{\alpha_j}{\sum_k(\sigma)_{jk}} + \frac{\sum_k(\sigma^{-1/2})_{jk} i(M_j - x_j)}{\sum_k(\sigma^{1/2})_{jk}}\Bigg) \\
&\quad \Bigg(\frac{\alpha_k}{\sum_k(\sigma)_{jk}} + \frac{\sum_k(\sigma^{-1/2})_{jk} i(M_k - x_k)}{\sum_k(\sigma^{1/2})_{jk}}\Bigg)\Bigg]\frac{1}{\sum_N(\sigma^{1/2})_{jk}}(d\alpha_1\ldots d\alpha_N) \\
&= (2\pi)^{-N}\int\ldots\int exp\Bigg[-\frac{1}{2}\alpha^2 - \sum_j(\sigma^{-1})(M_j - x_j)(M_k - x_k) \\
&\quad + \frac{\sum_{jk}(\sigma^{-1})_{jk}(M_j - x_j)(M_k - x_k)}{2}\Bigg](d\alpha_1\ldots d\alpha_N) \\
&= (2\pi)^{-N}\int\ldots\int exp\Bigg[-\frac{\alpha^2}{2} - \frac{\sum_{jk}(\sigma^{-1})_{jk}(M_j - x_j)(M_k - x_k)}{2}\Bigg](d\alpha_1\ldots d\alpha_N) \qquad (3.32)
\end{aligned}$$

Because the jacobian

$$\frac{dk_1\ldots dk_N}{d\alpha_1\ldots d\alpha_N} = \frac{d\alpha_1\ldots d\alpha_N}{dk_1\ldots dk_N} = (Det\sigma_{jk})^{-1/2}$$

$$\begin{aligned}
G_t(\{x\},t|\{x'\},t') &= (2\pi)^{-N}\frac{1}{(Det\sigma_{jk})^{1/2}}\Bigg(\int\ldots\int exp(\frac{-\alpha^2}{2})d\alpha_1\ldots d\alpha_N\Bigg) \\
&\quad \times exp\Bigg[-\frac{1}{2}\sum_{jk}(\sigma^{-1})_{jk}(M_j - x_j)(M_k - x_k)\Bigg] \\
&= (2\pi)^{-N}\frac{1}{(Det\sigma_{jk})^{1/2}}\Bigg(\int exp(\frac{-\alpha^2}{2})d\alpha\Bigg)^N exp\Bigg[-\frac{1}{2}\sum_{jk}(\sigma^{-1})_{jk}(M_j - x_j)(M_k - x_k)\Bigg] \\
&= (2\pi)^{-N/2}(Det\sigma_{jk})^{-1/2} exp\Bigg[-\frac{1}{2}\sum_{jk}(\sigma^{-1})_{jk}(x_j - M_j)(x_k - M_k)\Bigg] \qquad (3.33)
\end{aligned}$$

but $M_j(t-t') = T_{jk}(t-t')x'_k$ where $T_{jk}(t) = \delta_{ij}$.

Hence the general solution is:

$$G_t(\{x\},t|\{x'\},t') = (2\pi)^{-N/2}(Det\sigma_{jk})^{-1/2}exp\Big[-\frac{1}{2}\sum_{jk}(\sigma^{-1})_{jk}(x_j - T_{jk}(t-t')x'_k)(x_k - T_{kl}(t-t')x'_l)\Big] \quad (3.34)$$

Since $\{x\}$ and $\{x'\}$ are vectors of co-ordinates $\begin{pmatrix} x \\ v \end{pmatrix}$ and $\begin{pmatrix} x_0 \\ v_0 \end{pmatrix}$ and $N = 2$ then the general solution is written:

$$\begin{aligned} G_t(\{x\},t|\{x\},t') &= (2\pi)^{-1}(Det\sigma_{jk})^{-1/2}exp\Big[-\frac{1}{2}(\sigma^{-1})_{xx}(x-x(t))(x-x(t)) - \frac{1}{2}(\sigma^{-1})_{xv}(x-x(t)) \\ &\quad (v-v(t)) - \frac{1}{2}(\sigma^{-1})_{vx}(v-v(t))(x-x(t)) - \frac{1}{2}(\sigma^{-1})_{vv}(v-v(t))(v-v(t))\Big] \quad (3.35) \end{aligned}$$

where σ_{xx}, σ_{vv} ,σ_{xv} and σ_{vx} are the moments of order 2.

The Green function or propagator or probability density for propagation from the initial values x_0, v_0 to x, v in a time t will play a central role in our calculations of the residence time. Calculations of averages $<\Delta x>$, $<\Delta v>$, $<(\Delta x)^2>$, $<(\Delta v)^2>$.

$$\begin{aligned} \langle \Delta x \rangle &= \langle x(t) - x_0 \rangle \\ &= v_0 t + \int_0^t (t-t')\langle \eta(t') \rangle dt' \\ &= v_0 t \end{aligned} \quad (3.36)$$

$$\begin{aligned} \langle \Delta v \rangle &= \langle v(t) - v_0 \rangle \\ &= \int_0^t (t-t')\langle \eta(t')dt' \rangle \\ &= 0 \end{aligned} \quad (3.37)$$

$$\begin{aligned} \langle (\Delta x)^2 \rangle &= \langle (x(t)-x_0)^2 \rangle \\ &= \langle (v_0 t + \int_0^t (t-t')\eta(t')dt')(v_0 t + \int_0^t (t-t_1)\eta(t_1)dt_1) \rangle \\ &= (v_0 t)^2 + \int_0^t dt' \int_0^t (t-t')(t-t_1)\langle \eta(t')\eta(t_1)dt_1 \rangle \\ &= (v_0 t)^2 + 2\gamma \int_0^t dt'(t-t')^2 \\ &= (v_0 t)^2 + \frac{2\gamma t^3}{3} \end{aligned} \quad (3.38)$$

$$\begin{aligned}\langle(\Delta v)^2\rangle &= \langle(v(t)-v_0)^2\rangle \\ &= \langle(\int_0^t \eta(t')dt')(\int_0^t \eta(t_1)dt_1)\rangle \\ &= \int_0^t dt' \int_0^t \langle\eta(t')\eta(t_1)dt_1\rangle \\ &= 2\gamma t \end{aligned} \tag{3.39}$$

$$\begin{aligned}\sigma_{ij} &= \langle(x_i - \langle x_i\rangle)(x_j - \langle x_j\rangle)\rangle \\ &= \langle x_i x_j\rangle - \langle x_i\rangle\langle x_j\rangle\end{aligned}$$

Thus,

$$\begin{aligned}\sigma_{xx} &= \langle(\Delta x)^2\rangle - (\langle\Delta x\rangle)^2 \\ &= \frac{2\gamma t^3}{3}\end{aligned} \tag{3.40}$$

$$\begin{aligned}\sigma_{vv} &= \langle(\Delta v)^2\rangle - (\langle\Delta v\rangle)^2 \\ &= 2\gamma t\end{aligned} \tag{3.41}$$

$$\begin{aligned}\sigma_{xv} &= \langle(\Delta x\Delta v)\rangle - \langle\Delta x\rangle\langle\Delta v\rangle \\ &= \langle(v_0 t + \int_0^t (t-t')\eta(t')dt')(\int_0^t \eta(t_1)dt')\rangle \\ &= v_0 t\int_0^t \langle\eta(t_1)\rangle dt' + \int_0^t dt' \int_0^t (t-t')\langle\eta(t')\eta(t_1)\rangle dt' \\ &= 2\gamma t^2\end{aligned} \tag{3.42}$$

then $\sigma_{xv} = \sigma_{vx} = 2\gamma t^2$

Thus

$$\sigma = \begin{pmatrix} \sigma_{xx} & \sigma_{xv} \\ \sigma_{vx} & \sigma_{vv} \end{pmatrix}$$

$$\sigma = \begin{pmatrix} \frac{2\gamma t^3}{3} & \gamma t^2 \\ \gamma t^2 & 2\gamma t \end{pmatrix} \tag{3.43}$$

$$\begin{aligned}Det\sigma &= \sigma_{xx}\sigma_{vv} - \sigma_{xv}\sigma_{vx} \\ &= \frac{\gamma^2 t^4}{3}\end{aligned}$$

