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Field Theories for Stochastic Processes

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Declaration of Originality

I declare that all of the research presented here is the result of my own original work unless otherwise stated.

This thesis is to large parts a collection of research work that has been obtained through joint work with my collaborators and is partly published in peer-reviewed journals. Wherever it applies, I state clearly whether the text is taken from a published paper or manuscript in any form. Throughout the presentation of collaborative work, I indicate clearly which parts I did or did not do and transparently outline which contributions I have or have not made. I have sought and found the explicit approval of all my collaborators to cite our joint work which is reproduced at the end of this thesis. Academic citations are in accordance with standard practice.

Benjamin Walter, 31 March 2020.

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Abstract

This thesis is a collection of collaborative research work which uses field-theoretic techniques to approach three different areas of stochastic dynamics: Branching Processes, First-passage times of processes with are subject to both white and coloured noise, and numerical and analytical aspects of first-passage times in fractional Brownian Motion.

Chapter 1 (joint work with Rosalba Garcia Millan, Johannes Pausch, and Gunnar Pruessner, appeared in Phys. Rev. E **98** (6):062107) contains an analysis of non-spatial branching processes with arbitrary offspring distribution. Here our focus lies on the statistics of the number of particles in the system at any given time. We calculate a host of observables using Doi-Peliti field theory and find that close to criticality these observables no longer depend on the details of the offspring distribution, and are thus universal.

In Chapter 2 (joint work with Ignacio Bordeu, Saoirse Amarteifio, Rosalba Garcia Millan, Nanxin Wei, and Gunnar Pruessner, appeared in Sci. Rep. **9**:15590) we study the number of sites visited by a branching random walk on general graphs. To do so, we introduce a fieldtheoretic tracing mechanism which keeps track of all already visited sites. We find the scaling laws of the moments of the distribution near the critical point.

Chapter 3 (joint work with Gunnar Pruessner and Guillaume Salbreux, submitted, arXiv: 2006.00116) provides an analysis of the first-passage time problem for stochastic processes subject to white and coloured noise. By way of a perturbation theory, I give a systematic and controlled expansion of the moment generating function of first-passage times.

In Chapter 4, we revise the tracing mechanism found earlier and use it to characterise three different extreme values, first-passage times, running maxima, and mean volume explored. By formulating these in field-theoretic language, we are able to derive new results for a class of non-Markovian stochastic processes.

Chapter 5 and 6 are concerned with the first-passage time distribution of fractional Brownian Motion. Chapter 5 (joint work with Kay Wiese, appeared in Phys. Rev. E 101 (4):043312) introduces a new algorithm to sample them efficiently. Chapter 6 (joint work with Maxence Arutkin and Kay Wiese, submitted, arXiv:1908.10801) gives a field-theoretically obtained perturbative result of the first-passage time distribution in the presence of linear and non-linear drift.

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Chapter 0

Introduction

Stochastic processes are indispensable for the study of biological processes, chemical reaction kinetics, or complex systems. But why?

When studying systems comprised of many interacting agents, it is helpful to distinguish a single degree of freedom, the *particle*, and to observe its evolution in time. In doing so, all of the remaining degrees of freedom are subsumed into the *bath*. The ambition of this approach is to infer from observation of the particle the properties of the entire system. Methodically, this isn't unlike a biologist counting dragon flies to gauge the health of a pond.

Creating the potentially arbitrary distinction between the particle and the bath reduces the enormous number of interactions that are hidden to two: the *forcing* with which the bath acts on the particle, and the *feedback* with which the particle influences the dynamics of the bath. It is customary in physics to ignore the feedback entirely and to assume that the bath evolves fully independently of the particle. This then sets the stage for the great conceptual leap, brought about amidst the late 19th century, which is that the evolution of the bath no longer needs to be deterministically understood but is assumed to be *random*. The substitution of the bath's very many deterministic degrees of freedom by a single random force, however, is a delicate issue and I shall avoid expanding on it.

Instead, I would like to elaborate on the transition between deterministic and random evolution. I consider this transition to be the domain of *memory*. Memory stands at the centre of this thesis, and features in each chapter, in some more visibly than in others. How to think of it? Suppose, I use a microscope to measure the forcing exerted by a bath onto a particle over a large number of subsequent, very short time intervals. Within each of these very short time intervals, the forcing may still wildly fluctuate; this is no concern since I simply take note of, say, the average forcing within each of these very short time intervals. Through this procedure, I obtain a time series for the values of the forcing along every time interval. This time series is unpredictable in the deterministic sense, but empirically one may construct an a posteriori random distribution from which the values are drawn. In itself such a distribution may already illuminate some of the internal physics. To progress, however, it is worthwhile to analyse the data for correlations between different values of the time series. The usual paradigm in this case is white noise which declares that no two distinct points of the series are correlated to each other – a bold assumption! If such correlations exist, however, they are physically interpreted as *memory* of the bath. The emergence of memory is a sign that the width of the time interval

has been chosen small enough to be comparable to the timescale along which the bath evolves according to its hidden microscopic, and therefore deterministic, rules. The bath then retains some information about its internal state as it evolves from one time interval to the next. Memory in complex environments is therefore most of all a statement of time scales, and a feature of the interpolation between the deterministic and the random picture we make of it. As we zoom in, the gas is replaced by a spring, so to speak, and the different time intervals hang together more and more causally.

The question of how to address a potentially infinite number of interacting degrees of freedom acting on a *particle* is not reserved to stochastic dynamics. To the contrary: it caused the emergence of a second great conceptual advance in theoretical physics, *field theory*. Historically developed for the study of high energy particle physics, (quantum) field theory deals with the effective large scale behaviour of theories described at the microscopic level. At its core it operates with path integrals which generate every possible future (and past) evolution of a quantum field and assign to it a probabilistic weight. In constructing this weight, all possible interactions of the field (including with itself) are taken into account. Its fundamental structure therefore lends itself to the study of statistical mechanics, to which it was soon adapted in the form of statistical field theory. The renormalisation group method, oen of the most impressive machineries of theoretical physics, soon led to rapid advances in the study of universality and critical phenomena in many-body systems in and out of thermodynamic equilibirum.

In this tradition, I suggest to consider field theory as a precious tool for the study of stochastic processes. Field theory, re-interpreted, is a sophisticated way to calculate correlation functions of *nearly* Gaussian random variables. In its language, certain connections between stochastic processes and theoretical physics become very transparent. Examples are the link between a free particle and Brownian Motion, between particle interactions and correlations, or between thermodynamic equilibirum and the central limit theorem, to name but a few. Field theory is therefore a very capable tool to study stochastic evolutions in complex systems. Much of its power is derived from the many decades that physicists have improved and explored its abilities in its various domains of applications. To bring field theory and stochastic processes together therefore also means to build bridges of understanding to other areas of physics.

In this thesis, I will provide an overview on ways how to use field theory to study stochastic processes. In most of the chapters, the field-theory is employed to perturbatively compute certain observables for processes with memory (Chps. 3, 4, and 6). In two more chapters (Chps. 1 and 2), I demonstrate how branching processes can be considered field-theoretically. Chp. 5 is the exception to the rule in that it presents a purely numerical research project with no immediate connection to field theory. The work presented in this thesis is the result of many collaborative research projects that I had the pleasure to work on during my PhD at Imperial College (October 2016 to March 2020), including my six-month visit at École Normale Superiéure from October 2018 to March 2019.

Structure

This thesis is a **collective thesis** – every chapter is either a near verbatim copy of a peerreviewed journal article, or a manuscript eventually intended for publication. Depending on the particular chapter, I have either been co-author or main author. The precise correspondence

between chapters and publications is outlined in Tab. 0.1. At the beginning of every chapter I explain my individual contribution and what parts of the research I did or did not do. Where applicable, I have sought, and found, my co-authors' and publishers' permission to cite our joint work in full length. Throughout the thesis I have taken utmost care to highlight all citations as such. Every figure and table is credited properly, where appropriate.

In presenting this thesis as a collection of manuscripts and articles, I also follow the advice of my supervisor (*cf.* Gunnar Pruessner's response stated in A.1). The format of a collective thesis best represents the way in which this research took place: in collaborations, in projects, with different senior PIs and at two different institutions. All six chapters are independent works, yet still connected by common themes: field theory, stochastic processes, memory, extreme values etc. In their respective overviews, I point out the links to other chapters and how they influence each other. Finally, a conclusion shows future research directions which follow from this work.

This thesis is divided into three parts each covering a different aspect of my work: Branching processes, First-passage times, and fractional Brownian Motion.

In the first part, Branching Processes, I present two peer-reviewed journal articles of which I am a co-author. These two chapters were each the result of collaborations with fellow PhD students in my group under joint supervision of Gunnar Pruessner. In both projects, we develop a field theory that models branching processes, with and without spatial embedding, and use it to study certain characteristics with field-theoretic tools.

In the first chapter, Field theory of Branching Processes, we focus on a branching process with no spatial embedding. The system is initiated with one particle. Every particle has an exponentially distributed lifetime after which it either dies out or branches into k new indistinguishable particles with probability p_k . Each offspring undergoes the same rule ad infinitum. If, on average, the particle creates more than one offspring upon expiring, the expected total number of particles in the system grows exponentially. If the average number of offspring is less than one, it is certain that the system will die out within a finite amount of time. Once no particle is alive, no new ones can be created. This empty state is therefore called an absorbing phase. If the average number of offspring per particle is one, the system is referred to be at the critical point. We investigate the behaviour of the branching process at, or in the vicinity of, the critical point. By calculating various different observables, we show that at or close to criticality the precise details of the offspring distribution $\{p_k\}$ do not matter. Instead, we find that these observables can be expressed universally, *i.e.* with no recurrence to the precise offspring distribution.

The second chapter, Branching Random Walks on General Graphs, deals with a spatially embedded branching random walk. As in the previous chapter, a particle placed on a lattice undergoes branching or extinction events after an exponentially distributed life time but, concurrent to these, further hops onto neighboured lattice sites. Each particle therefore performs a random walk on the lattice connecting the site at which it was created to the one at which it expired. If one marked every site which is visited by any of these random walks up to a given time t, one obtains the so-called "trace" of the branching random walk. It is of great interest, in particular in times of a pandemic, to understand how the number of such sites grows with time. In this chapter, we answer this question for a branching random walk at criticality, *i.e.* when the expected number of offspring per particle is one.

The second part, First-passage times, contains research I have worked on in collaboration with Guillaume Salbreux at the Francis Crick Institute and together with Gunnar Pruessner. This work has been developed over almost four years and has not yet been published. Both chapters in this part address the question of first-passage time distributions (and related extreme values) for stochastic processes whose increments are weakly short-range correlated.

In the third chapter, Fist passage time distribution of active thermal particles, I present a framework with which one can compute perturbative corrections to the moment generating function of first-passage times. Based on a renewal type equation for Markovian processes, I introduce its perturbative expansion and compute the first-order correction explicitly for two systems in order to illustrate its validity. The class of processes this framework is capable to handle are particles which are subject to an external potential, some white noise, and, mediated by a small coupling constant in which the perturbation takes place, a second driving noise term with non-vanishing self-correlation. The additional driving by a second self-correlated noise induces correlations in the particles stochastic increments, therefore breaking its Markovianity.

The fourth chapter, Field Theory for Extreme Values in Stochastic Processes, is less technical and acts as a summary bringing together different pieces of work I have been involved in. It acts as a hinge between Chp. 2 and Chp. 3 in that it takes the field-theoretic trace-mechanism from Chp. 2 and re-interprets it in a way that makes it useful to study extreme values of stochastic processes. The field-theoretic formulation further allows for an additional driving noise, equivalent to the one introduced in the previous chapter, and leads to a diagrammatic correction of the moment-generating function of first-passage times, for instance, which is fully equivalent to the one obtained previously with different means. In fact, it retraces the "history" of the project in that we initially derived the key result in this field-theoretic manner. At a later stage of the project, I then developed the interpretation and new derivation that is presented in Chp. 3. The use of inverse functionals and functional expansions that is new to this chapter, and the linking of different extreme values to one "trace" function introduced in 4 were both inspired by the collaboration with Kay Wiese, thus linking both chapters of this part to the third part of my thesis.

In the third part, Fractional Brownian Motion, I present the outcomes of my collaboration with Kay Wiese which occurred during and after my visit at École Normale Supérieure in Paris from October 2018 to March 2019. At the time I joined Kay Wiese, he and his former PhD student Maxence Arutkin had already worked on calculating the first-passage time distribution of fractional Brownian Motion using perturbative field theory. Their work therefore perfectly complemented my earlier interests, outlined in the second part. Fractional Brownian Motion is characterised by its long-range correlated increments, and the type of perturbative expansion I have been working on previously does not apply to such cases. I therefore had the chance to learn about the field-theoretic machinery developed by them and collaborators over the last decade.

One of the obstacles met at the time of my visit was the numerical validation of the fieldtheoretic predictions of certain scaling functions of first-passage times in fractional Brownian Motion. This is due to the computational complexity associated with generating large sequences of correlated random variables. In order to sample large numbers of first-passage times with great numerical accuracy, we developed a new kind of algorithm which we refer to as "adaptive

Chapter	Publication Status	Arxiv preprint	Main author?
1	Published in Phys. Rev. E. 98 (6):062107	1808.08418	No
2	Published in Sci. Rep. 9 :15590	1909.00471	No
3	Submitted for publication	2006.00116	Yes
4	In preparation		Yes
5	Published in Phys. Rev. E $101(4):043312$	1908.11634	Yes
6	In review (Phys. Rev. E)	1908.10801	No

Table 0.1.: Overview of chapters and publications

bisection" and which is outlined in the chapter Adaptive Bisections, a verbatim citation of the journal article which has been recently accepted for publication.

Equipped with this algorithm, we were able to confirm the predictions made earlier, which led to a second manuscript which is at the time of writing still under peer-review and presented in the chapter Extreme values of Fractional Brownian Motion. This chapter uses a field-theory of fractional Brownian Motion to calculate the first-passage time density in the presence of a linear and/or a non-linear drift.

The three parts together showcase three different ways in which field theory, or closely related perturbative techniques, can be applied to the study of stochastic processes. They can be used to describe global observables, such as first-passage times, or avalanche shapes, which require knowledge of the full path. They are capable of encapsulating memory, here defined as correlation between the stochastic increments of a path. Using different flavours of field theory, these correlations can either be short-ranged or long-ranged and enter as a perturbation around a free field theory which is associated to Brownian motion. Many of the technologies developed in this thesis are new, and will certainly benefit further work which is necessary to strengthen the connection between field theory and stochastic processes.

List of peer-reviewed publications resulting from this thesis

- I. BORDEU, S. AMARTEIFIO, R. GARCIA-MILLAN, B. WALTER, N. WEI, AND G. PRUESS-NER. Volume explored by a branching random walk on general graphs. *Sci. Rep.* 9(1):15590, 2019. arXiv:1909.00471
- R. GARCIA-MILLAN, J. PAUSCH, B. WALTER, AND G. PRUESSNER. Field-theoretic approach to the universality of branching processes. *Phys. Rev. E* **98**(6):062107, 2018. arXiv:1808.08418
- B. WALTER AND K. J. WIESE. Sampling first-passage times of fractional brownian motion using adaptive bisections. *Phys. Rev. E* **101**:043312, 2020. arXiv:1908.11634

Further, the implementation of the algorithm discussed in Chp. 5 has been published as

• B. WALTER AND K. WIESE. Monte Carlo sampler of first passage times for fractional Brownian motion using adaptive bisections: Source code, 2019. HAL:02270046

Part I.

Branching Processes



Kleiner Baum im Spätherbst, Egon Schiele (1911), Leopold Museum Wien. The work of art depicted in this image and the reproduction thereof are in the public domain.

Chapter 1

Field-theoretic approach to the universality of branching processes

Abstract

"Branching processes are widely used to model phenomena from networks to neuronal avalanching. In a large class of continuous-time branching processes, we study the temporal scaling of the moments of the instant population size, the survival probability, expected avalanche duration, the so-called avalanche shape, the *n*-point correlation function and the probability density function of the total avalanche size. Previous studies have shown universality in certain observables of branching processes using probabilistic arguments, however, a comprehensive description is lacking. We derive the field theory that describes the process and demonstrate how to use it to calculate the relevant observables and their scaling to leading order in time, revealing the universality of the moments of the population size. Our results explain why the first and second moment of the offspring distribution are sufficient to fully characterise the process in the vicinity of criticality, regardless of the underlying offspring distribution. This finding implies that branching processes are universal. We illustrate our analytical results with computer simulations."

Cited from

R. GARCIA-MILLAN, J. PAUSCH, B. WALTER, AND G. PRUESSNER. Field-theoretic approach to the universality of branching processes. *Phys. Rev. E* **98**(6):062107, 2018. arXiv:1808.08418

Overview

In this chapter, I present a near verbatim copy of the peer-reviewed journal article

R. GARCIA-MILLAN, J. PAUSCH, B. WALTER, AND G. PRUESSNER. Field-theoretic approach to the universality of branching processes. *Phys. Rev. E* **98**(6):062107, 2018. arXiv:1808.08418. DOI: https://doi.org/10.1103/PhysRevE.98.062107

This paper was the outcome of a reading group led by Gunnar Pruessner and attended by Rosalba Garcia-Millan, Johannes Pausch and myself. Its initial motivation was to better understand the Doi-shift, a fundamental step in the derivation of a Doi-Peliti field theory (see main text below), and how it simplifies certain calculations. For the toy model we studied, a simple branching process, we found ways to express a wide-ranging variety of observables as field-theoretic expectation values which are represented diagrammatically. Near criticality, certain terms, or diagrams, can be neglected and the calculations simplify; the observables become universal, *i.e.* they no longer depend on the details of the underlying offspring distribution. The field-theory and its diagrammatics provide a very intuitive understanding of how the universality is attained. Not all of the observables are new in the literature, but the way field-theory allows for their computation is new and intuitive. Further, this chapter provides an hands-on introduction into the way Doi-Peliti field theories can be set up for non-spatial stochastic processes.

For a clearly written and very instructive guidance to Doi-Peliti field theory, not only in the context of branching processes, I refer the interested reader to Johannes Pausch' PhD thesis [181]. For a more mathematical take, I further recommend [3].

Statement of Contribution

I contributed to the construction and derivation of the field theory. I also wrote, ran, and evaluated the numerical simulations. The calculations concerning the moments, avalanche shape, and expected avalanche duration were **not** performed by me. The manuscript was written by Rosalba Garcia-Millan. It was further read, commented and approved by all the co-authors.

Acknowledgement

I would like to thank my collaborators very much for their permission to present our joint work as a part of my PhD thesis. I have obtained their approval which is shown in App. A.1.

Further, this work has benefited from fruitful discussions with Nanxin Wei, Stephanie Miller, Kay Wiese, Ignacio Bordeu Weldt, Eric Smith, David Krakauer, and Nicholas Moloney. We would like to extend our gratitude to Andy Thomas for invaluable computing support.

"Branching processes [116] are widely used for modelling phenomena in many different subject areas, such as avalanches [257, 148, 99], networks [98, 99, 148, 78], earthquakes [163, 45], family names [198], populations of bacteria and cells [129, 79], nuclear reactions [253, 185], cultural evolution [201] and neuronal avalanches [211, 13]. Because of their mathematical simplicity they play an important role in statistical mechanics [231] and the theory of complex systems [45].

Branching processes are a paradigmatic example of a system displaying a second-order phase transition between extinction (absorbing state) with probability one and non-zero probability of survival (non-absorbing state) in the infinite time limit. The critical point in the parameter region at which this transition occurs is where branching and extinction rates exactly balance, namely when the expected number of offspring per particle is exactly unity [116, 45].

In the present work we study the continuous-time version of the Galton-Watson branching process [116], which is a generalisation of the birth-death process [95, 104]. In the continuous-time branching process, particles go extinct or replicate into a number of identical offspring at random and with constant Poissonian rates. Each of the new particles follows the same process. The difference between the original Galton-Watson branching process and the continuous-time branching process we consider here, lies in the waiting times between events. In the original Galton-Watson branching process, updates occur in discrete time steps, while in the continuous-time process share many asymptotics [116, 231], and therefore we regard the continuous-time branching process as the continuum limit of the Galton-Watson branching process.

By using field-theoretic methods, we provide a general framework to determine universal, finite-time scaling properties of a wide range of branching processes close to the critical point. The main advantages of this versatile approach are, on the one hand, the ease with which observables are calculated and, on the other hand, the use of diagrammatic language, which allows us to manipulate the sometimes cumbersome expressions in a neat and compact way. Other methods in the literature developed to study problems related to branching processes, in particular relating branching processes to different forms of motion, include the formalism based on the Pal-Bell equation [175, 14, 130].

Moreover, our framework allows us to determine systematically observables that are otherwise complicated to manipulate if possible at all. To illustrate this point, we have calculated in closed form a number of observables that describe different aspects of the process in the vicinity of the critical point: we have calculated the moments of the population size as a function of time, the probability distribution of the population size as a function of time, the avalanche shape, the two-time and n-time correlation functions, and the total avalanche size and its moments.

Our results show that branching processes are universal in the vicinity of the critical point [144, 2] in the sense that exactly three quantities (the Poissonian rate and the first and second moments of the offspring distribution) are sufficient to describe the asymptotics of the process regardless of the underlying offspring distribution.

The contents of this paper are organised as follows. In Sec. 1.2 we derive the field theory of the continuous-time branching process. In Sec. 1.3 we use our formalism to calculate a number of observables in closed form, and in Sec. 1.4 we discuss our results and our conclusions. Further

details of the calculations can be found in the appendices.

1.2 Field Theory of the continuous-time branching process

The continuous-time branching process is defined as follows. We consider a population of N(t) identical particles at time $t \ge 0$ with initial condition N(0) = 1. Each particle is allowed to branch independently into κ offspring with Poissonian rate s > 0, where $\kappa \in \{0\} \cup \mathbb{N}$ is a random variable with probability distribution $P(\kappa = k) = p_k \in [0, 1]$ [95], Fig. 1.1. In the language of chemical reactions, this can be written as the reaction $A \to \kappa A$.

To derive the field theory of this process following the methods by Doi and Peliti [73, 186, 67, 231], we first write the master equation of the probability P(N, t) to find N particles at time t,

$$\frac{\mathrm{d}P(N,t)}{\mathrm{d}t} = s \sum_{k} p_k (N-k+1) P(N-k+1,t) - s N P(N,t), \tag{1.1}$$

with initial condition $P(N,0) = \delta_{N,1}$. Following work by Doi [73], we cast the master equation in a second quantised form. A system with N particles is represented by a Fock-space vector $|N\rangle$. We use the ladder operators a^{\dagger} (creation) and a (annihilation), which act on $|N\rangle$ such that $a |N\rangle = N |N-1\rangle$ and $a^{\dagger} |N\rangle = |N+1\rangle$, and satisfy the commutation relation $[a, a^{\dagger}] = aa^{\dagger} - a^{\dagger}a = 1$. The probabilistic state of the system is given by

$$|\Psi(t)\rangle = \sum_{N} P(N,t) |N\rangle, \qquad (1.2)$$

and its time evolution is determined by Eq. (1.1),

$$\frac{\mathrm{d}\left|\Psi(t)\right\rangle}{\mathrm{d}t} = s\left(f\left(a^{\dagger}\right) - a^{\dagger}\right)a\left|\Psi(t)\right\rangle,\tag{1.3}$$

using the probability generating function of κ ,

$$f(z) = \sum_{k=0}^{\infty} p_k z^k = \langle z^{\kappa} \rangle , \qquad (1.4)$$

where $\langle \bullet \rangle$ denotes expectation. We define the mass r as the difference between the extinction and the net branching rates,

$$r = sp_0 - s \sum_{k \ge 2} (k - 1)p_k = s (1 - \langle \kappa \rangle), \qquad (1.5)$$

and the rates q_i as

$$q_j = s \sum_k \binom{k}{j} p_k = s \left\langle \binom{\kappa}{j} \right\rangle = \frac{s}{j!} f^{(j)}(1), \qquad (1.6)$$

where $f^{(j)}(1)$ denotes the *j*th derivative of the probability generating function Eq. (1.4) evaluated at z = 1. We assume that the rates q_j are finite. In this notation, the time evolution in



Figure 1.1.: Typical avalanche profiles N(t) of a binary branching process (blue) and a branching process with geometric distribution of the number of offspring (orange), both at criticality r = 0, and with Poissonian rate s = 1. This figure has been published in [94] and is reproduced here with the permissions of the right holder stated in App. A.1

Eq. (1.3) can be written as

$$\tilde{\mathcal{A}} |\Psi(t)\rangle = \frac{\mathrm{d}}{\mathrm{d}t} |\Psi(t)\rangle \text{ and thus } |\Psi(t)\rangle = e^{\tilde{\mathcal{A}}t} |\Psi(0)\rangle,$$
(1.7)

where $\tilde{\mathcal{A}}$ is the operator

$$\tilde{\mathcal{A}} = \sum_{j \ge 2} q_j \tilde{a}^j a - r \tilde{a} a, \tag{1.8}$$

and \tilde{a} denotes the Doi-shifted creation operator, $a^{\dagger} = 1 + \tilde{a}$.

The sign of the mass r, Eq. (1.5), determines in which regime a particular branching process is in; if r = 0 the process is at the critical point, if r > 0 the process is in the subcritical regime and if r < 0 the process is in the supercritical regime. Subcritical and critical processes are bound to go extinct in finite time, whereas supercritical process have a positive probability of survival [116].

Following the work by Peliti [186], Eq. (1.3) can be cast in path integral form. Here, the creation and annihilation operators a^{\dagger} and a are transformed to time-dependent creation and annihilation fields $\varphi^{\dagger}(t)$ and $\varphi(t)$ respectively. Similarly, the Doi-shifted operator \tilde{a} is transformed to the time-dependent Doi-shifted field $\tilde{\varphi}(t) = \varphi^{\dagger}(t) - 1$. The action functional of the resulting field theory is given by

$$\mathcal{A}[\tilde{\varphi},\varphi] = \int_{-\infty}^{\infty} dt \left\{ \sum_{j\geq 2} q_j \tilde{\varphi}^j(t) \varphi(t) - \tilde{\varphi}(t) \left(\frac{d}{dt} + r\right) \varphi(t) \right\}.$$
(1.9)

1. Field theory of Branching Processes

Using the Fourier transform

$$\varphi(t) = \int d\omega \,\varphi(\omega) e^{-i\omega t} \quad \text{with} \quad d\omega = \frac{d\omega}{2\pi},$$
 (1.10a)

$$\varphi(\omega) = \int dt \,\varphi(t) e^{i\omega t},$$
 (1.10b)

and identically for $\tilde{\varphi}(t)$, the action Eq. (1.9) becomes local in ω and the bilinear, *i.e.* the Gaussian part

$$\mathcal{A}_0[\tilde{\varphi},\varphi] = -\int \mathrm{d}\omega \,\tilde{\varphi}(-\omega)(-i\omega + r)\varphi(\omega) \tag{1.11}$$

of the path integral can be determined in closed form. The Gaussian path integral is well-defined only when the mass is positive, r > 0. The non-linear terms, $j \ge 2$ in Eq. (1.9) are then treated as a perturbation about the Gaussian part, as commonly done in field theory [231, 232].

1.3 Observables

We use the field theory described above to calculate a number of observables that have received attention in the literature in various settings. In Table 1.1 we list all the observables that we have calculated in closed form and the degree of approximation of our analytical result. Some results are exact for any kind of branching process and other results are only exact for binary branching processes. Those results that are an approximation have the exact asymptotic behaviour.

All observables are constructed on the basis of the probability vector $|\Psi(t)\rangle$ which evolves according to Eq. (1.7). If the initial state, t = 0, consists of a single particle, then $|\Psi(0)\rangle = a^{\dagger} |0\rangle$ and $|\Psi(t)\rangle = \exp(\tilde{A}t) a^{\dagger} |0\rangle$. Probing the particle number requires the action of the operator $a^{\dagger}a$, whose eigenvectors are the pure states $|N\rangle$, such that $a^{\dagger}a |N\rangle = N |N\rangle$. The components of the vector $a^{\dagger}a \exp(\tilde{A}t) a^{\dagger} |0\rangle$ are thus the probability that the process has generated N particles weighted by N. To sum over all states, we further need the projection state

$$\langle \mathfrak{P} | = \sum_{N=0}^{\infty} \langle N | = \sum_{N=0}^{\infty} \frac{1}{N!} \langle 0 | a^N = \langle 0 | e^a .$$

$$(1.12)$$

The expected particle number at time t may thus be written as

$$\langle N(t) \rangle = \langle \mathfrak{P} | \, a^{\dagger} a \, e^{\tilde{\mathcal{A}}t} a^{\dagger} \, | 0 \rangle \quad . \tag{1.13}$$

More complicated observables and intermediate temporal evolution can be compiled following the same pattern [232]. To perform any calculations, the operators need to be normal ordered and then mapped to fields as suggested above, $a^{\dagger} \rightarrow \varphi^{\dagger}(t) = 1 + \tilde{\varphi}(t)$ and $a \rightarrow \varphi(t)$, where the time t corresponds to the total time the system has evolved for, Eq. (1.7). The expectation in Eq. (1.13) can thus be written as

$$\langle N(t)\rangle = \left\langle \varphi^{\dagger}(t)\varphi(t)\,\varphi^{\dagger}(0)\right\rangle,\tag{1.14}$$

bservable	Symbol	Equation	$\mathbf{Expression}$	Regime	Figure
Ioments of the number of particles $N(t)$	$\langle N^n(t) angle$	(1.37), (1.38)	exact asymptote	$r \in \mathbb{R}$	1.2
foments of the number of particles $N(t)$	$\langle N^n(t) angle,\ n\in\{1,2,3\}$	(1.67)	exact	$r\in\mathbb{R}$	1.2
Ioment generating function of $N(t)$	${\cal M}_N(z)$	(1.40)	exact asymptote	$r\in\mathbb{R}$	
robability distribution of $N(t)$	P(N,t)	(1.43)	exact for binary bp	$r\in \mathbb{R}$	
robability of survival	$P_{ m s}(t)$	(1.44), (1.45)	exact for binary bp	$r\in\mathbb{R}$	1.3
is tribution of the avalanche duration ${\cal T}$	$\mathcal{P}_{T}(t)$	(1.46), (1.47)	exact for binary bp	$r \ge 0$	
xpected avalanche duration	$\langle T angle$	(1.48)	exact for binary bp	$r \ge 0$	1.4
valanche shape	V(t,T)	(1.54), (1.55)	exact for binary bp	$r\in\mathbb{R}$	1.5a
veraged avalanche shape	$\langle V(au) angle_T$	(1.78)	exact for binary bp	$r\in\mathbb{R}$	1.5b
wo-point connected correlation function	$\operatorname{Cov}\left(N(t_1),N(t_2) ight)$	(1.58)	exact	$r\in \mathbb{R}$	1.6
hree-point correlation function	$\langle N(t_1)N(t_2)N(t_3) angle$	(1.71)	exact	$r\in \mathbb{R}$	
Λ oments of the total avalanche size S	$\langle S^n angle$	(1.62), (1.63)	exact asymptote	$r \ge 0$	
loment generating function of S	${\cal M}_S(z)$	(1.65)	exact asymptote	$r \ge 0$	
istribution of S	$\mathcal{P}_{S}\left(x ight)$	(1.66)	exact asymptote	$r \ge 0$	1.7

critical and subcritical $(r \ge 0)$ or all encompassing $(r \in \mathbb{R})$. This table has been published in [94] and is reproduced here with the permissions of the either: exact, exact for binary branching processes (i.e. for other branching process, our result is the leading order in q_2/r for small r at fixed rt), or provide exact asymptotes (that is, our result is the leading order for any kind of branching process). The regime of validity near criticality is either Summary of observables including their equation number and what cases and limits are exact. The expressions referred to are, in the limit $r \to 0$, right holder stated in App. A.1

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where $\langle \mathcal{O} \rangle$ denotes the path integral

$$\langle \mathcal{O} \rangle = \int \mathcal{D}\left[\tilde{\varphi}, \varphi\right] \mathcal{O}e^{\mathcal{A}\left[\tilde{\varphi}, \varphi\right]}.$$
(1.15)

The resulting expressions are most elegantly expressed in terms of Feynman diagrams [231]. The bare propagator of the field φ is read off from the bilinear part of the action which, in Fourier space, is

$$\langle \varphi(\omega)\widetilde{\varphi}(\omega')\rangle = \frac{\delta(\omega+\omega')}{-\imath\omega+r} \hat{=}$$
 (1.16)

where $\delta(\omega + \omega') = 2\pi\delta(\omega + \omega')$ denotes the scaled Dirac- δ function. Diagrammatically, the bare propagator is represented by a straight directed line. The directedness of the propagator reflects the causality (see Eq. (1.17)) of the process in the time domain as a particle has to be created before it can be annihilated but not vice versa. By convention, in our Feynman diagrams time proceeds from right to left.

Using the fact that the mass r is strictly positive for the Gaussian path integral to converge, we write the propagator in real time by Fourier transforming,

$$\left\langle \varphi(t)\widetilde{\varphi}(t')\right\rangle = \int_{-\infty}^{\infty} \mathrm{d}\omega \,\frac{\delta(\omega+\omega')}{-\imath\omega+r} e^{-\imath\omega t} e^{-\imath\omega't'} = \Theta(t-t')e^{-r(t-t')},\tag{1.17}$$

where Θ is the Heaviside step function. If r < 0, the integral in Eq. (1.17) is only convergent for t < t', which violates causality and therefore yields an unphysical result. For this reason, we will assume r > 0 and we will take the limit $r \to 0$ where possible. Therefore, in this paper, the analytical results obtained through this field theory hold for the critical and subcritical regimes only $(r \ge 0)$. However, in some cases we may be able to use probabilistic arguments that allow us to extend our results to the supercritical case (r < 0), see Section 1.3.2. Furthermore, we will drop the cumbersome Heaviside Θ functions, assuming suitable choices for the times, such as t > t' above.

Each of the interaction terms of the form $\tilde{\varphi}^{j}\varphi$ with $j \geq 2$ in the non-linear part of the action Eq. (1.8) come with individual couplings q_{j} , Eq. (1.6). These are to be expanded perturbatively in. Following the canonical field theoretic procedure [232, 231, 186], they are represented by (tree-like) amputated vertices such as

These vertices are *not* to be confused with the underlying branching process, because after the Doi-shift, lines are not representative of particles, but of their correlations. For example, the vertex with coupling q_2 in Eq. (1.18), accounts for density-density correlations due to *any* branching or extinction, just like the propagator Eq. (1.16) accounts for all particle density due to *any* branching or extinction. After Fourier transforming, these processes are accounted for regardless of when they take place.

The directionality of the diagrams allows us to define *incoming* legs and *outgoing* legs of a vertex [231]. In the present branching process, all vertices have one incoming leg and j outgoing legs. We will refer to diagrams that are constructed solely from q_2 vertices as *binary*

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tree diagrams. The most basic such diagram is \succ , which in real time reads

$$\left\langle \varphi^{2}(t)\varphi^{\dagger}(0)\right\rangle = 2 \right\rangle^{q_{2}} = 2q_{2} \int d\omega_{1}d\omega_{1}'d\omega_{2}d\omega_{2}d\omega_{3}d\omega_{3}' e^{-i\omega_{2}t}e^{-i\omega_{3}t} \\ \times \delta\left(\omega_{1}+\omega_{2}'+\omega_{3}'\right)\frac{\delta\left(\omega_{1}+\omega_{1}'\right)}{-i\omega_{1}+r}\frac{\delta\left(\omega_{2}+\omega_{2}'\right)}{-i\omega_{2}+r}\frac{\delta\left(\omega_{3}+\omega_{3}'\right)}{-i\omega_{3}+r} \\ = 2\frac{q_{2}}{r}e^{-rt}\left(1-e^{-rt}\right),$$

$$(1.19)$$

where the pre-factor 2 is the combinatorial factor of this diagram.

The various observables that we calculate in the following are illustrated by numerics for two different kinds of continuous-time branching processes. Firstly, the binary branching process with probabilities $p_0, p_2 \ge 0$ such that $p_0 + p_2 = 1$, and secondly, the branching process with geometric offspring distribution $p_k = p(1-p)^k$ with $p \in [0, 1]$. The mass r (1.5) and the rates of the couplings q_j (1.6) are, in each case,

(binary)
$$r_B = s(1 - 2p_2),$$
 (1.20a)
 $q_{B2} = sp_2 = \frac{s - r_B}{2}, q_{Bj} = 0 \text{ for } j \ge 3,$
(geometric) $r_G = s\frac{2p - 1}{p},$ (1.20b)
 $q_{Gj} = s\left(\frac{1 - p}{p}\right)^j = s\left(1 - \frac{r_G}{s}\right)^j.$

Fig. 1.1 shows typical trajectories for each case.