The inverses of σ gives:

$$\sigma^{-1} = \frac{1}{Det\sigma}\begin{pmatrix} \sigma_{vv} & -\sigma_{xv} \\ -\sigma_{vx} & \sigma_{xx} \end{pmatrix}$$

$$\sigma^{-1} = \begin{pmatrix} \frac{6}{\gamma t^3} & -\frac{3}{\gamma t^2} \\ -\frac{3}{\gamma t^2} & 2\gamma t \end{pmatrix} \tag{3.44}$$

Thus according to the equation (3.35) elements of the diffusion coefficient D are:

$$\mathbf{D} = \frac{1}{2}\begin{pmatrix} (\sigma^{-1})_{xx} & (\sigma^{-1})_{xv} \\ (\sigma^{-1})_{vx} & (\sigma^{-1})_{vv} \end{pmatrix}$$

and taking into account the fact that $\{x\}$ and $\{x'\}$ are vectors of co-ordinates $\begin{pmatrix} x \\ v \end{pmatrix}$ and $\begin{pmatrix} x_0 \\ v_0 \end{pmatrix}$ and $N = 2$ and also that $x(t) =< x >= x_0 + v_0 t$ and $v(t) =< v >= v_0$ the general solution of the Fokker-Planck equation (3.35) at several variables is written:

$$\begin{aligned} G_t(\{x\}|\{x'\}) &= (2\pi)^{-1}(3)^{1/2}\gamma^{-1}t^{-2}exp\Big[-\frac{3}{\gamma t^3}(x - x_0 - v_0 t)^2 - \frac{3}{\gamma t^2}(x - x_0 - v_0 t)(v - v_0) - \frac{1}{\gamma t}(v - v \\ &= (2\pi)^{-1}(3)^{1/2}\gamma^{-1}t^{-2}exp\Big\{ -\frac{3t^{-3}}{\gamma}\Big[(x - x_0 - v_0 t)(x - x_0 - vt) + \frac{t^2}{3}(v - v_0)^2\Big]\Big\} \end{aligned} \tag{3}$$

which is the free propagator or the Green function for our process and γ is the damping coefficient.

For $\gamma = 1$ then the Green function takes the form:

$$\begin{aligned} G_t(\{x\}|\{x'\}) &= (2\pi)^{-1}(3)^{1/2}t^{-2}exp\Big[-\frac{3}{t^3}(x - x_0 - v_0 t)^2 - \frac{3}{t^2}(x - x_0 - v_0 t)(v - v_0) - \frac{1}{t}(v - v_0)^2\Big] \\ &= (2\pi)^{-1}(3)^{1/2}t^{-2}exp\Big\{ -3t^{-3}\Big[(x - x_0 - v_0 t)(x - x_0 - vt) + \frac{t^2}{3}(v - v_0)^2\Big]\Big\} \end{aligned} \tag{3.46}$$

3.2.1 Solution of the moment equations

Observe that Eq. (3.24) have the same structure, namely,

$$\frac{\partial}{\partial t}\langle T_A^m\rangle_t(x_0, v_0) = v_0\frac{\partial}{\partial x_0}\langle T_A^m\rangle_t(x_0, v_0) + \gamma\frac{\partial^2}{\partial v_0^2}\langle T_A^m\rangle_t(x_0, v_0) + a(x_0, v_0, t) \tag{3.47}$$

where $a(x_0; v_0; t) = mV(x_0)\langle T_A^{m-1}\rangle_t$ is a source term depending at most on moments of order $m - 1$ is a source term depending at most on moments of order $m - 1$. The initial

condition is $\langle T_A^m \rangle_0(x_0, v_0) = 0$, stemming from $T_A(t = 0|x0; v0) = 0$. Equations of this form have an explicit solution

$$\langle T_A^m \rangle(x_0, v_0) = \int_0^t dt' \int dx' \int dv' a(x', v', t) G_{t-t'}(x', v'; x_0, v_0). \tag{3.48}$$

where $G_t(x; v; x0; v0)$ is the Green's function satisfying

$$\frac{\partial}{\partial t} G_t(x, v; x_0, v_0) = v_0 \frac{\partial}{\partial x_0} G_t(x, v; x_0, v_0) + \gamma \frac{\partial^2}{\partial v_0^2} G_t(x, v; x_0, v_0), \tag{3.49}$$

with initial condition $G_t(x, v; x_0, v_0) = \delta(x - x_0)\delta(v - v_0)$ and boundary conditions on x_0 and v_0 depending on the problem at hand.

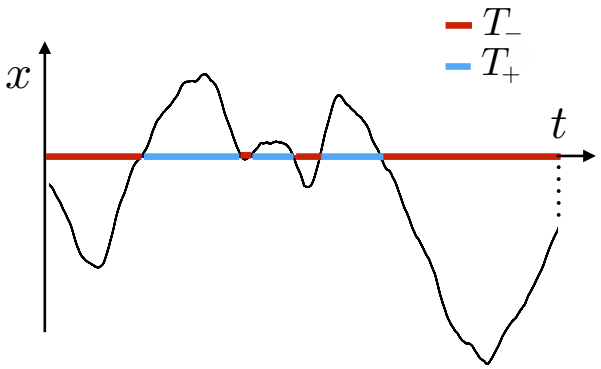

Figure 3.1: Possible trajectory of a randomly accelerated particle moving on the x axis with position x_0 and velocity v_0 at $t_0 = 0$. The residence time $T_+(t|x_0, v_0)$ of the trajectory is the time spent by the particle on the positive half axis in a total time of observation t. Note that $T_- = t - T_+$.

3.2.2 Moments of the residence time on the half-line

To fix the ideas, we would like to compute the moments of the residence time in the positive half-axis for a random acceleration process starting from arbitrary x_0 and v_0. A sketch of this process is given in Fig. 3.1. By identifying each term in the equations above, for the average residence time $\langle T_+ \rangle_t(x_0; v_0)$ we have

$$\langle T_+ \rangle_t(x0; v0) = \int_0^t dt' \int dx' \int dv' G_{t-t'}(x', v'; x_0, v_0) \tag{3.50}$$

The integrals over x' and v' can be carried out, which yields

$$\langle T_+ \rangle_t(x_0, v_0) = \frac{t}{2} + \frac{1}{2} \int_0^t dt' \mathrm{erf} \left[\frac{\sqrt{3}\,(v_0(t - t') + x_0)}{2\sqrt{\gamma}(t - t')^{3/2}} \right]. \tag{3.51}$$

For the special case where $x_0 = 0$ and $v_0 = 0$, we obtain

$$\langle T_+ \rangle_t (x_0 = 0, v_0 = 0) = \frac{t}{2}, \tag{3.52}$$

as expected on physical grounds because of the apparent symmetry of the process around the starting point.

As for the second moment, the calculations are more involved. The expression reads

$$\langle T_+^2 \rangle_t (x_0; v_0) = \frac{t}{2} \int_0^t dt' \int dx' \int dv' \int_0^{t'} dt'' \int dx'' \int dv'' G_{t'-t''}(x'', v''; x', v') G_{t-t'}(x', v'; x_0, v_0), \tag{3.53}$$

For the special case where $x_0 = 0$ and $v_0 = 0$, the calculation can be carried out explicitly. One has to first integrate over dv'' and dv' (which is made possible by resorting to the fact that the Green's function has a Gaussian shape and that integral of the product of Gaussian functions is still a Gaussian function), and then over dx'' and dx'. This yields

$$\langle T_+^2 \rangle_t (x_0 = 0; v_0 = 0) = \frac{t^2}{4} + \frac{1}{\pi} \int_0^t dt' \int_0^{t'} dt'' tan^{-1} \left[\frac{\sqrt{\frac{t-t'}{3t-t'-4t''}} (2t - t' - 3t'')}{t - t'} \right] \tag{3.54}$$

The integral over t'' and t' can be also performed explicitly, and the final result reads

$$\langle T_+^2 \rangle_t (x_0 = 0; v_0 = 0) = \frac{3\sqrt{3}}{4\pi} t^2 \simeq 0.413497 t^2. \tag{3.55}$$

It is interesting to compare the exact results (3.52) and (3.55) for the first and second moments of the residence time T_+ with the corresponding moments of the time T_m at which the randomly accelerated particle makes its maximum excursion. As mentioned above, for regular Brownian motion the cumulative distributions of T_+ and T_m coincide and are given by Lévy's arcsine law [46].

In [45], the cumulative distribution of T_m was derived analytically for the class of trajectories of a randomly accelerated particle which begin and end with velocity $v_i = v_f = 0$. For this class of trajectories the random acceleration process corresponds to the integral of a Brownian bridge, and the cumulative distribution of the rescaled variable $z = T_m/t$ is given by

$$I_{\frac{1}{4},\frac{1}{4}}(z) = \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{4})} B_z \left(\frac{1}{4}, \frac{1}{4} \right) \tag{3.56}$$

in terms of the incomplete beta function $B_z(p, q) = \int_0^z x^{p-1}(1-x)^{q-1} dx$. The nth moment of T_m for this cumulative distribution is

$$\langle T_m^n \rangle = t^n \int_0^1 dz z^n \frac{d}{dz} I_{\frac{1}{4},\frac{1}{4}}(z) = \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2}+n)} \frac{\Gamma(\frac{1}{4}+n)}{\Gamma(\frac{1}{4})} t^n, \tag{3.57}$$

which implies

$$\langle T_m \rangle = \frac{t}{2}, \qquad \langle T_m^2 \rangle = \frac{5}{12} t^2 \simeq 0.416667 t^2 \tag{3.58}$$

for the first and second moments. Comparing equations (3.52), (3.55) and (3.58), we see that the first moments of T_+ and T_m coincide and that the second moments differ, but by a small amount, less than $1^\circ/_\circ$. Clearly, the cumulative distribution of T_+/t is not given exactly by the expression in equation (3.56), even though it appears to provide a very good approximation. The comparison between the distribution of the occupation time T_+ and the beta distribution has been considered by other researchers in the past ([120, 121]).

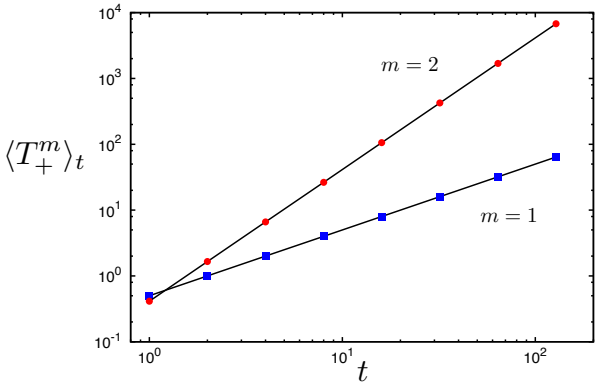

Figure 3.2: First two moments of the residence time T_+ for a randomly accelerated particle with initial conditions $x_0 = 0$ and $v_0 = 0$ as a function of the total time of observation t. The square and round points show our Monte Carlo results for the first and second moments, respectively, for $t = 2^0, \ldots, 2^7$. Each point represents an average over 10^6 realizations, and the error bars are smaller than the sizes of the points. The solid lines indicate the analytical predictions given by Eq.(3.52) and Eq.(3.55) for the first two moments.

3.3 Numerical results of the residence time

To illustrate the results derived in the subsection 3.2.2, we have also studied the residence time T_+ of a randomly accelerated particle with Monte Carlo simulations. In the simulations the particle moves according to a discrete version of equations (3.1) and (3.2) given by

$$x_{t'+\Delta t} = x_{t'} + v_{t'}\Delta t \tag{3.59}$$
$$v_{t'+\Delta t} = v_{t'} + \eta_{t'}\Delta t. \tag{3.60}$$

where $\eta_{t'}$ are independant and identically distributed(i.i.d). Gaussian numbers with zero mean and variance $2\gamma\Delta t = 10^{-4}$. Let us set $\gamma = 1$ in the simulations. Initial conditions are chosen in agreement with the definitions above, namely, $x_{t=0} = v_{t=0} = 0$. Our Monte Carlo results for the first two moments of the residence time, based on 10^6 realizations are compared with the exact analytical results in equations (3.52) and (3.55) in Fig. 3.2. The agreement is excellent.

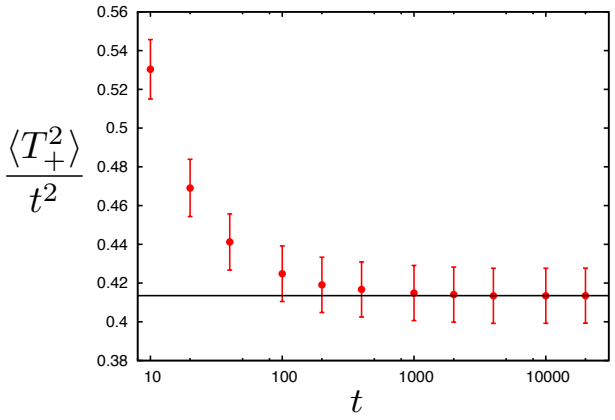

Figure 3.3: Results for the prefactor of the second moment T_+^2. We computed the ratio T_+^2/t^2 for larger value of t from Monte Carlo simulations, as described in Sec. 3.3. The points indicate the averages of 10^6 realizations, and the solid line shows the prefactor $3\sqrt{3}/(4\pi)$ in Eq. (3.55).

The non-trivial prefactor (3.55) for the second moment has been carefully checked by resorting to Monte Carlo simulation. Setting $\Delta t = 1$ in equations (3.59) and (3.60) and performing 10^6 realizations, we have numerically computed the ratio T_+^2/t^2 for the discretized version of the random acceleration model with the same initial conditions as above and 10^6 realizations. By setting $dt = 1$ and letting t grow, the ratio asymptotically saturates for large t at the predicted value indistinguishable from $3\sqrt{3}/(4\pi)$ given by (3.55), as shown in Fig. 3.3.

As a final numerical test concerning the residence time distribution, we have computed by Monte Carlo simulation the complete cumulative distribution $P(z)$ of the rescaled residence time $z = T_+/t$ numerically. In a previous work [45], Alberto Rosso et al. had explicitly computed the cumulative distribution for the time at which the maximum excursion occurs in a random acceleration process with a condition on the final velocity v_f of the process, namely $v_f = 0$. In this case, the random acceleration process corresponds

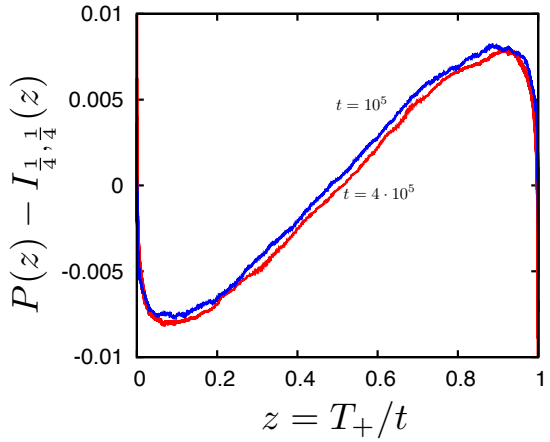

Figure 3.4: Difference of the cumulative distribution $P(z)$ of the rescaled residence time $z = T_+/t$, obtained by Monte Carlo simulations, and the distribution $I_{1/4,1/4}(z)$ given in Eq. (3.61). By refining the mesh size for the Monte Carlo simulations (blue: 10^4 steps; red: 4×10^4 steps), the difference converges to an asymptotic shape and does not shrink to zero.

to the integral of a Brownian bridge, and the cumulative distribution reads $I_{1/4,1/4}(z)$ for the rescaled variable $z = T_m/t$, $I_{1/4,1/4}(z)$ being the normalized incomplete Beta function

$$I_{1/4,1/4}(z) = \frac{\Gamma(1/2)}{\Gamma^2(1/4)} B_z(1/4, 1/4), \tag{3.61}$$

with $B_z(p,q) = \int_0^z x^{p-1}(1-x)^{q-1}dx$ the incomplete Beta function. The difference between the Monte Carlo result for $P(z)$ and the cumulative distribution $I_{1/4,1/4}(z)$ in equation (3.61) is plotted in figure 3.4. From the figure it is clear that the two distributions are different but that the difference is small.