1.3.1 Moments $\langle N^n(t) \rangle$ and their universality

In the following we will calculate the moments of the number of particles N(t), which can be determined using the particle number operator $a^{\dagger}a$, as introduced above. The *n*th moment of N(t) can be expressed as

$$\langle N^{n}(t) \rangle = \left\langle \bigotimes \left| \left(a^{\dagger} a \right)^{n} \right| \Psi(t) \right\rangle$$

$$= \sum_{\ell=0}^{n} \left\{ n \atop \ell \right\} \left\langle \bigotimes \left| a^{\ell} \right| \Psi(t) \right\rangle$$

$$= \sum_{\ell=0}^{n} \left\{ n \atop \ell \right\} \left\langle \varphi^{\ell}(t) \widetilde{\varphi}(0) \right\rangle,$$

$$(1.21)$$

where ${n \\ \ell}$ denotes the Stirling number of the second kind for ℓ out of n^{-1} . We define the dimensionless function $\hat{g}_n(t)$ as the expectation

$$\hat{g}_n(t) = \langle \varphi^n(t) \tilde{\varphi}(0) \rangle \stackrel{\circ}{=} n \qquad (1.22)$$

with $\hat{g}_0(t) = \langle \tilde{\varphi}(0) \rangle = 0$ and $\hat{g}_1(t) = \langle \varphi(t) \tilde{\varphi}(0) \rangle = e^{-rt}$. The black circle in the diagram of Eq. (1.22) represents the sum of all possible intermediate nodes, allowing for internal lines. For instance,

$$\hat{g}_1(t) \doteq - - - - , \qquad (1.23a)$$

$$\hat{g}_2(t) = 2$$
, (1.23b)

$$\hat{g}_3(t) = - = 6 + 12$$
, (1.23c)

$$\hat{g}_4(t) = 24 + 48$$
 (1.23d)

$$+72 \rightarrow +24 \rightarrow +96 \rightarrow --,$$

where the coefficient in front of each diagram is its symmetry factor, which is included in the representation involving the black circle, Eq. (1.22).

The tree diagrams follow a pattern, whereby \hat{g}_n involves all \hat{g}_m with m < n. For $n \ge 2$ this can be expressed as the recurrence relation

$$\hat{g}_{n}(t) \stackrel{\text{a}}{=} \sum_{k=2}^{n} \sum_{m_{1},\dots,m_{k}=1} \binom{n}{m_{1},\dots,m_{k}} m_{2} \stackrel{m_{1}}{\underset{m_{k}}{\longrightarrow}} , \qquad (1.24)$$

where $\binom{n}{m_1,\ldots,m_k}$ denotes the multinomial coefficient with the implicit constraint of $m_1 + \ldots + m_k = n$. Including $\hat{g}_1(t)$ from Eqs. (1.23a) and (1.17), this may be written as

$$\hat{g}_n(t) = \delta_{n,1} e^{-rt} + \left(\sum_{k=2}^n q_k \sum_{m_1,\dots,m_k} \binom{n}{m_1,\dots,m_k} \int_0^t \mathrm{d}t' \, e^{-r(t-t')} \hat{g}_{m_1}(t') \hat{g}_{m_2}(t') \cdots \hat{g}_{m_k}(t')\right) \,, \quad (1.25)$$

where the integral accounts for the propagation up until time $t - t' \in [0, t]$ when a branching into (at least) k particles takes place, each of which will branch into (at least) m_k particles at some later time within [t - t', t].

$$\binom{n}{\ell} = \frac{1}{\ell!} \sum_{j=0}^{\ell} (-1)^{\ell-j} \binom{\ell}{j} j^n.$$

 $^{^{1}}$ The Stirling numbers of the second kind can be calculated using the expression

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We proceed by determining the leading order behaviour of \hat{g}_n in small r, starting with a dimensional argument. Since

$$\langle N^n(t)\rangle = \sum_{\ell=0}^n \left\{ {n \atop \ell} \right\} \hat{g}_\ell(t) \tag{1.26}$$

from Eqs. (1.21) and (1.22), $\langle N^n(t) \rangle$ being dimensionless implies the same for $\hat{g}_n(t)$. Our notation for the latter obscures the fact that $\hat{g}_n(t)$ is also a function of r and all q_j , which, by virtue of s, are rates and thus have the inverse dimension of t. We may therefore write

$$\hat{g}_n(t) = \overline{g}_n(rt; \overline{q}_2, \overline{q}_3, \dots) \tag{1.27}$$

where $\overline{q}_j = q_j/r$ are dimensionless couplings. Dividing q_j by any rate renders the result dimensionless, but only the particular choice of dividing by r ensures that all couplings only ever enter multiplicatively (and never as an inverse), thereby enabling us to extract the asymptote of $\hat{g}_n(t)$ in the limit of small r, as we will see in the following.

Writing Eq. (1.25) as

$$\overline{g}_{n}(y;\overline{q}_{2},\overline{q}_{3},\ldots) = \delta_{n,1}e^{-y} + \left(\sum_{k=2}^{n} \overline{q}_{k}\sum_{m_{1},\ldots,m_{k}} \binom{n}{m_{1},\ldots,m_{k}} \int_{0}^{y} \mathrm{d}y' \, e^{-(y-y')} \overline{g}_{m_{1}}(y';\overline{q}_{2},\ldots) \overline{g}_{m_{2}}(y';\ldots) \cdots \overline{g}_{m_{k}}(y';\ldots)\right)$$

$$(1.28)$$

the dominant terms in small r and fixed y = rt are those that contain products involving the largest number of factors of $\bar{q}_j \propto r^{-1}$. Since each \bar{q}_j corresponds to a branching, diagrammatically these terms are those that contain the largest number of vertices, *i.e.* those that are entirely made up of binary branching vertices q_2 . This coupling, $q_2 = \langle \kappa(\kappa - 1) \rangle/2$, cannot possibly vanish if there is any branching taking place at all. From Eqs. (1.27) and (1.28) it follows that $\hat{g}_n(t) \propto (q_2/r)^{(n-1)}$ to leading order in small r at fixed y = rt. Terms of that order are due to binary tree diagrams, whose contribution we denote by $g_n(t)$ in the following. For instance, $g_1(t) = \hat{g}_1(t), g_2(t) = \hat{g}_2(t)$,

$$g_3(t) \stackrel{\circ}{=} 12$$
, (1.29a)

$$g_4(t) = 24 + 96$$
 (1.29b)

To summarise, $\hat{g}_n(t)$ is dominated by those terms that correspond to binary tree diagrams, which are the trees g_n that have the largest number of vertices for any fixed n, *i.e.*

$$\langle \varphi^n(t)\widetilde{\varphi}(0)\rangle = \hat{g}_n(t) = g_n(t) + \mathcal{O}\left(\left(1 - \langle \kappa \rangle\right)^{-(n-2)}\right), \tag{1.30}$$

where the correction in fact vanishes for n < 3.

In what follows, we describe the asymptotic behaviour of various averages and densities near

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the critical point at r = 0. To simplify the notation, we denote

$$f(t) \simeq f_{\text{asymp}}(t) \tag{1.31}$$

if f(t) tends to $f_{asymp}(t)$ in the joint limit

$$\lim_{r \downarrow 0} \lim_{t \uparrow \infty} f(t) = f_{\text{asymp}}(t)$$
(1.32)

where $y = rt \gg 1$ is kept constant.

As far as the asymptote in small r is concerned, we may thus replace \hat{g}_{ℓ} in Eq. (1.26) by g_{ℓ} . Among the $\hat{g}_{\ell} \sim r^{-(\ell-1)}$ with $\ell = 0, 1, \ldots, n$, the dominating term is g_n so that the *n*th moment of the particle number N is, to leading order,

$$\langle N^n(t) \rangle \simeq g_n(t),$$
 (1.33)

although exact results, as shown in Eq. (1.67), are easily derived using Eqs. (1.21), (1.22), (1.23), and (1.25). On the basis of (1.25) the recurrence relation of g_n is give by

$$g_n(t) = \delta_{n,1} e^{-rt} + q_2 \sum_{m=1}^{n-1} \binom{n}{m} \int_0^t dt' e^{-r(t-t')} g_m(t') g_{n-m}(t'), \qquad (1.34)$$

whose exact solution is

$$g_n(t) = n! e^{-rt} \left(\frac{q_2}{r} \left(1 - e^{-rt}\right)\right)^{n-1}.$$
 (1.35)

We draw two main conclusions from our results. Firstly, that near the critical point r = 0, the branching process is solely characterised by the two parameters r and q_2 . We therefore conclude that this process displays *universality*, in the sense that its asymptotics are exactly the same for any given r and q_2 regardless of the underlying offspring distribution. In particular, certain ratios of the moments of the particle number are universal constants (they do not depend on any parameters nor variables). For $k, \ell \in \mathbb{N}$ and $m \in 0, \ldots, k-1$, we find the constant ratios

$$\frac{\left\langle N^{k}(t)\right\rangle \left\langle N^{\ell}(t)\right\rangle}{\left\langle N^{k-m}(t)\right\rangle \left\langle N^{\ell+m}\right\rangle} = \frac{k!\ell!}{(k-m)!(\ell+m)!}.$$
(1.36)

Secondly, our results show that the scaling form of the moments is

$$\langle N^n(t) \rangle \simeq (q_2 t)^{n-1} \mathcal{G}_n(rt), \qquad (1.37)$$

where \mathcal{G}_n is the scaling function

$$\mathcal{G}_n(y) = n! e^{-y} \left(\frac{1 - e^{-y}}{y}\right)^{n-1},$$
(1.38)

and the argument y = rt is the rescaled time, Fig. 1.2. The asymptotes of $\mathcal{G}_n(y)$ characterise


Figure 1.2.: Data collapse of the moments $\langle N(t) \rangle$, $\langle N^2(t) \rangle$ and $\langle N^3(t) \rangle$, as a function of rescaled time rt as of Eq. (1.37). Symbols show results for the binary branching process (blue) and the branching process with geometric distribution of offspring (orange), both with $r \in \{10^{-3}, 10^{-2}, 10^{-1}\}$ and s = 1. Solid lines indicate the exact solution in Eq. (1.67) and dashed lines indicate our approximation in Eq. (1.33). This figure has been published in [94] and is reproduced here with the permissions of the right holder stated in App. A.1

the behaviour of the branching process in each regime,

$$\mathcal{G}_n(y) \simeq \begin{cases} n! & \text{for } y = 0, \\ n! \, y^{-(n-1)} e^{-y} & \text{for } y \to \infty. \end{cases}$$
(1.39)

Moreover, from Eq. (1.37), we find that the moment generating function $\mathcal{M}_N(z) = \langle e^{Nz} \rangle$ is

$$\mathcal{M}_N(z) \simeq 1 + \frac{ze^{-rt}}{1 + z\frac{q_2}{r} (e^{-rt} - 1)}.$$
 (1.40)

1.3.2 Probability distribution of N(t), probability of survival $P_s(t)$ and expected avalanche duration $\langle T \rangle$

Using Eq. (1.21) and the identity ² of Stirling numbers of the second kind, we deduce that the falling factorial moments of N(t) are

$$\left\langle \varphi^{\ell}(t)\widetilde{\varphi}(0) \right\rangle = \left\langle N(t)(N(t)-1)\dots(N(t)-\ell+1) \right\rangle.$$
 (1.41)

$$N^{n} = \sum_{\ell=0}^{n} {\binom{n}{\ell}} N(N-1)\dots(N-\ell+1).$$

² The Stirling numbers of the second kind satisfy the identity

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Therefore, the probability generating function of N(t) is

$$\mathcal{P}_{N(t)}(z) = \sum_{\ell=0}^{\infty} \langle N(t)(N(t)-1)\dots(N(t)-\ell+1)\rangle \frac{(z-1)^{\ell}}{\ell!}$$
$$= \sum_{\ell=0}^{\infty} \left\langle \varphi^{\ell}(t)\widetilde{\varphi}(0) \right\rangle \frac{(z-1)^{\ell}}{\ell!}, \qquad (1.42)$$

and the probability distribution of N(t) is, using Eqs. (1.30) and (1.35),

$$P(N,t) = \frac{1}{N!} \frac{\mathrm{d}^N}{\mathrm{d}z^N} \left(\mathcal{P}_{N(t)}(z) \right) \Big|_{z=0}$$
(1.43a)

$$\simeq \sum_{\ell=N}^{\infty} {\ell \choose N} \frac{(-1)^{\ell-N}}{\ell!} g_{\ell}(t)$$
(1.43b)

$$= \begin{cases} 1 - \frac{e^{-rt}}{1 + \frac{q_2}{r}(1 - e^{-rt})} & \text{if } N = 0, \\ \frac{e^{-rt} \left(\frac{q_2}{r} \left(1 - e^{-rt}\right)\right)^{N-1}}{\left(1 + \frac{q_2}{r}(1 - e^{-rt})\right)^{N+1}} & \text{if } N > 0, \end{cases}$$
(1.43c)

which satisfies the initial condition $P(N, 0) = \delta_{N,1}$ and is an exact result for binary branching processes, consistent with [185].

It is straightforward to check that Eq. (1.43) satisfies the master equation (1.1) and the initial condition in the binary branching case. Due to the uniqueness of solutions of a system of coupled linear ordinary differential equations, the solution in Eq. (1.43) is the only solution. In particular, this solution holds in the supercritical case, r < 0. Reconstructing back the path that has lead us here, we find that $g_{\ell}(t)$ is the ℓ th falling factorial moment of N(t), $\langle N(t)(N(t)-1)\dots(N(t)-\ell+1)\rangle$, for binary branching processes including the supercritical case and, therefore, most expressions derived from $g_{\ell}(t)$ can be extended to r < 0. In what follows, we will specify which expressions hold in the supercritical case.

The probability of survival $P_s(t)$ is the probability that there is at least one particle at time $t, i.e. P_s(t) = P(N(t) \ge 1)$. Therefore, from Eq. (1.43),

$$P_{\rm s}(t) = 1 - P(0,t) = \frac{e^{-rt}}{1 + \frac{q_2}{r} \left(1 - e^{-rt}\right)},\tag{1.44}$$

and at the critical point,

$$\lim_{r \to 0} P_{\rm s}(t) \simeq \frac{1}{1 + q_2 t},\tag{1.45}$$

which is consistent with [93, 245, 46], Fig. 1.3.

We define the avalanche duration T as the exact time where an avalanche dies, *i.e.* the time t when the process reaches the absorbing state, $T = \min\{t|N(t) = 0\}$. The probability of survival $P_{\rm s}(t)$ gives the probability that T > t. Thus, $1 - P_{\rm s}(t)$ is the cumulative distribution function of the time of death and its probability density function is

$$\mathcal{P}_{T}(t) = -\frac{dP_{s}(t)}{dt} \simeq \frac{re^{rt}\left(1 + \frac{q_{2}}{r}\right)}{\left(\frac{q_{2}}{r} - e^{rt}\left(1 + \frac{q_{2}}{r}\right)\right)^{2}},$$
(1.46)



Figure 1.3.: Probability of survival as a function of rescaled time rt as of Eq. (1.44). Symbols show numerical results for the binary branching process (blue) and the branching process with geometric distribution of offspring (orange), both with $r \in$ $\{10^{-3}, 10^{-2}, 10^{-1}\}$ and s = 1. Lines indicate the result in Eq. (1.44), which is exact for binary branching (solid lines) and approximate otherwise (dashed lines). As rgets closer to the critical value, r = 0, the curves $P_{\rm s}(t)$ flatten and resemble the power law in Eq. (1.45), which has exponent -1. This figure has been published in [94] and is reproduced here with the permissions of the right holder stated in App. A.1

and at the critical point,

$$\lim_{r \to 0} \mathcal{P}_T(t) \simeq \frac{q_2}{(1+q_2 t)^2},\tag{1.47}$$

see Fig. 1.4. It follows from (1.46) that the expected avalanche duration is

$$\langle T \rangle \simeq \frac{1}{q_2} \ln \left(1 + \frac{q_2}{r} \right).$$
 (1.48)

Because the derivation of Eq. (1.46) relies on a finite termination time, we cannot assume that it remains valid in the supercritical case, and similarly for (1.48).

1.3.3 Avalanche shape V(t,T)

The avalanche shape V(t,T) is defined as the average of the temporal profiles N(t) conditioned to extinction at time T [99, 72, 213, 178, 10, 254, 142]. Closed form expressions of the avalanche shape have been calculated in other models such as avalanches in elastic interfaces [72], the Barkhausen noise [178], the discrete-time Ornstein-Uhlenbeck process [10]. An implicit expression of avalanche shape of branching processes is given in [99].

To produce an explicit expression we first calculate the expected number of particles at time t of a branching process conditioned to being extinct by time T, $\langle N(t) | N(T) = 0 \rangle$. In terms of ladder operators,

$$\left\langle N(t) \middle| N(T) = 0 \right\rangle = \left\langle 0 \middle| e^{\hat{\mathcal{A}}(T-t)} a^{\dagger} a e^{\hat{\mathcal{A}}t} a^{\dagger} \middle| 0 \right\rangle,$$
(1.49)

which means that a particle is created from the vacuum, the system is allowed to evolve for time t, the number of particles is measured, and the system evolves further for time T - t. Finally,



Figure 1.4.: Probability density function of the avalanche duration $\mathcal{P}_T(t)$ for the binary branching process with $r \in \{0, 10^{-3}, 10^{-2}, 10^{-1}\}$ and s = 1. Solid lines represent our result in Eqs. (1.46) and (1.47), which is exact for binary branching. Symbols show numerical results. This figure has been published in [94] and is reproduced here with the permissions of the right holder stated in App. A.1

all possible trajectories are "sieved" so that only those avalanches are taken into account whose number of particles is 0 at time T The path integral expression of Eq. (1.49) is

$$\left\langle N(t) \middle| N(T) = 0 \right\rangle = \left\langle e^{-\varphi(T)} \varphi^{\dagger}(t) \varphi(t) \varphi^{\dagger}(0) \right\rangle$$

$$= \left\langle \varphi(t) \widetilde{\varphi}(0) \right\rangle + \sum_{n \ge 1} \frac{(-1)^n}{n!} \times \left(\left\langle \varphi^n(T) \varphi(t) \widetilde{\varphi}(0) \right\rangle + \left\langle \varphi^n(T) \widetilde{\varphi}(t) \varphi(t) \widetilde{\varphi}(0) \right\rangle \right).$$

$$(1.50)$$

The two terms in the bracket have asymptotes

$$\langle \varphi^n(T)\varphi(t)\tilde{\varphi}(0)\rangle \simeq \sum_{k=1}^n \sum_{m_1,\dots,m_k} \binom{n}{m_1,\dots,m_k} \frac{1}{k!} g_{m_1}(T-t)\cdots g_{m_k}(T-t)g_{k+1}(t), \quad (1.51)$$

and

$$\left\langle \varphi^{n}(T)\widetilde{\varphi}(t)\varphi(t)\widetilde{\varphi}(0)\right\rangle \simeq \sum_{k=1}^{n} \sum_{m_{1},\dots,m_{k}} \binom{n}{m_{1},\dots,m_{k}} \frac{1}{(k-1)!} g_{m_{1}}(T-t)\cdots g_{m_{k}}(T-t)g_{k}(t), \quad (1.52)$$

with the constraint $m_1 + \ldots + m_k = n$ in both cases. Both expressions are exact in case of binary branching. Their diagrammatic representation and closed form expressions can be found in Appendix 1.B. Using the expression of $g_n(t)$ in Eq. (1.35) and the number of combinations of n legs into k groups, we have

$$\left\langle N(t) \middle| N(T) = 0 \right\rangle = e^{-rt} - P_{\rm s}(T) \left[1 + \frac{q_2}{r} \left(1 - e^{-rt} \right) \left(2 - \frac{P_{\rm s}(T)}{P_{\rm s}(t)} \right) \right],$$
 (1.53)

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where $P_{\rm s}(t)$ is given in Eq. (1.44).

In order to account solely for those instances that become extinct exactly at time T, the expectation $\langle N(t) | N(T) = 0 \rangle$ is to be differentiated with respect to T, and in order to account for the factor due to conditioning to extinction, we need to divide the result by $-\frac{d}{dt}P_s(t)$, yielding,

$$V(t,T) = \frac{\frac{\mathrm{d}}{\mathrm{d}T} \langle N(t) | N(T) = 0 \rangle}{-\frac{\mathrm{d}}{\mathrm{d}t} P_{\mathrm{s}}(t)}$$
$$\simeq 1 + 2\frac{q_2}{r} \left(1 - e^{-rt}\right) \left(1 - \frac{P_{\mathrm{s}}(T)}{P_{\mathrm{s}}(t)}\right), \qquad (1.54)$$

Fig. 1.5a. Since the observable V(t,T) suitably incorporates the condition N(T) = 0, the result in Eq. (1.54) holds for the supercritical case as well. At criticality, the avalanche shape is the parabola [99, 178, 10, 254]

$$\lim_{r \to 0} V(t,T) \simeq 1 + 2 \frac{(q_2 T)^2}{1 + q_2 T} \left(1 - \frac{t}{T}\right) \frac{t}{T}.$$
(1.55)

The avalanche shape V(t,T) in Eq. (1.54) is a symmetric function with its maximum at t = T/2, which is bounded [10] by

$$\lim_{T \to \infty} V\left(\frac{T}{2}, T\right) \simeq 1 + 2\frac{q_2}{r}.$$
(1.56)

1.3.4 Connected correlation function $Cov(N(t_1), N(t_2))$

To calculate the expectation $\langle N(t_1)N(t_2)\rangle$ we assume $0 < t_1 < t_2$ without loss of generality,

$$\langle N(t_1)N(t_2)\rangle = \left\langle \bigotimes \left| a^{\dagger}ae^{-\hat{\mathcal{A}}(t_2-t_1)}a^{\dagger}ae^{-\hat{\mathcal{A}}t_1}a^{\dagger} \right| 0 \right\rangle$$
(1.57a)

$$= \left\langle \varphi(t_2)\varphi^{\dagger}(t_1)\varphi(t_1)\varphi^{\dagger}(0) \right\rangle$$
(1.57b)

$$= \langle \varphi(t_2)\widetilde{\varphi}(t_1)\varphi(t_1)\widetilde{\varphi}(0) \rangle + \langle \varphi(t_2)\varphi(t_1)\widetilde{\varphi}(0) \rangle$$

$$\hat{=} - + 2 \rangle - . \qquad (1.57c)$$

The diagram on the left consists of two separate components. We refer to diagrams of that kind as disconnected diagrams, in contrast to connected diagrams that only consist of one component as the one appearing on the right. The connected correlation function is

$$\operatorname{Cov}\left(N(t_1), N(t_2)\right) = \left\langle N(t_1)N(t_2)\right\rangle - \left\langle N(t_1)\right\rangle \left\langle N(t_2)\right\rangle$$
$$= \left(2\frac{q_2}{r} + 1\right)e^{-r(t_1+t_2)}\left(e^{rt_1} - 1\right)$$
(1.58)

which is an exact result independent of the type of branching process, (i.e. irrespective of the offspring distribution), Fig. 1.6. In particular, the variance is $\operatorname{Var}(N(t)) = \operatorname{Cov}(N(t), N(t))$ [231].



Figure 1.5.: In Fig. 1.5a, avalanche shape V with rescaled time $\tau = t/T$ for different times of extinction T, $r = 10^{-1}$ and $q_2 = 0.45$ as of Eq. (1.54). The shapes are symmetric and flatten as T increases with the upper bound given in Eq. (1.56). However, this observable is numerically inaccessible because it is computationally unfeasible to obtain a large enough sample of avalanches in the subcritical regime conditioned to extinction at large times. Instead, in Fig. 1.5b we show an observable that is accessible both numerically and analytically, the **averaged avalanche shape** $\langle V(\tau) \rangle_T$, that is for each r, avalanches are rescaled in time to the interval [0, 1], their shapes are averaged and normalised regardless of their extinction times T. Numerical results shown as symbols are for the binary branching process with $r \in$ $\{10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}\}$ and s = 1, and are in agreement with Eq. (1.78) (solid lines), which is an exact expression for binary branching processes. We find that the shape tends to a parabola as r approaches the critical point. This figure has been published in [94] and is reproduced here with the permissions of the right holder stated in App. A.1



Figure 1.6.: Two-point correlation function $\operatorname{Cov}(N(t_a), N(t_b))$ of the binary continuoustime branching process with $r = 10^{-1}$ and s = 1. Our numerical results shown as symbols are in perfect agreement with the exact expression in Eq. (1.58) with $t_1 = \min(t_a, t_b)$ and $t_2 = \max(t_a, t_b)$ (solid lines). We also show $\operatorname{Var}(N(t)) =$ $\operatorname{Cov}(N(t), N(t))$, which is the envelope. This figure has been published in [94] and is reproduced here with the permissions of the right holder stated in App. A.1

1.3.5 *n*-point correlation function

We call $\zeta_n(t_1, \ldots, t_n)$, with $0 < t_1, \ldots, t_n$ (not necessarily in order), the contribution of all binary, and therefore connected, diagrams to the *n*-point correlation function, where the error term is controlled as

$$\langle N(t_1)\dots N(t_n)\rangle = \zeta_n(t_1,\dots,t_n) + \mathcal{O}\left((1-\langle\kappa\rangle)^{-(n-2)}\right).$$
(1.59)

The leading order contribution ζ_n satisfies the following recurrence relation,

$$\zeta_{n}(t_{1},...,t_{n}) = \sum_{m=1}^{n-1} \sum_{\substack{\sigma \subset \{t_{1},...,t_{n}\} \\ |\sigma|=m}} \left\{ \begin{array}{c} \sigma \\ & & \\ \sigma \\ \\ \sigma \\ \end{array} \right\}$$

$$= q_{2} \sum_{m=1}^{n-1} \sum_{\substack{\sigma \subset \{t_{1},...,t_{n}\} \\ |\sigma|=m}} \int_{0}^{t_{\min}} \zeta_{m}(t_{\sigma(1)} - t', \dots, t_{\sigma(m)} - t')$$

$$\times \zeta_{n-m}(t_{\sigma^{c}(m+1)} - t', \dots, t_{\sigma^{c}(n)} - t')e^{-rt'}dt',$$

$$(1.60)$$

with $\zeta_0 = 0$ and $\zeta_1(t) = e^{-rt}$, and $t_{\min} = \min\{t_1, \ldots, t_n\}$. Here, σ is a subset of the set of times $\{t_1, \ldots, t_n\}$, whose size is $|\sigma|$, and $\sigma(1), \ldots, \sigma(m)$ is a list of its distinct elements. Its complementary set is $\sigma^c = \{t_1, \ldots, t_n\} \setminus \sigma$, which contains the elements $\sigma^c(m+1), \ldots, \sigma^c(n)$. Eq. (1.61) is symmetric under exchange of any permutation of the times t_1, \ldots, t_n , see the 3-point correlation function in Appendix 1.A.

This approximation is two-fold. First, it neglects higher order branching vertices proportional to $q_{j\geq3}$, and secondly, it neglects contributions from disconnected diagrams, cf. Eq. (1.57). Latter contributions are dominant only when $t_{\max} = \max\{t_1, \ldots, t_n\}$ is smaller than s^{-1} . For times in $(0, s^{-1})$, the branching process has typically not yet undergone a change in the particle number.

1.3.6 Distribution of the total avalanche size S

We define the total avalanche size as the time-integrated activity $S = s \int dt N(t)$. Using $\langle N(t) \rangle = e^{-rt}$ and Eq. (1.58), the first and second moments of the total avalanche size [45, 47] read

$$\langle S \rangle = s \int dt \langle N(t) \rangle = \frac{s}{r} = \frac{1}{1 - \langle \kappa \rangle},$$
 (1.62a)

$$\langle S^2 \rangle = s^2 \int dt_1 dt_2 \langle N(t_1)N(t_2) \rangle = \frac{s^2}{r^2} \left(\frac{q_2}{r} + 1\right).$$
 (1.62b)

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To calculate $\langle S^n \rangle$ close to criticality, we use the approximation to the *n*-point correlation function defined in Eq. (1.59) and find the following recurrence relation,

$$\langle S^n \rangle \simeq s^n \int \mathrm{d}t_1 \dots \mathrm{d}t_n \,\zeta_n(t_1, \dots, t_n)$$
 (1.63a)

$$\simeq \frac{q_2}{r} \sum_{m=1}^{n-1} \binom{n}{m} \langle S^m \rangle \langle S^{n-m} \rangle \tag{1.63b}$$

$$\simeq \frac{s^n q_2^{n-1}}{r^{2n-1}} 2^{n-1} (2n-3)!!, \qquad (1.63c)$$

see Appendix 1.D for a proof by induction of Eq. (1.63). Similarly to Eq. (1.36), we find the universal constant ratios of the moments of S,

$$\frac{\left\langle S^k \right\rangle \left\langle S^\ell \right\rangle}{\left\langle S^{k-m} \right\rangle \left\langle S^{\ell+m} \right\rangle} = \frac{(2k-3)!!(2\ell-3)!!}{(2(k-m)-3)!!(2(\ell+m)-3)!!} \tag{1.64}$$

with $k, \ell \in \mathbb{N}$ and $m \in \{0, \ldots, k-1\}$. The moment generating function of S is

$$\mathcal{M}_S(z) \simeq 1 + \frac{r - \sqrt{r^2 - 4sq_2z}}{2q_2},$$
 (1.65)

and its probability density function $\mathcal{P}_{S}(x)$ is the inverse Laplace transform of $\mathcal{M}_{S}(-z)$,

$$\mathcal{P}_{S}(x) \simeq \frac{1}{2} \sqrt{\frac{s}{q_{2}\pi}} x^{-\frac{3}{2}} e^{-\frac{r^{2}x}{4q_{2}s}}, \qquad (1.66)$$

which is a power law with exponent -3/2 with exponential decay, Fig. 1.7. At criticality, this distribution is a pure power law.

The approximation used to derive these results, Eq. (1.59), consists in neglecting contributions of disconnected diagrams to the *n*-point correlation function. This approximation is unjustified for total avalanche sizes corresponding those realisations of branching processes that underwent no branching but a single extinction event, and whose sizes are therefore typically smaller than 1, because their *n*-point correlation functions $\langle N(t_1) \dots N(t_n) \rangle$ vanish for $t_{\max} \gtrsim s^{-1}$. Consequently, the *n*-point correlation functions are dominated by purely disconnected diagrams (cf. Sec. 1.3.5). We therefore expect a breakdown of our approximation around x = 1. All three features of the distribution of the total avalanche size, the power-law behaviour, the exponential cutoff, and the breakdown of the approximation for x < 1, are in good agreement with numerical simulations as shown in Fig. 1.7.

1.4 Discussion and conclusions

In this paper we study the continuous-time branching process following a field-theoretic approach. We build on the wealth of existing results in the literature obtained through other methods. Here, we demonstrate that the Doi-Peliti field theory provides an elegant, intuitive, and seemingly natural language for continuous-time branching processes.

We illustrate how to use the field theory to calculate a number of relevant observables, listed in Table 1.1. Our results are valid for any offspring distribution in the vicinity of the critical

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Figure 1.7.: Probability density function of the total avalanche size $\mathcal{P}_S(x)$ for the binary branching process (blue) and the branching process with geometric distribution of offspring (orange), with $r \in \{0, 10^{-3}, 10^{-2}, 10^{-1}\}$ and s = 1. Dashed lines indicate our approximation in Eq. (1.66). This approximation is not valid for small times, which explains the disagreement between the numerical results and the dashed lines for small values of x. This figure has been published in [94] and is reproduced here with the permissions of the right holder stated in App. A.1

point and at large times. However, many of the results are exact for the binary branching process and others are exact for any branching process. In principle, many observables can be calculated systematically using the field theory for any offspring distribution, for any time and any parameter set.

In this paper, we extend the existing results in the literature by finding explicit scaling functions and universal moment ratios for any offspring distribution. We find that all the scaling laws derived above depend on two parameters only, namely r and q_2 . Therefore, one may argue that the master equation of any branching process close to the critical point and asymptotically in large times is captured by the action Eq. (1.8) with couplings r and q_2 only.

Having established the field-theoretic ground work, in particular the basic formalism and range of relevant observables, we may now proceed by extending the basic branching process into more sophisticated models of natural phenomena.

Appendix

1.A Exact expressions

The continuous-time branching process is exactly solvable, that is, in principle, all moments and correlation functions can be calculated in exact form if all the terms in the (possibly infinite) sums are taken into account. Here we show some exact expressions. The exact first three moments of N(t) are

$$\langle N(t)\rangle = e^{-rt},\tag{1.67}$$

$$\left\langle N^{2}(t)\right\rangle = e^{-rt} \left(1 + \frac{2q_{2}}{r} \left(1 - e^{-rt}\right)\right),$$
(1.68)

$$\left\langle N^{3}(t)\right\rangle = e^{-3rt} \left(\frac{6q_{2}^{2}}{r^{2}} - \frac{3q_{3}}{r}\right) - e^{-2rt} \left(\frac{12q_{2}^{2}}{r^{2}} + \frac{6q_{2}}{r}\right) + e^{-rt} \left(\frac{6q_{2}^{2}}{r^{2}} + \frac{3q_{3}}{r} + \frac{6q_{2}}{r} + 1\right), \quad (1.69)$$

and therefore the variance is

$$\operatorname{Var}(N(t)) = \left(1 + 2\frac{q_2}{r}\right) e^{-rt} \left(1 - e^{-rt}\right), \qquad (1.70)$$

which is consistent with Eq. (1.58) and [67, 231, 245, 116, 185]. The three-point correlation function is, assuming $0 \le t_1 \le t_2 \le t_3$ and using Eq. (1.61),

$$\langle N(t_1)N(t_2)N(t_3)\rangle \simeq \zeta(t_1, t_2, t_3)$$

$$= 2\left(\frac{q_2}{r}\right)^2 e^{-r(t_1+t_2+t_3)} \left(\left(e^{rt_1}-1\right)\left(2e^{rt_1}+e^{rt_2}\right)-\frac{3}{2}\left(e^{2rt_1}-1\right)\right).$$
(1.71)

1.B Diagrammatic representation and closed form expressions of

Eqs. (1.51) and (1.52)

Defining

$$a = \frac{e^{-r(T-t)} - e^{-rT}}{1 - e^{-r(T-t)}},$$
(1.72)

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we have, firstly (1.51),

$$\langle \varphi^{n}(T)\varphi(t)\tilde{\varphi}(0)\rangle = \sum_{k=1}^{n} \sum_{m_{1},\dots,m_{k}} \binom{n}{m_{1},\dots,m_{k}} g_{m_{1}}(T-t)\cdots g_{m_{k}}(T-t)g_{k+1}(t)\frac{1}{k!}$$
(1.73)
$$\hat{=} \sum_{k=1}^{n} \sum_{m_{1},\dots,m_{k}} \binom{n}{m_{1},\dots,m_{k}} \begin{cases} m_{1} \\ m_{k} \\ m_{k$$

and secondly (1.52),

$$\langle \varphi^n(T)\widetilde{\varphi}(t)\varphi(t)\widetilde{\varphi}(0)\rangle = \sum_{k=1}^n \sum_{m_1,\dots,m_k} \binom{n}{m_1,\dots,m_k} g_{m_1}(T-t)\cdots g_{m_k}(T-t)g_k(t)\frac{1}{(k-1)!}$$

$$\hat{=} \sum_{k=1}^{n} \sum_{m_1,\dots,m_k} \binom{n}{m_1,\dots,m_k} \begin{cases} m_1 \\ m_2 \\ m_2 \\ m_k \\ m_$$

1.C Averaged avalanche shape

In Section 1.3.3, we derive analytically the expected avalanche shape V(t,T) for a specific time of death T. However, direct comparison with numerics is computationally very expensive as specific large times of death occur rarely for subcritical branching processes. Here we describe an observable that is accessible both analytically and numerically: the averaged avalanche shape $\langle V(\tau) \rangle_T$. For a fixed parameter set, we first rescale time $\tau = t/T$ and then average all the avalanche profiles irrespectively of T. Finally, to achieve convergence to a shape comparable across parameter settings, we normalise the result by area [254],

$$\langle V(\tau) \rangle_T = \frac{1}{N_V} \int_0^\infty \mathrm{d}T \mathcal{P}_T(T) V(\tau T, T),$$
 (1.77a)

$$N_V = \int_0^1 \int_0^\infty d\tau dT \mathcal{P}_T(T) V(\tau T, T). \qquad (1.77b)$$

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The result [255] can be expressed with the Gaussian hypergeometric function ${}_2F_1(a, b, c, z)$,

$$\langle V(\tau) \rangle_T = \frac{1}{N_V} + \tau(\tau - 1) \frac{q_2 F(\tau, q_2, r)}{(q_2 + r) N_V},$$
(1.78)

where

$$F(\tau, q_2, r) = \frac{2F_1\left(1, 2 - \tau, 3 - \tau, \frac{q_2}{q_2 + r}\right)}{\tau - 2} - \frac{2F_1\left(1, 1 + \tau, 2 + \tau, \frac{q_2}{q_2 + r}\right)}{\tau + 1}.$$
(1.79)

Both F and N_V diverge at the critical point with the limit

$$\lim_{r \to 0} \frac{F(\tau, q_2, r)}{N_V} = 6.$$
(1.80)

1.D Proof of Eq. (1.63)

Eq. (1.63) can be proved by induction. In Eq. (1.62) we see that it applies to $\langle S \rangle$. The approximation of binary tree diagrams of $\langle N(t_1)N(t_2)\rangle$ gives $\langle S^2 \rangle = s^2 q_2/r^3$, which also satisfies Eq. (1.63). The induction step is verified by

$$\langle S^n \rangle = \frac{q_2}{r} \sum_{m=1}^{n-1} \binom{n}{m} \left(\frac{s^m q_2^{m-1} 2^{m-1} (2m-3)!!}{r^{2m-1}} \right) \left(\frac{s^{n-m} q_2^{n-m-1} 2^{n-m-1} (2(n-m)-3)!!}{r^{2(n-m)-1}} \right)$$

$$= \frac{s^n q_2^{n-1}}{r^{2n-1}} 2^{n-2} \sum_{m=1}^{n-1} \binom{n}{m} (2m-3)!! (2(n-m)-3)!!.$$
(1.81)

This sum is equivalent to

$$\sum_{m=1}^{n-1} \binom{n}{m} (2m-3)!!(2(n-m)-3)!! = \frac{1}{n-1} \sum_{m=1}^{n-1} \binom{n}{m} (2m-3)!!(2(n-m)-1)!!$$
$$= \frac{1}{n-1} \sum_{k=0}^{n-2} \binom{n}{k+1} (2k-1)!!(2(n-k)-3)!!$$
$$= 2(2n-3)!!, \qquad (1.82)$$

where we have used the identity [34],

$$\sum_{k=0}^{n-1} \binom{n}{k+1} (2k-1)!!(2(n-k)-3)!! = (2n-1)!!.$$
(1.83)

Using Eq. (1.82) in Eq. (1.81) reproduces Eq. (1.63), thereby completing the proof."