3.4 Conclusion

In summary, in this chapter, we presented the results and discussions made on the study of the residence time of the random acceleration process. We have considered the residence time statistics of a randomly accelerated particle moving in one dimension. After deriving evolution equations for the generating function and moments of the residence time; we calculated the first two moments of the time T_+ on the positive half line exactly. Comparing these exact results with those for the first and second moments of the time T_m at which the particle makes its maximum excursion, we conclude that the distributions of T_+ and T_m are very similar but not identical, in contrast to the case of ordinary Brownian motion. Our Monte Carlo simulations of randomly accelerated motion are in excellent

agreement with our analytical results for the first two moments of T_+ and confirm the conclusion that T_+ and T_m have very similar but not identical distributions.

General Conclusion

Main results

In this thesis, the focus has been on the statistics of the residence time of the random acceleration model. To undertake our study of residence time statistics, we have used as an analytical tool, the Fokker-Planck equation associated with the natural and absorbing boundary conditions, in order to have a well defined problem. From these boundary conditions, we have found the solution of the probability density or Greenś function(propagator) for the Fokker-Planck equation in the phase space (x, v) for propagation from (x_0, v_0) to (x, v) in a time t.

As another analytical tool, we have used Feynman-Kac formulas which are useful to investigate properties of partial differential equations in terms of appropriate stochastic models, as well as to study probabilistic properties of Markov processes, by means of related partial differential equations. In this part of our thesis, we have presented, as numerical tools, the Monte Carlo methods, which are methods allowing us to solve many insoluble problems such as, for example the evaluation of integrals on complex and/or large-sized fields; the calculation of functional stochastic process, or exploration of complex probability distributions.

In this thesis, we have considered the residence time statistics of a randomly accelerated particle moving in one dimension. After deriving evolution equations for the generating function and moments of the occupation time, we have calculated the first two moments of the residence time T_+ on the positive half line exactly. Comparing these exact results with those for the first and second moments of the time T_m, at which the particle makes its maximum excursion, we conclude that the distributions of T_+ and T_m are very similar but unidentical, in contrast to the case of ordinary Brownian motion. Our Monte Carlo simulations of randomly accelerated motion are in excellent agreement with our analytical results for the first two moments of T_+, and has confirmed the conclusion that T_+ and Tm have very similar but not identical distributions. This conclusion follows from the exact results for the moments of the distributions and is also consistent with our Monte Carlo simulations.

Future works

At the end of the work done in this thesis, there emerges and suggests several interesting perspectives for further investigation. It is natural to wonder what happens to residence time statistics of the random acceleration model at the higher order. From this point of view, it would be interesting to continue our study by calculating the higher moments of the residence time T_+ and its exact distribution.

Thanks to the knowledge of Fokker-Planckś equations, it would also be interesting in the future to study this new track, namely the dynamics of DNA bubbles formed in double stranded DNA, of which we began the developments without completing it(see Appendix A.2), as well as its distribution.

Appendix A

Additional Proofs

Contents

A.1 Appendix to Chapter 3

A.1.1 Feynman-Kac equation for the generating function

Let us start with a single particle in x_0 with velocity v_0 at time $t = 0$. Consider a total observation time $t + dt$, with dt arbitrary small. Since the process is Markovian with respect the extended phase space (x, v), we can decompose the total observation time $[0, t + dt]$ in a first interval between $t = 0$ and $t = dt$, and then a second interval between dt and the final time $t + dt$, which yields

$$\begin{aligned} Q_{t+dt}(s|x_0, v_0) &= \langle e^{-sT_A(t+dt|x_0,v_0)} \rangle \\ &= \langle e^{-s\int_0^{dt} V(x(t'))dt'} e^{-s\int_{dt}^{t+dt} V(x(t'))dt'} \rangle. \end{aligned} \tag{A.1}$$

By supposing that dt is small, the first term can be evaluated to be

$$e^{-s\int_0^{dt} V(x(t'))dt'} \simeq e^{-sV(x(dt))dt} = e^{-sV(x_0)dt}. \tag{A.2}$$

We realize that this term is actually completely deterministic and can be then singled out from the bracket signs:

$$Q_{t+dt}(s|x_0, v_0) = e^{-sV(x_0)dt} \langle e^{-s\int_{dt}^{t+dt} V(x(t'))dt'} \rangle. \tag{A.3}$$

We can then rearrange the integral by translating back by dt the time interval:

$$\begin{aligned} Q_{t+dt}(s|x_0,v_0) &= e^{-sV(x_0)dt}\langle e^{-s\int_0^t V(x(t'))dt'}\rangle \\ &= e^{-sV(x_0)dt}\langle Q_t(s|x_0+\Delta x, v_0+\Delta v)\rangle, \end{aligned} \tag{A.4}$$

where Δx is the displacement of the coordinate x from the initial condition x_0, and similarly Δv is the velocity increment from the initial condition v_0 during the time interval dt. We can now use the Taylor expansion of the function $Q_t(s|x_0+\Delta x, v_0+\Delta v)$ for small Δx and Δv: we have

$$\begin{aligned} Q_t(s|x_0+\Delta x, v_0+\Delta v) = Q_t(s|x_0,v_0) + \Delta x\frac{\partial}{\partial x_0}Q_t(s|x_0,v_0) \\ +\Delta v\frac{\partial}{\partial v_0}Q_t(s|x_0,v_0) + \frac{1}{2}(\Delta v)^2\frac{\partial^2}{\partial v_0^2}Q_t(s|x_0,v_0) + \cdots \end{aligned}$$

Observe that $\langle \Delta x\rangle = v_0 dt$, $\langle \Delta v\rangle = 0$ and $\langle (\Delta v)^2\rangle = \gamma dt$. Then, by taking the limit for $dt \to 0$ and retaining the terms of the order of dt at most, Eq. A.4 finally yields

$$\frac{\partial}{\partial t}Q_t = v_0\frac{\partial}{\partial x_0}Q_t + \gamma\frac{\partial^2}{\partial v_0^2}Q_t - sV(x_0)Q_t, \tag{A.5}$$

which is a backward equation, the derivatives acting on the initial coordinates x_0 and v_0.

A.2 Appendix to section future works

A.2.1 Dynamics of a bubble formed in double stranded DNA.

We study the dynamics of a tagged base-pair in double stranded DNA; we calculate the drift force which acts on the tagged base-pair using a potential model that describes interactions at base pairs level and use it to construct a Fokker-Planck equation. We use the simple potential model of Joyeux-Buyukdagli(JB) [122] to represent the interaction in dsDNA at base pairs level. The potential of the model is written as

$$U(y^N) = D\sum_n(1-e^{-\alpha y_n})^2 + \frac{\Delta H}{2}\sum_n\{1-e^{-b(y_n-y_{n-1})^2}\} + K_b(y_n-y_{n-1})^2. \tag{A.6}$$

where N is the number of base pairs, summation on the r.h.s is over all base pairs of the molecule and $y^N = \{y_n\}$, the set of relative base pairs separation. The first term of Eq.(A.7) is the Morse potential [1] that represents the stacking interaction between the bases of the opposite strands and the second term is the JB potential [2].

[1] D denotes the dissociation energy; the parameter α homogeneous to the inverse of a length; and y_n is the displacement that stretches the hydrogen bonds.

[2] this potential represents the stacking interaction between adjacent base pairs. $\frac{\Delta H}{2}$ is a Gaussian hole of depth; K_b is a constant.

The potential felt by the tagged base pair at a separation y from the ground state $y = 0$ is found from the relation

$$V(y) = -k_B T[\ln Z_n(y_0) - \ln Z_n(0)]. \tag{A.7}$$

where

$$\begin{aligned} Z_n(y) &= \int \prod_{i=1}^{N} dy_i \delta(y_n - y) exp[-\beta U(y^N)] \\ Z_n(0) &= \int \prod_{i=1}^{N} dy_i \delta(y_n - 0) exp[-\beta U(y^N)] \\ \delta(y_n - y) &= \sum_i \Phi_i^*(y_N)\Phi_i(y_0). \end{aligned}$$

are the constrained partition function integrals; δ is the Dirac function and $\beta = (k_B T)^{-1}$.