Chapter 2

Volume Explored by a Branching Random Walk on General Graphs

Abstract

"Branching processes are used to model diverse social and physical scenarios, from extinction of family names to nuclear fission. However, for a better description of natural phenomena, such as viral epidemics in cellular tissues, animal populations and social networks, a spatial embedding—the branching random walk (BRW)—is required. Despite its wide range of applications, the properties of the volume explored by the BRW so far remained elusive, with exact results limited to one dimension. Here we present analytical results, supported by numerical simulations, on the scaling of the volume explored by a BRW in the critical regime, the onset of epidemics, in general environments. Our results characterise the spreading dynamics on regular lattices and general graphs, such as fractals, random trees and scale-free networks, revealing the direct relation between the graphs' dimensionality and the rate of propagation of the viral process. Furthermore, we use the BRW to determine the spectral properties of real social and metabolic networks, where we observe that a lack of information of the network structure can lead to differences in the observed behaviour of the spreading process. Our results provide observables of broad interest for the characterisation of real world lattices, tissues, and networks."

Cited from

I. BORDEU, S. AMARTEIFIO, R. GARCIA-MILLAN, B. WALTER, N. WEI, AND G. PRUESS-NER. Volume explored by a branching random walk on general graphs. *Sci. Rep.* **9**(1):15590, 2019. arXiv:1909.00471

Overview

In this chapter, I present a near verbatim copy of the peer-reviewed journal article

I. BORDEU, S. AMARTEIFIO, R. GARCIA-MILLAN, B. WALTER, N. WEI, AND G. PRUESSNER. Volume explored by a branching random walk on general graphs. *Sci. Rep.* **9**(1):15590, 2019. arXiv:1909.00471.

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This paper addresses the question how many sites a branching random walker visits over time and how this number depends on the properties of the underlying graph, notably its (spectral) dimension. It is based on a Doi-Peliti field theory of a tracing mechanism, and serves as an introduction into this method, initially put forward in [171], that will be drawn upon in Chp. 4. The field-theoretic incorporation of the branching is very similar to the one introduced in Chp. 1, with the difference that in this chapter the fields are space-dependent since the branching process is embedded into space. A further difference to Chp. 1 are the observables studied; Instead of studying the statistical properties of the particle number of active walkers, the focus here lies on the ability of a branching random walk to explore its spatial surrounding. Although the branching random walk evolves by fully local rules only, the scaling of its explored volume over time reveals global geometric properties of its embedding space, namely the spectral dimension of the graph.

Statement of Contribution

All of the authors were involved in setting up the field theory, which is presented in the appendices 2.A to 2.C. IB is the main author of this work who, together with GP, wrote the draft and managed the collaboration. Once the key results, given in Sec. 2.3, were obtained, numerical validation was necessary. SA wrote the simulation code which generates the branching random walkers on regular lattices in arbitrary dimension and some further general graphs such as Sierpiński carpets, random trees, and preferential-attachment networks. My main involvement was to run the simulations and to analyse the data, except for the case of d = 1 which was dealt with separately by RGM. To that end, I wrote several routines which fitted the conjectured scaling functions to the data on a defined range and which are described in App. 2.F. Further, I assisted NW in working out the conditions under which this field theory is applicable to general graphs, as discussed in Appendix 2.4.

Acknowledgement

I would like to thank all my collaborators for kindly allowing me to share our joint research work as a near verbatim citation as a part of my thesis. *Their approval is shown in App. A.2.* Further, all authors thank Aman Pujara, Brandon Annesi, Kin Tat Yiu, Henry Grieve, and Henry Wilkes for their contributions at an earlier stage of this project. We thank Renaud Lambiotte and Erwin Frey for their useful comments. We would also like to thank Andy Thomas and Nemar Porats for their tireless computing support.

2.1 Introduction

"Modern models of disease propagation incorporate spatial interaction by allowing a pathogen to be passed on only to the neighbours of an infected host [84, 179]. A virus may multiply at a host cell and then infect any of the neighbouring ones at random [208]. The total number of infected cells therefore corresponds to the number of distinct sites visited by a branching random walk (BRW) [76], also referred to as the Branching Wiener Sausage [171, 19]. In this process active random walkers spontaneously produce descendants that carry on hopping from site to site. At the same time, the walkers are subject to spontaneous extinction, for example, by immune-response, healing or decay. The average number of descendants produced during any of these events, branching and extinction, is known to control a transition from a subcritical phase, where the disease ultimately infects only a finite number of sites, to a supercritical phase, where the exponential growth of the virus eventually engulfs almost all available tissue [116]. The expected fraction of distinct sites visited or the size of the epidemic outbreak can be seen as the order parameter of the process.

The characterisation of the distribution of distinct sites visited by a BRW is a long-standing problem of branching processes and random walk theory [209, 76, 195] and is closely related to the problem of distinct sites visited by a simple random walk (*i.e.* no branching events). For simple random walks in regular lattices of general dimension, the problem of distinct visited sites has been initially studied in [80, 237, 170]. In this case, the critical dimension, above which the number of distinct sites grows lienarly in time (corresponding to the mean field behaviour), is $d_c = 2$. Further, fluctuations around the asymptotic result for a simple random walker have been found in [234]. In [141], the authors consider the distinct sites visited by N independent random walkers for which three different scaling regimes in time are characterised. This result is further developed in [157], where the average number of distinct sites visited *jointly* by all of the N random walkers is studied. In d = 1, the work of [138] provides the exact distribution of both the distinct sites visited and the common visited sites of N random walkers. These preceding articles illustrate the broader interest in distinct sites visited and its study in the context of indepent simple random walks. In this chapter, however, we study branching random walks which are qualitatively different to N independent random walkers: the particle number is not conserved (and wildly fluctuates at the critical point), the walkers are spawned off at random sites, and the system features two phases (sub- and supercitical branching, cf. Chp. 1) with the effective reproduction rate r playing the role of the tuning parameter.

For the number of distinct sites visited by a branching random walk, exact results have been obtained for one-dimensional systems [195]. However, extending such results to higher dimensional lattices and networks is met with major technical obstacles, some of which have been addressed over the past decade [76, 145, 146]. In two dimensions [76] derived the properties of the area and perimeter of the convex hull of the cluster of visited sites, and related it to the spreading of animal epidemics. In three dimensions and below, results have been obtained for a related system, the so-called tree-indexed random walk [145, 146].

In the present work, we characterise analytically and, to confirm our findings, numerically the epidemic spreading in general graphs, including regular lattices, fractal, and artificial and real complex networks, at the onset of epidemics. At this point fluctuations are of crucial



Figure 2.1.: Tracing the path of a branching random walker. a, The active walkers, Hänsel and Gretel, leave a trace of breadcrumbs along their way to mark the path they have taken. Birds slowly remove the breadcrumbs, as if they were subject to decay (regularisation, see main text). b, Time evolution of branching random walkers (red) and the cloud of visited sites on a 3d regular lattice at times $t_1 \sim 10^2$, $t_2 \sim 10^3$, and $t_3 \sim 10^4$. Scale bars are equal for all time points. This figure has been published in [25] and is reproduced here under the creative commons licence as stated in App. A.2

importance, dominating the dynamics.

2.2 The model

We model the epidemic as a Poisson process by considering a reaction-diffusion system of a population of active (mobile, branching, spawning) walkers that hop from their current location \mathbf{x} on a graph to any adjacent site \mathbf{y} with rate H, and have occupation numbers $n_{\mathbf{x}}$. Walkers are further subject to two concurrent Poisson processes, namely extinction with rate e and binary branching with rate s, thereby producing **descendants**, which are indistinguishable from their ancestors.

To extract the number of distinct sites visited, we introduce an immobile **tracer** particle species with occupation numbers m_x . They are spawned as **offspring** by the active walkers with rate γ at the sites they are visiting, thereby leaving a trail of tracers behind, similar to the breadcrumbs left by Hänsel and Gretel [103], Fig. 2.1a. We impose the constraint that at most a single tracer can reside at any given site, which means that the spawning of a tracer is suppressed in the presence of another tracer. It is that suppression that generates significant complications from the point of view of the stochastic process. Yet, only with this restriction in place is the number of tracers a measure of the number of distinct sites visited by the walkers, as pictured by the *cloud* of visited sites in Fig. 2.1b.

There is no interaction between active and tracer particles, other than at the spawning of immobile tracers by active walkers. In principle, the spawning (attempt) rate γ has to diverge in order to mark every single site visited by the walkers. However, it turns out that this limit is irrelevant as far as the asymptotic features of this process at large system sizes and long times are concerned [171].

By definition, the sets $\{n\}$ and $\{m\}$ of occupation numbers n_x and m_x , respectively, for



Figure 2.1.: Distinct sites visited on regular lattices. Scaling of the moments of the numbers of distinct sites visited in time (left) and system size (right) for \mathbf{a} , d = 1, \mathbf{b} , d = 2, \mathbf{c} , d = 3, and \mathbf{d} , d = 5 regular lattices. Solid black lines represent the theoretical exponents given by Eq. (2.2) for d < 4, and Eq. (2.3) for d > 4. Simulations parameters: H = 0.1, s = e = 0.45, $\epsilon' = 0$, and $\gamma \to \infty$. This figure has been published in [25] and is reproduced here under the creative commons licence as stated in App. A.2

each site **x** of a given graph, are Markovian and a master equation can be written for the joint probability $\mathcal{P}(\{n\}, \{m\}; t)$ to find the graph in a certain configuration of occupation numbers at time t

$$\dot{\mathcal{P}} = \dot{\mathcal{P}}_s + \dot{\mathcal{P}}_e + \dot{\mathcal{P}}_{\epsilon'} + \dot{\mathcal{P}}_H + \dot{\mathcal{P}}_{\gamma}, \tag{2.1}$$

where $\dot{\mathcal{P}}$ corresponds to the time derivative of the (joint) probability $\mathcal{P}(\{n\},\{m\};t)$, and the terms on the right-hand side, $\dot{\mathcal{P}}_{\bullet} = \dot{\mathcal{P}}_{\bullet}(\{n\},\{m\};t)$, indicate the contributions from branching s, extinction of active walkers e and tracer particles ϵ' , hopping H and deposition γ , respectively (see Sec. 2.A for details). We constructed a statistical field theory from the master Eq. (2.1) using the ladder operators introduced by Doi [73] and Peliti [186] (Sec. 2.6.1). To regularise the propagators of the immobile particles in the field theory, we allow for the extinction of immobile particles with rate ϵ' in Eq. (2.1), not dissimilar to the birds that foiled Hänsel and Gretel's plans (Fig. 2.1a). The propagators for active and tracer particles do not renormalise, and the limit $\epsilon' \to 0$ is taken before any observable is evaluated. Through field-theoretic renormalisation in dimensions $d = 4 - \varepsilon$ we can then determine the exact scaling behaviour of the number of distinct sites visited by the walkers.

The branching process described by Eq. (2.1) has three regimes, as becomes evident in the field-theoretic formulation, where a *net* extinction rate r = e - s appears. This net extinction rate is not renormalised in the field-theory and therefore no mass shift appears. The BRW is subcritical for r > 0, critical for r = 0 (onset of epidemics) and supercritical for r < 0. Hereafter, we focus on the critical case, where fluctuations dominate the dynamics, and the behaviour becomes unpredictable and highly volatile. Furthermore, for both analytical and numerical computations we consider the initial condition of a single walker at t = 0. Extensions to different initial conditions are straight-forward.

2.3 Results for regular lattices

Following the field theoretic approach (details in Secs. 2.6.1 and 2.B) of the bulk critical behaviour in the continuum limit, where hopping is replaced by diffusion by introducing a diffusion constant D, we find that in the thermodynamic limit at long times t, the expected number of distinct sites visited or the volume explored, $\langle a \rangle (t, L)$, scales like $t^{(d-2)/2}$ in dimensions d < 4. In dimensions d < 2 this volume remains finite in large t. The scaling of the p-th moment of the number of distinct sites visited follows,

$$\langle a^p \rangle (t,L) \propto t^{(pd-2)/2} \quad \text{for} \quad Dt \ll L^2$$

$$(2.2a)$$

$$\langle a^p \rangle (t,L) \propto L^{(pd-2)} \quad \text{for} \quad Dt \gg L^2$$

$$(2.2b)$$

in d < 4 provided that pd - 2 > 0. The gap-exponent [188] of $\langle a^{p+1} \rangle / \langle a^p \rangle$ for the scaling in L, which can be thought of as the effective dimension of the cluster of visited sites, is therefore d in dimensions less than $d_c = 4$. These results describe the numerical observations on regular lattices in dimensions d = 1, 2, and 3 (see Sec. 2.6.2.A, as shown in Fig. 2.2, where, after an initial transient, the moments scale according to Eq. (2.2) in time and system size (see Tabs. 2.F.1 and 2.F.2). The process is *free* beyond $d_c = 4$ dimensions, where the probability of any walker



Figure 2.1.: Probability distribution of the number of visited sites, a for regular lattices of dimensions d = 1, 2, 3 and 5, and for b Sierpiński carpet, random tree, and a preferential attachment (scale-free) networks. The solid black lines represent the predicted scaling given by Eq. (2.4). Simulations parameters: H = 0.1, s = e =0.45, $\epsilon' = 0$, and $\gamma \to \infty$. This figure has been published in [25] and is reproduced here under the creative commons licence as stated in App. A.2

or any of its ancestors or descendants ever to return to a previously visited site drops below unity, and the scaling becomes independent of the dimension,

$$\langle a^p \rangle (t,L) \propto t^{2p-1} \quad \text{for} \quad Dt \ll L^2$$
 (2.3a)

$$\langle a^p \rangle (t,L) \propto L^{4p-2} \quad \text{for} \quad Dt \gg L^2$$
 (2.3b)

with logarithmic corrections in $d = d_c = 4$. The gap-exponent in dimensions greater than $d_c = 4$ is thus 4, as confirmed by numerical observations in dimension d = 5 (see Fig. 2.2 and Tab. 2.F.2). As correlations become irrelevant, this is usually referred to as mean-field behaviour. The set of sites visited may thus be regarded as a four-dimensional object, projected into the *d*-dimensional lattice considered. Focusing on dimensions below $d_c = 4$, the distribution of the number of distinct sites visited, *a*, follows a power law,

$$\mathcal{P}(a) = Aa^{-(1+2/d)}\mathcal{G}(a/a_c) \tag{2.4}$$



Figure 2.2.: Scaling on general graphs on a, the Sierpinski carpet, b, random tree and, c, preferential attachment networks. The top row shows representative states (full Sierpinski carpet shown on inset), indicating walkers (red), visited sites (grey) and non-visited sites (black). The bottom row shows the scaling of moments of the number of distinct sites visited as a function of time, and linear system size (inset), or number of nodes, in the case of networks. The solid black lines represent the predicted scaling from Eqs. (2.5). Simulation parameters: H = 0.1, s = e = 0.45, $\epsilon' = 0$, and $\gamma \to \infty$. This figure has been published in [25] and is reproduced here under the creative commons licence as stated in App. A.2

with metric factor A and cutoff $a_c \sim (Dt)^{d/2}$ for $Dt \ll L^2$ and $a_c \sim L^d$ otherwise. These results show how increasing the dimensionality of the lattice promotes the appearance of larger events, evidencing the relevance of dimension on the spreading.

In dimensions $d \ge d_c = 4$ the resulting scaling of the distribution is that of Eq. (2.4) at d = 4, where the probability distribution decays like $a^{-3/2}$. Numerically, we recorded, for each realisation, the total number of distinct sites visited by the process in order to construct the distribution, $\mathcal{P}(a)$, of sites visited. The numerical results coincide with our theoretical predictions, as shown in Fig. 2.1.

The exponents found above for d = 1 are in agreement with the exact solution by Ramola et al. [195], where $\mathcal{P}(a)$ decays as a^{-3} . In two dimensions the power-law tail decays as a^{-2} , which coincides with the decay of the 2d convex hull area distribution [76].

2.4 Extension to general graphs

In the field theoretic approach followed to find the scaling in Sec. 2.3 the spatial dimension of the lattice enters only in as far as its spectral dimension is concerned, which characterises the density of eigenvalues of the Laplace operator on the graph given. Our results extend

naturally to all translational invariant lattices and graphs, by replacing the dimension d of the lattice in Eqs. (2.2), (2.3) and (2.4) by the spectral dimension d_s of the graph, as detailed in Sec. 2.E. This holds true more generally as long as the lattice Laplacian itself does not undergo renormalisation, *i.e.* in the absence of an anomalous dimension [31]. In the study of networks the number of nodes N, is a more natural measure of the size of the network than the linear size L. Using $L \sim N^{1/d_s}$ we can write the scaling of the BRW in time and number of nodes as

$$\langle a^p \rangle (t, N) \propto t^{(pd_s-2)/2} \quad \text{for} \quad Dt \ll N^{2/d_s}$$
 (2.5a)

$$\langle a^p \rangle (t, N) \propto N^{(p-2/d_s)} \quad \text{for} \quad Dt \gg N^{2/d_s}.$$
 (2.5b)

Here, the gap-exponent for the scaling in number of nodes is always unity. This extension to graphs allowed us to predict the behavior of the BRW spreading in both artificial networks relevant for social and biological sciences, and complex systems in general [12, 1, 179, 243], as well as real networks. To illustrate this, we considered first the Sierpiński carpet (SCs) (Fig. 2.3, Sec. 2.6.2.B), and random trees (RTs) (Fig. 2.3 and Sec. 2.6.2.C). Both of these graphs are widely applied in the context of porous media [256] and percolation [151], and have known spectral dimension: $d_s \approx 1.86$ for the SC [244], and $d_s = 4/3$ for RTs [65]. Considering Eq. (2.2) with $d = d_s$, for the SC, and (2.5) for the RT we obtain accurate predictions for the spreading dynamics as confirmed by numerical simulations, Figs. 2.3 and 2.3. These theoretical predictions extend also to the distribution of visited sites (see Fig. 2.1), by setting $d = d_s$ in (2.4).

Furthermore, we studied the BRW behaviour on a class of scale free networks [11]. Since their introduction, scale free graphs have been observed to describe a plethora of natural phenomena, including the World-Wide-Web [12], transportation [108], and metabolic networks [125], to name but a few. We considered a preferential attachment scheme [11] (Fig. 2.3, see Sec. 2.6.2.D), to construct networks with power-law degree distribution (Fig. 2.F.1). The existence of a finite spectral gap in these networks, which indicates slow decay of return times [205, 165], suggested that the BRW process is bound to exhibit mean-field behaviour, i.e. $d_s \ge 4$. This was confirmed by numerical simulations, where the probability distribution of visited sites (Fig. 2.1) has a power-law decay with exponent $-1.52(2) \approx -3/2$, and the scaling in time and system size (Fig. 2.3 and Tab. 2.F.1) follow mean-field behaviour as predicted by (2.5) for $d_s = 4$.

The spectral dimension gives information on the behaviour of dynamical processes on graphs. Here we use the BRW to characterise real-world networks through the power-law decay of the distribution of visited sites $\mathcal{P}(a)$, which according to Eq. (2.4) is $a^{-(1+2/d_s)}$ provided $d_s \leq 4$. For example, the BRW exhibits near mean field-behaviour on a subset of the Facebook network, which has been characterised as scale-free [238]. Hence, we derived a large effective (spectral) dimension, $d_s = 3.9(1)$, indicating a fast spreading of the viral process in this network (see Fig. 2.1).

We should emphasize that the spectral dimension is sensitive to changes in network topology and connectivity. To exemplify this we have considered two publicly available datasets for the yeast protein interaction network (see Fig. 2.1). We found that even though both network describe subsets of the same biochemical network, namely the complete yeast protein interactome, the spectral dimensions in both cases are significantly different, $d_s = 3.0(1)$ for the network with



Figure 2.1.: Probability distribution of number of distinct sites visited $\mathcal{P}(a)$, for the Facebook network (L = 63730 nodes) [238], and yeast protein interaction networks with L = 1870 [124], and L = 2559 nodes [92]. The data was obtained from simulations of the BRW on each graph, with parameters H = 0.1, s = e = 0.45, $\epsilon' = 0$, and $\gamma \to \infty$. This figure has been published in [25] and is reproduced here under the creative commons licence as stated in App. A.2

N = 1870 nodes [124], and $d_s = 3.8(1)$ for the larger network of N = 2559 nodes [92], leading to differences in properties of the spreading process among the two. The discrepancy points to differences in the connectivities of both networks and shows the importance of having access to the complete network in order provide a reliable analysis of its properties, which may have biological implications [112, 226].

2.5 Outlook

The results presented above for the binary branching process, where walkers branch into exactly two new walkers, apply equally to more general branching processes, where the number of offspring in each birth event is given by a distribution (for details see Sec. 2.D). This can be seen, for example, in real-world scenarios where a single infected individual or device infects a whole neighbourhood around them, or in the case of signal propagation in protein networks, where the activation of one node (or chemical reaction) can in turn activate a whole fraction of its neighboring nodes.

While the scaling behaviour does not depend on the initial position \mathbf{x}_0 of a walker, provided it is located in the bulk and remains there as the thermodynamic limit is taken, the field theory has to be adjusted to account for more complicated boundary conditions [171] or the walker starting close to any such boundary. It may also be interesting to consider the case of initialising each site with an independent Poisson distributions of walkers [39].

The approach followed in the present work provides a quantitative measure to explore and

determine the spectral dimension of artificial and real networks. This is of particular interest when the spectral dimension is greater or equal to 2, where the traditional approach of exploring graphs, based on simple random walks [217, 165], fails. When simulating the BRW we made the observation that robust scaling is more easily obtained on small lattices if the hopping rate His clearly smaller than the rates of branching s and extinction e. For large values of the hopping rate particles leave the system during the initial transient, as seen in Fig. 2.1, thus boundary effects appear before any robust scaling can be observed. In graphs such as the PA network (Fig. 2.2), that does not have any boundaries, these artefacts are much less pronounced. In summary our results shed new light on the properties of spatial branching processes on general graphs, and their applicability in the study of real complex networks, and provide observables of broad interest for the characterisation of real world lattices, tissues, and networks.

2.6 Methods

2.6.1 Field theory of the BRW

In order to derive the main results for the scaling of distinct sites visited by the BRW (Sec. 2.3) we work along established lines [232], casting the master equation in a field theory of the annihilation fields $\varphi(\mathbf{x}, t)$ and $\psi(\mathbf{x}, t)$ for the active and the immobile particles, respectively, and of the corresponding (Doi-shifted) creation fields $\tilde{\varphi}(\mathbf{x}, t)$ and $\tilde{\psi}(\mathbf{x}, t)$. The governing Liouvillian $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1$ consists of a harmonic part,

$$\mathcal{L}_0(\varphi,\psi,\tilde{\varphi},\tilde{\psi}) = -\tilde{\varphi}\partial_t\varphi + D\tilde{\varphi}\nabla^2\varphi - r\tilde{\varphi}\varphi - \tilde{\psi}\partial_t\psi - \epsilon'\tilde{\psi}\psi + \tau\tilde{\psi}\varphi, \qquad (2.6)$$

and a non-linear part,

$$\mathcal{L}_1(\varphi,\psi,\tilde{\varphi},\tilde{\psi}) = s\tilde{\varphi}^2\varphi + \sigma\tilde{\psi}\tilde{\varphi}\varphi - \lambda\tilde{\psi}\psi\varphi - \xi\tilde{\psi}^2\psi\tilde{\varphi}\varphi - \kappa\tilde{\psi}\psi\tilde{\varphi}\varphi - \chi\tilde{\psi}^2\psi\varphi, \qquad (2.7)$$

where we have taken the continuum limit. The space and time integrated Liouvillian produces the field-theoretic action $\mathcal{A} = \int d^d x dt \mathcal{L}$, whose exponential $e^{\mathcal{A}}$ enters into the path integral formulation. The couplings in the Liouvillian are related to the rates in the master equation as follows: D is a diffusion constant $D = H\Delta x^2$, where Δx is the lattice spacing, and $H \propto \Delta x^{-2}$ when the limit $\Delta x \to 0$ is taken, in order to maintain finite diffusivity. At bare level the non-linear couplings, with the exception of the branching rate s, are equal to spawning rate γ , i.e. $\tau = \sigma = \lambda = \xi = \kappa = \chi = \gamma$. This follows from translating the master Eq. (2.1) into field-theoretic language (see Sec. 2.A for details).

At the same time the *net* extinction rate r = e - s, the field-theoretic mass of the walkers, has to be kept finite. In this parameterisation, there are three regimes, as described in the main text: a subcritical one for r > 0, a critical for r = 0 and a supercritical for r < 0. In the field theory, all large scale (infrared) phenomena will be controlled by $r \to 0^+$, which corresponds to the onset of epidemics, the limit studied in this work. The mass of the tracers, ϵ' , serves merely as a regularisation, and is removed by taking the limit $\epsilon' \to 0$. The bare transmutation rate τ , corresponding to γ on the lattice, and the bare branching rate s of the active particles (s on the lattice) are the two processes that we expect will govern all infrared behaviour in all dimensions

and are therefore assumed to be dimensionless. These two choices determine the engineering dimension [231] of all other bare couplings, resulting in ξ , κ and χ being infrared irrelevant. Together with λ , these four couplings are due to the suppression of the spawning of tracers when a site is occupied already. At the upper critical dimension, $d_c = 4$, the coupling λ is marginally relevant, being infrared irrelevant above and relevant below. The minimal subtraction scheme [231] we have used will produce results in terms of $\varepsilon = 4 - d$.

The Liouvillian constructed above is the object that allows the exact calculation of the scaling exponents of the *p*-th moment of the volume explored by a branching random walk $\langle a^p \rangle(t, L)$, in time *t*, and linear system size *L*. Initialising the system at time $t_0 = 0$ with a single active walker at position \mathbf{x}_0 , field-theoretically implemented by the creation field $\tilde{\varphi}(\mathbf{x}_0, 0)$, the ensemble average $\langle a \rangle(t, L)$ of the volume explored by the BRW is determined by

$$\langle a \rangle (t,L) = \int \mathrm{d}^d x \, \langle \psi(\mathbf{x},t) \tilde{\varphi}(\mathbf{x}_0,0) \rangle \,,$$
 (2.8)

where the density of tracers particles at position \mathbf{x} and time t > 0 is measured by $\psi(\mathbf{x}, t)$ and integrated over all space. Similarly [171], higher moments are dominated by integrals of the form

$$\langle a^p \rangle (t,L) \sim \int \mathrm{d}^d x_p \dots \mathrm{d}^d x_1 \langle \psi(\mathbf{x}_p,t) \dots \psi(\mathbf{x}_1,t) \tilde{\varphi}(\mathbf{x}_0,0) \rangle,$$
 (2.9)

or equivalently, by evaluating the Fourier transform at spatial momentum $\mathbf{k} = 0$. These are functions of the couplings introduced above, but to leading order not of the walker's initial position \mathbf{x}_0 , provided it is located in the bulk. We implement this numerically by always placing the walker initially at the centre site of odd-sized regular lattices, see Sec. 2.6.2.A. The average $\langle \bullet \rangle$ introduced on the right hand side of Eq. (2.8) correspond to the path integral

$$\langle \psi(\mathbf{x}_p, t) \dots \psi(\mathbf{x}_1, t) \tilde{\varphi}(\mathbf{x}_0, 0) \rangle = \int \mathcal{D}\Pi \left(\psi(\mathbf{x}_p, t) \dots \psi(\mathbf{x}_1, t) \tilde{\varphi}(\mathbf{x}_0, 0) \right) e^{\int d^d x dt \mathcal{L}} , \qquad (2.10)$$

which measures the *p*-point correlation function of tracers at (\mathbf{x}_i, t) , i = 1, 2, ..., p in response to the creation of a walker at $(\mathbf{x}_0, t = 0)$. Here, the integration measure is $\mathcal{D}\Pi = \mathcal{D}\varphi \mathcal{D}\tilde{\varphi} \mathcal{D}\psi \mathcal{D}\tilde{\psi}$. Field theoretic renormalisation in dimensions $d = 4 - \varepsilon$ then allows us to derive the scaling of the number of distinct sites visited (see Sec. 2.B for more details).

2.6.2 Numerical implementation

In the numerical implementation, an active particle is allowed to diffuse by hopping from the site it resides on to a nearest neighbouring site with rate H, branch with rate s by placing an identical offspring at the present site or become extinct with rate e. Each distinct site visited is recorded, equivalent to taking the limit $\gamma \to \infty$ in the theory. The instantaneous number a(t, L) of distinct sites visited up to time t is therefore the number of sites recorded. Parameters were chosen such that H + s + e = 1, H was set to 0.1, and e = s = 0.45. If M walkers are present in the system at a given time the waiting time for the next event (hopping, branching or extinction) is determined by $-\ln(1-u)/M$ where $[0, 1) \ni u \sim U(0, 1)$ is a uniformly distributed random variable. For every lattice size we performed 10^6 to 10^9 realisations of the process.

2.6.2.A Regular, integer-dimensional lattices

The regular lattices studied here are hypercubic *d*-dimensional lattices, characterised by their linear size $L = 2^m - 1$, $m \ge 4$, which is chosen to be odd so that it contains a well-defined centre site, on which the single active walker is initially placed. To study finite-size scaling, absorbing boundary conditions were applied. However, we observed that the boundary conditions have no effect on the scaling (data not shown). The numerical results were fitted to a power-law as described in Sec. 2.F, to obtain the values in Tabs. 2.F.1 and 2.F.2.

2.6.2.B Sierpinski carpet

The Sierpinski carpets were constructed from two dimensional lattices of linear dimension 3^m , $m \ge 2$. The lattice was divided into 3^2 equal sub-squares each of size 3^{m-1} , the central square was removed, leaving $3^2 - 1$ sub-squares. The procedure is iterated over the remaining sub-squares. The spectral dimension of the Sierpinski carpet has been estimated to be $d_s = 1.86$ [244, 53]. A random point around the central hole of the fractal was used as the initial location of the walker in every realisation.

2.6.2.C Random trees

The critical random tree networks [64] were constructed as a critical Galton-Watson process, where every node has either 0, 1, or 2 descendants, such that the mean degree of the network is 2. We generated networks with 2⁶ to 2¹² nodes. These graphs have no closed loops. The spectral dimension of the random tree ensemble is $d_s = 4/3$ [65]. For every realisation of the process, a new random tree was generated, and a node was selected at random as the starting location of the initial walker.

2.6.2.D Preferential-attachment network

A preferential attachment (PA) network is a class of scale-free networks, characterised by a power-law degree distribution. We followed the BarabÃąsiâĂŞAlbert model of preferential attachment [11] initialised with a single node to generate networks with 2^{12} to 2^{19} nodes. The networks have power-law degree distribution with exponent -2.9 and mean degree $\langle k \rangle = 6.3$ (see Fig. 2.F.1). For every realisation of the process, a new network was constructed, and a node was selected at random as the starting location of the initial walker.

Appendix

2.A Master equation for the branching random walk

In the following we describe the contributions to the master Eq. (2.1) from each of the processes the branching random walk comprises. The contribution to the master equation for the joint probability $\mathcal{P}(\{n\},\{m\};t)$ from the spawning of immobile tracer particles by active walkers must take into account the finite carrying capacity \bar{m}_0 of each lattice site. To account for a finite carrying capacity an effective deposition rate is introduced that decays linearly with the number of tracer particles already present at the site of interest [171],

$$\gamma_{\rm eff} = \gamma \frac{\bar{m}_0 - m_{\mathbf{x}}}{\bar{m}_0}.$$

To study the number of distinct sites visited \bar{m}_0 is set to 1. With this constraint in place, each site visited is *marked* with a tracer particle at most once, so that their total number is that of *distinct* sites visited by the BRW. With these considerations, the contributions to the master equation from deposition of tracer particles read

$$\dot{\mathcal{P}}_{\gamma}(\{n\},\{m\};t) = \gamma \sum_{\mathbf{x}} \left((1 - (m_{\mathbf{x}} - 1))n_{\mathbf{x}} \mathcal{P}(\{n\},\{\dots,m_{\mathbf{x}} - 1,\dots\};t) - (1 - m_{\mathbf{x}})n_{\mathbf{x}} \mathcal{P}(\{n\},\{m\};t) \right), \quad (2.11)$$

where $n_{\mathbf{x}}$ and $m_{\mathbf{x}}$ correspond to the number of active and immobile particles at site \mathbf{x} . The sum $\sum_{\mathbf{x}}$ runs over all lattice sites. The contribution from branching of active walkers reads

$$\dot{\mathcal{P}}_{s}(\{n\},\{m\};t) = s \sum_{\mathbf{x}} \left((n_{\mathbf{x}} - 1)\mathcal{P}(\{\dots, n_{\mathbf{x}} - 1, \dots\}, \{m\};t) - n_{\mathbf{x}}\mathcal{P}(\{n\},\{m\};t) \right).$$
(2.12)

The contributions from extinction are

$$\dot{\mathcal{P}}_e(\{n\},\{m\};t) = e \sum_{\mathbf{x}} \left((n_{\mathbf{x}}+1)\mathcal{P}(\{\dots,n_{\mathbf{x}}+1,\dots\},\{m\};t) - n_{\mathbf{x}}\mathcal{P}(\{n\},\{m\};t) \right)$$
(2.13)

for active particles, and

$$\dot{\mathcal{P}}_{\epsilon'}(\{n\},\{m\};t) = \epsilon' \sum_{\mathbf{x}} \left((m_{\mathbf{x}}+1)\mathcal{P}(\{n\},\{\dots,m_{\mathbf{x}}+1,\dots\};t) - m_{\mathbf{x}}\mathcal{P}(\{n\},\{m\};t) \right)$$
(2.14)

for immobile particles. Finally, the contribution to the joint probability from the hopping of active walkers reads

$$\dot{\mathcal{P}}_{H}(\{n\},\{m\};t) = \frac{H}{q} \sum_{\mathbf{x}} \sum_{\mathbf{y}.nn.\mathbf{x}} \left((n_{\mathbf{y}}+1)\mathcal{P}(\{\dots,n_{\mathbf{x}}-1,\dots,n_{\mathbf{y}}+1,\dots\},\{m\};t) - n_{\mathbf{x}}\mathcal{P}(\{n\},\{m\};t) \right), \quad (2.15)$$

where the sum $\sum_{\mathbf{v}.nn.\mathbf{x}}$ runs over all q nearest neighbouring (nn) sites \mathbf{y} of \mathbf{x} .

Combining the contributions from all the subprocesses, the master equation for the joint probability $\mathcal{P} = \mathcal{P}(\{n\}, \{m\}; t)$ reads

$$\dot{\mathcal{P}} = \dot{\mathcal{P}}_s + \dot{\mathcal{P}}_e + \dot{\mathcal{P}}_{\epsilon'} + \dot{\mathcal{P}}_H + \dot{\mathcal{P}}_{\gamma}.$$
(2.16)

as shown in Eq. (2.1).

2.B Field-theory of the BRW

In the following, we show the details of the field-theoretical calculations performed to obtain the main results of the article, Eqs. (2.2), (2.3), and (2.4). In Sec. 2.B.1 we describe the dimensional analysis of the bare couplings. In Sec. 2.B.3, we introduce a diagrammatic representation of the propagators and couplings, and in Sec. 2.B.4 we determine the relevant interactions. In Sec. 2.B.5, we perform the renormalisation of the couplings, and finally calculate the higher order correlations that give rise to the scaling of the moments of the number of distinct sites visited in Sec. 2.B.7.

2.B.1 Dimensional analysis of the bare couplings

To compute the critical dimension of the process described by the Liouvillian $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1$, Eqs. (2.6) and (2.7), and to extract the relevant interactions, i.e the couplings that remain relevant in every spatial dimension, we study the engineering dimensions (here, represented by [·]) of every coupling in the action. We expect that the long range physics in time and space is governed by three processes: diffusion with constant D, branching with rate s, and transmutation with rate τ . Introducing three independent dimensions, namely A, B and C, we impose

$$[\tau] = \mathbf{A}, \quad [s] = \mathbf{B}, \quad \text{and} \quad [D] = \mathbf{C}.$$
 (2.17)

With $[\mathbf{x}] = \mathbf{L}$, $[t] = \mathbf{T}$, and $[\partial_t] = [D\nabla^2]$ it follows that $\mathbf{T} = \mathbf{C}\mathbf{L}^2$ is not an independent dimension. As the action, $\mathcal{A} = \int d^d x dt \mathcal{L}$, itself must be dimensionless, i.e. $[\mathcal{A}] = 1$, we obtain $[r] = \mathbf{T}^{-1} = \mathbf{C}\mathbf{L}^{-2}$ and

$$[\tilde{\varphi}] = \mathbf{B}^{-1}\mathbf{C}\mathbf{L}^{-2}, \qquad [\varphi] = \mathbf{B}\mathbf{C}^{-1}\mathbf{L}^{2-d}, \qquad \left[\tilde{\psi}\right] = \mathbf{A}^{-1}\mathbf{B}^{-1}\mathbf{C}^{2}\mathbf{T}^{-2}, \qquad [\psi] = \mathbf{A}\mathbf{B}\mathbf{C}^{-2}\mathbf{L}^{4-d} \qquad (2.18)$$

for the fields in real time and space, such that $[\tilde{\varphi}\varphi] = [\tilde{\psi}\psi] = L^{-d}$. The engineering dimensions of the couplings follow:

$$[\lambda] = \mathsf{B}^{-1}\mathsf{C}^{2}\mathsf{L}^{d-4} \qquad [\sigma] = \mathsf{A}\mathsf{B}\mathsf{C}^{-1}\mathsf{L}^{2} \qquad [\chi] = \mathsf{A}\mathsf{L}^{d} \tag{2.19a}$$

$$[\kappa] = CL^{d-2} \qquad [\xi] = ABC^{-1}L^{d+2}. \tag{2.19b}$$

Setting $\mathbf{A} = \mathbf{B} = \mathbf{C} = 1$, we find a critical dimension $d_c = 4$, above which all of these interactions become irrelevant. At the critical dimension $d = d_c = 4$ the couplings σ , χ , κ , and ξ remain irrelevant, while λ becomes marginal. To regularise the ultraviolet we work in dimensions $d = 4 - \epsilon < 4$.

As a point of discussion, we note that other choices of independent dimensions are possible, limited only by the symmetries to be preserved. Initially we considered σ , rather than τ to have an independent dimension. The resulting (very messy) field theory depends on the non-universal, bare value of s and produces no renormalisation of τ , which, however, must renormalise as $\langle a \rangle (t, L) \sim \tau_{\text{eff}} L^2$ (see Section 2.B.5) and cannot scale faster than the volume of the system, L^d .

A coupling with independent dimension is saved from changing relevance and thus from possible irrelevance in the infrared limit of large space and long time. The choice of dimensions is therefore a choice of interactions that ultimately govern the infrared. If the stochastic process under consideration takes place on the lattice, this may be determined by taking the continuum limit, provided the process does not possess any competing scales, in which case the continuum limit coincides with the thermodynamic limit of infinite system size. However, as soon as different processes and scales compete, such as hopping, branching, spawning and extinction rates in the present case, the continuum limit is a mere approximation of the original process on the lattice and the choice of (independent) dimensions becomes a claim about which interactions govern the infrared. For example, considering a biased random walk, letting space scale linear in time preserves a drift but removes diffusion, while letting space scale quadratically in time preserves the latter, while the drift velocity diverges.

2.B.2 Fourier transform

Throughout the manuscript, we denote the Fourier transform $\mathcal{F}[f(\mathbf{x},t)]$ of a function $f(\mathbf{x},t)$ in space \mathbf{x} and time t simply as $f(\mathbf{k},\omega)$, where the spatial momentum \mathbf{k} is the conjugate of the position \mathbf{x} , and the frequency ω is the conjugate of time t. The direct Fourier transform is defined as

$$f(\mathbf{k},\omega) = \int e^{i\omega t - i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{x},t) \mathrm{d}^d \mathbf{x} \mathrm{d}t, \qquad (2.20)$$

so that the inverse Fourier transform is

$$f(\mathbf{x},t) = \int e^{-i\omega t + i\mathbf{k}\cdot\mathbf{x}} f(\mathbf{k},\omega) \mathrm{d}^d \mathbf{k} \mathrm{d}\omega, \qquad (2.21)$$

where $d^d \mathbf{k} = (1/2\pi)^d d\mathbf{k}$, $d\omega = (1/2\pi) d\omega$, and d is the spatial dimension.

2.B.3 Propagators and couplings

We begin by considering the field-theoretic action $\mathcal{A} = -\int d^d x dt \mathcal{L}$, where the terms in the Liouvillian $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1$ are given by Eqs. (2.6) and (2.7), respectively. In order to render the Laplacian term local the action is rewritten in Fourier space, where the momentum **k** is the conjugate of position **x** and the frequency ω is the conjugate of time t (as defined in Sec. 2.B.2).

The perturbative renormalisation scheme starts by reading off the propagators from the bilinear part, introducing a diagrammatic language as we proceed. For the walkers the bare propagator reads

$$\langle \varphi(\mathbf{k},\omega)\tilde{\varphi}(\mathbf{k}',\omega')\rangle_0 = \frac{\delta(\mathbf{k}+\mathbf{k}')\delta(\omega+\omega')}{-\iota\omega+Dk^2+r} \triangleq$$
 (2.22)

where $\delta(\mathbf{k} + \mathbf{k}') = (2\pi)^d \delta(\mathbf{k} + \mathbf{k}')$ denotes a scaled *d*-dimensional Dirac- δ function, and correspondingly for $\delta(\omega + \omega')$. Diagrammatically, the bare propagator is shown as a straight line. For the tracers the bare propagator becomes

$$\left\langle \psi(\mathbf{k},\omega)\tilde{\psi}(\mathbf{k}',\omega')\right\rangle_{0} = \frac{\delta(\mathbf{k}+\mathbf{k}')\delta(\omega+\omega')}{-\iota\omega+\epsilon'} \triangleq \cdots ,$$
 (2.23)

diagrammatically shown as a wavy line. Both bare propagators carry a positive mass, r = e - sin Eq. (2.22) and ϵ' in Eq. (2.23), which guarantees causality as the inverse Fourier transform will generate a Heaviside- θ function in time. Both propagators Eqs. (2.22) and (2.23) do not undergo renormalisation. Finally, the transmutation vertex features in

$$\left\langle \psi(\mathbf{k},\omega)\tilde{\varphi}(\mathbf{k}',\omega')\right\rangle_{0} = \tau \frac{\delta(\mathbf{k}+\mathbf{k}')\delta(\omega+\omega')}{(-\imath\omega+\epsilon')(-\imath\omega+Dk^{2}+r)} \triangleq \checkmark$$
(2.24)

and signals the appearance of a tracer in response to the presence of a walker, as time is to be read from right to left. The non-linear part of the Liouvillian, \mathcal{L}_1 , contributes with six interaction vertices, which diagrammatically read

$$\sum^{s} \frac{\sigma}{z^{s}}$$
(2.25)

$$\frac{\chi\xi}{\zeta^{5}\chi}$$
 $\frac{\kappa}{\zeta^{5}\chi}$ (2.26)

$$\chi$$
 $-\lambda$ (2.27)

Finally, the observables of the form of Eq. (2.10) have the diagrammatic structure

$$p\left(\begin{array}{c} & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ \end{array} \right)$$
 (2.28)

Their scaling in time and finite-size can be extracted from the scaling of the vertex generating function, which is the standard object of field-theoretic renormalisation. In the next section we describe all possible infrared-relevant interactions.

2.B.4 Relevant interactions

Whether a particular interaction is allowed by the basic process introduces above is a matter of some topological constraints, which we will discuss in the first part of this section. Whether it is infrared-relevant is determined by its engineering dimension, which we discuss in the second part of this section. Combining topological and engineering constraints will then produce a finite number of interaction vertices to consider. Constraints that avoid certain, otherwise relevant

vertices from being generated are preserved under renormalisation.

The general proper vertex

are the one-particle irreducible graphs of the amputated correlation function

$$G^{\begin{bmatrix} m & n \\ p & q \end{bmatrix}}(r, D, \tau, s, \sigma, \lambda, \kappa, \chi, \xi; \{\mathbf{k}_{1}, \dots, \mathbf{k}_{m+n+p+q}; \omega_{1}, \dots, \omega_{m+n+p+q}\}) = \left\langle \underbrace{\varphi(\mathbf{k}_{1}, \omega_{1}) \dots \varphi(\mathbf{k}_{m}, \omega_{m})}_{m \text{ terms}} \underbrace{\psi \dots \psi}_{p \text{ terms}} \underbrace{\tilde{\varphi} \dots \tilde{\varphi}}_{n \text{ terms}} \underbrace{\tilde{\psi} \dots \tilde{\psi}}_{q \text{ terms}} \right\rangle$$
(2.30)

Denoting, where applicable, terms of higher order in non-linear couplings by h.o.t., the bare couplings are the tree-level contributions to the proper vertices:

$$\tau = \Gamma \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} + \text{h.o.t.} \qquad s = \Gamma \begin{bmatrix} 2 & 1 \\ 0 & 0 \end{bmatrix} \qquad \lambda = \Gamma \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} + \text{h.o.t.}$$
(2.31a)

$$\sigma = \Gamma^{\begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}} + \text{h.o.t.} \qquad \chi = \Gamma^{\begin{bmatrix} 0 & 1 \\ 2 & 1 \end{bmatrix}} + \text{h.o.t.} \qquad \kappa = \Gamma^{\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}} + \text{h.o.t.} \qquad \xi = \Gamma^{\begin{bmatrix} 1 & 1 \\ 2 & 1 \end{bmatrix}} + \text{h.o.t.} \quad (2.31b)$$

Every proper vertex has a number of topological constraints, since any such term needs to arise from the perturbative expansion of the action as a one-particle irreducible (connected, amputated) diagram made from the bare vertices available in the theory. By inspection, we found the following constraints, which we will use to determine all relevant, possible couplings below: Firstly, all non-linear vertices in the field theory (all diagrams except the bare propagator of the tracer particles) have at least one straight leg coming in, $n \ge 1$. Secondly, all vertices have at least as many wavy legs coming out, as come in, $p \ge q$. Thirdly, there are at least as many outgoing legs (wavy or straight), as there are incoming straight legs, $m + p \ge n$.

The engineering dimension of the general proper vertex can be determined from the considerations at the beginning of Section 2.B.1, using the fact that each proper vertex may be seen as an effective coupling, which, after integration over real time and space, gives rise to a dimensionless contribution to the action, $L^d T[\Gamma[\frac{m \ n}{p \ q}]\tilde{\varphi}^m \tilde{\psi}^p \varphi^n \psi^q] = 1$, so that

$$[\Gamma^{\left[\frac{m}{p} q\right]}] = \mathsf{L}^{d(n+q-1)+2(m-n+2p-2q-1)} \mathsf{A}^{p-q} \mathsf{B}^{m-n+p-q} \mathsf{C}^{n-m-2p+2q+1}.$$
(2.32)

Demanding that (effective) transmutation τ , branching s and diffusion D may remain relevant at any scale (which amounts to a suitable continuum limit), we set the independent dimensions A, B and C, respectively, to unity A = B = C = 1. The (marginally) infrared-relevant couplings are those whose engineering dimension (in L) is non-positive. At the upper critical dimension $d = d_c = 4$, the inequality $d(n + q - 1) + 2(m - n + 2p - 2q - 1) \leq 0$ gives

$$m + n + 2p \le 3.$$
 (2.33)

The field theory needs to include all vertices $\Gamma^{\left[\frac{m}{p},\frac{n}{q}\right]}$ with (non-negative) integers m, n, p and q that fulfill Eq. (2.33) together with the topological constraints $n \ge 1, p \ge q$ and $m + p \ge n$. To

find them, we distinguish two cases for Eq. (2.33):

• $p = 0 \xrightarrow{p \ge q} q = 0$, then $m + n \le 3$. Under the topological constraint $m + p \ge n$ there are only two viable solutions: m = n = 1, or m = 2 and n = 1, that correspond to

$$---$$
 and \nearrow , (2.34)

the bare propagator for active walkers, and branching of active walkers, respectively.

• $p = 1 \implies m + n \le 1$. Only the propagator of the immobile particles allows for n = 0. Otherwise, $n \ge 1$ requires m = 0. The constraint $p \ge q$ leaves only q = 0 and q = 1. As a result, there are three viable combinations: Firstly, m = n = 0 and q = 1, secondly, m = q = 0 and n = 1, thirdly, m = 0 and n = q = 1, which correspond to

$$\gamma$$
, γ and γ , (2.35)

the bare propagator of immobile tracer particles, the transmutation vertex and hindrance of spawning, respectively.

Together with the propagators, the vertices in (2.34) and (2.35) represent all (marginally) relevant couplings at $d = d_c = 4$, consisting of the (bilinear) transmutation, τ , and the interaction vertices s of branching and $-\lambda$ of suppression of spawning.

In the following we perform the renormalisation of the couplings τ and $-\lambda$.

2.B.5 Renormalisation of the couplings

As far as the observables in the present work are concerned, the only couplings to consider are τ and λ . Both are renormalised by the same set of loops

$$\tau_R \triangleq \checkmark = \tau + \checkmark + \checkmark + \checkmark + \checkmark + \cdots \checkmark + \cdots \qquad (2.36)$$

and

where all diagrams are amputated. The subscript R indicates a renormalised quantity, which may still be dimensionfull as in the expression above. Only the non-crossing loop diagrams, such as the first three in Eqs. (2.36) and (2.37), are easily calculated (see Sec. 2.C for details). Of the diagrams in Eqs. (2.36) and (2.37), the non-crossing ones are summed over by virtue of field-theoretic renormalisation. The last diagram in both Eq. (2.36) and Eq. (2.37), on the other hand, require further explicit calculation and subsequent summation. The same applies to an infinite number of further crossing diagrams. And yet, because of the Ward-identity (Sec. 2.B.6)

$$\frac{\partial \tau_R}{\partial \tau} = \frac{\lambda_R}{\lambda} \tag{2.38}$$

all exponents can be determined without calculating any of the diagrams explicitly.

As usual in perturbative field theory [231, 143], the governing non-linearity, here λ , becomes spatially dimensionless by multiplying it by $\mu^{-\epsilon}$, where μ is an arbitrary inverse length scale. In fact, any dimensionless coupling involving λ , τ , s, D and μ is proportional to a power of $\lambda s D^{-2} \mu^{-\epsilon}$. Introducing $g = \lambda s \mathcal{U} \mu^{-\epsilon} D^{-2} \Gamma(\epsilon/2)$ with suitable numerical factor \mathcal{U} , both couplings λ and τ renormalise identically

$$\tau_R = \tau Z(g)$$
 and $\lambda_R = \lambda Z(g)$ (2.39)

with Z(g) governing the renormalisation of both λ and τ . To one loop and with suitable \mathcal{U} , the Z-factor becomes Z(g) = 1 - g, see Eqs. (2.36) and (2.37), and Sec. 2.C. However, there is no need to determine the precise dependence of Z on g as far as scaling is concerned. It suffices to know that the renormalised, dimensionless

$$g_R = \lambda_R s \mathcal{U} \mu^{-\epsilon} D^{-2} \Gamma(\epsilon/2) \tag{2.40}$$

$$= Z\lambda s \mathcal{U}\mu^{-\epsilon} D^{-2} \Gamma(\epsilon/2) \tag{2.41}$$

has β -function

$$\beta_g = \frac{\mathrm{d}g_R}{\mathrm{d}\ln\mu} = -\epsilon g_R + g_R \frac{\mathrm{d}\ln Z}{\mathrm{d}\ln\mu} \tag{2.42}$$

which implies $d \ln Z/d \ln \mu = \epsilon$ at the root $\beta_g(g = g^*) = 0$, irrespective of \mathcal{U} and therefore irrespective of the presence or absence of the crossing diagrams. It follows that $Z \sim \mu^{\epsilon}$ in $d \leq 4$ and therefore the effective transmutation rate is $\tau_{\text{eff}} \sim \tau Z \sim \mu^{\epsilon}$. In the limit of $t \to \infty$, for systems of linear size L, the characteristic scale is $\mu \sim L^{-1}$ and thus $\tau_{\text{eff}} \sim L^{-\epsilon}$. With open boundary conditions, the branching walkers visit $\sim L^2$ sites during the course of their lifetimes, leaving behind $\sim \tau_{\text{eff}} L^2 \sim L^{2-\epsilon}$ immobile tracer particles in dimensions greater than 2, so that $\langle a \rangle (t, L) \sim L^{d-2}$. This average is bounded from below by a constant, as at least one site is always visited, so that $\langle a \rangle (t, L)$ approaches a constant below 2 dimensions. As for the timedependence, the characteristic inverse scale μ is proportional to $t^{-1/2}$ because the dynamical exponent z = 2 in $\mu \sim t^{-1/z}$ remains unchanged. It follows that $\langle a \rangle (t, L) \sim t^{(d-2)/2}$.

In the following section, the mean $\langle a \rangle (t, L)$ and higher moments are calculated in greater detail.

To see this, we introduce a dimensionless coupling $g = \lambda s \mathcal{U} \mu^{-\epsilon} D^{-2} \Gamma(\epsilon/2)$ with suitable numerical factor \mathcal{U} and arbitrary inverse length scale μ . Both couplings therefore renormalise identically,

$$\tau_R = \tau Z$$
 and $\lambda_R = \lambda Z$ (2.43)

with Z = 1 - g governing the renormalisation of both renormalised τ and λ . The β -function of g,

$$\beta_g = \frac{\mathrm{d}g}{\mathrm{d}\ln\mu}$$

in d < 4 always produces a root g^* such that $\gamma_{\tau} = d \ln Z/d \ln \mu = \epsilon = 4 - d$ when $g = g^*$, irrespective of \mathcal{U} and therefore irrespective of the presence or absence of the crossing diagrams. Because the Z-factor for λ is identical to that of τ , the latter scales in the inverse scale μ like μ^{ϵ} . As the dynamical exponent z = 2 remains unchanged, it follows that in the long time $t \to \infty$, and large system size $L \to \infty$ limits, the volume visited $\langle a \rangle (t, L)$ by a walker by time t scales

like $t^{(d-2)/2}$ in dimensions d < 4. It remains finite in dimensions d < 2, as discussed in the main text.

2.B.6 Ward identity

To identify the Ward-identity, we first state the action

$$\mathcal{A}\left([\varphi,\psi,\tilde{\varphi},\tilde{\psi}];D,r,\epsilon',\tau,s,\lambda\right)$$
$$=\int \mathrm{d}^{d}x\mathrm{d}t\,\left(-\tilde{\varphi}\partial_{t}\varphi+D\tilde{\varphi}\nabla^{2}\varphi-r\tilde{\varphi}\varphi-\tilde{\psi}\partial_{t}\psi-\epsilon'\tilde{\psi}\psi+\tau\tilde{\psi}\varphi+s\tilde{\varphi}^{2}\varphi-\lambda\tilde{\psi}\psi\varphi\right) \quad (2.44)$$

after having removed the irrelevant couplings from the Liouvillian $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1$, Eqs. (2.6) and (2.7). The Ward-identity Eq. (2.38) is rooted in a symmetry of the action under shifting $\psi(\mathbf{x}, t)$ by a constant Σ ,

$$\mathcal{A}\left([\varphi,\psi+\Sigma,\tilde{\varphi},\tilde{\psi}];D,r,\epsilon',\tau,s,\lambda\right) = \mathcal{A}\left([\varphi,\psi,\tilde{\varphi},\tilde{\psi}];D,r,\epsilon',\tau-\lambda\Sigma,s,\lambda\right) + \Sigma \int \mathrm{d}^d x \mathrm{d}t \left(-\epsilon'\right) \tilde{\psi}(\mathbf{x},t) , \quad (2.45)$$

where the last term amounts to a source term, which maintains a density of Σ of immobile particles throughout time and space, as they are subject to continuous decay with (matching) rate ϵ' . To ease notation we write

$$\mathcal{A} = \mathcal{A}\left([\varphi, \psi, \tilde{\varphi}, \tilde{\psi}]; D, r, \epsilon', \tau, s, \lambda\right)$$
(2.46)

$$\mathcal{A}' = \mathcal{A}\left([\varphi, \psi + \Sigma, \tilde{\varphi}, \tilde{\psi}]; D, r, \epsilon', \tau, s, \lambda\right)$$
(2.47)

$$\mathcal{A}'' = \mathcal{A}\left([\varphi, \psi, \tilde{\varphi}, \tilde{\psi}]; D, r, \epsilon', \tau - \lambda \Sigma, s, \lambda\right)$$
(2.48)

so that

$$\mathcal{A}' = \mathcal{A}'' - \epsilon' \Sigma \int \mathrm{d}^d x \mathrm{d}t \, \tilde{\psi}(\mathbf{x}, t) \,, \qquad (2.49)$$

as well as

$$\left\langle \bullet \right\rangle_{\mathcal{A}} = \int \mathcal{D}\Pi \, \bullet e^{\mathcal{A}} \,, \tag{2.50}$$

and similarly for the actions \mathcal{A}' and \mathcal{A}'' . Since ψ is only a dummy variable in this path integral, any expectation over the action \mathcal{A} of an observable involving the field ψ , is identical to the expectation of an observable involving the shifted field $\psi + \Sigma$ over the action \mathcal{A}' , for example

$$\left\langle \psi(\mathbf{x}_3, t_3)\psi(\mathbf{x}_2, t_2)\tilde{\psi}(\mathbf{x}_1, t_1)\tilde{\varphi}(\mathbf{x}_0, t_0)\right\rangle_{\mathcal{A}} = \left\langle \left(\psi(\mathbf{x}_3, t_3) + \Sigma\right)\left(\psi(\mathbf{x}_2, t_2) + \Sigma\right)\tilde{\psi}(\mathbf{x}_1, t_1)\tilde{\varphi}(\mathbf{x}_0, t_0)\right\rangle_{\mathcal{A}'} \right\rangle$$
(2.51)

To derive the Ward-identity (2.38), we consider

$$\langle \psi(\mathbf{x},t)\tilde{\varphi}(\mathbf{x}_{0},t_{0})\rangle_{\mathcal{A}} = \langle (\psi(\mathbf{x},t)+\Sigma)\tilde{\varphi}(\mathbf{x}_{0},t_{0})\rangle_{\mathcal{A}'} = \langle \psi(\mathbf{x},t)\tilde{\varphi}(\mathbf{x}_{0},t_{0})\rangle_{\mathcal{A}'} + \Sigma \langle \tilde{\varphi}(\mathbf{x}_{0},t_{0})\rangle_{\mathcal{A}'}$$
$$= \left\langle \psi(\mathbf{x},t)\tilde{\varphi}(\mathbf{x}_{0},t_{0})e^{-\epsilon'\Sigma\int d^{d}xdt\,\tilde{\psi}(\mathbf{x},t)}\right\rangle_{\mathcal{A}''}$$
(2.52)

using $\langle \tilde{\varphi}(\mathbf{x}_0, t_0) \rangle_{\mathcal{A}'} = 0$ and Eq. (2.49) in the last line. Differentiation with respect to Σ and evaluating at $\Sigma = 0$ then gives

$$0 = -\lambda \partial_{\tau} \left\langle \psi(\mathbf{x}, t) \tilde{\varphi}(\mathbf{x}_0, t_0) \right\rangle_{\mathcal{A}} - \epsilon' \int \mathrm{d}^d x' \mathrm{d}t' \left\langle \psi(\mathbf{x}, t) \tilde{\varphi}(\mathbf{x}_0, t_0) \tilde{\psi}(\mathbf{x}', t') \right\rangle$$
(2.53)

as $\mathcal{A}'' = \mathcal{A}$ at $\Sigma = 0$ and the left-hand side of Eq. (2.52) is independent of Σ . The integral is most efficiently evaluated after Fourier-transforming, as $\int d^d x' dt' \tilde{\psi}(\mathbf{x}', t') = \tilde{\psi}(\mathbf{k} = 0, \omega = 0)$ and noting that

$$\left\langle \psi(\mathbf{k}',\omega')\tilde{\psi}(\mathbf{k}=0,\omega=0)\right\rangle = \frac{1}{\epsilon'}\delta(\omega')\delta(\mathbf{k}')$$
 (2.54)

whenever $\tilde{\psi}(\mathbf{k} = 0, \omega = 0)$ is paired up with any internal field $\psi(\mathbf{k}', \omega')$. Dividing out two bare propagators, the right-hand side of Eq. (2.53) consists of the amputated diagrams shown in Eq. (2.36) and Eq. (2.37), so that

$$0 = -\lambda \partial_\tau \tau_R + \frac{\epsilon'}{\epsilon'} \lambda_R , \qquad (2.55)$$

the desired identity Eq. (2.38).

2.B.7 Calculating scaling of higher-order correlation functions

The scaling of higher-order correlation functions is derived, within the field theory, from the solution of theallanâĂŞSymanzik equation [231] for the general proper vertex Eq. (2.29), from which the scaling of the moments of the total number of distinct sites visited follow, Eq. (2.2). From dimensional analysis (Sec. 2.B.1), and by introducing a bare scale μ_0 , related to μ by $\mu = \mu_0 \ell$, the general proper vertex, Eq. (2.29), then satisfies

$$\Gamma^{\left[\frac{m}{p}\frac{n}{q}\right]}(r, D, \tau, s, \sigma, \lambda, \kappa, \chi, \xi; \{\mathbf{k}; \omega\}) = \ell^{-d(n+q-1)-2(m-n+2p-2q-1)+(p-q)\gamma_{\tau}} \Gamma^{\left[\frac{m}{p}\frac{n}{q}\right]}\left(\frac{r}{\ell^2}, D, \tau, s, \sigma, \lambda, \kappa, \chi, \xi; \left\{\frac{\mathbf{k}}{\ell}; \frac{\omega}{\ell^2}\right\}\right), \quad (2.56)$$

asymptotically in small ℓ and provided that r is close enough to the critical point, $r_c = 0$. For the transmutation vertex, where p = n = 1 and q = m = 0, we find

$$\Gamma^{\begin{bmatrix} 0 \ 1 \\ 1 \ 0 \end{bmatrix}}(r, D, \tau, s, \sigma, \lambda, \kappa, \chi, \xi; \{\mathbf{k}; \omega\}) = \ell^{\gamma_{\tau}} \Gamma^{\begin{bmatrix} 0 \ 1 \\ 1 \ 0 \end{bmatrix}}\left(\frac{r}{\ell^2}, D, \tau, s, \sigma, \lambda, \kappa, \chi, \xi; \left\{\frac{\mathbf{k}}{\ell}; \frac{\omega}{\ell^2}\right\}\right), \quad (2.57)$$

with $\gamma_{\tau} = \varepsilon = 4 - d$. Generally, for observables of the form Eq. (2.28), where n = 1 and q = m = 0 we have

$$\Gamma^{\begin{bmatrix} 0 \ 1 \\ p \ 0 \end{bmatrix}}(r, D, \tau, s, \sigma, \lambda, \kappa, \chi, \xi; \{\mathbf{k}; \omega\}) = \ell^{4(1-p)+p\gamma_{\tau}} \Gamma^{\begin{bmatrix} 0 \ 1 \\ p \ 0 \end{bmatrix}} \left(\frac{r}{\ell^2}, D, \tau, s, \sigma, \lambda, \kappa, \chi, \xi; \{\frac{\mathbf{k}}{\ell}; \frac{\omega}{\ell^2}\}\right).$$
(2.58)

The scaling of the first moment of the number of distinct sites visited, $\langle a(t) \rangle$, as function of time, t, can be obtained by analysing the scaling of

$$\langle a(t) \rangle = \int d^d \mathbf{x} \langle \psi(\mathbf{x}, t) \tilde{\varphi}(\mathbf{x}_0, 0) \rangle$$
 (2.59)

$$\triangleq \int \mathrm{d}\omega \mathrm{d}\omega_0 e^{-i\omega t} \cdots \Big|_{\mathbf{k}=0}$$
(2.60)

$$= \int \mathrm{d}\omega e^{-i\omega t} \frac{1}{-i\omega + \epsilon'} \Gamma^{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}} \frac{1}{-i\omega + r}.$$
 (2.61)

According to Eq. (2.57), $\Gamma_{10}^{\left[\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right]}$ scales like

$$\Gamma^{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}(L^{-2}, D, \tau, s, \sigma, \lambda, \kappa, \chi, \xi; \{\mathbf{k}; \omega\}) = L^{-\gamma_{\tau}} \Gamma^{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}} \left(1, D, \tau, s, \sigma, \lambda, \kappa, \chi, \xi; \{\mathbf{k}L; \omega L^2\}\right),$$
(2.62)

if we identify $r \sim L^{-2}$ and $\ell \sim L^{-1}$, which means that the effective transmutation rate scales like $L^{-\varepsilon}$ in large linear system size L, as $\gamma_{\tau} = \varepsilon = 4 - d$. In long time t, the integral over ω in Eq. (2.61) has the effect of evaluating $\Gamma^{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}_{\frac{1}{i\omega+r}} \text{ at } \omega = 0$, because

$$\lim_{t \to \infty} \lim_{\epsilon' \to 0} \int_{-\infty}^{\infty} e^{-i\omega t} \frac{1}{-i\omega + \epsilon'} f(\omega) = f(0)$$
(2.63)

provided $f(\omega)$ has no pole at 0.

It follows that

$$\lim_{t \to \infty} \langle a(t) \rangle \propto L^{2-\epsilon}.$$
 (2.64)

For higher moments, on the basis of Eq. (2.58) we find

$$\lim_{t \to \infty} \langle a^p(t) \rangle \propto L^2 L^{pd-4} \Gamma^{\left[\begin{array}{c} 0 & 1 \\ p & 0 \end{array} \right]}(1, D, \tau, s, \sigma, \lambda, \kappa, \chi, \xi; \{0, 0\}).$$
(2.65)

We thus recover the finite-size scaling results Eqs. (2.2b) and (2.3b) of Section 2.3 for the *p*-th moment of the volume explored by a branching random walk

$$\lim_{t \to \infty} \langle a^p(t) \rangle \propto \begin{cases} L^{dp-2} & \text{if } \varepsilon > 0\\ L^{4p-2} & \text{if } \varepsilon < 0 \end{cases}$$
(2.66)

where $\varepsilon > 0$ and $\varepsilon < 0$ separate regions below and above the upper critical dimension, $d_c = 4$, respectively. The dimensionality of the embedding space enters only below the upper critical dimension. Above the upper critical dimension, fluctuations and interactions become asymptotically irrelevant and the process can be considered as free.

The above analysis is easily extended to scaling in time, using $t \propto \mu^{-z}$ with z = 2 as the relevant scale, thereby reproducing Eqs. (2.2a) and (2.3a).

2.C Loop integrals

The non-crossing diagrams, such as the first three in Eqs. (2.36) and (2.37), are calculated through the integral

$$I_{\tau} = \int d^{d}k d\omega \frac{\tau}{-i\omega + \epsilon'} \frac{1}{\omega^{2} + (Dk^{2} + r)^{2}} = \tau \frac{1}{2} \frac{r^{-\varepsilon/2}}{(4\pi D)^{d/2}} \Gamma(\varepsilon/2) , \qquad (2.67)$$

and (essentially identical)

$$I_{-\lambda} = -\lambda \int d^d k d\omega \frac{-\lambda}{-i\omega + \epsilon'} \frac{1}{\omega^2 + (Dk^2 + r)^2} = -\lambda \frac{1}{2} \frac{r^{-\varepsilon/2}}{(4\pi D)^{d/2}} \Gamma(\varepsilon/2) , \qquad (2.68)$$

where the lower part of the loop carries the coupling τ in case of contributing to τ or the coupling $-\lambda$ and an incoming wavy leg in case of contributing to λ . The integration measure is $d^d k d\omega = d^d k d\omega / (2\pi)^{d+1}$.

2.D Generalisation to k offspring

In this section we extend the field-theoretic results presented above to the case where the offspring number is a random number and show that it lies in the same universality class as binary branching [2, 144]. Instead of two distinct processes for branching into two active walkers (with rate s above) and getting extinguished (with rate e above) we consider the latter as branching into k = 0 walkers and generalise the former to branching into any number k of walkers. Each of these processes may occur with rate σ_k , which can always be written as $\sigma_k = \sigma p_k$ with p_k the normalised probability for branching into k walkers and σ the rate with which any such processes take place.

The two contributions \mathcal{P}_s , Eq. (2.12), and \mathcal{P}_e , Eq. (2.13), are thus subsumed and generalised by

$$\dot{\mathcal{P}}_{c}(\{n\},\{m\};t) = \sigma \sum_{k=0}^{\infty} \sum_{\mathbf{x}} p_{k} \Big((n_{\mathbf{x}} - k + 1) \mathcal{P}(\{\dots, n_{\mathbf{x}} - k + 1, \dots\}, \{m\};t) - n_{\mathbf{x}} \mathcal{P}(\{n\},\{m\};t) \Big),$$
(2.69)

which allows for p_1 , but the process of branching into a single particle has no bearing on the master equation.

In the field theory, the mass of the bare propagator for active walkers becomes [94]

$$r = -\sigma \sum_{k=0}^{\infty} p_k(k-1) = \sigma(1-\bar{k}), \qquad (2.70)$$

where $\bar{k} = \sum_{k=0}^{\infty} p_k k$ is the average offspring number, which again, defines a subcritical (r > 0), a critical (r = 0), and a supercritical (r < 0) regime.

In the case of generalised branching, the non-linear part of the action contains contributions of the form $\tilde{\varphi}^k \varphi$ for all $k \ge 2$ as soon as there is any $k \ge 2$ with $p_k > 0$ [94]. Terms with k > 2, however, turn out to be infrared irrelevant, as their couplings have dimension $\mathsf{B}^{k-1}\mathsf{C}^{2-k}\mathsf{L}^{2(k-2)}$. The field theoretic results above for binary branching therefore govern also branching processes with generalised offspring distribution.
2.E Extension to general graphs

In this section we provide further details about the extension of our results to general graphs. The loops integrated over in Eqs. (2.67) and (2.68) are in fact integrals over the spectrum of the Laplacian accounting for the diffusion on the graph considered. Generalising to arbitrary graphs, the Laplacian is to be replaced by a lattice-Laplacian and the integral in Eqs. (2.67)and (2.68) by a suitable sum or, equivalently, an integral with suitable spectral density. In fact, the d-dimensional integral in Eqs. (2.67) and (2.68) can be seen as an integral over all distinct eigenvalues \mathbf{k}^2 of the Laplacian entering with weight $w(k)dk = S_d k^{d-1}dk$ with $S_d =$ $2\pi^{d/2}/\Gamma(d/2)$. On regular lattices, their Hausdorff dimension d coincides with the spectral dimension d_s characteristing, in particular, the small k asymptote of $w(k) \sim k^{d_s-1}$. Replacing $\int d^d k$ by $\int dk w(k)$ suggests that the results derived above remain valid by replacing d by d_s , in order to recover the scaling of the various observables in arbitrary graphs with spectral dimension d_s . The replacement $d \to d_s$ hinges crucially on the fact that d_s characterises the scaling of the spectral density of the Laplacian. If this operator itself renormalises, then a different spectral density may be needed. In other words, d_s may not be the correct dimension if the Laplacian renormalises, *i.e.* if the anomalous dimension does not vanish, $\eta \neq 0$ [31]. This argument relies on the assumption that vertices such as Eq. (2.29) preserve momentum, that is integrals of the form

$$I_n(\mathbf{k}_1, \mathbf{k}_2, \dots, \mathbf{k}_n) = \int \mathrm{d}^d x \, u_{\mathbf{k}_1}(x) u_{\mathbf{k}_2}(x) \dots u_{\mathbf{k}_n}(x)$$
(2.71)

over eigenfunctions $u_{\mathbf{k}}(x)$ of the Laplacian with eigenvalue $\mathbf{k} \cdot \mathbf{k}$ vanish for off-diagonal terms, i.e. whenever $\mathbf{k}_1 + \mathbf{k}_2 + \ldots + \mathbf{k}_n \neq 0$. This condition can be further relaxed by demanding merely that off-diagonal terms are sub-leading as observed in the presence of boundaries [68, 171].