For the JB model, the calculation of a partition function integral reduces to multiplication of N matrices.

The dynamic of the base pair may described by the Langevin equation. Indeed,invoking Newtonś law of motion and neglecting the inertial effects, we obtain

$$\begin{aligned} \sum \vec{f}_{ext} = m\vec{a} \quad &\Longleftrightarrow \quad \vec{0} = \vec{F}_d + \vec{F}_{drift} + \vec{F}_f \\ &\Longleftrightarrow \quad \gamma \frac{dy}{dt} = F_{drift} + F_f \\ &\Longleftrightarrow \quad \frac{dy}{dt} = -\frac{1}{\gamma}\frac{dV(y)}{dy} + \xi \\ &\Longleftrightarrow \quad \frac{dy}{dt} = -\beta D + \xi(t); \qquad < \xi(t)\xi(t') >= 2D\delta(t - t') \end{aligned} \tag{A.8}$$

here $\frac{1}{\gamma}$ is a transport coefficient of dimension time/mass; β is a thermodynamic constant [3]an D is the diffusion coefficient. Eq.(A.8) describes a one-dimensional random walk in a potential V(y).

As we have seen before, the current corresponding to the above Langevin equation is

$$\begin{aligned} J &= J_{diff} + J_{drift} \\ &= \frac{F_c}{\gamma}\rho(y,t) - D\frac{\partial \rho(y,t)}{\partial y} \end{aligned} \tag{A.9}$$

Using the continuity equation $\frac{\partial \rho(y,t)}{\partial t} + \frac{\partial J}{\partial y} = 0$ this then leads to the following equation for $\rho(y,t)$

[3] $\beta = \frac{1}{k_B T}$ where $k_B$is the Boltzmann constant; and T the temperature.

$$\frac{\partial\rho(y,t)}{\partial t} = -\frac{\partial}{\partial y}\Big[\frac{F_c}{\gamma}\rho(y,t) - D\frac{\partial\rho(y,t)}{\partial y}\Big]$$
$$\Rightarrow \frac{\partial\rho(y,t)}{\partial t} = -\frac{\partial}{\partial y}\Big\{\beta D\Big[\frac{\partial V(y)}{\partial y}\rho(y,t)\Big] - D\frac{\partial\rho(y,t)}{\partial y}\Big\}$$
$$\Rightarrow \frac{\partial\rho(y,t)}{\partial t} = D\Big\{\frac{\partial}{\partial y}\Big[-\frac{\partial\beta V(y)}{\partial y}\rho(y,t)\Big] + \frac{\partial^2\rho(y,t)}{\partial y^2}\Big\} \tag{A.10}$$

then the Fokker-Planck equation corresponding to A.10 is found to be

$$\frac{\partial\rho(y,t)}{\partial t} = D\Big\{\frac{\partial}{\partial y}\Big[-\frac{\partial\beta V(y)}{\partial y}\rho(y,t)\Big] + \frac{\partial^2\rho(y,t)}{\partial y^2}\Big\} \tag{A.11}$$

where $\rho(y, y_0; t)$ is the probability density of the random walkers.

We assume that if separation y reduces to zero at time t', it will not contribute to autocorrelation function defined as $\mathcal{C}(t) =< y(t)y(0) > - < y >^2$ for t>t' and similarly any new fluctuational opening which appear after $t = 0$ will not contribute to $\rfloor(t)$.

Thus for purposes of computing the autocorrelation function we place an absorbing wall at $y = 0$, i.e. $\rho(y = 0, t) = 0$. In addition to this, we may require $\rho(y = L, t) = 0$, where L depends on the size of the double stranded DNA molecule or on any other condition which limits the size of the bubble.

The problem of calculating the autocorrelation function $\mathcal{C}(t)$ therefore reduces to finding how many walkers of an ensemble of random walkers distributed according to thermal equilibrium at $t = 0$ are still present at time t and have not been absorbed by the wall at $y = 0$.

We express $\rho(y, y_0; t)$ in terms of eigenfunctions.

let us set

$$\rho(y,t) = exp[-\beta V(y)/2]\psi(y,t) \tag{A.12}$$

and use it in Eq.(A.11) we have

$$-\frac{\partial\psi}{\partial t} = \mathcal{L}\psi, \qquad \mathcal{L} = -\frac{\partial^2}{\partial y^2} + v(y) \tag{A.13}$$

where

$$v(y) = \frac{1}{4}\Big[\frac{\partial\beta V(y)}{\partial y}\Big]^2 - \frac{1}{2}\Big[\frac{\partial^2\beta V(y)}{\partial y^2}\Big] \tag{A.14}$$

Which is the time Schrödinger equation for a particle of mass 1/2 in the potential v(y). Let ϕ_k denote the eigenfunctions of the operator $\mathcal{L}$, $\mathcal{L}\phi_k = E_k\phi_k$, with $\phi_k(y = 0) = 0$ and $\int dy\phi_k^*(y)\phi_{k'}(y) = \delta_{kk'}$.

Then

$$\psi(y,t) = \Sigma_k a_k\phi_k e^{-E_k t} \tag{A.15}$$

where

$$a_k = \int_0^\infty \psi(y, t=0)\phi_k^*(y)dy \tag{A.16}$$

If we start with a random walker at $y = y_0$ at $t = 0$, then $\rho(y, t = 0) = \delta(y - y_0$, and, from Eq.(A.12), $\psi(y, t = 0) = e^{V(y)/2}\delta(y - y_0)$. Equation (A.16) then gives $a_k = exp[V(y_0)/2]\phi_k^*(y_0)$. The Green's function, i.e., the probability density that this random walker will be at position y at time t, is found to be

$$\begin{aligned}\rho(y, t|y_0, t = 0) &= e^{-\beta V(y)/2}\psi(y, t|y_0, t = 0) \\ &= \sum_k e^{-\beta[V(y)-V(y_0)]/2}\phi_k^*(y_0)\phi_k(y)e^{-E_k t}.\end{aligned} \tag{A.17}$$

For an initial distribution, we choose the Boltzmann function

$$B(y) = Aexp(-\beta V(y)), \tag{A.18}$$

where $A = 1/\int_0^L dyexp(-\beta V(y))$ is a normalization factor. If we start with the equilibrium function at time $t = 0$, the distribution function at time t, $\rho(y, t)$ is

$$\rho(y, t) = \int_0^L dyG(y, t|y_0, t) \tag{A.19}$$

where $G(y, t|y_0, t)$ is the weighted Green's function define by

$$\begin{aligned}G(y, t|y_0, t) &\equiv Ae^{-\beta V(y)}\rho(y, t|y_0, t = 0) \\ &= Ae^{-\beta[V(y)-V(y_0)]/2}\sum_k \phi_k^*(y_0)\phi_k(y)e^{-E_k t}.\end{aligned} \tag{A.20}$$

Then the survival probability for this random walker is

$$\begin{aligned}P(y, t) &= \int_0^L dy\rho(y, t|y_0, t) \\ &= A\sum_k e^{-E_k t}\int_0^L dy_0 exp\Big[-\beta\frac{V(y) + V(y_0)}{2}\Big].\end{aligned} \tag{A.21}$$

The weighted survival probability is

$$\bar{P}(y, t) \equiv Ae^{-\beta V(y)}P(y, t) = \int_0^L dyG(y, t|y_0, t), \tag{A.22}$$

where $P(y, t)$ is the unweighted survival probability given in Eq.(A.23). The right-hand sides of Eqs.(A.19) and (A.22) are equal to each other, thus $\bar{P}(y, t) = \rho(y = y_0, t)$,

because of the symmetry in $G(y, y_0; t)$, where we found the autocorrelation function as follows

$$\begin{aligned}\mathcal{C}(t) &= \int_0^L dy \bar{P}(y,t) \\ &= \int_0^L dy \rho(y,t) \\ &= A \sum_k e^{-E_k t} \left| \int_0^L e^{-\beta V(y)/2} \phi_k(y) dy \right|^2 . \end{aligned} \tag{A.23}$$

The values of $\phi_k(y)$ and E_k of the operator $\mathcal{L}$ in equation (A.13) are determined numerically using the numerical matrix multiplication (NMM) method developed in [123].

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Occupation time statistics of the random acceleration model

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Abstract. The random acceleration model is one of the simplest non-Markovian stochastic systems and has been widely studied in connection with applications in physics and mathematics. However, the occupation time and related properties are non-trivial and not yet completely understood. In this paper we consider the occupation time T_+ of the one-dimensional random acceleration model on the positive half-axis. We calculate the first two moments of T_+ analytically and also study the statistics of T_+ with Monte Carlo simulations. One goal of our work was to ascertain whether the occupation time T_+ and the time T_m at which the maximum of the process is attained are statistically equivalent. For regular Brownian motion the distributions of T_+ and T_m coincide and are given by Lévy's arcsine law. We show that for randomly accelerated motion the distributions of T_+ and T_m are quite similar but not identical. This conclusion

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follows from the exact results for the moments of the distributions and is also consistent with our Monte Carlo simulations.

Keywords: Brownian motion, exact results

Contents

1. Introduction

A variety of systems in physics, in the life and social sciences, and in engineering can be modeled in terms of particles traveling in a host medium which randomly change their state (position, direction, energy, etc) in collisions with other particles or with the medium itself. The nature of the randomness may vary widely from one system to another. It may result either from the intrinsic stochastic nature of the underlying process or from uncertainty [1]. Some transport phenomena, while originating in deterministic and reversible events, can in practice only be described by resorting to the laws of probability.

A prominent example of such a stochastic system is the random acceleration model, which has been studied both in physics and mathematics. In physics it appears, for example, in the continuum description of the equilibrium statistics of a semiflexible polymer chain with non-zero bending energy [2]. It also describes the steady state profile of a $(1 + 1)$-dimensional Gaussian interface [3] with dynamical exponent $z = 4$ in the continuum version of the Golubovic–Bruinsma–Das Sarma–Tamborenea model [4]. In addition, the random acceleration process arises in the description of the statistical properties of the Burgers equation with Brownian initial velocity [5].

The random acceleration model is a non-trivial, non-Markov model, which is both relevant to real-world applications and simple enough so that it can be studied analytically. The first-passage properties and related properties have been investigated extensively

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over the last few decades [2, 3, 6–14]. Recently, the extreme-value statistics of the process was analyzed, with special emphasis on the global maximum in a given time interval [2, 15, 16] and the time at which the global maximum is reached [17]. However, the occupation time statistics of random acceleration is still not understood in detail.

The occupation time in stochastic systems was first considered by mathematicians [18–21] and has more recently been investigated in physical systems with continuous degrees of freedom and in connection with persistence (see [22, 23] and references therein). In this paper we consider a randomly accelerated particle moving in one dimension on the infinite x axis and study the occupation time T_+ on the positive x axis. We calculate the first two moments of T_+ analytically and also study the statistics of T_+ with Monte Carlo simulations. One of our aims was to learn whether the occupation time T_+ of the randomly accelerated particle and the time $T_{\rm m}$ at which it attains its maximum displacement are statistically equivalent. Both our analytical and Monte Carlo results indicate that this is not the case. This is in contrast to regular Brownian motion, where the distributions of T_+ and $T_{\rm m}$ coincide and are given by Lévy's celebrated arcsine law [18, 24].

The paper is structured as follows: in section 2, we derive partial differential equations which determine the moment generating function and the moments of the occupation time. In section 3 the first two moments of the occupation time T_+ are calculated explicitly and compared with the corresponding moments of the time $T_{\rm m}$ at which the randomly accelerated particle makes its maximum excursion. In section 4 we study the moments of T_+ and its distribution with Monte Carlo simulations and compare the results with our analytic predictions for the first two moments of T_+ and with exact results [17] for the distribution of $T_{\rm m}$. Section 5 contains concluding remarks. Some calculational details pertaining to section 2 are given in the appendix.

2. Differential equations for analyzing the occupation time

The randomly accelerated particle we consider moves in one dimension according to the equations of motion

$$\frac{{\rm d}x}{{\rm d}t} = v, \tag{1}$$

$$\frac{{\rm d}v}{{\rm d}t} = \eta(t). \tag{2}$$

Here $x(t)$ is the position of the particle, $v(t)$ is its velocity, and $\eta(t)$ is Gaussian white noise, with $\langle\eta(t)\rangle = 0$ and $\langle\eta(t)\eta(t')\rangle = 2\gamma\delta(t-t')$, $\gamma > 0$. The initial conditions at time $t = 0$ are $x(0) = x_0$ and $v(0) = v_0$.

The occupation time $T_A(t|x_0, v_0)$, i.e. the time the particle spends in a region A during a total time of observation t, is formally expressed by the random variable

$$T_A(t|x_0, v_0) = \int_0^t V_A(x(t')){\rm d}t', \tag{3}$$

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where the marker function $V_A(x(t)) = 1$ if $x(t) \in A$ and vanishes otherwise. In studying the statistics of $T_A(t|x_0, v_0)$, it is convenient to introduce the moment generating function

$$Q_t(s|x_0, v_0) = \langle \mathrm{e}^{-sT_A(t|x_0, v_0)} \rangle, \tag{4}$$

where s is the variable conjugate to T_A and has the dimensions of inverse time. The moments of the occupation time can be obtained by differentiating equation (4) with respect to s and then setting $s = 0$, according to

$$\langle T_A^n \rangle_t(x_0, v_0) = (-1)^n \frac{\partial^n}{\partial s^n} Q_t(s|x_0, v_0)|_{s=0}. \tag{5}$$

The evolution of $Q_t(s|x_0, v_0)$ is governed by a backward partial differential equation of the Fokker–Planck type, which is derived in the appendix and is given by

$$\frac{\partial}{\partial t} Q_t = v_0 \frac{\partial}{\partial x_0} Q_t + \gamma \frac{\partial^2}{\partial v_0^2} Q_t - s V_A(x_0) Q_t. \tag{6}$$

Taking derivatives of equation (6) with respect to s and making use of equation (5) leads to the corresponding differential equation

$$\frac{\partial}{\partial t} \langle T_A^n \rangle_t = v_0 \frac{\partial}{\partial x_0} \langle T_A^n \rangle_t + \gamma \frac{\partial^2}{\partial v_0^2} \langle T_A^n \rangle_t + n V_A(x_0) \langle T_A^{n-1} \rangle_t \tag{7}$$

for the nth moment of the occupation time. Note that the rightmost term or source term in equation (7) depends on the moment of order $n - 1$.

With the initial condition $\langle T_A^n \rangle_0(x_0, v_0) = 0$, stemming from $T_A(t = 0|x_0, v_0) = 0$, differential equation (7) has the explicit solution

$$\langle T_A^n \rangle_t(x_0, v_0) = n \int_0^t \mathrm{d}t' \int_{-\infty}^{\infty} \mathrm{d}x' \int_{-\infty}^{\infty} \mathrm{d}v' V_A(x') \langle T_A^{n-1} \rangle_{t'}(x', v') G_{t-t'}(x', v'; x_0, v_0). \tag{8}$$

Here $G_t(x, v; x_0, v_0)$ is the Green's function satisfying

$$\frac{\partial}{\partial t} G_t(x, v; x_0, v_0) = v_0 \frac{\partial}{\partial x_0} G_t(x, v; x_0, v_0) + \gamma \frac{\partial^2}{\partial v_0^2} G_t(x, v; x_0, v_0), \tag{9}$$

with initial condition $G_0(x, v; x_0, v_0) = \delta(x - x_0)\delta(v - v_0)$ and with boundary conditions that depend on the problem of interest.

The hierarchical relation (8) is the main result of this section that we will need below. It generates all the moments $\langle T_A^n \rangle_t(x_0, v_0)$ for positive integer n recursively from the zeroth moment

$$\langle T_A^0 \rangle_t(x_0, v_0) = Q_t(s|x_0, v_0)|_{s=0} = 1 \tag{10}$$

implied by equations (4) and (5). We note that equation (8) also follows, without recourse to the differential equations (6) and (7), from the definition (3) of T_A and the interpretation of $G_t(x, v; x_0, v_0)$ as the probability density in the phase space (x, v) for propagation from (x_0, v_0) to (x, v) in a time t.