Considering only graphs which are translationally invariant such that the indices \mathbf{j}_m of the q neighbours $m = 1, \ldots, q$ of any node \mathbf{i} can be determined by adding the same set of translational lattice vectors, $\mathbf{d}_1, \ldots, \mathbf{d}_q$, such that $\mathbf{j}_m = \mathbf{i} + \mathbf{d}_m$, it is easy to show that the Laplacian has exponential eigenfunctions and any of their products are an eigenfunction as well, so that $I_n(\mathbf{k}_1, \mathbf{k}_2, \ldots, \mathbf{k}_n) = I_2(\mathbf{k}_1, \mathbf{k}_2 + \ldots + \mathbf{k}_n)$, which vanishes by orthogonality for any $\mathbf{k}_1 + \mathbf{k}_2 + \ldots + \mathbf{k}_n \neq \mathbf{0}$, i.e. the assumption of momentum conservation mentioned above is fulfilled.

2.F Numerics for the scaling of moments

The scaling of the moments $\langle a^p \rangle(t, L)$ for p = 1, 2, 3, ..., 5, as function of time t in the limit $L \to \infty$, and as function of the system size L in the limit $t \to \infty$ were obtained from numerical Monte Carlo simulations and fitted against a power-law

$$f(x) = Ax^B \tag{2.72}$$

and a power-law with corrections of the form

$$g(x) = Ax^B + Cx^{B-1/2}. (2.73)$$

The fitting parameter B in Eqs. (2.72) and (2.73) provides the estimates of the exponents that characterise the scaling of the moments in time t and sistem size L (or N, see main text), by fitting the numerical estimates against f(x) and g(x), with x replaced by t and L, respectively. At large times the moments display plateauing due to finite-size effects.

For the scaling in system size L, we fitted the data for the latest time point available against Eq. (2.72) and used the estimates of A and B as the initial values for a fit against Eq. (2.73), which gave the final estimates of the finite-size scaling exponents.

For the scaling in time t, we fitted data for the largest system, of size $L = L_{\text{max}}$. The fitting range in t for each moment was determined systematically as follows:

- To remove the time-point affected by the finite-size effects, we defined the upper bound of the fitting range as the time t^{up} for which the lowest moment displaying algebraic divergence $(p = p_{\text{low}})$ reached a value of half the maximum value in the plateau, *i.e.* $\langle a^{p_{\text{low}}} \rangle (t^{\text{up}}, L_{\text{max}}) = \max_{t} (\langle a^{p_{\text{low}}} \rangle (t, L_{\text{max}}))/2$. For the preferential attachment network the plateau was observed to occur at an earlier time point than t^{up} , probably due to the high connectivity of the networks, so we set the upper bound to $t^{\text{up}}_{pa} = (1/5) \max(\langle a^k \rangle)$, in this case.
- To find the lower bound t_{low} of the fitting range in t we iterate over an auxiliary time t^* starting at a value that is close to, but smaller than, t_{up} . For each t^* , we fit both equations, (2.72) and (2.73), to the data for L_{max} . We define $\hat{f}_{[t^*,t^{\text{up}}]}(t)$ and $\sigma_{[t^*,t^{\text{up}}]}^{\hat{f}}(t)$ as the values and errors, respectively, of fitting Eq. (2.72) to the data in the range $t \in [t^*, t^{\text{up}}]$, and $\hat{g}_{[t^*,t^{\text{up}}]}(t)$ as the values and errors, respectively, of fitting Eq. (2.72) to the data in the range $t \in [t^*, t^{\text{up}}]$, to the same data set and range. Further, we define $N_{[t^*,t^{\text{up}}]}$ as the number of data points within the fitting interval $[t^*, t^{\text{up}}]$. In each iteration step, we lower t^* by one time-step (as given by the simulation data). The iteration halts at the earliest time at which both fitting models (2.72) and (2.73) agree within errors. This earliest time defines the lower bound t_{low} . Formally, this expression reads

$$t_{\text{low}} = \min_{0 < t^* < t_{\text{up}}} \left\{ t^* : |\hat{f}_{[t^*, t^{\text{up}}]}(t^*) - \hat{g}_{[t^*, t^{\text{up}}]}(t^*)| \le \sqrt{N_{[t^*, t^{\text{up}}]}} \max\left(\sigma^f_{[t^*, t^{\text{up}}]}(t^*), \sigma^g_{[t^*, t^{\text{up}}]}(t^*)\right) \right\}.$$
(2.74)

Where we account for correlations between estimates of moments by rescaling the error by the square root of the number of data points in the fitting range, $N_{[t^*,t^{up}]}$. The exponents characterising the time dependence of the moments are determined by fitting the data in the range $[t^*, t^{up}]$ against Eq. (2.73).

The fitting of the power laws, Eqs. (2.72) and (2.73), was done by means of the Levenberg-Marquardt algorithm [194]. In table 2.F.1 and 2.F.2 we report the numerical results for the asymptotic scaling in time, $\langle a^p \rangle(t) \sim t^{\alpha_p}$, and in system size, $\langle a^p \rangle(t) \sim L^{\beta_p}$, provided these observables display an algebraic divergence."



Figure 2.F.1.: **Degree distribution of the preferential attachment networks** used for the simulations presented in Sec. 2.4. This figure has been published in [25] and is reproduced here under the creative commons licence as stated in App. A.2

					-			F
Table 2.F.1.: Scaling of visited sites in time	P.A.	theo		с,	ъ	2	9	2
		mum	1.0(1)	2.8(2)	4.8(4)	6.6(5)	8.5(9)	1.9(4)
	R.T.	$_{\mathrm{theo}}$		1/3	1	5/3	7/3	2/3
		num		0.35(7)	0.9(1)	1.6(2)	2.2(4)	0.6(2)
	S.C.	theo		0.86	1.79	2.72	3.66	0.93
		unu		0.81(5)	1.71(7)	2.62(10)	3.54(14)	0.91(9)
	d=5	theo	-	n	ى ت	2	6	2
		unu	1.0(2)	2.9(3)	4.8(4)	6.7(7)	9(1)	2.0(5)
	d=3	theo	1/2	2	7/2	ы	13/2	3/2
		mum	0.47(2)	2.0(1)	3.5(1)	5.0(2)	6.4(2)	1.5(2)
	d=2	theo			2		4	
		mum		0.98(3)	2.0(1)	2.9(1)	3.9(1)	1.0(1)
	d=1	$_{\mathrm{theo}}$			1/2	-	3/2	1/2
		mum			0.48(4)	1.0(1)	1.5(1)	0.5(1)
	ownon on t		α_1	α_2	α_3	α_4	α_5	mean gap

and for the Sierpinski carpet (S.C., $d_s \approx 1.86$), the random tree (R.T., $d_s = 4/3$), and preferential attachment (P.A., $d_s > 4$) networks. The columns marked num shows the numerical results, the columns marked theo show theoretical results according to Eqs. (2.2a) with d replaced by the spectral Scaling in time, $\langle a^p \rangle (t) \sim t^{\alpha_p}$, of the *p*-th moment of the number of distinct sites visited for regular lattices of integer dimension, *d*, as indicated, dimension d_s where applicable. The row marked mean gap show the average gap-exponent, $(1/p) \sum_{i=1}^{p} (\alpha_{i+1} - \alpha_i)$, for the corresponding lattice. This table has been published in [25] and is reproduced here under the creative commons licence as stated in App. A.2

Table 2.F.2.: Scaling of visited sites by a BRW as function of the system size	P.A.	1 theo	(1) 1/2	(1) 3/2	(2) 5/2	(2) 7/2	(2) 9/2	(2) 1	$-1, 2^{19} - 1$
		unu	0.49	1.49	2.49	3.49	4.49	1.00	$[2^{14}]$
	R.T.	theo		1/2	3/2	5/2	7/2	-1	$2^{12} - 1$]
		unu		0.58(6)	1.6(1)	2.6(2)	3.7(2)	1.0(1)	$[2^6 - 1,$
	S.C.	theo		1.72	3.59	5.45	7.31	1.86	43]
		unu		1.9(1)	3.8(2)	5.7(3)	7.5(4)	1.9(3)	[9, 2
	d=5	$_{\mathrm{theo}}$	2	9	10	14	18	4	31]
		unu	$1.9(2)^{*}$	$5.7(5)^{*}$	10(1)	14(2)	17(3)	4(1)	[7,
	d=3	theo	, - 1	4	7	10	13	3	2
		unu	0.97(4)	$3.9(1)^{*}$	$6.8(2)^{*}$	$9.8(3)^{*}$	$12.7(4)^*$	2.9(2)	[7, 12
	d=2	$_{\mathrm{theo}}$		2	4	9	∞	2	[27]
		unu		2.1(2)	4.2(3)	6.1(3)	8.1(4)	2.0(3)	[15,
	d=1	$_{\mathrm{theo}}$			1	2	33	1	095]
		mum			0.96(4)	1.93(7)	2.93(8)	0.9(1)	[255, 4]
	ownon ont		β_1	β_2	β_3	β_4	β_5	mean gap	fit range

 $(1/p)\sum_{i=1}^{p}(\beta_{i+1}-\beta_i)$, for the corresponding lattice. *Goodness of fit < 0.05. This table has been published in [25] and is reproduced here under the dimension d as indicated and for the Sierpinski carpet (S.C., $d_s \approx 1.86$). The columns marked num show the numerical results, the columns marked theo show theoretical results according to Eq. (2.2b), for regular lattices, and S.C. (with d replaced by the spectral dimension d_s), and according to Scaling, $\langle a^p \rangle(t) \sim L^{\beta_p}$, of the *p*-th moment of the number of distinct sites visited as function of the system size L, for regular lattices of integer Eq. (2.5) for random tree (R.T.) and preferential attachment (P.A.) The row marked mean gap shows the average gap-exponent, creative commons licence as stated in App. A.2

2. Branching Random Walks on General Graphs

Part II.

First-passage times



Wein. Fennin. Oliander. (Geografisch und Algebraische Hefte), Adolf Wölfli (1914). The work of art depicted in this image and the reproduction thereof are in the public domain.

Chapter 3

Fist passage time distribution of active thermal particles

Abstract

We introduce a perturbative method to calculate all moments of the first-passage time distribution in stochastic one-dimensional processes which are subject to both white and coloured noise. This class of non-Markovian processes is at the centre of the study of thermal active matter, that is self-propelled particles subject to diffusion. The perturbation theory about the Markov process considers the effect of self-propulsion to be small compared to that of thermal fluctuations. To illustrate our method, we apply it to the case of active thermal particles (i) in a harmonic trap (ii) on a ring. For both we calculate the first-order (or one-loop) correction of the moment-generating function of first-passage times, and thus to all its moments. Our analytical results are compared to numerics.

Overview

In this chapter, I present a near verbatim copy of a preprint that is currently undergoing review

B. WALTER, G. PRUESSNER, AND G. SALBREUX. First passage time distribution of active thermal particles in potentials 2020. Submitted, arXiv:2006.00116

This Chapter contains a summary of a research project I conducted with Gunnar Pruessner and Guillaume Salbreux (Francis Crick Institute). At its centre stand first-passage times. The first-passage time, the time a stochastic process takes to attain a certain value, is a key concept in stochastic dynamics and will be the central object of interest in the remaining four chapters of this thesis. Here, we focus on the problem of first-passage times of stochastic processes with small short-range correlated increments.

The way we approach the problem is by decomposing the process into a sum of two stochastic contributions. The first contribution is a fully Markovian process. The second contribution, which is assumed to be small compared to the first, is a stationary self-correlated noise which drives the first and is therefore referred to as driving noise. The sum of both contributions therefore inherits correlated increments from the driving noise. Since the driving noise is considered to be small, the first-passage time distribution of the full process will be "close" to the Markovian first-passage time distribution of the undriven first process. The meaning of closeness will be made more precise in the main text.

In this work, we find a way to calculate the difference between the Markovian and the driven first-passage time distribution. It is not an exact result, simply because we cannot expect there is one, but it is a systematic and controllable approximation scheme and therefore the best one can hope for in such a situation.

This chapter is a slightly edited version of a manuscript submitted for publication.

Statement of Contribution

I have done all of the analytical and numerical work whilst being regularly and fruitfully supervised and adviced by Gunnar Pruessner and Guillaume Salbreux. I also wrote the manuscript except subsection 3.2.2.B which was written by GP and slightly adapted by me.

Acknowledgement

I would like to thank Gunnar and Guillaume for their approval in using our manuscript as a part of my thesis. I have obtained their approval which is shown in App. A.3.

I would like to thank the Francis Crick Institute for their hospitality, Kay Wiese for fruitful discussions, and Greg Pavliotis and Asher Mullokandov for their valuable feedback.



Figure 3.1.: A particle in a potential (orange parabola) subject to both white and coloured noise (see Eq. (3.1)). While the white noise models a thermal environment whose timescale of correlation is negligibly small, the driving term models hidden degrees of freedom which are correlated over timescales comparable to those of the particle's stochastic dynamics. Those driving forces induce correlations (**pink correlation kernel**) in the particle's increments and therefore break its Markovianity. In this work, we study first-passage times τ_{x_0,x_1} ; the time such a random walker (**blue rough path**) takes to first reach x_1 starting from x_0 (**dashed lines**).

3.1 Introduction and Main results

3.1.1 Introduction

Understanding the statistical properties of first-passage times (FPTs), the time a stochastic process takes to first reach a prescribed target, has fuelled research in stochastic dynamics for over a century. Thanks to its wide-ranging applications it has enjoyed increased attention over the last decade [127, 197, 166]. First-passage times are often used as a key characteristic of complex systems, such as chemical reactions [227], polymer-synthesis [221], intra-cellular events [97], neuronal activity [230] or financial systems [42]. Besides their dynamical information, FPTs are helpful to understand spatial properties of complex networks [233], extreme values of stochastic processes [117] and characteristic observables in out-of-equilibrium statistical physics [30].

Historically, the first settings in which FPT-problems were studied were Markovian processes in one spatial dimension. Schrödinger approached this problem first by integrating over the probability density with absorbing boundary conditions [210]. Pontryagin et al. introduced a method which casts the mean first-passage time (MFPT) into an ODE derived from the Kolmogorov backward equation [193, 114]. Further, Siegert and Darling introduced a method to obtain the moment-generating function of the FPT starting from a renewal equation [215, 52]. These three key advances of the first "classical" period suggest that, despite the innocent looking simplicity of the problem, even Markovian processes do generally not allow for a closed form expression of the full distribution of FPT. Expectations alone, the MFPT, are difficult enough to compute in very simple systems.

In a parallel development, and sparked by the work of Kramers [131], much effort was put into investigating the rate with which fluctuating particles escape from metastable potentials. The forces the surrounding heat bath exerts on the particle, usually inter-molecular collisions, were modelled as white noise ξ_t with correlator $\langle \xi_s \xi_t \rangle = 2D_x \delta(s-t)$. This correlator implies that the timescale on which the particle evolves is infinitely separated from the heat bath's correlations [127]. In this setup, the fluctuation-dissipation theorem (FDT) [35, 137] identifies the diffusivity D_x with a fixed temperature T of the surrounding heat bath. Particles subject to white noise follow Markovian (memoryless) trajectories and are immersed in a heat bath in thermodynamical equilibrium (e.g. [150]).

In many systems, the paradigm of white noise is a drastic over-simplification. Coloured noise, *i.e.* noise with non-uniform power spectrum, was introduced to account for correlations due to the heat bath [113, 136]. Coloured noise is usually assumed to have a correlator that decays exponentially with some characteristic inverse rate β^{-1} , sometimes referred to as the "colour" of the noise. White noise corresponds to the limit of $\beta \to \infty$. Escape rate problems with coloured noise were a highly active area of research in the late 1980s and early 1990s, when various approximation methods to calculate the MFPT were developed [164, 139, 140, 196, 81, 126]. There contradictory predictions initially led to a considerable degree of confusion [89]. Many of these developments are reviewed in [113].

More recently, coloured noise was suggested as a model for "active" swimmers which are selfpropelled and whose energy-consumption is fuelled by the environment [228]. In these systems, the fluctuation-dissipation theorem does not hold (*e.g.* [159]) such that no thermodynamic equilibrium can be assumed. Ensembles of non-interacting "active swimmers" have been intensively studied over the last five years in the light of their non-equilibrium features [152, 207, 36, 37]. Notably, their first-passage time distributions have been recognised as one of their characterising properties [158].

Over the last twenty years or so, first-passage times have regained interest independently of escape problems, and new methods have been developed to extend older techniques into the realm of non-Markovian stochastic processes. The classic approaches of Schrödinger (cf. [147, 71, 224]), Pontryagin (cf. [223, 235]) and Siegert (cf. [221]) have been successfully employed to a plethora of non-Markovian systems such as generalised Langevin and Fokker-Planck equations and coupled oscillator chains. Further approaches have been found in [236, 29, 16, 15, 105]. The vast majority of that work is concerned with MFPT, also because in many cases higher moments or the full distribution contain prohibitively complicated expressions. And yet, the MFPT has recently been criticised as insufficient or misleading in characterising the timescale of a dynamics. Therefore a more precise understanding of the full distribution poses a pressing current challenge [100, 101].

In attacking the problem of first-passage times for non-Markovian processes, various perturbative methods have been successfully established in the past. One such example is the calculation of the persistence (see [155, 30]) of non-Markovian Gaussian stochastic processes in [156]. In some similarity to the methods developed in Chp. 6, a path-integral formalism is used to characterise Gaussian processes and to calculate constrained propagators. The result is a perturbative expansion of the large time behaviour of the persistence probability, thus encapsulating the tail of the first-passage time distribution. Similar perturbative approaches have since been developed to calculate persistence exponents in critical dynamics in various lattice models near the upper critical dimension using renormalisation group methods [33, 180], again treating fluctuations as non-Markovian Gaussian processes. This illustrates not only the scientific context of this chapter but also the overarching claim of this thesis, namely that field-theoretically inspired perturbation schemes have greatly advanced the understanding of non-Markovian Gaussian processes, for instance the large-time scaling of their first-passage time distribution.

In this chapter, however, we depart in two ways from the work following the lines of [155, 156, 33, 180] and others: First, we do not study any critical dynamics, that means there is neither an assumption of scale invariance nor a notion of a phase (transition). Secondly, we develop a perturbation theory for the moment generating function instead of the large time scaling, such that our result is a priori equally valid (in a perturbative sense) at any timescale.

In this work, we address this challenge and compute the full moment-generating function of a class of non-Markovian stochastic processes perturbatively. In doing so, we obtain all moments of the distribution to the same order in the perturbative expansion. To our knowledge, this is the first time the full distribution is obtained systematically in the presence of correlated driving noise and white thermal noise for a wide range of settings, including a potential. The formulas we obtain order by order are exact, and the results we obtain for two systems, as an illustration, are in excellent agreement with numerical simulation.

3.1.2 Outline

In the following, we study the first-passage time distribution of non-interacting *active* particles subject to *thermal* noise in an external potential. Particles which are driven by coloured noise alone, such as those studied in [87, 159], are used as a model for self-propelled particles, but do not have a coupling to a thermal heat bath; Such systems are referred to as active and athermal [229]. More recent models contain an active force term to capture self-propulsion in addition to thermal white noise which represents the heat bath, *e.g.* [37, 212, 51]. Additionally, a conservative force may be considered stemming from an external potential. Particles which are driven by both white and non-white noise and are embedded in potentials are also considered in the context of Brownian motors, see [183].

Together, for a particle moving in a 1D space, this class of *thermal and active* models is characterised by a single degree of freedom x_t satisfying a Langevin-type equation [127, 51] (see Fig. 3.1 for a graphical representation)

$$\dot{x}_t = -V'(x_t) + \xi_t + \varepsilon y(t); \tag{3.1}$$

Here, V(x) denotes a potential, ξ_t a white noise with $\langle \xi_s \xi_t \rangle = 2D_x \delta(t-s)$ and D_x a diffusivity fixed by the FDT. The second, stochastic term y(t) in Eq. (3.1) denotes an additional coloured noise, in the following referred to as *driving noise*, which we assume to be stationary and of zero mean. Since there are two noise-terms, we introduce the *driving* average $\overline{\bullet}$ over all realisations of y(t), as opposed to the *thermal* average $\langle \bullet \rangle$ over realisations of ξ_t . The central result of this work consists in finding the doubly averaged moment-generating function of first-passage times $\langle \overline{\exp(-s\tau_{x_0,x_1})} \rangle$ perturbatively in ε .

Since y(t) is self-correlated, x_t by itself is no longer Markovian; Our framework therefore provides a tool to study FPT-distributions of non-Markovian processes. On the other hand, this work stands in the context of recent efforts to approach active thermal systems with fieldtheoretic methods. As will be reported elsewhere, the process Eq. (3.1) can be mapped to a non-equilibrium field-theory from which a variety of observables can be deduced. In the present work, we focus on first-passage times, for which a simpler setup is sufficient in which we use functional perturbation theory instead of a fully-fledged field theory.

The perturbation takes place in the regime where $\varepsilon y(t)$ is small compared to ξ_t , that means where thermal fluctuations dominate. In our perturbation theory, we will emphasise this point by controlling the amplitude of the driving noise term via ε which is chosen small. Since ε carries the dimension of an inverse time, we will later introduce ν which is a dimensionless perturbation parameter whose precise form depends on the particular process in question. A priori no assumption is made about the noise-colour β^{-1} and we recover all moments at once to equal perturbative order. Our framework is based on the established renewal approach [215, 52], but uses functional expansions to circumvent the problem of non-Markovianity of Eq. (3.1).

3.1.3 Main results

The central result of the present work concerns the moment-generating function of first-passage times of x_t ,

$$F(s) = \left\langle \overline{e^{-s\tau_{x_0,x_1}}} \right\rangle = 1 - s \left\langle \overline{\tau_{x_0,x_1}} \right\rangle + \frac{s^2}{2} \left\langle \overline{(\tau_{x_0,x_1})^2} \right\rangle + \dots$$
(3.2)

where τ_{x_0,x_1} is the first-passage time of x_t defined as

$$\tau_{x_0, x_1} \coloneqq \inf_{t>0} \left\{ t : x_t = x_1 | x_{t=0} = x_0 \right\}.$$
(3.3)

The following argument is based on two assumptions. First, we assume the moment-generating function F(s) is known for $\varepsilon = 0$. The case of $\varepsilon = 0$ corresponds to the case of a purely "passive" particle with no self propulsion. The particle behaves Markovian in this case, and already established techniques can be applied (see Introduction). We refer to this state as *in equilibrium*. Secondly, we assume that around this state F(s) is analytic in ε or, to be more precise, in a dimensionless parameter ν which is of order $\mathcal{O}(\varepsilon^2)$. This means that the moment generating function of first-passage times has an expansion in ν of the form

$$F(s) = \left\langle \overline{\exp(-s\tau_{x_0,x_1})} \right\rangle = \mathcal{M}_0(x_0, x_1; s) + \nu \mathcal{M}_1(x_0, x_1, ...; s) + \mathcal{O}(\nu^2).$$
(3.4)

where \mathcal{M}_0 and \mathcal{M}_1 are the coefficients of expansion of F(s) in ν around $\nu = 0$. The equilibrium component, \mathcal{M}_0 , can be found by classical methods such as the Darling-Siegert method which is discussed in the next subsection. The first-order contribution, \mathcal{M}_1 , requires some deeper analysis. Much of what follows is dedicated to the calculation of \mathcal{M}_1 , which to our knowledge is new in the literature. In principle, the method we present here is capable of calculating coefficients $\mathcal{M}_2, \mathcal{M}_3, ...$ of arbitrarily high order of ν for arbitrarily coloured noise (cf. Eq. (3.69)) as long as the autocorrelations can be integrated suitably. Further the potentials V(x) are arbitrary, as long as an associated differential operator can be diagonalised (Sec. 3.3 and [9]),



(a) Numerical validation of first order correction to FPT moment generating function M₁ (cf. Eq. (3.4)) of a particle in a harmonic potential V(x) = α/2 x² subject to white noise of diffusivity D_x and coloured Gaussian noise with correlator y
{t1}y{t2} = D_yβ⁻¹ exp(-β|t₁ - t₂|)) (see Eq. (3.81) and Sec. 3.3.1 for discussion). The result is calculated in Eq. (3.109). Numerical Simulations are shown for various values of ν = D_yε²/(D_xαβ) (plot marks). For small values of ν agreement with theoretical first-order correction (black line) is excellent. For larger values of ν the deviation increases. The rescaled deviation, M₂ (see Eq. (3.111)), (inset) collapse and thus confirm that these deviations are systematic higher-order corrections. See (3.3.1.B) for further results and discussion.



- (b) Numerical validation of first order correction to FPT moment generating function \mathcal{M}_1 of a Brownian Motion on a ring of radiues r additionally driven by coloured Gaussian noise with correlator $\overline{y_{t_1}y_{t_2}} = D_y\beta^{-1}\exp(-\beta|t_1 - t_2|))$ (see Eq. (3.115) and Sec. 3.3.2 for discussion). The moment generating functions were sampled for $D_x = 1$, $\alpha = 1$, $D_y = 1$, $\beta = \frac{1}{2}$ and varying values of $\nu = \varepsilon^2 D_y r^2 / (D_x\beta^2)$ (plot marks). For small values of ν agreement with theoretical first-order correction (black line) is very good. For larger values of ν the deviation increases. The rescaled deviations, $\tilde{\mathcal{M}}_2$ (see Eq. (3.141)), (inset) collapse and thus confirm that these deviations are systematic higher-order corrections. See (3.3.2.B) for further results and discussion. ε .
- Figure 3.2.: First order corrections to the moment-generating function of first-passage times as found by the framework presented in this work for two example processes.

otherwise it needs to be treated perturbatively as well.

We further illustrate our framework by explicitly computing \mathcal{M}_0 and \mathcal{M}_1 for two cases each of which are additionally driven by coloured Gaussian noise, *i.e.* y(t) is Gaussian and has correlator $\overline{y(t_1)y(t_2)} = D_y\beta^{-1}\exp(-\beta|t_1-t_2|))$ with some diffusivity D_y and correlation time β^{-1} . In the first case, the particle is places in a harmonic potential, $V(x) = \frac{\alpha}{2}x^2$. This particular model has been studied in, *e.g.*, [51]. While \mathcal{M}_0 (see Eq. (3.105)) has been long known, \mathcal{M}_1 (see Eq. (3.109)) is a new result. The first-order contribution is compared to numerical simulations in Fig. 3.2a. Further, we calculate \mathcal{M}_0 and \mathcal{M}_1 for the case of a Brownian Motion on a ring of radius r. The first-order contribution is compared to numerical results in Fig. 3.2b.

Our method is *systematic* since it allows its user to calculate in principle corrections to arbitrary order, and it is *controllable* in the sense that the error can be made arbitrarily small. Further *all moments* are available at once. It is also valid for arbitrary noise colours β^{-1} .

The paper is structured as follows. In Sec. 3.2 we give detailed account of how to calculate F(s) for small ν . First, we reproduce the Darling-Siegert argument in the equilibrium case $(\nu = \varepsilon = 0)$. Next, we introduce a perturbative version of the Darling-Siegert equation. Then, we obtain, as an intermediate result, a formula for F(s) which is still a functional of the coloured noise y(t). In the last step, we need to average over the stationary distribution of y(t) to arrive at the explicit formula Eq. (3.78) which is the main result of our work. In the subsequent section 3.3, we calculate all quantities required for the case of a harmonic potential and a Brownian motion with periodic boundary conditions and arrive at the first-order correction to the moment-generating function of first-passage times Eq. (3.109). Section 3.4 concludes with a discussion of our findings.

3.2 Perturbation Theory

As outlined above, in this work we present a way to calculate the moment-generating function of first-passage times of stochastic processes which are close to an equilibrium state. The underlying assumption is that moment-generating function varies smoothly as ε , the coupling to the self-propelling force, is switched on. The moment-generating function of the equilibrium version of the process ($\varepsilon = 0$) is assumed to be known in closed form, as is for instance justified for the Ornstein-Uhlenbeck process or Brownian Motion ([9]). This exact form is then corrected by terms in the spirit of a perturbative expansion which is controlled by powers of a dimensionless parameter describing the distance to equilibrium. First, we revise the arguments given by Darling and Siegert for the equilibrium case ([215, 52]). Next, we outline our perturbative approach to the active case.

3.2.1 Notation

We introduce some notations. The transition probability density of progressing from x_0 at t_0 to x_1 at t_1 is denoted by

$$T(x_0, x_1; t_0, t_1) = T(t_0, t_1)$$
(3.5)

where the subscripts x_0 and x_1 are dropped wherever confusion can be avoided for the sake of easier notation and where we use hats on symbols to indicate that the function depends on two variables. Analogously the return probability at x_1 , $T(x_1, x_1; t_0, t_1)$ is denoted by

$$R(x_1; t_0, t_1) = R(t_0, t_1) = T(x_1, x_1; t_0, t_1)$$
(3.6)

Further, the first-passage time density to first reach x_1 starting from x_0 is denoted by

$$F(x_0, x_1; t_0, t_1) = F(t_0, t_1)$$
(3.7)

In the following, we denote the Fourier transform of a function f(t) by a hat as follows:

$$\hat{f}(\omega) = \int_{-\infty}^{\infty} dt \ e^{-i\omega t} f(t) , \qquad (3.8)$$

with inverse

$$f(t) = \int_{-\infty}^{\infty} d\omega \, e^{i\omega t} \hat{f}(\omega), \qquad (3.9)$$

where $d\omega = \frac{d\omega}{2\pi}$. In the same spirit, we introduce

$$\delta(\omega) = 2\pi\delta(\omega) = \int_{-\infty}^{\infty} dt \, e^{-i\omega t} \,, \qquad (3.10)$$

chosen so that we will not encounter any powers of 2π due to the Fourier-transform.

Functions of more than one time, say $f(t_0, t_1, t_2)$, which depend on the difference $t_1 - t_0$ and $t_2 - t_0$ only, say $f(t_0, t_1, t_2) = g(t_1 - t_0, t_2 - t_0)$ we will refer to as *diagonal*. Their Fourier-transforms, then also referred to as diagonal, pick up a δ pre-factor as discussed below, Section 3.2.2.B.

3.2.1.A Equilibrium case: The Darling-Siegert solution

We here consider the equilibrium case of Eq. (3.1) defined by setting $\varepsilon = 0$. As x_t is Markovian, the functions F and T satisfy the following renewal equation:

$$T(x_0, x_1; t_0, t_1) = \int_{t_0}^{t_1} \mathrm{d}t' \, F(x_0, x_2; t_0, t') T(x_2, x_1; t', t_1) \tag{3.11}$$

for all $x_2 \in (x_0, x_1]$.

Applying a Fourier transform to Eq. (3.11), the time-homogeneity of both $T(t_0, t_1)$ and $F(t_0, t_1)$ translates into diagonality in frequencies and turns the convolution into a product, such that the result can be stated at the level of the amplitudes alone. Rearranging the terms and choosing $x_2 = x_1$ results in

$$\hat{F}(\omega) = \frac{\hat{T}(\omega)}{\hat{R}(\omega)}$$
(3.12)

Since the Fourier transform of a probability density equals its characteristic function, Eq. (3.12) recovers all moments of the first passage time provided \hat{T} is known. Further, setting $\omega = -is$ for some $s \in \mathbb{R}_+$ turns the Fourier transforms into Laplace transforms and the characteristic function into the moment generating function. This recovers the Darling-Siegert equation in its original form in which the Laplace transform of transition and return probabilities is linked to the moment-generating function of first-passage times.

3.2.1.B Out-of-equilibrium: A perturbative approach

The argument made by Darling and Siegert breaks down when $\varepsilon \neq 0$: indeed when averaging over the driving noise y(t), the renewal equation Eq. (3.11) no longer is true. The approach we take in this paper, consists of three steps (with some of the notation introduced in the subsequent section 3.2.2)

1. Fix a particular realisation y(t), and expand transition and return probabilities of x_t as functional expansion around $y(t) \equiv 0$ of the form

$$\hat{T}(\omega_0,\omega_1,[\hat{y}]) = \sum_{n=0}^{\infty} \varepsilon^n \int d\tilde{\omega}_1 ... d\tilde{\omega}_n \delta\left(\omega_0 + \omega_1 + \sum_{i=1}^n \tilde{\omega}_i\right) \times T^{(n)}\left(\omega_1,\tilde{\omega}_1,...,\tilde{\omega}_n\right) \hat{y}(-\tilde{\omega}_1) ... \hat{y}(-\tilde{\omega}_n) . \quad (3.13)$$

- 2. As long as y(t) is fixed, the process, when understood as conditioned on this particular driving, satisfies a renewal equation of the type Eq. (3.11). Inserting the perturbative transition and return probabilities from the previous step, gives a perturbative series for the first-passage time density $\hat{F}(\omega_0, \omega_1; [y])$ of x_t conditioned on a particular y(t).
- 3. Averaging over the ensemble of driving noises. For simplicity, we here assume that the correlation function of the driving noise is given by

$$\overline{y(t_1)y(t_2)} = \frac{D_y}{\beta} \exp\left(-\beta |t_2 - t_1|\right)$$
(3.14)

where β is the inverse correlation time. Generally, when computing the term of order ε^n , the first *n* moments of y(t) need to be known.

This procedure leads to the central result of this work: the moment-generating function of first-passage times to second order in ε reads

$$F(\omega) = \underbrace{\frac{T^{(0)}(\omega)}{R^{(0)}(\omega)}}_{=:\mathcal{M}_{0}(x_{0},x_{1};\omega)} + \frac{\varepsilon^{2}D_{y}}{\beta} \left[\frac{T^{(2)}(\omega;i\beta,-i\beta)}{R^{(0)}(\omega)} - \frac{T^{(1)}(\omega-i\beta,i\beta)R^{(1)}(\omega,i\beta)}{R^{(0)}(\omega-i\beta)R^{(0)}(\omega)} + \frac{T^{(0)}(\omega)R^{(1)}(\omega-i\beta,i\beta)R^{(1)}(\omega,i\beta)}{(R^{(0)}(\omega))^{2}R^{(0)}(\omega-i\beta)} - \frac{T^{(0)}(\omega)R^{(2)}(\omega;i\beta,-i\beta)}{(R^{(0)}(\omega))^{2}} \right] + \mathcal{O}(\varepsilon^{4}).$$
(3.15)

In the next sections, we derive this relation in more details.

3.2.2 Perturbative Darling-Siegert equation

3.2.2.A Expression for the first-passage time distribution

By imposing an additional driving noise y(t), the transition probability and FPT probability density of x_t depend on a particular realisation of y(t). Accordingly, we introduce the transition

probability density $T(t_0, t_1, [y])$ and FPT probability density $F(t_0, t_1, [y])$ as the densities of the process x_t conditioned on y(t) given. The conditional densities are explicitly dependent on t_0 and t_1 rather than their difference $t_1 - t_0$ because y(t) is an explicit function of time.

For y fixed, the process remains Markovian and therefore Eq. (3.11) still applies and gives rise to

$$T(x_0, x_1; t_0, t_1; [y]) = \int_{-\infty}^{\infty} \mathrm{d}t' \, F(x_0, x_1; t_0, t'; [y]) \times R(x_1; t', t_1; [y]) \tag{3.16}$$

where the dependency of the functions on the spatial values x_0 , x_1 has been made explicit for clarity, and we have used the fact that $F(t_0, t'; [y])$ vanishes for $t' < t_0$ and $R(t', t_1)$ vanishes for $t' > t_1$ to integrate over the full real axis.

It is no longer possible to directly invert this equation in Fourier space to solve for F, as done in Eq. (3.12), since neither terms in the integral are diagonal, *i.e.* they depend explicitly on both t_0, t' and t', t_1 . However, introducing the inverse functional R^{-1} which is defined by the implicit equation

$$\int_{-\infty}^{\infty} \mathrm{d}t \, R^{-1}(t_0, t; [y]) R(t, t_1; [y]) = \delta(t_1 - t_0) \tag{3.17}$$

the renewal equation can be formally solved by the relation:

$$F(x_0, x_1; t_0, t_1; [y]) = \int_{-\infty}^{\infty} \mathrm{d}t \, T(x_0, x_1; t_0, t; [y]) R^{-1}(x_1; t, t_1; [y])$$
(3.18)

Our approach is then to perform a functional expansion of the quantities involved in Eq. (3.18) in the function y, around the Markovian case $y \equiv 0$.

3.2.2.B Functional expansion of the transition and return probability densities

We start by spelling out the Taylor expansion in $\hat{y}(\omega)$ about $\hat{y} \equiv 0$ of the transition probability $T(t_0, t_1; [y])$ or equivalently its Fourier transform $\hat{T}(\omega_0, \omega_1; [y])$

$$\hat{T}(\omega_0,\omega_1;[y]) = \sum_{n=0}^{\infty} \int d\tilde{\omega}_1 \dots d\tilde{\omega}_n \left. \frac{1}{n!} \left. \frac{\delta^n \hat{T}(\omega_0,\omega_1;[y])}{\delta \hat{y}(-\tilde{\omega}_1) \dots \delta \hat{y}(-\tilde{\omega}_n)} \right|_{\hat{y}\equiv 0} \times \hat{y}(-\tilde{\omega}_1) \dots \hat{y}(-\tilde{\omega}_n) , \quad (3.19)$$

where we have chosen the sign of the $\tilde{\omega}_i$ in anticipation of the signs convenient below. As we show in the following, the functional derivatives with respect to $\hat{y}(\omega)$ all carry a Dirac- δ in ω , which simplifies the expressions considerably.