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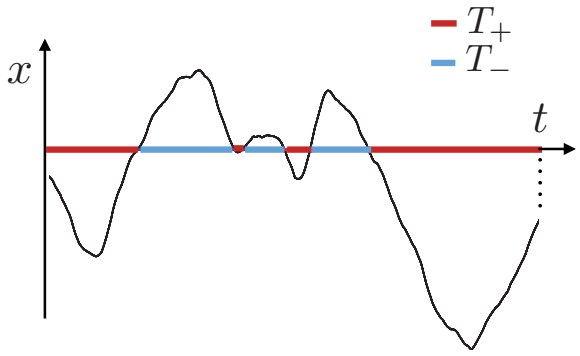

Figure 1. Possible trajectory of a randomly accelerated particle moving on the x axis with position x_0 and velocity v_0 at $t_0 = 0$. The occupation time $T_+(t|x_0, v_0)$ of the trajectory is the time spent by the particle on the positive half axis in a total time of observation t. Note that $T_- = t - T_+$.

3. Occupation time on the half-line

For a particle which is free to move on the entire real axis, the Green's function in equations (8) and (9) is given by [2]

$$G_t(x, v; x_0, v_0) = \frac{3^{1/2}}{2\pi\gamma t^2} \times \exp\{-[3(x - x_0 - vt)(x - x_0 - v_0 t)/(\gamma t^3) + (v - v_0)^2/(\gamma t)]\}. \tag{11}$$

Let us focus on the occupation time $T_+(t|x_0, v_0)$ that a randomly accelerated particle with initial position and velocity x_0 and v_0 spends on the positive half-axis $A = [0, +\infty)$ in a total time of observation t. The occupation time T_+ for a possible trajectory of the particle is illustrated in figure 1. Combining equations (8), (10) and (11), we obtain

$$\langle T_+\rangle_t(x_0, v_0) = \int_0^t \mathrm{d}t' \int_0^\infty \mathrm{d}x' \int_{-\infty}^\infty \mathrm{d}v' G_{t-t'}(x', v'; x_0, v_0) \tag{12}$$

for the average occupation time. The integrals over x' and v' can be evaluated explicitly, yielding

$$\langle T_+\rangle_t(x_0, v_0) = \frac{t}{2} + \frac{1}{2}\int_0^t \mathrm{d}t' \mathrm{erf}\left[\frac{\sqrt{3}}{2}\frac{x_0 + v_0(t - t')}{\sqrt{\gamma}(t - t')^{3/2}}\right]. \tag{13}$$

In the special case $x_0 = 0$ and $v_0 = 0$, we obtain

$$\langle T_+\rangle_t(x_0 = 0, v_0 = 0) = \frac{1}{2}t, \tag{14}$$

as expected on physical grounds because of the symmetry of the process around the starting point.

According to equations (8) and (12), the second moment of T_+ is given by

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$$\langle T_+^2\rangle_t(x_0, v_0) = 2\int_0^t \mathrm{d}t' \int_0^\infty \mathrm{d}x' \int_{-\infty}^\infty \mathrm{d}v' \int_0^{t'} \mathrm{d}t'' \times \int_0^\infty \mathrm{d}x'' \int_{-\infty}^\infty \mathrm{d}v'' G_{t'-t''}(x'', v''; x', v') G_{t-t'}(x', v'; x_0, v_0). \tag{15}$$

In the special case where $x_0 = 0$ and $v_0 = 0$, the integrals may be evaluated explicitly. First evaluating the Gaussian integrals over v'' and v' and then integrating over x'' and x', we obtain

$$\langle T_+^2\rangle_t(x_0 = 0, v_0 = 0) = \frac{t^2}{4} + \frac{1}{\pi}\int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}t'' \tan^{-1}\left[\frac{2t + t' - 3t''}{t' - t''}\sqrt{\frac{t - t'}{3t + t' - 4t''}}\right]. \tag{16}$$

The integrals over t'' and t' can also be evaluated explicitly, and the final result is

$$\langle T_+^2\rangle_t(x_0 = 0, v_0 = 0) = \frac{3^{3/2}}{4\pi} t^2 \simeq 0.413\,497 t^2. \tag{17}$$

It is interesting to compare the exact results (14) and (17) for the first and second moments of the occupation time T_+ with the corresponding moments of the time T_m at which the randomly accelerated particle makes its maximum excursion. As mentioned above, for regular Brownian motion the cumulative distributions of T_+ and T_m coincide and are given by Lévy's arcsine law [18].

In [17], the cumulative distribution of T_m was derived analytically for the class of trajectories of a randomly accelerated particle which begin and end with velocity $v_\mathrm{i} = v_\mathrm{f} = 0$. For this class of trajectories the random acceleration process corresponds to the integral of a Brownian bridge, and the cumulative distribution of the rescaled variable $z = T_\mathrm{m}/t$ is given by

$$I_{\frac{1}{4},\frac{1}{4}}(z) = \frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{1}{4}\right)^2} B_z\left(\frac{1}{4}, \frac{1}{4}\right), \tag{18}$$

in terms of the incomplete beta function $B_z(p, q) = \int_0^z x^{p-1}(1-x)^{q-1}\mathrm{d}x$. The nth moment of T_m for this cumulative distribution is

$$\langle T_\mathrm{m}^n\rangle = t^n \int_0^1 \mathrm{d}z\; z^n \frac{\mathrm{d}}{\mathrm{d}z} I_{\frac{1}{4},\frac{1}{4}}(z) = \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2}+n)} \frac{\Gamma(\frac{1}{4}+n)}{\Gamma(\frac{1}{4})}\; t^n, \tag{19}$$

which implies

$$\langle T_\mathrm{m}\rangle = \frac{1}{2}t, \qquad \langle T_\mathrm{m}^2\rangle = \frac{5}{12}t^2 \simeq 0.416\,667 t^2 \tag{20}$$

for the first and second moments. Comparing equations (14), (17) and (20), we see that the first moments of T_+ and T_m coincide and that the second moments differ, but by a small amount, less than 1%. Clearly, the cumulative distribution of T_+/t is not given exactly by the expression in equation (18), even though it appears to provide a very good approximation. The comparison between the distribution of the occupation time T_+ and the beta distribution has been considered by other researchers in the past: see, e.g. [26, 27].

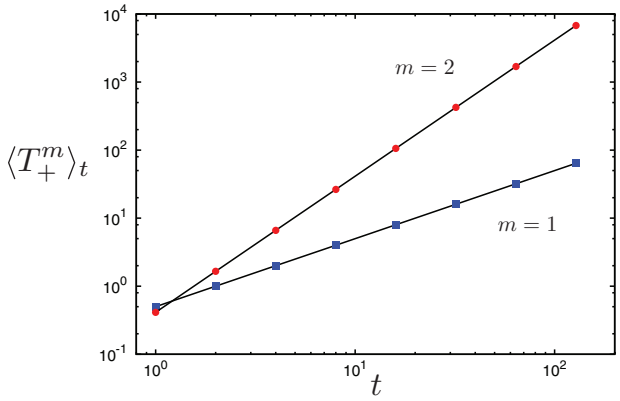

Figure 2. First two moments of the occupation time T_+ for a randomly accelerated particle with initial conditions $x_0 = 0$ and $v_0 = 0$ as a function of the total time of observation t. The square and round points show our Monte Carlo results for the first and second moments, respectively, for $t = 2^0, \ldots, 2^7$. Each point represents an average over 10^6 realizations, and the error bars are smaller than the sizes of the points. The solid lines indicate the analytical predictions (14) and (17) for the moments.