The derivative with respect to the Fourier-transformed $\hat{y}(-\omega)$ is the Fourier-transform of the derivative with respect to y(t), which can be seen by a functional chain rule:

$$\frac{\delta}{\delta\hat{y}(-\tilde{\omega})}\Big|_{\hat{y}\equiv0} \hat{T}(\omega_0,\omega_1;[y]) \\
= \int d\tilde{t} \left. \frac{\delta}{\delta y(\tilde{t})} \right|_{y\equiv0} \hat{T}(\omega_0,\omega_1;[y]) \frac{\delta y(\tilde{t})}{\delta\hat{y}(-\tilde{\omega})} = \int d\tilde{t} \left. \frac{\delta}{\delta y(\tilde{t})} \right|_{y\equiv0} \hat{T}(\omega_0,\omega_1;[y]) \exp\left(-i\tilde{\omega}\tilde{t}\right) \quad (3.20)$$

as

$$\frac{\delta y(\tilde{t})}{\delta \hat{y}(-\tilde{\omega})} = \exp\left(-i\tilde{\omega}\tilde{t}\right) \tag{3.21}$$

according to Eq. (3.9) and using that the inverse Fourier-transform of $\hat{y} \equiv 0$ is $y \equiv 0$. Higher order derivatives follow obviously the pattern of Eq. (3.20).

The Dirac- δ in ω of the functional derivatives implicitly present in Eq. (3.19) is found by returning to direct time. All observables governed by Eq. (3.1) are time (-translational) invariant after averaging over the white noise, provided y(t) is constant. To see this more clearly for $T(t_0, t_1; [y])$ and its functional derivatives, we notice that for arbitrary shifts of time by t^* , the transition probability obeys

$$T(t_0, t_1; [y]) = T(t_0 - t^*, t_1 - t^*; [\hat{y}])$$
(3.22)

with suitably shifted $\hat{y}(t - t^*) = y(t)$, so that

$$\frac{\delta}{\delta y(\tilde{t})} T(t_0, t_1; [y]) = \int \mathrm{d}t' \frac{\delta \hat{y}(t')}{\delta y(\tilde{t})} \frac{\delta}{\delta \hat{y}(t')} T(t_0 - t^*, t_1 - t^*; [\hat{y}]) = \frac{\delta}{\delta \hat{y}(\tilde{t} - t^*)} T(t_0 - t^*, t_1 - t^*; [\hat{y}]) \quad (3.23)$$

using $\delta \hat{y}(t')/\delta y(\tilde{t}) = \delta(t' + t^* - \tilde{t})$ in the functional chain rule. Higher order derivatives produce corresponding results.

Eq. (3.23) holds for any t^* with the additional caveat that $\hat{y}(t-t^*) = y(t)$, implying a different transformation of y to \hat{y} for each t^* . Making the particular choice of $t^* = t_0$ renders the right hand side of Eq. (3.23) dependent on only two time *differences*. Defining therefore T_0 such that

$$T(t_0, t_1; [y]) = T_0(t_1 - t_0; [\hat{y}_0]) \text{ with } \hat{y}_0(t - t_0) = y(t) , \qquad (3.24)$$

the functional derivative in Eq. (3.23) can be written in terms of T_0 after a suitable transform of y to \hat{y}_0 . This transform, however, becomes the identity for $y(t) \equiv 0$ or equivalently $\hat{y} \equiv 0$ as needed in Eq. (3.19). The functional derivative on the right of Eq. (3.20) may thus be written as

$$\frac{\delta^n}{\delta y(\tilde{t}_1)\dots\delta y(\tilde{t}_n)}\Big|_{y\equiv 0} T(t_0, t_1; [y]) = \frac{\delta^n}{\hat{y}_0(\tilde{t}_1 - t_0)\dots\delta\hat{y}_0(\tilde{t}_n - t_0)}\Big|_{y\equiv 0} T_0(t_1 - t_0; [\hat{y}_0])$$
(3.25)

$$=T_0^{(n)}(t_1-t_0,\tilde{t}_1-t_0,\ldots,\tilde{t}_n-t_0;[0]) .$$
(3.26)

On the right hand side of this equation all dependence on t_0 features explicitly in the arguments and not in \hat{y}_0 , because y(t) = const. means $\hat{y}_0(t) = \text{const.}$ without any dependence on t_0 . The right hand side is a *function* rather than a functional of n + 1 arguments. Taking the Fourier

transform in t_0, t_1 , as well as $\tilde{t}_1, \ldots \tilde{t}_n$ of Eq. (3.25) thus gives

$$\frac{\delta^{n}}{\delta \hat{y}(-\tilde{\omega}_{1})\dots\delta \hat{y}(-\tilde{\omega}_{n})}\Big|_{\hat{y}\equiv 0} \hat{T}(\omega_{0},\omega_{1};[y]) \tag{3.27}$$

$$= \int dt_{0}dt_{1}d\tilde{t}_{1}\dots d\tilde{t}_{1} \frac{\delta}{\tilde{\omega}(\tilde{\omega}) - \tilde{\omega}(\tilde{\omega})}\Big| \quad T(t_{0},t_{1};[y])\exp(-i(\omega_{0}t_{0}+\omega_{1}t_{1}+\tilde{\omega}_{1}\tilde{t}_{1}+\dots+\tilde{\omega}_{n}\tilde{t}_{n}))$$

$$= \int \mathrm{d}t_0 \mathrm{d}t_1 \mathrm{d}t_1 \dots \mathrm{d}t_1 \left. \frac{\delta y(\tilde{t}_1) \dots \delta y(\tilde{t}_n)}{\delta y(\tilde{t}_1) \dots \delta y(\tilde{t}_n)} \right|_{y \equiv 0} T(t_0, t_1; [y]) \exp(-i(\omega_0 t_0 + \omega_1 t_1 + \tilde{\omega}_1 t_1 + \dots + \tilde{\omega}_n t_n))$$
(3.28)

$$= \int dt_0 dt_1 d\tilde{t}_1 \dots d\tilde{t}_1 T_0^{(n)}(t_1 - t_0, \tilde{t}_1 - t_0, \tilde{t}_2 - t_0, \dots, \tilde{t}_n - t_0; [0]) \\ \times \exp(-i(\omega_0 t_0 + \omega_1 t_1 + \tilde{\omega}_1 \tilde{t}_1 + \dots + \tilde{\omega}_n \tilde{t}_n)) \\ = \delta(\omega_0 + \omega_1 + \tilde{\omega}_1 + \dots + \tilde{\omega}_n) \hat{T}_0^{(n)}(\omega_1, \tilde{\omega}_1, \tilde{\omega}_2, \dots, \tilde{\omega}_n; [0])$$
(3.29)

combining Eqs. (3.25) and (3.20). To ease notation we introduce $T^{(n)}$ as

$$T^{(n)}(\tilde{\omega}_1,\ldots,\tilde{\omega}_n) = \frac{1}{\varepsilon^n} \hat{T}_0^{(n)}(\omega_1,\tilde{\omega}_1,\tilde{\omega}_2,\ldots,\tilde{\omega}_n;[0])$$
(3.30)

which includes the factor $1/\varepsilon^n$ to make the orders of ε explicit in the functional expansion. The derivation above may be repeated for the return probability R, which is obtained from the transition probability T by taking x_0 to x_1 . As a result, R is equally time-invariant. Introducing therefore

$$\delta(\omega_0 + \omega_1 + \tilde{\omega}_1 + \ldots + \tilde{\omega}_n) R^{(n)}(\omega_1, \tilde{\omega}_1, \ldots, \tilde{\omega}_n) = \frac{1}{\varepsilon^n} \left. \frac{\delta^n}{\delta \hat{y}(-\tilde{\omega}_1) \ldots \delta \hat{y}(-\tilde{\omega}_n)} \right|_{\hat{y} \equiv 0} \hat{R}(\omega_0, \omega_1; [y]) \quad (3.31)$$

we arrive at a new form of the functional expansions for the transition and the return probabilities

$$\hat{T}(\omega_{0},\omega_{1},[\hat{y}]) = \sum_{n=0}^{\infty} \varepsilon^{n} \int d\tilde{\omega}_{1} \dots d\tilde{\omega}_{n} \delta\left(\omega_{0} + \omega_{1} + \sum_{i=1}^{n} \tilde{\omega}_{i}\right) \\ \times T^{(n)}\left(\omega_{1},\tilde{\omega}_{1},...,\tilde{\omega}_{n}\right) \hat{y}(-\tilde{\omega}_{1}) \dots \hat{y}(-\tilde{\omega}_{n})$$
(3.32a)
$$\hat{R}(\omega_{0},\omega_{1},[\hat{y}]) = \sum_{n=0}^{\infty} \varepsilon^{n} \int d\tilde{\omega}_{1} \dots d\tilde{\omega}_{n} \delta\left(\omega_{0} + \omega_{1} + \sum_{i=1}^{n} \tilde{\omega}_{i}\right) \\ \times R^{(n)}\left(\omega_{1},\tilde{\omega}_{1},...,\tilde{\omega}_{n}\right) \hat{y}(-\tilde{\omega}_{1}) \dots \hat{y}(-\tilde{\omega}_{n}) .$$
(3.32b)

3.2.2.C Functional expansion of the inverse of the return probability density

We now turn to the expansion of R^{-1} in Eq. (3.18). The analysis of the previous subsection still applies and one obtains the expansion

$$\hat{R}^{-1}(\omega_0,\omega_1,[\hat{y}]) = \sum_{n=0}^{\infty} \varepsilon^n \int d\tilde{\omega}_1 ... d\tilde{\omega}_n \delta\left(\omega_0 + \omega_1 + \sum_{i=1}^n \tilde{\omega}_i\right)$$

$$\times (R^{-1})^{(n)}(\omega_1,\tilde{\omega}_1,...,\tilde{\omega}_n)\hat{y}(-\tilde{\omega}_1)...\hat{y}(-\tilde{\omega}_n)$$
(3.33)

where again we simplify the notation of the expansion terms in direct analogy to Eq. (3.32). We then obtain by applying a Fourier transform to Eq. (3.17):

$$\int \mathrm{d}\omega \hat{R}^{-1}(\omega_0,\omega;[\hat{y}])\hat{R}(-\omega,\omega_1;[\hat{y}]) = \delta(\omega_0+\omega_1) .$$
(3.34)

This relation allows to relate the functions $(R^{-1})^{(n)}$ to the functions $R^{(n)}$, by repeatedly taking derivatives with respect to $\hat{y}(-\tilde{\omega}_i)$ and identifying the terms on the left hand side, which need to vanish. The first three expansion terms thus read

$$(R^{-1})^{(0)}(\omega) = \frac{1}{R^{(0)}(\omega)}$$
(3.35)

$$(R^{-1})^{(1)}(\omega,\tilde{\omega}_1) = -\frac{R^{(1)}(\omega,\tilde{\omega}_1)}{R^{(0)}(\omega)R^{(0)}(\omega+\tilde{\omega}_1)}$$
(3.36)

$$(R^{-1})^{(2)}(\omega,\tilde{\omega}_{1},\tilde{\omega}_{2}) = \frac{1}{R^{(0)}(\omega+\tilde{\omega}_{1}+\tilde{\omega}_{2})R^{(0)}(\omega)} \left\{ \frac{2R^{(1)}(\omega+\tilde{\omega}_{2},\tilde{\omega}_{1})R^{(1)}(\omega,\tilde{\omega}_{2})}{R^{(0)}(\omega+\tilde{\omega}_{2})} - R^{(2)}(\omega,\tilde{\omega}_{1},\tilde{\omega}_{2}) \right\}$$
(3.37)

3.2.2.D Second-order expansion of the first passage time distribution

Equipped with these expansions, one now can expand the first-passage time density expression (3.18) to obtain a functional expansion of the first-passage density in ε , involving the functions $\hat{T}^{(n)}$ and $\hat{R}^{(n)}$ which are simpler to calculate. We first state the Fourier-transformed version of the key relation (3.18):

$$\hat{F}(\omega_0, \omega_2; [\hat{y}]) = \int_{-\infty}^{\infty} \mathrm{d}\omega \, \hat{T}(\omega_0, \omega_1; [\hat{y}]) \hat{R}^{-1}(-\omega_1, \omega_2; [\hat{y}]) \,. \tag{3.38}$$

where the dependency on x_0 , x_1 is here implicit. Performing an expansion of this relation in ε , the result reads to second order:

$$\begin{aligned} \hat{F}(\omega_{0},\omega_{2};[\hat{y}]) &= \frac{\hat{T}^{(0)}(\omega_{2})}{R^{(0)}(\omega_{2})} \delta(\omega_{0} + \omega_{2}) \end{aligned} \tag{3.39} \\ &+ \varepsilon \left[-\frac{T^{(0)}(-\omega_{0}) R^{(1)}(\omega_{2}, -\omega_{0} - \omega_{2})}{R^{(0)}(-\omega_{0}) R^{(0)}(\omega_{2})} + T^{(1)}(\omega_{2}, -\omega_{0} - \omega_{2}) \frac{1}{R^{(0)}(\omega_{2})} \right] \hat{y}(\omega_{0} + \omega_{2}) \\ &+ \frac{1}{2} \varepsilon^{2} \int d\tilde{\omega} \left[\frac{T^{(2)}(\omega_{2}, \tilde{\omega}, -\omega_{0} - \omega_{2} - \tilde{\omega})}{R^{(0)}(\omega_{2})} - \frac{2T^{(1)}(-\tilde{\omega} - \omega_{0}; \tilde{\omega}) R^{(1)}(\omega_{2}, -\omega_{0} - \omega_{2} - \tilde{\omega})}{R^{(0)}(\omega_{2}) R^{(0)}(-\tilde{\omega} - \omega_{0})} \right. \\ &+ \frac{T^{(0)}(-\omega_{0})}{R^{(0)}(-\omega_{0}) R^{(0)}(\omega_{2})} \\ &\left. \left\{ \frac{2R^{(1)}(-\tilde{\omega} - \omega_{0}; \tilde{\omega}) R^{(1)}(\omega_{2}, -\omega_{0} - \omega_{2} - \tilde{\omega})}{R^{(0)}(-\tilde{\omega} - \omega_{0})} - R^{(2)}(\omega_{2}, \tilde{\omega}, -\omega_{0} - \omega_{2} - \tilde{\omega})} \right\} \right] \\ &\times \hat{y}(-\tilde{\omega})\hat{y}(\omega_{0} + \omega_{2} + \tilde{\omega}) + \dots \end{aligned}$$

At this stage, we have obtained a perturbative expansion of the first-passage time density for a particular realisation of y, and only in terms of the expansion coefficients of transition and return probability T and R. Before we turn to give a more explicit expression of the latter, we discuss driving noise averaging.

3.2.3 Driving noise averaging

As was set out initially, the quantity of interest is the first-passage time density when averaged over all driving noises (even if the quantity given above might be of interest in itself). The average over driving noise realisations y(t) is an average different to the average over the underlying stochastic process x_t , in that sense akin to "quenched disorder averages" which replace a stochastic background field by an effective deterministic correction to observables. The expansion in Eq. (3.39) is a power series in orders of ε , where contributions of order ε^n contain an internal integration over n-1 free frequencies. The expansion terms which stand in front of the y terms, those denoted within square brackets, are independent of y. They may be interpreted as the *n*th order response functionals of the first-passage time distribution (in s) to perturbations in the driving noise y. To calculate the y-average of $\hat{F}(\omega_0, \omega_2; [y])$, each term in Eq. (3.39) is integrated over the path-measure of y, $\mathcal{P}[y]$. The order of internal integration and y-averaging can be swapped. Consequently, since $\langle y \rangle = 0$ by assumption, all terms in first order in y vanish. To second order, correlations of y come into play. We introduce the correlation function

$$\hat{C}_2(\tilde{\omega}_2)\delta(\tilde{\omega}_1 + \tilde{\omega}_2) = \overline{\hat{y}(\tilde{\omega}_1)\hat{y}(\tilde{\omega}_2)} = \int \mathcal{D}[y]\mathcal{P}[y]\hat{y}(\tilde{\omega}_1)\hat{y}(\tilde{\omega}_2), \qquad (3.40)$$

which by assumption of stationarity in time is diagonal in Fourier space and symmetric in $\tilde{\omega} \mapsto -\tilde{\omega}$. Averaging then amounts to an integral over the remaining free variable. We illustrate the averaging using the simplest term of second order appearing in Eq. (3.39) which reduces to

$$\int d\tilde{\omega} \frac{T^{(2)}(\omega_2, \tilde{\omega}, \omega_0 + \omega_2 - \tilde{\omega})}{R^{(0)}(\omega_2)} \overline{\hat{y}(-\tilde{\omega})\hat{y}(+\omega_0 + \omega_2 + \tilde{\omega})}$$
$$= \int d\tilde{\omega} \frac{T^{(2)}(\omega_2, \tilde{\omega}, -\tilde{\omega})}{R^{(0)}(\omega_2)} \hat{C}_2(\tilde{\omega})\delta(\omega_0 + \omega_2).$$

The last integral is irreducible and needs to be calculated for the corresponding correlator. In this fashion, all terms in Eq. (3.39) are averaged and result in

$$\begin{aligned} \overline{\hat{F}(\omega_{0},\omega_{2};[y])} &= \frac{T^{(0)}(\omega_{2})}{R^{(0)}(\omega_{2})} \delta(\omega_{0} + \omega_{2}) \\ + \varepsilon^{2} \left[-\underbrace{\int d\tilde{\omega} \frac{T^{(0)}(\omega_{2}) R^{(2)}(\omega_{2},\tilde{\omega},-\tilde{\omega})}{(R^{(0)}(\omega_{2}))^{2}} \hat{C}_{2}(\tilde{\omega})}_{=:(I)} + \underbrace{2 \int d\tilde{\omega} \frac{T^{(0)}(\omega_{2}) R^{(1)}(\omega_{2} + \tilde{\omega},\tilde{\omega}) R^{(1)}(\omega_{2},-\tilde{\omega})}{(R^{(0)}(\omega_{2}))^{2} R^{(0)}(\omega_{2} + \tilde{\omega})} \hat{C}_{2}(\tilde{\omega})}_{=:(II)} \right] \\ -\underbrace{2 \int d\tilde{\omega} \frac{T^{(1)}(\omega_{2} + \tilde{\omega},\tilde{\omega}) R^{(1)}(\omega_{2},-\tilde{\omega})}{R^{(0)}(\omega_{2}) R^{(0)}(\tilde{\omega} - \omega_{2})} \hat{C}_{2}(\tilde{\omega})}_{=:(II)} + \underbrace{\int d\tilde{\omega} \frac{T^{(2)}(\omega_{2},\tilde{\omega},-\tilde{\omega})}{R^{(0)}(\omega_{2})} \hat{C}_{2}(\tilde{\omega})}_{=:(IV)}}_{=:(IV)} \int d\omega_{0} + \underbrace{\int d\tilde{\omega} \frac{T^{(2)}(\omega_{2},\tilde{\omega},-\tilde{\omega})}{R^{(0)}(\omega_{2})} \hat{C}_{2}(\tilde{\omega})}_{=:(IV)}}_{=:(IV)} \right] \delta(\omega_{0} + \omega_{2}) + \dots \end{aligned}$$

$$(3.41)$$

The first term, of zeroth order, represents the Darling-Siegert solution (3.12). This is consistent with our expansion around the base-point of no driving noise (fully Markovian process). Once

averaged, the second-order contribution is again diagonal (*i.e.* proportional to $\delta(\omega_0 + \omega_2)$) indicating that the *y*-averaged first-passage distribution is again invariant under time-shifts. The four correction terms featuring in the second order expansion in ε are labelled (*I*) to (*IV*), and need to be calculated explicitly. This requires to find explicit expressions for the coefficients of expansion $T^{(n)}(\omega_1, \tilde{\omega}_1, ..., \tilde{\omega}_n)$ and $R^{(n)}(\omega_1, \tilde{\omega}_1, ..., \tilde{\omega}_n)$. These expressions are derived in the following section.

3.2.4 Finding the coefficient terms for probability densities in the functional expansion

In this section we show how the functional expansion of transition and return probability are obtained perturbatively in terms of some suitable eigenfunctions.

The transition probability $T(t_0, t_1)$ of the undriven process, characterised by Langevin equation (3.1) for $\varepsilon = 0$, depends on the time-difference only and can therefore be shortened to $T(t_0, t_1) = T^{(0)}(t_1 - t_0)$. The transition density solves the Kolmogorov forward equation

$$\begin{cases} \partial_t T^{(0)}(t) &= \mathcal{L}^{x_1} T^{(0)}(t) & t > 0 \\ T^{(0)}(t=0) &= \delta(x_1 - x_0) \end{cases}$$
(3.42)

where we introduce the forward evolution operator \mathcal{L} as

$$\mathcal{L}f = \partial_x (V'(x)f) + D_x \partial_x^2 f, \qquad (3.43)$$

where f is a twice differentiable test function, and may denote the forward operator as \mathcal{L}^{x_1} to indicate its gradient terms are acting on x_1 where necessary to avoid confusion. Correspondingly, the L^2 -adjoint operator \mathcal{L}^{\dagger} , also referred to as backward operator, is

$$\mathcal{L}^{\dagger}f = -V'(x)\partial_x f + D_x \partial_x^2 f.$$
(3.44)

The forward operator \mathcal{L} has a countable set of eigenfunctions $\{u_n(x)\}\$ and a non-positive spectrum $0 \ge -\lambda_0 > -\lambda_1 > \dots$ [184],

$$\mathcal{L}u_n(x) = -\lambda_n u_n(x) \qquad n \in \mathbb{N}_0 \tag{3.45}$$

but is a priori not self-adjoint in $L^2(\mathbb{R})$. In fact, one can show [184] that \mathcal{L} is self-adjoint on $L^2(u_0)$, the space of square-integrable functions weighted by the stationary solution

$$u_0(x) = \mathcal{N} \exp\left(-\frac{V(x)}{D_x}\right) \tag{3.46}$$

with \mathcal{N} a suitable normalisation constant. In what follows, however, we will discuss eigenfunctions in the unweighted L^2 space. To that end, we need to slightly modify the operator to ensure that our choice of adjoint eigenfunctions is still a suitable bi-orthogonal base of L^2 . It is straightforward to show [200] that the operator

$$\mathfrak{L} = (u_0(x))^{-\frac{1}{2}} \mathcal{L} (u_0(x))^{\frac{1}{2}} = \exp\left(\frac{V(x)}{2D_x}\right) \mathcal{L} \exp\left(-\frac{V(x)}{2D_x}\right)$$
(3.47)

is indeed self-adjoint in (unweighted) L^2 and that therefore the family of

$$\left\{\exp\left(\frac{V(x)}{2D_x}\right)u_n(x)\right\}_{n=0}^{\infty},\tag{3.48}$$

as eigenfunctions of \mathfrak{L} , form an orthogonal set of eigenfunctions spanning $L^2(\mathbb{R})$. Defining $u_n(x)$ as right eigenfunctions, and

$$v_n(x) = e^{\frac{V(x)}{D_x}} u_n(x)$$
(3.49)

as left eigenfunctions, satisfying

$$\mathcal{L}^{\dagger} v_n(x) = -\lambda_n v_n(x), \qquad (3.50)$$

we obtain a bi-orthogonal set which after suitable normalisation fulfils

$$\int \mathrm{d}x \, v_m(x) u_n(x) = \delta_{m,n}. \tag{3.51}$$

This is useful to solve the forward equation; taking the Fourier transform in time of Eq. (3.43), one obtains

$$i\omega T^{(0)}(\omega) = \mathcal{L}T^{(0)}(\omega) + \delta(x_1 - x_0).$$
 (3.52)

Inserting the ansatz

$$T^{(0)}(\omega) = \sum_{n} T_{n}^{(0)}(x_{0};\omega) u_{n}(x_{1})$$
(3.53)

into Eq. (3.52) and using Eq. (3.45) leads to

$$\sum_{n} (i\omega + \lambda_n) T_n^{(0)}(x_0; \omega) u_n(x_1) = \sum_{n} v_n(x_0) u_n(x_1)$$
(3.54)

where we made use of the decomposition of unity,

$$\delta(x_0 - x_1) = \sum_n v_n(x_0) u_n(x_1). \tag{3.55}$$

Since the $u_n(x_1)$ are linearly independent, their prefactors in Eq. (3.54) need to agree. Therefore,

$$T_n^{(0)}(x_0;s) = \frac{v_n(x_0)}{i\omega + \lambda_n}$$
(3.56)

implying, together with Eq. (3.53),

$$T(s) = \sum_{n} \frac{v_n(x_0)u_n(x_1)}{i\omega + \lambda_n}.$$
(3.57)

Turning to the case of $\varepsilon \neq 0$, the translation probability of the driven Langevin equation (3.1)

solves the forward equation

$$\begin{cases} \partial_{t_1} \hat{T}(t_0, t_1; [y]) = (\mathcal{L}^{x_1} + \varepsilon y(t_1) \partial_{x_1}) \, \hat{T}(t_0, t_1; [y]) \\ \hat{T}(t_0, t_0; [y]) = \delta(x_1 - x_0) \end{cases}$$
(3.58)

where time-homogeneity can no longer be assumed. Under Fourier transform, this forward equation becomes

$$(i\omega_1 - \mathcal{L}^{x_1})\hat{T}(\omega_0, \omega_1; [y]) = \delta(x_1 - x_0) + \varepsilon \partial_{x_1} \int d\tilde{\omega}_1 \, \hat{y}(\tilde{\omega}_1)\hat{T}(\omega_0, \omega_1 - \tilde{\omega}_1; [y])$$
(3.59)

where the y-dependent term turns from a product into a convolution under the Fourier transform. We develop a perturbative solution of $\hat{T}(\omega_0, \omega_1; [y])$ in powers of y, akin to previous perturbative approaches for externally driven Fokker-Planck equations as developed in [183]. Following functional expansion ansatz (3.32), and using zeroth order result (3.57), we assume

$$\hat{T}(\omega_0,\omega_1;[y]) = \sum_n \frac{v_n(x_0)u_n(x_1)\delta(\omega_0+\omega_1)}{i\omega_1+\lambda_n} + \varepsilon \int d\tilde{\omega}_1 T^{(1)}(\omega_1,\tilde{\omega}_1)\,\hat{y}(\tilde{\omega}_1)\delta(\omega_0+\omega_1+\tilde{\omega}_1) + \dots$$
(3.60)

Since the $u_n(x)$ span the L^2 -space, in analogy to ansatz (3.53), we assume that the first-order correction too can be written as a sum

$$T^{(1)}(\omega_1, \tilde{\omega}_1) = \sum_n T_n^{(1)}(x_0; \omega_1, \tilde{\omega}_1) u_n(x_1).$$
(3.61)

Re-inserting this ansatz into Eq. (3.59) causes all terms to zeroth order in y to cancel, and one obtains an equation relating the contributions proportional to ε ,

$$\sum_{n} (i\omega_1 + \lambda_n) \int d\tilde{\omega}_1 T_n^{(1)}(x_0; \omega_1, \tilde{\omega}_1) \, \hat{y}(\tilde{\omega}_1) u_n(x) = \int d\tilde{\omega}_1 \sum_{n} \frac{v_n(x_0) \partial_{x_1} u_n(x_1)}{i(\omega_1 - \tilde{\omega}_1) + \lambda_n} \hat{y}(\tilde{\omega}_1). \quad (3.62)$$

The right hand side, which is the convolution of $T^{(0)}(\omega)$ and $\hat{y}(\omega)$, no longer sums over $u_n(x_1)$ but their derivative $\partial_{x_1}u_n(x_1)$. In order to compare both left and right terms, we need to express this sum as a sum over the linearly independent $u_n(x_1)$ again. The decomposition of the derivative in terms of $u_n(x_1)$ is given by

$$\partial_x u_n(x_1) = \sum_k \Delta_{nk} u_k(x_1) \tag{3.63}$$

where we refer to the Δ_{nk} as derivative coupling matrix whose entries, as follows from biorthogonality, are

$$\Delta_{nk} = \int \mathrm{d}x \, v_k(x) \partial_x u_n(x). \tag{3.64}$$

Using this notation, inserting the sum (3.63) into Eq. (3.62), and resolving the ansatz (3.61),

one yields

$$T^{(1)}(\omega_1, \tilde{\omega}_1) = \sum_{n,k} \frac{v_k(x_0) \Delta_{kn} u_n(x_1)}{(i(\omega_1 - \tilde{\omega}_1) + \lambda_k)(i\omega_1 + \lambda_n)}$$
(3.65)

In a similar way, the second order correction can be found: Using

$$\hat{T}(\omega_0,\omega_1;[y]) = \left[\sum_n \frac{v_n(x_0)u_n(x_1)\delta(\omega_0+\omega_1)}{\omega_1+\lambda_n} + \varepsilon \sum_{n,k} \frac{v_k(x_0)\Delta_{kn}u_n(x_1)}{(-\omega_0+\lambda_k)(\omega_1+\lambda_n)}\hat{y}(\omega_0+\omega_1) + \varepsilon^2 \iint d\tilde{\omega}_1 d\tilde{\omega}_2 T^{(2)}(\omega_1,\tilde{\omega}_1,\tilde{\omega}_2)\,\hat{y}(\tilde{\omega}_1)\hat{y}(\tilde{\omega}_2)\delta(\omega_0+\omega_2+\tilde{\omega}_1+\tilde{\omega}_2)\right] + \cdots \quad (3.66)$$

as ansatz, with the results from Eqs. (3.57) and (3.65) to zeroth and first order, inserting this ansatz into the forward equation (3.59) gives, following in complete analogy to the previous steps,

$$T^{(2)}(\omega_1, \tilde{\omega}_1, \tilde{\omega}_2) = \sum_{n,m,k} \frac{v_n(x_0)\Delta_{nk}\Delta_{km}u_m(x_1)}{(i(\omega_1 - \tilde{\omega}_1 - \tilde{\omega}_2) + \lambda_n)(i(\omega_1 - \tilde{\omega}_1) + \lambda_k)(i\omega_1 + \lambda_n)}.$$
(3.67)

Following this method, it is straightforward to generate the perturbative terms of T(n) to arbitrary order in n,

$$T^{(n)}(\omega_1, \tilde{\omega}_1, ..., \tilde{\omega}_n) = \sum_{k_0, ..., k_n} \frac{v_{k_0}(x_0) \Delta_{k_0 k_1} \cdot ... \cdot \Delta_{k_{n-1} k_n} u_{k_n}(x_1)}{\prod_{j=0}^n \left(i(\omega_1 - \sum_{\ell=0}^j \tilde{\omega}_\ell) + \lambda_{k_j} \right)}.$$
(3.68)

Finally, choosing $x_0 = x_1$ in any of the expressions (3.57), (3.65), (3.67) and (3.68) gives the corresponding terms for the return probability coefficients $R^{(0)}(\omega)$, $R^{(1)}(\omega, \tilde{\omega}_1)$, Equipped with these expressions, we are able to compute the relevant integrals in the formula for the *y*-averaged first-passage time density Eq. (3.41).

3.2.5 The full one-loop correction to the moment-generating function

So far, in our derivation of the second-order correction to the first-passage time density, Eq. (3.41), we only demanded the active driving noise to be stationary, with finite correlations and vanishing mean. In what follows, we specify y(t) to be Gaussian coloured noise. This choice is almost canonical in the study of coloured noise, in our case it greatly simplifies the necessary integrals. It is, however, possible to use any other correlation functions as long as the integrals remain manageable. Generally, to compute the perturbative contribution of *n*th order in *y*, the *n*-point correlation function of y(t) needs to be known; For Gaussian processes all higher moments follow from the two-point correlation function which simplifies the calculation of potential higher order corrections. Since the correlation function of coloured noise is an exponential, the results obtained in this section hold *for any* noise with such autocorrelation up to order $\mathcal{O}(\varepsilon^2)$. In particular, this implies that the results developed in the following hold to this perturbative order for telegraphic noise as is used in the run-and-tumble process [40] for which recently first-passage time statistics have been found in [66]. In difference to the typical run-and-tumble process, however, the active thermal processes studied in this chapter are dominated by the thermal noise contribution ξ_t , and the perturbation takes place in the magnitude of the active noise. The run-and-tumble process therefore is at the opposite end of the thermal-active spectrum of stochastic processes.

Gaussian coloured noise is defined by its exponential correlator,

$$\overline{y(t_1)y(t_2)} = D_y \beta^{-1} \exp\left(-\beta |t_1 - t_2|\right), \qquad (3.69)$$

which in Fourier space reads (Eq. (3.40))

$$\hat{C}_2(\tilde{\omega}) = \frac{2D_y}{\tilde{\omega}^2 + \beta^2} \tag{3.70}$$

With the explicit expressions (3.57), (3.65), (3.67), we perform the loop-integral of (I) (see Eq. (3.41) for notation) in eigenfunction-representation,

$$(I) = \int d\tilde{\omega} \frac{T^{(0)}(\omega_2) R^{(2)}(\omega_2, \tilde{\omega}, -\tilde{\omega})}{(R^{(0)}(\omega_2))^2} \hat{C}_2(\tilde{\omega})$$
(3.71)
$$= 2D_y \frac{T^{(0)}(\omega_2)}{(R^{(0)}(\omega_2))^2} \int d\tilde{\omega} \frac{R^{(2)}(\omega_2, \tilde{\omega}, -\tilde{\omega})}{\beta^2 + \tilde{\omega}^2}$$

$$= 2D_y \frac{T^{(0)}(\omega_2)}{(R^{(0)}(\omega_2))^2} \sum_{n,m,k}$$
$$\times \int_{-\infty}^{\infty} d\tilde{\omega} \frac{v_n(x_1)\Delta_{nk}\Delta_{km}u_m(x_1)}{(i\omega_2 + \lambda_n)(i(\omega_2 - \tilde{\omega}) + \lambda_k)(i\omega_2 + \lambda_m)} \frac{1}{\tilde{\omega}^2 + \beta^2}$$

$$= \frac{D_y}{\beta} \frac{T^{(0)}(\omega_2) R^{(2)}(\omega_2, -i\beta, i\beta)}{(R^{(0)}(\omega_2))^2}.$$
(3.72)

where in the last equality we employed Cauchy's residue theorem closing the contour in the lower half-plane containing the simple pole at $\tilde{\omega} = -i\beta$. Likewise, we find

$$(IV) = \int d\tilde{\omega} \frac{T^{(2)}(\omega_2, \tilde{\omega}, -\tilde{\omega})}{R^{(0)}(\omega_2)} \hat{C}_2(\tilde{\omega})$$

$$= 2D_y \frac{1}{R^{(0)}(\omega_2)} \sum_{n,m,k}$$

$$\times \int_{-\infty}^{\infty} d\tilde{\omega} \frac{v_n(x_0)\Delta_{nk}\Delta_{km}u_m(x_1)}{(i\omega_2 + \lambda_n)(i(\omega_2 - \tilde{\omega}) + \lambda_k)(i\omega_2 + \lambda_m)} \frac{1}{\tilde{\omega}^2 + \beta^2}$$

$$= \frac{D_y}{\beta} \frac{T^{(2)}(\omega_2, -i\beta, i\beta)}{R^{(0)}(\omega_2)}$$

$$(3.73)$$

where again the integral is evaluated by closing the contour in the lower half-plane enclosing the pole at $\tilde{\omega} = -i\beta$.