4. Monte Carlo simulations

We have also studied the statistics of the occupation time T_+ of a randomly accelerated particle with Monte Carlo simulations. In the simulations the particle moves according to a discrete version of equations (1) and (2) given by

$$x_{t'+\Delta t} = x_{t'} + v_{t'}\Delta t, \tag{21}$$

$$v_{t'+\Delta t} = v_{t'} + \eta_{t'}\Delta t. \tag{22}$$

Here the $\eta_{t'}$ are independent and identically distributed (i.i.d.) Gaussian variables with zero mean and variance $2\gamma\Delta t = 10^{-4}$. We set $\gamma = 1$ in the simulations and chose the initial conditions $x_{t=0} = 0$ and $v_{t=0} = 0$ considered above. Our Monte Carlo results for the first two moments of the occupation time, based on 10^6 realizations are compared with the exact analytical results in equations (14) and (17) in figure 2. The agreement is excellent.

We have also checked the prediction (17) for the second moment in another way. Setting $\Delta t = 1$ in equations (21) and (22) and performing 10^6 realizations, we computed the ratio T_+^2/t^2 for larger and larger values of t. As shown in figure 3, the ratio saturates for large t at a value indistinguishable from $3^{3/2}/(4\pi)$, in agreement with equation (17).

In addition to these studies of the first and second moments, we have determined the complete cumulative distribution $P(z)$ of the rescaled occupation time $z = T_+/t$ numerically, from Monte Carlo simulations. The difference between the Monte Carlo result for $P(z)$ and the cumulative distribution $I_{\frac{1}{4},\frac{1}{4}}(z)$ in equation (18) is plotted in figure 4. From the figure it is clear that the two distributions are different but that the difference is small. This is the same conclusion we reached in section 3 on comparing exact results for the first and second moments of T_+ and $T_{\rm m}$.

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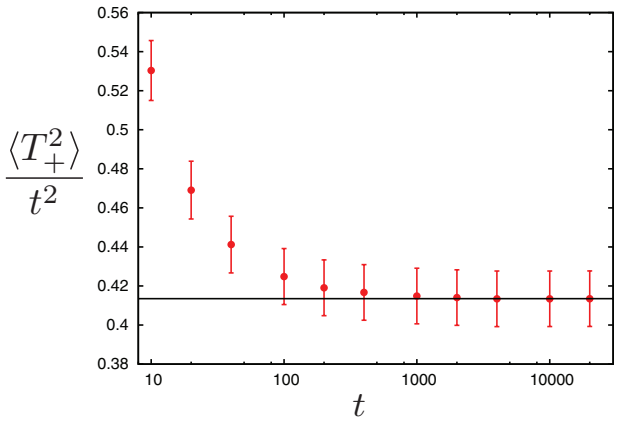

Figure 3. Results for the pre-factor of the second moment T_+^2. We computed the ratio T_+^2/t^2 from Monte Carlo simulation, as described in section 4. The points indicate the averages of 10^6 realizations, and the solid line shows the prefactor $3^{3/2}/(4\pi)$ in equation (17).

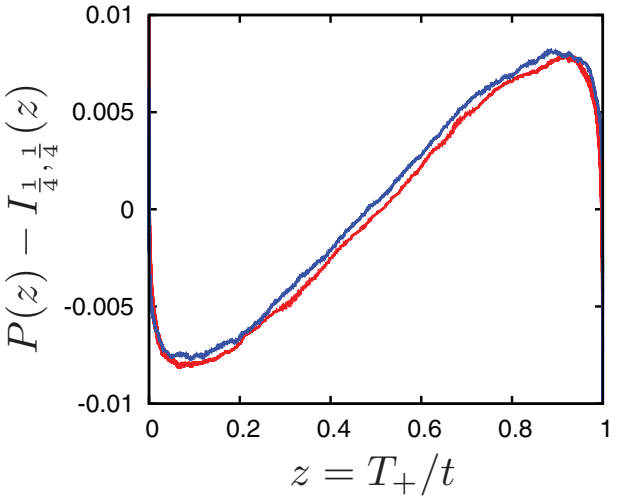

Figure 4. Difference of the cumulative distribution $P(z)$ of the rescaled occupation time $z = T_+/t$, determined by Monte Carlo simulations, and the cumulative distribution $I_{\frac{1}{4},\frac{1}{4}}(z)$ given in equation (18). On increasing the number of steps in the Monte Carlo simulations (blue: 10^4 steps; red: 4×10^4 steps), the difference converges to a non-trivial asymptotic shape and does not shrink to zero.

5. Conclusions

In this paper we have considered the occupation time statistics of a randomly accelerated particle moving in one dimension. After deriving evolution equations for the generating function and moments of the occupation time, we calculated the first two moments of the occupation time T_+ on the positive half line exactly. Comparing these exact results with those for the first and second moments of the time $T_{\rm m}$ at which the particle makes its maximum excursion, we conclude that the distributions of T_+ and $T_{\rm m}$ are very similar but not identical, in contrast to the case of ordinary Brownian motion. Our Monte Carlo simulations of randomly accelerated motion are in excellent

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agreement with our analytical results for the first two moments of T_+ and confirm the conclusion that T_+ and $T_{\rm m}$ have very similar but not identical distributions. The calculation of higher moments of T_+ and its exact distribution are challenging problems for future study.

Appendix. Derivation of differential equation (6) for the generating function

Considering a particle with position x_0 and velocity v_0 at time $t=0$ and following standard steps in deriving differential equations satisfied by path integrals (see, for example, [2, 19, 25]), we decompose the total observation time $[0, t+{\rm d}t]$ in a first interval from $t=0$ to ${\rm d}t$ and a second interval from ${\rm d}t$ to $t+{\rm d}t$. Since the random acceleration process is Markovian in the two-dimensional phase space $(x,\, v)$, equations (1) and (2) imply

$$Q_{t+{\rm d}t}(s|x_0,\, v_0) = \langle {\rm e}^{-sT_A(t+{\rm d}t|x_0,v_0)}\rangle = \langle {\rm e}^{-s\int_0^{\rm d} tV_A(x(t')){\rm d}t'} {\rm e}^{-s\int_{\rm d}^{t+{\rm d}t} V_A(x(t')){\rm d}t'}\rangle. \tag{A.1}$$

For infinitesimal ${\rm d}t$ the quantity

$${\rm e}^{-s\int_0^{\rm d} tV_A(x(t')){\rm d}t'} \to {\rm e}^{-sV_A(x_0){\rm d}t} \tag{A.2}$$

in equation (A.1) is completely deterministic and can be placed outside the angular brackets, yielding

$$Q_{t+{\rm d}t}(s|x_0,\, v_0) = {\rm e}^{-sV_A(x_0){\rm d}t}\langle {\rm e}^{-s\int_{{\rm d}t}^{t+{\rm d}t} V_A(x(t')){\rm d}t'}\rangle. \tag{A.3}$$

Translating the time in the integral on the right back by ${\rm d}t$, we obtain

$$Q_{t+{\rm d}t}(s|x_0,\, v_0) = {\rm e}^{-sV_A(x_0){\rm d}t}\langle {\rm e}^{-s\int_0^{t} V_A(x(t')){\rm d}t'}\rangle = {\rm e}^{-sV_A(x_0){\rm d}t}\langle Q_t(s|x_0+\Delta x,\, v_0+\Delta v)\rangle, \tag{A.4}$$

where Δx and Δv are the changes in position and velocity in the time interval from $t=0$ to ${\rm d}t$. On expanding the right-hand side for small Δx, Δv, and ${\rm d}t$, equation (A.4) takes the form

$$Q_{t+{\rm d}t}(s|x_0,\, v_0) - Q_t(s|x_0,\, v_0) = \left[-sV_A(x_0) + \Delta x\frac{\partial}{\partial x_0} + \Delta v\frac{\partial}{\partial v_0} + \frac{1}{2}(\Delta v)^2\frac{\partial^2}{\partial v_0^2} + \cdots\right] Q_t(s|x_0,\, v_0). \tag{A.5}$$

Substituting $\langle \Delta x\rangle = v_0{\rm d}t$, $\langle \Delta v\rangle = 0$ and $\langle (\Delta v)^2\rangle = \gamma{\rm d}t$ into equation (A.5) and dividing the equation by ${\rm d}t$ leads to the partial differential equation (6) for the evolution of the generating function. Since the derivatives on the right-hand side of equation (6) act on the initial coordinates x_0 and v_0, it is an example of a 'backward' evolution equation.

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