The diagrams (II) and (III), featuring $\tilde{\omega}$ -dependent denominators, require some more careful

analysis. We have

$$(II) = 2 \int d\tilde{\omega} \frac{T^{(0)}(\omega_2) R^{(1)}(\omega_2 + \tilde{\omega}, \tilde{\omega}) R^{(1)}(\omega_2, -\tilde{\omega})}{(R^{(0)}(\omega_2))^2 R^{(0)}(\omega_2 + \tilde{\omega})} \hat{C}_2(\tilde{\omega})$$

$$= 4D_y \frac{T^{(0)}(\omega_2)}{(R^{(0)}(\omega_2))^2}$$

$$\int_{-\infty}^{\infty} d\tilde{\omega} \frac{\sum_{mnk\ell} \frac{v_m(x_1)\Delta_{mn}u_n(x_1)}{(i\omega_2 + \lambda_m)(i(\omega_2 + \tilde{\omega}) + \lambda_n)} \cdot \frac{v_k(x_1)\Delta_{k\ell}u_\ell(x_1)}{(i(\omega_2 + \tilde{\omega}) + \lambda_k)(i\omega_2 + \lambda_\ell)}}}{\left(\sum_j \frac{v_j(x_1)u_j(x_1)}{i(\omega_2 + \tilde{\omega}) + \lambda_j}\right) (\tilde{\omega}^2 + \beta^2)}$$
(3.74)

Again, the numerator's poles all lie in the upper half-plane with the exception of the pole at $\tilde{\omega} = -i\beta$ stemming from the correlator. Before evaluating the integral by closing the contour in the lower half-plane, however, one needs to confirm that the denominator $R^{(0)}(\omega_2 + \tilde{\omega})$ does not have any roots for $\Im(\tilde{\omega}) < 0$ as these would lead to further poles. That this is indeed the case can be shown as follows. Using relation (3.49), one finds that $v_j(x_1)u_j(x_1) = e^{-V(x_1)/D}u_j(x_1)^2$. Since the $u_j(x)$ span the L^2 , there cannot be a x_1 for which all $u_j(x_1) = 0$. It follows that all $v_j(x_1)u_j(x_1)$ are all real and non-negative, and at least one is strictly positive. Further, by assumption $\Im(\tilde{\omega}) < 0$, $\lambda_j \geq 0$ and $\Im(\omega_2) < 0$ (for convergence of Eq. (3.8)). Therefore, $\Re(i(\omega_2 + \tilde{\omega}) + \lambda_j) > 0$. Finally, the real part of a positive real number divided by a number with positive real part is positive. Therefore, $R^{(0)}(\omega_2 + \tilde{\omega})$ has strictly positive real part in the lower half-plane and thus no roots. The contour can safely be closed in the lower half-plane and, invoking Cauchy's residue formula the integral is given by

$$(II) = 2\frac{D_y}{\beta} \frac{T^{(0)}(\omega_2) R^{(1)}(\omega_2 - i\beta, i\beta) R^{(1)}(\omega_2, i\beta)}{(R^{(0)}(\omega_2))^2 R^{(0)}(\omega_2 - i\beta)} .$$
(3.75)

By analogous reasoning one obtains

$$(III) = 2 \int d\tilde{\omega} \frac{T^{(1)}(\omega_2 + \tilde{\omega}, \tilde{\omega}) R^{(1)}(\omega_2, -\tilde{\omega})}{R^{(0)}(\omega_2) R^{(0)}(\tilde{\omega} - \omega_2)} \hat{C}_2(\tilde{\omega})$$
(3.76)

$$=2\frac{D_y}{\beta}\frac{T^{(1)}(\omega_2 - i\beta, i\beta)R^{(1)}(\omega_2, i\beta)}{R^{(0)}(\omega_2)R^{(0)}(\omega_2 - i\beta)}$$
(3.77)

All four terms together give a general formula for the moment generating function of firstpassage times for *arbitrary underlying processes and driving noises* provided the eigenfunctions and correlators are known. In the case of driving noise with exponentially decaying autocorrelation, the full formula for $\hat{F}(\omega_0, \omega_2) = F(\omega_2) \,\delta(\omega_0 + \omega_2)$, reads

$$F\left(\omega\right) = \frac{T^{\left(0\right)}\left(\omega\right)}{R^{\left(0\right)}\left(\omega\right)} \tag{3.78}$$

$$+ \frac{\varepsilon^2 D_y}{\beta} \left[-\frac{T^{(0)}(\omega) R^{(2)}(\omega, -i\beta, i\beta)}{\left(R^{(0)}(\omega)\right)^2} + 2\frac{T^{(0)}(\omega) R^{(1)}(\omega - i\beta, i\beta) R^{(1)}(\omega, i\beta)}{\left(R^{(0)}(\omega)\right)^2 R^{(0)}(\omega - i\beta)} \right] (3.79)$$

$$-2\frac{T^{(1)}(\omega - i\beta, i\beta) R^{(1)}(\omega, i\beta)}{R^{(0)}(\omega) R^{(0)}(\omega - i\beta)} + \frac{T^{(2)}(\omega, -i\beta, i\beta)}{R^{(0)}(\omega)}\right]$$
(3.80)

This general result concludes this section. In the next section, we consider two concrete examples to demonstrate how this perturbation theory can be turned into analytical results.

3.3 Results

3.3.1 Active Thermal Ornstein Uhlenbeck Process (ATOUP)

In this example we study the case of a particle in a harmonic potential driven by white and coloured noise described by the Langevin Equation

$$\dot{x}_t = -\alpha x_t + \xi_t + \varepsilon y(t) \tag{3.81}$$

with driving noise correlator (see Eq. (3.69))

$$\overline{y(t_1)y(t_2)} = D_y \beta^{-1} e^{-\beta|t_1 - t_2|}.$$
(3.82)

This process reduces to the simple Ornstein Uhlenbeck process when $\varepsilon = 0$ which models a particle in a harmonic potential $(V(x) = \frac{\alpha}{2}x^2)$ within a thermal bath. We consider, however, the process driven by an additional "active" term $\varepsilon y(t)$. We therefore refer to this process as active thermal Ornstein Uhlenbeck process (ATOUP). In the undriven case ($\varepsilon = 0$), the dynamics are characterised by the time and length-scales α^{-1} and

$$\ell = \sqrt{D_x \alpha^{-1}}.$$

3.3.1.A From eigenfunctions to the moment generating function of first-passage times

The Fokker-Planck equation associated (*cf.* Eq. (3.43)) to the Langevin Equation (3.81) has eigenvalues

$$\lambda_n = \alpha n \tag{3.83}$$

and is diagonalised by the (normalised) eigenfunctions

$$v_m(x) = \frac{1}{\sqrt{\sqrt{2\pi\ell} \cdot m!}} \operatorname{He}_m\left(\frac{x}{\ell}\right)$$
(3.84)

$$u_n(x) = \frac{1}{\sqrt{\sqrt{2\pi\ell} \cdot m!}} \operatorname{He}_m\left(\frac{x}{\ell}\right) \cdot \exp\left(-\frac{x^2}{2\ell^2}\right)$$
(3.85)

where we introduced Hermite polynomials using the convention

$$\operatorname{He}_{n}(x) = (-1)^{n} e^{\frac{x^{2}}{2}} \frac{\mathrm{d}^{n}}{\mathrm{d}x^{n}} e^{-\frac{x^{2}}{2}}$$
(3.86)

which satisfy the relation

$$\partial_x \operatorname{He}_n(x) = x \operatorname{He}_n(x) - \operatorname{He}_{n+1}(x)$$
(3.87)

such that the coupling matrix (cf. Eq. (3.64)) resolves to

$$\Delta_{mn} = -\frac{\sqrt{n}}{\ell} \delta_{m+1,n} \tag{3.88}$$

This time the coupling matrix is no longer diagonal, but instead incoming momentum n is upgraded to outgoing momentum n + 1 by the noise coupling. Just as in the case of Brownian motion, the amplitude of $\Delta_{m,n}$ grows like $|\Delta_{m,n}| \sim \sqrt{\lambda_m}$. For later use, we also note that

$$(x - \partial_x)v_n(x) = \sqrt{n+1} v_{n+1}(x)$$
(3.89)

$$\partial_x v_n(x) = \sqrt{n} \, v_{n-1}(x) \tag{3.90}$$

By L^2 -adjointness, it follows that the adjoint creation and annihilation operators are¹

$$-\partial_x u_n(x) = \sqrt{n+1} u_{n+1}(x) \tag{3.91}$$

$$(x + \partial_x)u_n(x) = \sqrt{n}u_{n-1}(x) \tag{3.92}$$

In order to compute the transition and return probabilities, the following identity [153]

$$\sum_{k=0}^{\infty} \frac{\operatorname{He}_{k}(x) \operatorname{He}_{k}(y) e^{-\frac{y^{2}}{2}}}{k!} z^{k}$$
(3.93)

$$= \frac{1}{\sqrt{1-z^2}} \exp\left(-\frac{1}{2} \frac{(y-zx)^2}{1-z^2}\right)$$
(3.94)

proves to be useful.

We introduce all quantities in dimensionless form, such as the reduced frequency σ and the reduced autocorrelation time β' as

$$\sigma = i\alpha^{-1}\omega \qquad \beta' = \alpha^{-1}\beta \tag{3.95}$$

By considering the Fourier transform at $\sigma = i\alpha^{-1}\omega$, we are effectively studying the Laplace transform. This is intended since our final observable is the moment generating function, the Laplace transform of the first-passage time distribution. Further, we denoted the lengths rescale by ℓ as

$$x_1' = \ell^{-1} x_1 \qquad x_0' = \ell^{-1} x_0. \tag{3.96}$$

In the discussion that follows, we analyse all densities as densities in these dimensionless quantities to simplify notation and calculations. Following Eq. (3.57), one obtains for the transition

¹It further follows that forward operator is $\mathcal{L} = -\partial_x(x + \partial_x)$ and $\mathcal{L}^{\dagger} = (x - \partial_x)\partial_x$, when interpreting them as number operators on a Fock space [3].

probability

$$T^{(0)}(\sigma) = \frac{1}{\sqrt{2\pi}\ell\alpha} \sum_{n=0}^{\infty} \frac{\operatorname{He}_{n}(x_{0}') \operatorname{He}_{n}(x_{1}') e^{-\frac{x_{1}'^{2}}{2}}}{n!(\sigma+n)}$$

$$= \frac{1}{\sqrt{2\pi}\ell\alpha} \int_{0}^{\infty} \mathrm{d}t \ e^{-\sigma t} \sum_{n=0}^{\infty} \frac{\operatorname{He}_{n}(x_{0}') \operatorname{He}_{n}(x_{1}') e^{-\frac{x_{1}'^{2}}{2}}}{n!} \left(e^{-t}\right)^{n}$$

$$= \frac{1}{\sqrt{2\pi}\ell\alpha} \int_{0}^{\infty} \mathrm{d}t \ \frac{e^{-\sigma t}}{\sqrt{1-e^{-2t}}} \exp\left[-\frac{(x_{1}'-x_{0}'e^{-t})}{2(1-e^{-2t})}\right]$$
(3.97)

where we used identity (3.94) setting $z = e^{-t}$. This choice suggests already that this integral is in fact the Laplace transform of the Ornstein-Uhlenbeck propagator (in $t \leftrightarrow \sigma$) the result of which is known in the literature to be ([52])

$$T^{(0)}(\sigma) = \begin{cases} \frac{\Gamma(\sigma)}{\sqrt{2\pi\ell\alpha}} \exp\left(\frac{{x'_0}^2 - {x'_1}^2}{4}\right) D_{-\sigma}(-x'_0) D_{-\sigma}(x'_1) & x'_0 < x'_1\\ \frac{\Gamma(\sigma)}{\sqrt{2\pi\ell\alpha}} \exp\left(\frac{{x'_0}^2 - {x'_1}^2}{4}\right) D_{-\sigma}(x'_0) D_{-\sigma}(-x'_1) & x'_0 > x'_1 \end{cases}$$
(3.98)

where we introduced the parabolic cylinder functions $D_{-\sigma}(x)$ ([102, 9.240]). By continuity, for $x'_0 \to x'_1$ it follows that

$$R^{(0)}(\sigma) = \frac{\Gamma(\sigma)}{\sqrt{2\pi\ell\alpha}} D_{-\sigma}(x_1') D_{-\sigma}(-x_1').$$
(3.99)

In order to compute $T^{(1)}(\sigma, -\beta')$, we use Eq. (3.65) and the derivative coupling matrix computed in (3.88) to find

$$T^{(1)}(\sigma, i\beta') = \frac{1}{\sqrt{2\pi}\ell^2 \alpha^2} \sum_n \frac{v_n(x_0')(-\sqrt{n+1})u_{n+1}(x_1')}{(\sigma+\beta'+n)(\sigma+n+1)}$$
(3.100)
$$= \frac{1}{\sqrt{2\pi}\ell^2 \alpha^2(1-\beta')} \partial_{x_1'} \sum_n v_n(x_0')u_n(x_1') \left[\frac{1}{\sigma+\beta'+n} - \frac{1}{\sigma+n+1}\right]$$
$$= \frac{\partial_{x_1'}}{\ell\alpha(1-\beta')} \left[T^{(0)}(\sigma+\beta') - T^{(0)}(\sigma+1)\right]$$

where we made use of relation (3.91) in the second equality. Letting $x'_0 \to x'_1$, one obtains $R^{(1)}(\sigma, -\beta')$. The counterpart, $T^{(1)}(\sigma + \beta', \beta')$, is similarly found to be

$$T^{(1)}\left(\sigma - i\beta', i\beta'\right) = \frac{\partial_{x_1'}}{\ell\alpha(1+\beta')} \left[\rho_{x_0', x_1'}^{(0)}(\sigma) - \rho_{x_0', x_1'}^{(0)}(\sigma+\beta'+1)\right]$$
(3.101)

This terms can be explicitly calculated and simplified. The rather lengthy but explicit expressions are given in appendix 3.C.

For the second order derivative term, using formula (3.67), one finds

$$T^{(2)}(\sigma, -i\beta', i\beta') = \frac{1}{\sqrt{2\pi}\ell^3 \alpha^3} \sum_{n=0}^{\infty} \frac{v_n(x_0')\sqrt{n+1}\sqrt{n+2}u_{n+2}(x_1')}{(\sigma+n)(\sigma+\beta'+n+1)(\sigma+n+2)}$$
(3.102)
$$= \frac{\partial_{x_1'}^2}{\sqrt{2\pi}\ell^3 \alpha^3} \sum_{n=0}^{\infty} \frac{v_n(x_0')u_n(x_1')}{(\sigma+n)(\sigma+\beta'+n+1)(\sigma+n+2)}$$
$$= \frac{\partial_{x_1'}^2}{\ell^2 \alpha^2} \left[\frac{1}{2(\beta'+1)} T^{(0)}(\sigma) - \frac{1}{2(\beta'-1)} T^{(0)}(\sigma+2) + \frac{1}{(\beta'^2-1)} T^{(0)}(\sigma+\beta'+1) \right]$$

Again, the evaluated terms, including for $x'_0 \to x'_1$ are given in appendix 3.C.

Equipped with the return and transition probabilities and its first two derivatives with respect to driving noise y (cf. (3.98)-(3.102)), we obtain the four diagrammatic contributions (3.71)-(3.77) which constitute the one-loop correction formula (3.78). Whilst all the explicit expressions are given in appendix 3.C, we here give the moment generating function in full as a undriven part and a perturbative correction, using $s = \alpha \sigma = i\omega$,

$$\left\langle \overline{e^{-s\tau_{x_0 \to x_1}}} \right\rangle = F(s)$$

$$= \mathcal{M}_0^{OU}\left(\frac{x_0}{\ell}, \frac{x_1}{\ell}, \alpha^{-1}s\right) + \underbrace{\frac{D_y \varepsilon^2}{D_x \alpha \beta}}_{=:\nu_{OU}} \mathcal{M}_1^{OU}\left(\frac{x_0}{\ell}, \frac{x_1}{\ell}, \alpha^{-1}\beta, \alpha^{-1}s\right) + \mathcal{O}(\nu_{OU}^2) \quad (3.103)$$

where we introduced the dimensionless parameter of expansion

$$\nu_{OU} = \frac{\varepsilon^2 D_y}{D_x \alpha \beta}.$$
(3.104)

As is already known from literature (e.g. [52]),

$$\mathcal{M}_{0}^{OU}(x_{0}', x_{1}', \sigma) = \begin{cases} \exp\left(\frac{{x_{0}'}^{2} - {x_{1}'}^{2}}{4}\right) \frac{D_{-\sigma}(-x_{0}')}{D_{-\sigma}(-x_{1}')} & x_{0}' < x_{1}' \\ \exp\left(\frac{{x_{0}'}^{2} - {x_{1}'}^{2}}{4}\right) \frac{D_{-\sigma}(x_{0}')}{D_{-\sigma}(x_{1}')} & x_{0}' > x_{1}'. \end{cases}$$
(3.105)

By symmetry $(x'_0, x'_1) \leftrightarrow (-x'_1, -x'_0)$ of the problem and symmetry of driving noise, it suffices to regard one case only, such that without loss of generality we assume $x'_0 < x'_1$. The central result of this section then is

$$\mathcal{M}_{1}^{OU}(x'_{0}, x'_{1}, \beta', \sigma) \tag{3.106}$$

$$= \frac{\sigma e^{\frac{\sigma}{4}}}{2\left(\beta'^{2}-1\right)D_{-\sigma}(-x_{1}')^{2}D_{-\beta'-\sigma}(-x_{1}')}$$

$$\times \left[(\beta'+1)\left(\sigma+1\right)\left(D_{-\sigma}(-x_{1}')D_{-\sigma}(-x_{1}')-D_{-\sigma}(-x_{1}')\right)D_{-\beta'-\sigma}(-x_{1}')\right]$$
(3.107)

$$\times \left[(\beta'+1) (\sigma+1) (D_{-\sigma}(-x_0) D_{-\sigma-2}(-x_1) - D_{-\sigma-2}(-x_0) D_{-\sigma}(-x_1)) D_{-\beta'-\sigma}(-x_1) \right]$$

$$(3.108)$$

$$2(\beta'+\sigma) D_{-\sigma}(-x') (D_{-\sigma}(-x') D_{-\sigma-2}(-x') - D_{-\sigma-2}(-x') D_{-\sigma}(-x')) D_{-\beta'-\sigma}(-x'))$$

$$-2(\beta'+\sigma)D_{-\sigma-1}(-x_1')\left(D_{-\sigma}(-x_0')D_{-\beta'-\sigma-1}(-x_1')-D_{-\sigma}(-x_1')D_{-\beta'-\sigma-1}(-x_0')\right)\right]$$
(3.109)

Using for instance a computer algebra system, all moments can be obtained by differentiation and evaluating the limit of $\sigma \to 0$ at which all derivatives have a removable singularity.

3.3.1.B Numerical Validation

In order to corroborate the closed form result of the first-order correction to the moment generating function of first-passage times, Eq. (3.109), we employ Monte Carlo simulations integrating the driven Langevin equation (3.81) $N \simeq 10^6$ times, numerically find the first-passage time $\tilde{\tau}_i$, and average the moment generating function $\tilde{\mathcal{M}} = \frac{1}{N} \sum_{i=1}^{N} \exp(-s\tilde{\tau}_i)$ over the range $s \in [0, 5]$. Throughout this work, the tilde denotes quantities that have been numerically obtained. Since we assume an expansion of the form $\mathcal{M}(\nu) = \mathcal{M}_0 + \nu \mathcal{M}_1 + \nu^2 \mathcal{M}_2 + ...$, we take the numerical first derivative

$$\tilde{\mathcal{M}}_1(\nu) = \frac{\tilde{\mathcal{M}}(\nu) - \mathcal{M}_0}{\nu}$$
(3.110)

which expands as $\tilde{\mathcal{M}}_1(\nu) = \mathcal{M}_1 + \nu \mathcal{M}_2 + \ldots$, to verify our analytic prediction of \mathcal{M}_1 . In Fig. 3.2a, the numerical estimate $\tilde{\mathcal{M}}_1$ is shown for various values of ν , together with the analytic expression Eq. (3.109) of the scaling function \mathcal{M}_1 . For small ν , the agreement is excellent. For larger values of ν , higher-order corrections become more visible. The next-higher contribution, which we did not calculate analytically but which can be found by following the framework to second order in ν , is numerically estimated by taking the second numerical derivative,

$$\tilde{\mathcal{M}}_2(\nu) = \frac{\tilde{\mathcal{M}}_1(\nu) - \mathcal{M}_1}{\nu},\tag{3.111}$$

and is shown in the inset of Fig. 3.2a. For $0.2 \leq \nu \leq 0.8$, the second-order corrections collapse, indicating that the deviations in the main figure are well accounted for by second-order corrections. For $\nu = 0.1$, $\tilde{\mathcal{M}}_2$ deviates slightly due to the statistical noise, since the second order correction is very small.

This numerical result therefore confirms the analytically obtained first-order correction to the moment-generating function; consequently, the correction to all moments has been gained. As an illustration, we further show the first and second moment of the Ornstein-Uhlenbeck process driven by coloured noise in Fig. 3.1a and Fig. 3.1b. In analogy to the moment-generating function, we measure the mean and mean square first passage times $\tilde{\mathcal{T}}^1 = \frac{1}{N} \sum_{i=1}^N \tilde{\tau}_i$, $\tilde{\mathcal{T}}^2 = \frac{1}{N} \sum_{i=1}^N \tilde{\tau}_i^2$, which we assume to expand in ν as $\mathcal{T}^1(\nu) = \mathcal{T}_0^1 + \nu \mathcal{T}_1^1 + \nu^2 \mathcal{T}_2^1 + \dots$ and $\mathcal{T}^2(\nu) = \mathcal{T}_0^2 + \nu \mathcal{T}_1^2 + \nu^2 \mathcal{T}_2^2 + \dots$ The first-order corrections introduced are obtained by differentiation wrt σ

$$\mathcal{T}_1^n = \frac{1}{n!} \left. \frac{\mathrm{d}^n}{\mathrm{d}(-\sigma)^n} \right|_{\sigma=0} \mathcal{M}_1 \tag{3.112}$$

using the result of Eq. (3.109) which is performed by a computer algebra system and evaluated exactly. Due to their lengthiness, we do not give their full expression here. In order to



(a) Correction to mean first passage time of active thermal Ornstein Uhlenbeck process (cf. Eq. (3.81)) as obtained from Eq. (3.113) versus target positions $x_1, x_0 = 0$ fixed, and various values of ν (plot marks) compared to theoretical result to first order in ν (black line) using Eq. (3.112) and the result obtained in (3.109). The inset shows the mean first-passage time τ_{x_0,x_1} as measured vs x_1 and its corrections for values of $\nu = 0.1$ to 0.8. Correction due to active driving noise increases MFPT for $x_1 \leq 1.6$ and decreases MFPT for $x_1 \gtrsim 1.6$. This behaviour is fully captured by the analytic result.



(b) Correction to mean squared first passage time of active thermal Ornstein Uhlenbeck process (cf. Eq. (3.81)) as obtained from Eq. (3.114) versus target positions x_1 , $x_0 = 0$ fixed, and various values of ν (plot marks) compared to theoretical result to first order in ν (black line) using Eq. (3.112) and the result obtained in (3.109). The inset shows the mean squared first-passage time τ_{x_0,x_1} as measured vs x_1 and its corrections for values of $\nu = 0.1$ to 0.8. Correction due to active driving noise increases MFPT for $x_1 \leq 1.6$ and decreases MFPT for $x_1 \gtrsim 1.6$. This behaviour is fully captured by the analytic result.

Figure 3.1.: First order correction to first and second moment of ATOUP.

numerically confirm these predictions, we measure the first order derivatives

$$\tilde{\mathcal{T}}_{1}^{1}(\nu) = \frac{\tilde{\mathcal{T}}_{1}^{1}(\nu) - \mathcal{T}_{0}^{1}}{\nu}$$
(3.113)

$$\tilde{\mathcal{T}}_{1}^{2}(\nu) = \frac{\tilde{\mathcal{T}}_{1}^{2}(\nu) - \mathcal{T}_{0}^{2}}{\nu}$$
(3.114)

and compare it to the result obtained from Eq. (3.112). In Fig. 3.1a and Fig. 3.1b, we show the resulting moments of first-passage times obtained for fixed start position $x_0 = 0$ (at the minimum of the potential) but varied $x_1 \in [0.05, 2]$. The figures show a clear agreement with the theoretical result and systematic deviations for larger ν . Further, we observe that in this setting the coloured noise increases the mean-first passage time for smaller distances ($x_1 \leq 1.6$) and decreases it for larger distances. This also holds true for the mean squared first-passage time. This example therefore further illustrates that the effect of coloured driving (or memory) on the Langevin dynamics is highly non-trivial, but yet our framework is to capture this effect. The insets in both figures show the measured moments $\tilde{\mathcal{T}}^1, \tilde{\mathcal{T}}^2$.

3.3.2 Active Thermal Brownian Motion on a ring (ATBM)

In this subsection, we consider the case of Brownian Motion x_t driven by coloured noise with periodic boundary conditions ($x \equiv x + 2\pi r$). The position of the particle satisfies the Langevin equation

$$\dot{x}_t = \xi_t + \varepsilon y(t) \tag{3.115}$$

with

$$\langle \xi_{t_1} \xi_{t_2} \rangle = 2D_x \delta(t_1 - t_2) \tag{3.116}$$

$$\langle y(t_1)y(t_2)\rangle = D_y \beta^{-1} e^{-\beta|t_1 - t_2|}.$$
 (3.117)

We refer to this system as Active Thermal Brownian Motion on a ring (ATBM). In analogy to the previous subsection, we derive the correction to the moment generating function of the first-passage time distribution.

3.3.2.A From eigenfunctions to the moment generating function of first-passage times

The eigenfunctions associated to the forward equation corresponding to Langevin Equation (3.115) are

$$u_n(x) = \frac{1}{\sqrt{2\pi r}} e^{i\frac{kx}{R}} \tag{3.118}$$

$$v_n(x) = \frac{1}{\sqrt{2\pi r}} e^{-i\frac{kx}{R}}$$
(3.119)

with corresponding eigenvalues

$$\lambda_n = D_x r^{-2} n^2 \qquad (n \in \mathbb{Z}). \tag{3.120}$$

The eigenfunctions are conjugate to each other since the forward operator of simple diffusion, $\mathcal{L} = D_x \partial_x^2$, is self-adjoint. From this follows that the noise-coupling matrix,

$$\Delta_{mn} = \frac{1}{2\pi r} \int_0^{2\pi r} \mathrm{d}x \; i \frac{n}{r} e^{i(n-m)\frac{x}{r}} = i \frac{n}{r} \delta_{mn} \tag{3.121}$$

is diagonal and purely imaginary. Because of scale-invariance and rotational symmetry, we simplify the following discussion by introducing the dimensionless angle

$$\theta \coloneqq \frac{x_1 - x_0}{r},\tag{3.122}$$

where we restrict ourselves to $\theta \in [0, 2\pi)$, and the diffusive timescale

$$\alpha^{-1} = \frac{r^2}{D_x}$$

with which we rescale the Fourier-frequency s to

$$\sigma = i\alpha^{-1}\omega, \tag{3.123}$$

again effectively evaluating the Laplace transform (cf. Eq. (3.8)) of the respective probability densities. With this simplified notation, the transition density to zeroth order reads

$$T^{(0)}(\sigma) = \frac{1}{2\pi\alpha r} \sum_{k=-\infty}^{\infty} \frac{e^{ik\theta}}{\sigma + k^2}$$
$$= \frac{1}{2\alpha r} \frac{\cosh\left((\theta - \pi)\sqrt{\sigma}\right)}{\sqrt{\sigma}\sinh\left(\pi\sqrt{\sigma}\right)},$$
(3.124)

and the return probability, setting $\theta = 0$, is

$$R^{(0)}(\sigma) = \frac{1}{2\alpha r} \frac{\cosh\left(\pi\sqrt{\sigma}\right)}{\sqrt{\sigma}\sinh\left(\pi\sqrt{\sigma}\right)}.$$
(3.125)

Assuming the y-averaged moment generating function has an expansion of

$$F(s) = \mathcal{M}_0\left(\frac{x_1 - x_0}{r}, \frac{r^2}{D_x}s\right) + \underbrace{\frac{D_y \varepsilon^2}{D_x \alpha \beta}}_{\nu_{BM}} \mathcal{M}_1\left(\frac{x_1 - x_0}{r}, \frac{r^2}{D_x}s, \frac{r^2 \beta}{D_x}\right) + \mathcal{O}(\nu_{BM}^2), \qquad (3.126)$$

where we introduced the dimensionless perturbative parameter

$$\nu_{BM} = \frac{D_y \varepsilon^2}{D_x \alpha \beta} = \frac{\varepsilon^2 D_y r^2}{D_x^2 \beta},\tag{3.127}$$

then the zeroth order contribution is, using the classic result Eq. (3.12), and the results in (3.124), (3.125),

$$\mathcal{M}_0(\theta, \sigma) = \frac{\cosh\left((\theta - \pi)\sqrt{\sigma}\right)}{\cosh\left(\pi\sqrt{\sigma}\right)} \tag{3.128}$$

which expands around $\sigma = 0$ as

$$\mathcal{M}_{0}(\theta,\sigma) = 1 + \left(\frac{\theta^{2}}{2} - \pi\theta\right)\sigma$$

$$+ \frac{1}{24}\left(\theta^{4} - 4\pi\theta^{3} + 8\pi^{3}\theta\right)\sigma^{2}$$

$$+ \frac{1}{720}\left(\theta^{6} - 6\pi\theta^{5} + 40\pi^{3}\theta^{3} - 96\pi^{5}\theta\right)\sigma^{3} + \dots$$
(3.129)

Being a moment generating function, the prefactors in front of σ^n correspond to the (rescaled) moments of the first-passage time $\frac{(-1)^n}{n!} \langle \tau_{x_0 \to x_1}^n \rangle \left(\frac{D_x}{r^2}\right)^n$.

We turn to higher orders in ε . To first order, the transition density

$$T^{(1)}(\sigma, i\beta') = \frac{1}{2\pi\alpha^2 r^2} \sum_{n=-\infty}^{\infty} \frac{-in}{(\sigma + \beta' + n^2)(\sigma + n^2)} = 0$$
(3.130)

vanishes since the sum is over terms odd in n. Here, we introduced

$$\beta' = \alpha^{-1}\beta \tag{3.131}$$

as the dimensionless correlation time-scale of the coloured noise. This implies that the contribution of diagrams (II) and (III), as given in Eq. (3.75) and (3.77), vanish, leaving only (I) and (IV) as correction terms. Indeed, the vanishing of the "odd" diagrams (II) and (III) is a consequence of the translational invariance of the system; all response functions of odd order $T^{(2n+1)}(\sigma; i\beta')$ need to vanish since to that order the response to a driving noise in a flat potential is invariant under $y(t) \to -y(t)$.

To second order, the transition density is

$$T^{(2)}\left(\sigma - i\beta', i\beta'\right) = -\frac{1}{2\pi\alpha^{3}r^{3}} \sum_{n=-\infty}^{\infty} \frac{n^{2}e^{in\theta}}{(\sigma + n^{2})(\sigma + \beta' + n^{2})(\sigma + n^{2})}$$

$$= -\frac{1}{2\pi\alpha^{3}r^{3}} \sum_{n=-\infty}^{\infty} \left[\frac{1}{\beta'^{2}} \frac{n^{2}e^{in\theta}}{\sigma + \beta' + n^{2}} - \frac{1}{\beta'^{2}} \frac{n^{2}e^{in\theta}}{\sigma + n^{2}} + \frac{1}{\beta'} \frac{n^{2}e^{in\theta}}{(\sigma + n^{2})^{2}}\right]$$

$$= \frac{1}{\alpha^{2}r^{2}} \cdot \frac{1}{\beta'^{2}} \partial_{\theta}^{2} \left[T^{(0)}\left(\sigma + \beta'\right) - T^{(0)}\left(\sigma\right) - \beta'\partial_{\sigma}T^{(0)}\left(\sigma\right)\right]$$

$$= \frac{1}{\alpha^{3}r^{3}} \cdot \frac{1}{4\beta'^{2}\sqrt{\sigma}} \left[\frac{\cosh\left((\theta - \pi)\sqrt{\sigma}\right)}{\sinh\left(\pi\sqrt{\sigma}\right)} \left(\pi\beta'\sqrt{\sigma}\coth\left(\pi\sqrt{\sigma}\right) - 2\sigma - \beta'\right) + \sqrt{\sigma} \left\{2\sqrt{\beta' + \sigma} \frac{\cosh\left((\theta - \pi)\sqrt{\sigma}\right)}{\sinh\left(\pi\sqrt{\beta' + \sigma}\right)} + \beta(\pi - \theta) \frac{\sinh\left((\theta - \pi)\sqrt{\sigma}\right)}{\sinh\left(\pi\sqrt{\sigma}\right)}\right\}\right]$$

$$(3.132)$$

where $\partial_{\theta} = r \partial_{x_1}$. Setting $\theta = 0$, one obtains the second order response of the return probability,

$$R^{(2)}(\sigma, -i\beta', i\beta')$$

$$= \frac{1}{4\alpha^3 \beta^2 r^3} \left[\pi\beta \coth^2(\pi\sqrt{\sigma}) - \frac{(\beta + 2\sigma) \coth(\pi\sqrt{\sigma})}{\sqrt{\sigma}} + 2\sqrt{\beta + \sigma} \coth(\pi\sqrt{\beta + \sigma}) - \pi\beta \right],$$
(3.133)
3. Fist passage time distribution of active thermal particles

Inserting these quantities into the FPT correction (3.78), gives

$$F(s = \alpha \sigma) = \left\langle \overline{e^{-s\tau_{x_0 \to x_1}}} \right\rangle$$
$$= \frac{\cosh\left((\theta - \pi)\sqrt{\sigma}\right)}{\cosh\left(\pi\sqrt{\sigma}\right)} + \frac{D_y \varepsilon^2}{D_x \alpha \beta} \cdot \frac{\sqrt{\sigma} \tanh\left(\pi\sqrt{\sigma}\right)}{2\beta'^2} \left[\frac{\cosh\left((\theta - \pi)\sqrt{\beta' + \sigma}\right)}{\sinh\left(\pi\sqrt{\beta' + \sigma}\right)} 2\sqrt{\beta' + \sigma} + \frac{\cosh\left(\pi\sqrt{\beta' + \sigma}\right)}{\cosh\left(\pi\sqrt{\sigma}\right)} \left(\pi\beta' - 2\sqrt{\beta' + \sigma} \coth\left(\pi\sqrt{\beta' + \sigma}\right)\right) + \frac{\sinh\left((\theta - \pi)\sqrt{\sigma}\right)}{\sinh\left(\pi\sqrt{\sigma}\right)}\beta'(\pi - \theta)\right]$$
(3.134)

This expression is the *full moment generating function up to second order in* ε in elementary functions. In line with our previous notation, we identify the dimensionless scaling functions

$$\mathcal{M}_{0}^{BM}\left(\theta,\sigma\right) = \frac{\cosh\left(\left(\theta-\pi\right)\sqrt{\sigma}\right)}{\cosh\left(\pi\sqrt{\sigma}\right)} \tag{3.135}$$

$$\mathcal{M}_{1}^{BM}\left(\theta,\sigma,\beta'\right) = \frac{\sqrt{\sigma}\tanh\left(\pi\sqrt{\sigma}\right)}{2\beta'^{2}} \left[\frac{\cosh\left((\theta-\pi)\sqrt{\beta'+\sigma}\right)}{\sinh\left(\pi\sqrt{\beta'+\sigma}\right)}2\sqrt{\beta'+\sigma}\right]$$
(3.136)

$$+ \frac{\cosh\left(\pi\sqrt{\beta'+\sigma}\right)}{\cosh\left(\pi\sqrt{\sigma}\right)} \left(\pi\beta' - 2\sqrt{\beta'+\sigma}\coth\left(\pi\sqrt{\beta'+\sigma}\right)\right) + \frac{\sinh\left((\theta-\pi)\sqrt{\sigma}\right)}{\sinh\left(\pi\sqrt{\sigma}\right)}\beta'\left(\pi-\theta\right)\right]$$

which together form the first-order correction of the moment-generating function

$$\left\langle \overline{\exp(-s\tau_{x_0,x_1})} \right\rangle = \mathcal{M}_0^{BM} \left(\frac{x_1 - x_0}{r}, \frac{r^2 s}{D_x} \right) + \frac{D_y r^2 \varepsilon^2}{D_x^2 \beta} \mathcal{M}_1^{BM} \left(\frac{x_1 - x_0}{r}, \frac{r^2 s}{D_x}, \frac{r^2 \beta}{D} \right) .$$
(3.137)

An expansion around $\sigma = 0$ gives corrections to all moments. The one-loop corrected mean first-passage time over an angle of θ , $\langle \tau_{0\to\theta} \rangle$, for instance reads

$$\alpha \left\langle \tau_{0,\theta} \right\rangle = \underbrace{\pi \theta - \frac{\theta^2}{2}}_{\mathcal{T}_0^1(\theta)} + \nu_{BM} \underbrace{\frac{1}{2\beta'^{3/2}} \left(\sqrt{\beta'} (2\pi - \theta)\pi - 2\pi \coth\left(\pi \sqrt{\beta'}\right) + 2\pi \frac{\cosh\left(\sqrt{\beta'}(\theta - \pi)\right)}{\sinh(\pi \sqrt{\beta'})} \right)}_{=:\mathcal{T}_1^1(\theta, \beta')}$$
(3.138)

where we indicated that the result can be written as the classical contribution (\mathcal{T}_0^1) times the dimensionless perturbative coefficient ν_{BM} (cf. Eq. (3.127)) and a dimensionless scaling function $\mathcal{T}_1^1(\theta, \beta')$. By successive derivation, any higher order moment may be obtained from Eq. (3.134).

3.3.2.B Numerical Validation

In order to validate the analytic result of the moment generating function of first-passage times Eq. (3.134) and the mean first-passage time Eq. (3.138), we follow the same steps as in the previous section 3.3.1.B. Using Monte-Carlo simulations, we sample the first-passage times τ_i of the integrated stochastic equation (3.115). To validate the moment-generating function, we average over $N \simeq 10^6$ to 10^7 iterations to sample

$$\tilde{\mathcal{M}} = \frac{1}{N} \sum_{i=1}^{N} \exp(-s\tau_i) \tag{3.139}$$



(a) Correction to mean first passage time of ATBM on a ring (cf. Eq. (3.115)) as obtained from Eq. (3.113) versus target position x_1 and various values of ν (plot marks cf. Eq. (3.127)). This is compared to theoretical result of Eq. (3.138) (solid blue line).



(b) Correction to mean squared first passage time of ATBM on a ring (cf. Eq. (3.115)) as obtained from Eq. (3.114) versus target position x_1 and various values of ν (plot marks cf. Eq. (3.127)). This is compared to theoretical result of twice differentiating Eq. (3.136) (solid blue line).

Figure 3.2.: First order correction to first and second moment of first-passage times of ATBM with periodic boundary conditions.

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for various values of ν (cf. Eq. (3.127)) and across $x'_1 - x'_0 \in (0, \pi]$ (with r = 1). Again, symbols with a tilde denote quantities which are measured numerically. To validate the theoretically predicted first-order correction Eq. (3.136), we subtract the $\nu = 0$ contribution, \mathcal{M}_0 (cf. Eq. (3.135)), and rescale by ν ,

$$\tilde{\mathcal{M}}_1(\nu) = \frac{\tilde{M}(\nu) - \mathcal{M}_0}{\nu} = \mathcal{M}_1 + \nu \mathcal{M}_2 + \dots = \mathcal{M}_1 + \nu \tilde{\mathcal{M}}_2$$
(3.140)

where we introduced, in analogy to Eq. (3.111),

$$\tilde{\mathcal{M}}_2 = \frac{\tilde{\mathcal{M}}_1(\nu) - \mathcal{M}_1}{\nu} = \mathcal{M}_2 + \nu \mathcal{M}_3 + \dots$$
(3.141)

as shorthand for numerically measured higher-order corrections. In Fig. 3.2b, we show the analytic result \mathcal{M}_1 (*cf.* Eq. (3.136)) and numerically obtained $\tilde{\mathcal{M}}_1(\nu)$ (*cf.* Eq. (3.140)) for various values of $0 \leq \nu \leq 0.8$. The agreement is again excellent, and the discrepancy between simulated result and theoretical first order correction grows, as expected, with larger values of ν . The rescaled discrepancy, $\tilde{\mathcal{M}}_2$, to leading order the second-order correction \mathcal{M}_2 (*cf.* Eq. (3.141)), is plotted in the inset and collapses, indicating that the discrepancy is systematic and confirming the validity of the result in Eq. (3.136).

In Figs. 3.2a and 3.2b, we show the first and second moment of first-passage times and how its deviation to the $\nu = 0$ case is captured by the first-order correction obtained using Eq. (3.113) and Eq. (3.114) with the result of Eq. (3.136). For the first and second moment, the agreement is again excellent, showing that the correction induced by the active driving noise is accurately captured to leading order. The insets of Figs. 3.2a and 3.2b show the respective moments of the FPT for various ν , indicating the systematic decrease for increased values of ν .

3.3.3 Limit Cases

The framework we introduce here allows to study coloured driving noises at any noise-colour β . In particular, this includes two limit cases of $\beta \to 0$ and $\beta \to \infty$. For appropriate re-scaling of D_y , the former limit corresponds to a particular quenched disorder model, and the latter to additional white noise. In what follows we discuss these limit cases in more detail.

3.3.3.A The white noise limit

For very small autocorrelation times β^{-1} the driving noise y(t) appears more and more as white noise. If increasing D_y in a way such that $\lim_{\beta\to\infty} D_y\beta^{-2} = w^2\beta^{-1}$ remains constant (w has units of length), then the correlator of y(t) tends towards

$$\langle y(t_1)y(t_2)\rangle = \frac{D_y}{\beta} e^{-\beta|t_1-t_2|} \to 2w^2 \beta^{-1} \delta(t_1-t_2), \qquad \beta \to \infty.$$
 (3.142)

In this limit, the driving noise features in the Langevin equation (3.1) as additional white noise and is absorbed as

$$\dot{x} = -V'(x_t) + \sqrt{2(D_x + \varepsilon^2 w^2 \beta^{-1})}\xi,$$
(3.143)

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such that effectively the diffusion constant is shifted by $D_x \mapsto D_x + \varepsilon^2 w^2$. In the white noise limit, the theory is Markovian and Eq. (3.12) may be applied using the shifted diffusivity to obtain exact results. The perturbation theory presented here, however, will effectively expand in

$$D_{\rm eff} = D_x + \varepsilon^2 w^2 = D_x \left(1 + \nu + \dots \right)$$
(3.144)

with $\nu = \varepsilon^2 w^2 \beta^{-1} D_x^{-1}$. This means that the first order correction term to $\mathcal{M}_0(x_0, x_1, ...; D_x)$ is

$$\lim_{\beta \to \infty} \mathcal{M}_1(x_0, x_1, ...; D_x) = \left(\frac{\partial}{\partial D_x} \mathcal{M}_0(x_0, x_1, ...; D_x)\right) D_x.$$
(3.145)

3.3.3.B Quenched Disorder limit

In the opposite limit of $\beta \to 0$, provided $D_y \beta^{-1} = w^2$ remains fixed, the driving noise "freezes" to a random constant since

$$\langle y(t_1)y(t_2)\rangle = \frac{D_y}{\beta} e^{-\beta|t_1-t_2|} \to 2w^2, \qquad \beta \to 0.$$
 (3.146)

Effectively, the Langevin equation (3.1) therefore turns into

$$\dot{x} = -V'(x_t) + \sqrt{2D_x}\xi_t + v \tag{3.147}$$

where v is a constant driving velocity which is normal distributed according to $v \sim \mathcal{N}(0, \varepsilon^2 w^2)$. The driving noise average $e^{-s\tau_{x_0,x_1}}$ then corresponds to a quenched average over the ensemble of normal distributed velocities v. If we treat \mathcal{M}_1 as a functional of the potential V(x) in which the particle is embedded, then formally

$$\lim_{\beta \to 0} \mathcal{M}_1(x_0, x_1, ...; [V(x)])$$
(3.148)

$$= \frac{1}{2} \underbrace{\varepsilon^2 w^2}_{=\overline{v^2}} \left. \partial_v^2 \right|_{v=0} \mathcal{M}(x_0, x_1, ...; [V(x) + vx]).$$
(3.149)

Our framework therefore predicts the first-order correction in $\overline{v^2}$.

Example: Brownian Motion with periodic boundary conditions and a random drift For Brownian Motion with periodic boundary conditions, as studied in Sec. 3.3.2, one can compute the moment generating function of first-passage times for a particular fixed drift vexactly (see Appendix 3.A and in particular Eq. (3.163) for the result. We could not find this result elsewhere in the literature.) On expanding this result in orders of the drift v and averaging v^2 over its distribution $\mathcal{N}(0, \varepsilon^2 w^2)$ we obtain a resulting quenched average approximation in orders of $\overline{v^2}$, $\overline{F(s;v)} = F(s;v=0) + \frac{1}{2} \partial_v^2|_{v=0} F(s;v) \cdot \overline{v^2} + \dots$ When employing our framework and letting $\beta \to 0$ in our general result Eq. (3.134) we recover precisely $\frac{1}{2} \partial_v^2|_{v=0} \hat{F}(s;v)$. The necessary calculations are given in App. 3.B and show that this is indeed the case. By way of this relation, our framework for instance returns the correction to the mean-first passage time of a Brownian motion with quenched disordered drift to first order in ν as (compare to Eq. (3.138))

$$\alpha \left\langle \overline{\tau_{0,\theta}} \right\rangle = \frac{\theta \left(2\pi - \theta\right)}{2} - \frac{\varepsilon^2 w^2}{\alpha^2 R^2} \cdot \frac{\theta^2 (\theta - 2\pi)^2}{24} + \dots \tag{3.150}$$

such that quenched disorder lowers the mean first-passage time for any choice of parameters. Further, for the mean squared first-passage time we obtain

$$\alpha^{2} \langle \overline{\tau_{0,\theta}} \rangle = \frac{1}{12} \theta \left(\theta - 2\pi \right) \left(\theta + 2\varphi \pi \right) \left(\theta - 2\pi + 2\varphi \pi \right) + \frac{\varepsilon^{2} w^{2}}{\alpha^{2} R^{2}} \frac{\theta (\theta - 2\pi) (\theta - \pi (1 + \psi^{+})) (\theta - \pi (1 - \psi^{+}))}{360} \cdot \left(\theta - \pi (1 + \psi^{-}) \right) (\theta - \pi (1 - \psi^{-})),$$
(3.151)

where $\varphi = \frac{1+\sqrt{5}}{2}$ is the golden ratio, and $\psi^{\pm} = \frac{1\pm\sqrt{10}}{\sqrt{3}}$.

3.4 Conclusion

In the present work, we introduce a perturbative approach to study the first-passage time distribution of stochastic processes which are driven both by white and coloured noise. This class of stochastic processes lies at the heart of the study of self-propelled particles in a thermal environment. The self-propulsion is modelled by a noise with exponential autocorrelation and characteristic timescale β^{-1} , while the thermal bath is modelled by white noise with diffusion constant D_x . The expansion parameter in which the perturbation takes place is a dimensionless quantity, ν , which indicates how strong the fluctuations of the self-propulsion are in comparison to the strength of thermal fluctuations.

Setting out from a renewal equation which gives the moment generating function of firstpassage times, we employ a functional expansion to obtain its perturbative corrections. This key equation (3.18) stands at the centre of this work. In order to solve it perturbatively, one needs to calculate the expansion terms (*cf.* Eqs. (3.32) and (3.33)) which involve the eigenfunctions of the Fokker Planck operator associated to the non driven process (*cf.* Eq. (3.45)). To first order in ν , we obtain an analytic result of the moment-generating function in terms of the associated eigenfunctions (cf. Eq. (3.78)). Higher order contributions can be obtained by further iterating the steps outlined in Sec. 3.2.4.

To illustrate the capabilities of our framework, we study two systems. First, we consider an active thermal particle in a harmonic potential, the Active Thermal Ornstein-Uhlenbeck Process. In Sec. 3.3.1.A, we calculate all necessary response functions to find the first order correction to the moment-generating function of first-passage times (cf. Eq. (3.109)). By taking derivatives, we could in principle obtain closed form expressions for the first order correction to any moment of the first-passage time distribution. We confirm these analytical results by numerical simulations. Sampling the experimental moment generating function, we obtain an excellent agreement with the first-order correction (see Fig. 3.2a). For larger values of ν , the perturbative parameter, the deviations systematically indicate higher-order corrections. Further, we compare the theoretically predicted correction to the first two moments of the firstpassage times to numerical results (see Figs. 3.1a and 3.1b) which are in excellent agreement.

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Secondly, we study Active Thermal Brownian Motion on a ring (see Sec. 3.3.2). Again, we illustrate our framework by finding the first-order correction to the moment generating function (*cf.* Eq. (3.134)). Numerical simulations show excellent agreement and systematic higher-order corrections (see Fig. 3.2b). Both first and second moment of the first-passage time are obtained from Eq. (3.134) and show good agreement with numerical simulations.

Further, since the perturbation theory we present makes no assumption on β^{-1} , we are able to recover the limiting cases for $\beta \to 0$ and ∞ , respectively. The case of $\beta \to 0$ is of particular interest since it recovers quenched disorder averages over processes with additional fixed and normal distributed drift (see Sec. 3.3.3).

The framework requires to find the eigenfunctions of a differential operator, and to express all transition and return densities as sums over these eigenfunctions. This often requires certain calculations that for more unusual eigenfunctions may be difficult to perform.

Our approach further allows for the presence of an external potential provided the associated differential operator (Eq. (3.43)) can be diagonalised. This significantly extends the range of systems our framework can be applied to. In this work, we focused on Fourier-modes and Hermite-polynomials which are suitable for flat and harmonic potentials. It is, however, also possible to study piece-wise combinations of the potentials using these eigenfunctions. This may be relevant when studying bi-stable processes for instance. Further, as long as Eq. (3.43) can be diagonalised, this framework also allows for a space-dependent thermal diffusivity by letting $D_x = D(x)$. For future work, for instance, it would be interesting to study first-passage time behaviour of particles at the boundary between two heat baths at different temperature $(e.g. D(x) = D_0 + \text{sgn}(x)\Delta D)$.

Moreover, the functional expansion in $\hat{y}(\omega)$ (cf. Eq. (3.32)) drastically simplifies in the case of y(t) being a periodic driving force. This framework therefore would not only be able to capture stochastic y, but also oscillating deterministic driving forces. This will possibly be addressed in future work

To first order in ν , the corrections, as given in Eqs. (3.71) to (3.77), involve simple complex integrals which can be solved by the residue theorem. For higher-order corrections, however, the integration runs over more than one free internal variable and will require more work. This corresponds to the problems of typical Feynman-diagrams of higher order in statistical field theories which often involve non-trivial integrals. To study higher orders, field theory therefore would provide the necessary toolbox to solve the required correction terms.

The results obtained in this work can be derived alternatively using field-theoretic methods. In fact, the field theoretic treatment allows for the study of a broader class of extreme events and will be reported in the subsequent chapter 4.

Appendix

3.A First passage times of Brownian Motion on a ring with drift

We calculate the first-passage time distribution of a Brownian Motion with drift v on a ring of radius R departing from the methods outlined in [48, Chp. V] although the explicit formula is not given there. Instead of considering the first passage event of transition $x_0 \rightarrow x_1$, we calculate the exit probability of a Brownian Motion on the real line over the absorbing boundaries at x_1 and $x_1 - 2\pi R$ where without loss of generality we chose $x_1 - 2\pi R < x_0 \leq x_1$. The transition density T(t) satisfies the Fokker-Planck Equation

$$\partial_t T(t) = D_x \partial_x^2 T(t) - v \partial_x T(t)$$
(3.152)

and the Kolmogorov backward equation

$$\partial_t T\left(t\right) = D_x \partial_{x_0}^2 T\left(t\right) + v \partial_{x_0} T\left(t\right) \tag{3.153}$$

with absorbing boundary conditions

$$T(x = x_1; t) = 0 \tag{3.154}$$

$$T(x = x_1 - 2\pi R; t) = 0 \tag{3.155}$$

and initial condition

$$T(t) = \delta(x - x_0) \tag{3.156}$$

As is outlined in more detail in [48], the moment generating function of the first-passage time $\tau_{x_0,x}$, $F(x_0, x; s) = F(s)$, satisfies the differential equation obtained by Fourier transform of Eq. (3.153),

$$D_x \partial_{x_0}^2 F\left(s\right) + v \partial_{x_0} F\left(s\right) = s F\left(s\right) \tag{3.157}$$

with boundary conditions

$$F(x_0 = x_1, x_1; s) = F(x_0 = x_1 - 2\pi R, x_1; s) = 1$$
(3.158)

since the process is immediately absorbed when started at either boundary, corresponding to a 1 under Laplace transformation. The ordinary differential equation in the starting point x_0 is

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solved by the exponential ansatz

$$F(x_0, x_1; s) = Ae^{\omega_1 x_0} + Be^{\omega_2 x_0}$$
(3.159)

Inserting this ansatz into (3.157) enforces

$$\omega_{1,2} = -\frac{v}{2D_x} \pm \frac{\sqrt{v^2 + 4D_x s}}{2D_x} \tag{3.160}$$

The boundary conditions (3.158) fix the normalising constants A, B to

$$A = e^{-\omega_1 x_1} (1 - Be^{\omega_2 x_1})$$
(3.161)

$$B = \frac{e^{-2\pi R\omega_1} - 1}{e^{\omega_2 x_1 - 2\pi R\omega_1} - e^{\omega_2 x_1 - 2\pi R\omega_2}}$$

$$= \frac{1 - \exp(\pi R(\omega_2 - \omega_1))}{2\sinh(\pi R(\omega_1 - \omega_2))}$$

$$= \frac{1 - \exp\left(-\pi R \frac{\sqrt{v^2 + 4D_x s}}{D_x}\right)}{2\sinh\left(\pi R \frac{\sqrt{v^2 + 4D_x s}}{D_x}\right)}$$
(3.162)

After some further simplifications one arrives at the v-dependent moment generating function

$$F(x_0, x_1; s; v) = \frac{1}{\sinh\left(\frac{r\sqrt{v^2 + 4D_x s}}{2D_x} 2\pi\right)} \times \left[\exp\left(\frac{rv}{2D_x}\left(\theta - 2\pi\right)\right) \sinh\left(\frac{r\sqrt{v^2 + 4D_x s}}{2D}\theta\right) - \exp\left(\frac{rv}{2D_x}\theta\right) \sinh\left(\frac{r\sqrt{v^2 + 4D_x s}}{2D_x}\left(\theta - 2\pi\right)\right)\right]$$
(3.163)

Indeed, for $v \to 0$,

$$\frac{r\sqrt{v^2 + 4D_x s}}{2D} \to \sqrt{\sigma} \tag{3.164}$$

(with notation from main text) and one recovers the undriven moment generating function

$$F(x_0, x_1; s; v = 0) = F(x_0, x_1; s) = \frac{\sinh\left(\theta\sqrt{\sigma}\right) - \sinh\left((\theta - 2\pi)\sqrt{\sigma}\right)}{\sinh\left(2\pi\sqrt{\sigma}\right)}$$
(3.165)

which after some hyperbolic identities reduces to

$$F(x_0, x_1; s) = \frac{\cosh\left((\theta - \pi)\sqrt{\sigma}\right)}{\cosh\left(\pi\sqrt{\sigma}\right)}$$
(3.166)

in agreement with the independently found expression (3.128). In App. 3.B, we show that to second order in v this result is identical to the first-order correction \mathcal{M}_1 from Eq. 3.134 in the limit of $\beta \to 0$.

3.B Equivalence of quenched averages

In this section, we provide a more detailed proof showing that Eq. (3.149) indeed holds for the case of Brownian Motion driven by coloured noise, *i.e.* that our framework perturbatively gives the correct moment generating function of first-passage times when taking the quenched average over Eq. (3.147) with normal distributed drift $v \sim \mathcal{N}(0, \sqrt{2\varepsilon^2 w^2})$. To that end, we take the $\beta \to 0$ limit of the analytically found \mathcal{M}_1 (Eq. (3.136)),

$$\lim_{\beta \to 0} \mathcal{M}_1 = \frac{1}{8\alpha^2 r^2 \sqrt{\sigma}} \Big\{ \theta \cosh\left(\theta \sqrt{\sigma}\right) \left(\theta \sqrt{\sigma} - \tanh\left(\pi \sqrt{\sigma}\right)\right)$$
(3.167)

$$+\sinh\left(\theta\sqrt{\sigma}\right)\left[-\left(\theta^{2}-2\pi\theta+2\pi^{2}\right)\sqrt{\sigma}\tanh\left(\pi\sqrt{\sigma}\right)\right.$$

$$+2\pi(\pi-\theta)\sqrt{\sigma}\coth\left(\pi\sqrt{\sigma}\right)+\pi\tanh^{2}\left(\pi\sqrt{\sigma}\right)+\theta-\pi\right]\left.\right\}.$$

$$(3.168)$$

In Eq. (3.149), it is claimed that this equals

$$\frac{1}{2} \int_{-\infty}^{\infty} \mathrm{d}v \, \frac{e^{-\frac{v^2}{2\varepsilon^2 w^2}}}{\sqrt{2\pi\varepsilon^2 w^2}} v^2 \left. \partial_v^2 \right|_{v=0} F\left(x_0, x_1; s; v\right) \ . \tag{3.169}$$

Evaluating this expression using the result from Eq. (3.163) and setting v = 0 results in

$$\frac{1}{2} \left. \partial_{v}^{2} \right|_{v=0} F\left(x_{0}, x_{1}; s; v\right) = \tag{3.170}$$

$$\frac{1}{8\alpha^{2}r^{2}\sqrt{\sigma}} \times \left\{ \frac{1}{\sinh\left(2\pi\sqrt{\sigma}\right)} \left[\sinh\left((\theta - 2\pi)\sqrt{\sigma}\right) \left(2\pi \coth\left(2\pi\sqrt{\sigma}\right) - \theta^{2}\sqrt{\sigma}\right) + \theta \cosh\left(\theta\sqrt{\sigma}\right) + \left(2\pi - \theta\right) \cosh\left((\theta - 2\pi)\sqrt{\sigma}\right) + \sinh\left(\theta\sqrt{\sigma}\right) \left((\theta - 2\pi)^{2}\sqrt{\sigma} - 2\pi \coth\left(2\pi\sqrt{\sigma}\right)\right) \right] \right\}.$$

The expressions in Eq. (3.167) and Eq. (3.170) are indeed equal as can be verified using for instance Mathematica.

3.C Explicit expressions for functional derivatives of transition probability densities of Ornstein-Uhlenbeck processes

Following the notation from Sec. 3.3.1.A, we here give the explicit expressions of $\rho_{x_0,x_1}^{(1)}, \rho_{x_0,x_1}^{(2)}$ as implicitly given in Eq. (3.100)-(3.102). We confine ourselves to the case of $x_0 < x_1$. Starting from the Fourier-transformed transition probability density (cf. Eq. (3.98)), all other functional derivatives are given as partial derivatives of this density. From formula (3.100), one obtains

$$T^{(1)}(\sigma, i\beta') = \frac{e^{\frac{x_0^2 - x_1^2}{4}}}{\sqrt{2\pi}(\beta' - 1)} \left[(\Gamma(\beta' + \sigma)D_{-\beta' - \sigma}(-x_0)D_{-\beta' - \sigma + 1}(x_1) - \Gamma(\sigma + 1)D_{-\sigma - 1}(-x_0)D_{-\sigma}(x_1)) \right]$$
(3.171)

where $\Gamma(\sigma)$ is the usual Gamma-function. Letting $x_0 \to x_1$, gives the first functional derivative of the return probability at x_1 ,

$$R^{(1)}(\sigma, i\beta') = \frac{\Gamma(\beta + \sigma)D_{-\beta - \sigma}(-x_1)D_{-\beta - \sigma + 1}(x_1) - \Gamma(\sigma + 1)D_{-\sigma - 1}(-x_1)D_{-\sigma}(x_1)}{\sqrt{2\pi}(\beta - 1)}$$
(3.172)

These results imply

$$T^{(1)}(\sigma - i\beta', i\beta') = \frac{e^{\frac{x_0^2 - x_1^2}{4}}(\Gamma(\beta' + \sigma + 1)D_{-\beta' - \sigma - 1}(-x_0)D_{-\beta' - \sigma}(x_1) - \Gamma(\sigma)D_{-\sigma}(-x_0)D_{1 - \sigma}(x_1))}{\sqrt{2\pi}(\beta' + 1)}$$
(3.173)

and

$$R^{(1)}(\sigma - i\beta', i\beta') = \frac{\Gamma(\beta + \sigma + 1)D_{-\beta - \sigma - 1}(-x_1)D_{-\beta - \sigma}(x_1) - \Gamma(\sigma)D_{1 - \sigma}(x_1)D_{-\sigma}(-x_1)}{\sqrt{2\pi}(\beta + 1)}$$
(3.174)

The second order derivative of the transition probability is

$$T^{(2)}(\sigma, i\beta') = \frac{e^{\frac{x_0^2 - x_1^2}{4}}}{2\sqrt{2\pi} \left(\beta'^2 - 1\right)} \left[2\Gamma(\beta' + \sigma + 1)D_{-\beta' - \sigma - 1}(-x_0)D_{-\beta' - \sigma + 1}(x_1) + (\beta' - 1)\Gamma(\sigma)D_{-\sigma}(-x_0)D_{2-\sigma}(x_1) - (\beta + 1)\Gamma(\sigma + 2)D_{-\sigma - 2}(-x_0)D_{-\sigma}(x_1))\right]$$
(3.175)

and of the return probability

$$R^{(2)}(\sigma, i\beta') = \frac{1}{2\sqrt{2\pi} \left(\beta'^2 - 1\right)} \left[2\Gamma(\beta' + \sigma + 1)D_{-\beta' - \sigma - 1}(-x_1)D_{-\beta' - \sigma + 1}(x_1) + (\beta' - 1)\Gamma(\sigma)D_{-\sigma}(-x_1)D_{2-\sigma}(x_1) - (\beta + 1)\Gamma(\sigma + 2)D_{-\sigma - 2}(-x_1)D_{-\sigma}(x_1))\right]$$
(3.176)

Chapter 4

Field Theory for Extreme Values in Stochastic Processes

Abstract

I introduce a field-theoretic method to calculate the full distribution of first-passage times, running maxima, and explored volume of one-dimensional stochastic processes which are subject to both white and coloured noise. All associated densities are expressed in terms of the transition probability of the process. In the case of only white noise, the expressions are exact. When coloured noise is added, I give a systematic field-theoretic correction.

Overview

This Chapter is more than any other chapter a synthesis of this thesis. It connects the tracing mechanism developed in Chp. 2 and re-interprets the vertex computed in Eq. (2.36) as a trace function in the spirit of the survival probability introduced later in Sec. 6.2.14 in Chp. 6. In doing so, one recovers the key results in Chp. 3 but with a clear field-theoretic interpretation of the rather abstract functional derivatives with respect to the driving noise used there.

This chapter, albeit relatively short, therefore has benefited from the many different influences I have gathered over the course of my PhD and illustrates the way I think field theory and stochastic processes are symbiotic.

Acknowledgement

The results included in this chapter are fruitful offshoots of my collaboration with Guillaume Salbreux and Gunnar Pruessner. I have tremendously benefited from discussions with members of the Non-Equilibrium Group. In particular I would like to thank Rosalba Garcia Millan for fruitful discussions.

4.1 Field Theory for Random Walkers

In this chapter, I widely follow the notation introduced in Chp. 3. I also assume some familiarity with the concepts introduced in Chp. 2, in particular the field theory for the trace particles introduced there. I consider one-dimensional continuous stochastic processes x_t which are either described by a Langevin Equation [127],

$$\dot{x}_t = -V'(x_t) + \xi_t \tag{4.1}$$

where $V'(x_t)$ is the gradient of a potential and ξ_t Gaussian white noise with correlator $\langle \xi_t \xi_{t'} \rangle = 2D_x \delta(t-t')$, or the equivalent Fokker Planck Equation [200, 127]

$$\begin{cases} \partial_t T(x,t) &= \partial_x \left(V'(x_t) T(x,t) \right) + D_x \partial_x^2 T(x,t) \\ T(x,t=t_0) &= \delta(x-x_0) \end{cases}$$
(4.2)

where $T(x,t) \equiv T(x_0, x; t_0, t)$ is the transition probability for the walker to travel from x_0 at time t_0 to x at time t. Where confusion can be avoided, I omit noting x_0 and t_0 explicitly. The second-order differential operator in the first line of Eq. (4.2) is referred to as *forward operator*, and is denoted by

$$\mathcal{L}(x) = V''(x) + V'(x)\partial_x + D_x\partial_x^2.$$
(4.3)

The partial differential equation (4.2) can be mapped to a Doi-Peliti field theory containing two fields, $\varphi(x,t)$ and $\tilde{\varphi}(x,t)$, satisfying [38, 231]

$$T(x,t) = \langle \varphi(x,t)(1+\widetilde{\varphi}(x_0,t_0)) \rangle_{\mathcal{S}_{\alpha}}, \qquad (4.4)$$

where $\langle \bullet \rangle_{S_{\varphi}}$ denotes the expectation over the joint stochastic distribution of the fields given by

$$\mathcal{P}[\varphi, \widetilde{\varphi}] = \exp\left(-\mathcal{S}_{\varphi}[\varphi, \widetilde{\varphi}]\right), \qquad (4.5)$$

where the random walker action S_{φ} featuring in the exponential is given by [231]

$$S_{\varphi} = \iint \mathrm{d}x \,\mathrm{d}t \,\tilde{\varphi}(\partial_t - \mathcal{L})\varphi = \iint \mathrm{d}x \,\mathrm{d}t \,\tilde{\varphi}\left(\partial_t - V''(x) - V'(x)\partial_x - D\partial_x^2\right)\varphi. \tag{4.6}$$

4.2 Tracing Mechanism

In order to keep track of the range already visited by x_t up to time t, I introduce the trace function,

$$\mathcal{Q}(x,t) = \mathbb{P}[x_s = x \text{ for at least one } s \le t]$$
(4.7)

which measures the probability with which the particle has been at x at or before time t, but does not keep track of how many times such a visit occurred. As is detailed in Chp. 2, the evolution of $\mathcal{Q}(x,t)$ can also be mapped to a Doi-Peliti field theory with two additional fields $\psi(x,t)$ and $\tilde{\psi}(x,t)$. To derive this field theory, I introduce a tracing mechanism that is described as follows and has been used in Chp. 2.

I consider a coarse-grained version \mathfrak{x}_t of the stochastic process x_t (cf. Eq. (4.1)) which only takes values on a lattice $\delta_a \mathbb{Z}$ (where δ_a is the lattice-spacing) and is defined as $\mathfrak{x}_t = \delta_a [\delta_a^{-1} x_t]$ where $[x] = \min_{n \in \mathbb{Z}} \{n : n \ge x - 1/2\}$. At any time, the random walker attempts to deposit a *trace* at \mathfrak{x}_t with Poissonian rate γ . If at this point a trace has already been deposited, any further deposition is suppressed such that every site of the lattice has either zero or one traces attached to it. Taking $\gamma \to \infty$, the particle will deposit trace particles everywhere given it has not done so before. In the limit of $\delta_a \to 0$, the process \mathfrak{x}_t tends to x_t , and the density of trace particles approaches $\mathcal{Q}(x, t)$.

Translating this reaction-diffusion like kinetics into a field theory leads to a joint probability distribution of the fields (*cf.* Eq. (2.7))

$$\mathcal{P}[\varphi, \tilde{\varphi}, \psi, \tilde{\psi}] = \lim_{\gamma \uparrow \infty} \exp\left(-\mathcal{S}_{\varphi}[\varphi, \tilde{\varphi}] - \mathcal{S}_{\psi}[\psi, \tilde{\psi}] + \gamma \mathcal{S}_{\gamma}[\varphi, \tilde{\varphi}, \psi, \tilde{\psi}]\right)$$
(4.8)

with S_{ψ} denoting the *trace action*

$$S_{\psi} = \int \mathrm{d}x \, \mathrm{d}t \, \widetilde{\psi}(\partial_t + \varepsilon) \psi, \qquad (4.9)$$

where $\varepsilon > 0$ is a regularising infrared-cutoff to be taken to $\varepsilon \to 0^+$ at the end of the calculation, and S_{γ} the *deposition action* S_{γ} (*cf.* Chp. 2)

$$S_{\gamma} = \iint \mathrm{d}x \,\mathrm{d}t \,\tau \widetilde{\psi} \varphi + \sigma \widetilde{\varphi} \widetilde{\psi} \varphi - \lambda \widetilde{\varphi} \varphi \psi - \kappa \widetilde{\varphi} \widetilde{\psi} \varphi \psi \tag{4.10}$$

where I introduced the couplings $\tau, \sigma, \kappa, \lambda$ which are nominally different to emphasize their (potentially) different renormalisations but at bare level are all given by¹

$$\tau = \sigma = \kappa = \lambda = 1. \tag{4.11}$$

The trace function $\mathcal{Q}(x,t)$ field-theoretically translates into the expectation value

$$\mathcal{Q}(x,t) = \lim_{\gamma \uparrow \infty} \langle \psi(x,t) \left(1 + \widetilde{\varphi}(x_0,t_0) \right) \rangle_{\mathcal{S}}$$
(4.12)

where $\langle \bullet \rangle_{\mathcal{S}}$ denotes the average with respect to the probability distribution given in Eq. (4.8). To calculate the trace function, in a first step I employ standard tools from field theory to perturbatively calculate Eq. (4.12) in small γ , and secondly evaluate the expressions for $\gamma \to \infty$. That this is in fact justified will be discussed later.

¹Note the slight difference to Chp. 2 where γ was absorbed into the couplings itself, see for instance Sec. 2.B.4.

4.3 Field-theoretic Calculation of Q(x, t)

I begin by studying the bilinear theory at $\gamma = 0$, *i.e.* in the absence of trace-deposition. I introduce the right and left eigenfunctions of the forward operator \mathcal{L} together with their eigenvalues

$$\mathcal{L}u_n(x) = -\lambda_n u_n(x) \tag{4.13}$$

$$\mathcal{L}^{\dagger} v_n(x) = -\lambda_n v_n(x) \tag{4.14}$$

where

$$\mathcal{L}^{\dagger} = -V'(x)\partial_x + D_x\partial_x^2. \tag{4.15}$$

is the L^2 -adjoint of \mathcal{L} [184]. In what follows, I will restrict myself to Fokker Planck operators with a unique stationary solution $u_0(x)$. The eigenfunctions are rescaled such that they satisfy the orthonormal relation

$$\int \mathrm{d}x \, u_m(x) v_n(x) = \delta_{mn},\tag{4.16}$$

$$\sum_{n} v_n(x_1)u_n(x_2) = \delta(x_1 - x_2) \tag{4.17}$$

Since they jointly form a bi-orthogonal basis of L^2 [200] (see also the remarks in previous Chp. 3 and [184] on adjointness in weighted L^2 spaces), every field $\varphi, \tilde{\varphi}, \psi, \tilde{\psi}$ has a unique decomposition into the $u_n(x), v_n(x)$ in space which, together with the Fourier transform in time, I introduce as

$$\varphi(x,t) = \int \mathrm{d}\omega \sum_{k} \varphi_k(\omega) u_k(x) e^{-i\omega t}$$
(4.18)

$$\tilde{\varphi}(x,t) = \int \mathrm{d}\omega \sum_{k} \tilde{\varphi}_{k}(\omega) v_{k}(x) e^{-i\omega t}, \qquad (4.19)$$

and analogously for $\psi, \tilde{\psi}$ with coefficients $\psi_k(\omega), \tilde{\psi}_k(\omega')$, respectively. This eigenfunction transform diagonalises the non-perturbative contributions to the action, S_{φ} and S_{ψ} (cf. Eq. (4.8)), which read

$$S_{\varphi}[\varphi, \widetilde{\varphi}] = \int \mathrm{d}\omega \sum_{n} \widetilde{\varphi}_{n}(\omega) \left(-i\omega + \lambda_{n}\right) \varphi_{n}(\omega) \tag{4.20}$$

$$\mathcal{S}_{\psi}[\psi, \widetilde{\psi}] = \int \mathrm{d}\omega \sum_{n} \widetilde{\psi}_{n}(\omega) \left(-i\omega + \varepsilon\right) \psi_{n}(\omega). \tag{4.21}$$

For $\gamma = 0$, the action in Eq. (4.8) is Gaussian and the bare propagators of both fields therefore immediately follow from Eqs. (4.20), (4.21),

$$\langle \varphi_n(\omega')\widetilde{\varphi}_m(\omega)\rangle = \frac{\delta_{m,n}\delta(\omega-\omega')}{-i\omega'+\lambda_n} = \frac{(m,\omega') \quad (n,\omega)}{-i\omega'+\lambda_n}$$
(4.22)

$$\langle \psi_n(\omega')\widetilde{\psi}_m(\omega)\rangle = \frac{\delta_{m,n}\delta(\omega-\omega')}{-i\omega'+\varepsilon} = \frac{(m,\omega')(n,\omega)}{2}, \qquad (4.23)$$

where I introduced a diagrammatic representation for both bare propagators. Using Eq. (4.4), and transforming back into real space and time using Eqs. (4.18)-(4.19), I obtain the transition probability

$$T(x,t) = \sum_{n} v_n(x_0) u_n(x) e^{-\lambda_n(t-t_0)} \Theta(t-t_0)$$
(4.24)

where $\Theta(t)$ is the Heaviside Θ -function. Crucially, I made use of the property [38]

$$\left\langle \widetilde{\varphi} \right\rangle_{\mathcal{S}} = 0. \tag{4.25}$$

such that $\langle \varphi(1+\widetilde{\varphi}) \rangle = \langle \varphi \widetilde{\varphi} \rangle$.

Turning to the trace function and its field-theoretic formula (4.4), I need to consider $\gamma \neq 0$. For $\gamma \neq 0$, the non-linear contributions of S_{γ} (Eq. (4.10)) enter into the path-action (4.8). Each of the four vertices is diagrammatically represented as

$$\overset{\tau}{\leadsto} \quad \overset{\sigma}{\overset{\tau}{\checkmark}} \quad \overset{-\lambda}{\overset{\tau}{\checkmark}} \quad \overset{-\kappa}{\overset{\tau}{\checkmark}} \quad (4.26)$$

and enters into the action multiplied by γ . It follows that the diagrammatic expansion of the trace function (4.12) is

$$\mathcal{Q}(x,t) = \lim_{\gamma \to \infty} \begin{array}{c} (x,t) & (x_0,t_0) \\ & & & \\ \end{array}$$
(4.27)

where the central dot stands for the renormalised coupling τ_R . This renormalisation is given by the diagrammatic expansion

$$\tau_R = \mathbf{\gamma} \mathbf{\varphi} - \gamma \mathbf{\varphi} + \gamma^2 \mathbf{\varphi} + \gamma^3 \mathbf{\varphi} + \gamma^3 \mathbf{\varphi} + \dots$$
(4.28)

The only possible diagrams contributing to this expansions are chains of the loop-diagram \sim . Considering the expansion in Fourier/eigenfunction transform (see Eqs. (4.18), (4.19) and App. 4.A for details), each diagram factorises into a product over the bubbles and I can employ the geometric sum to obtain the renormalised coupling (see App. 4.A for derivation)

$$\tau_R(\omega_0,\omega_1) = \frac{\gamma}{1 + \gamma R(x_1,\omega_1)} \delta(\omega_0 + \omega_1)$$
(4.29)

such that the effective trace function, in Fourier domain, is

$$\int dt \, e^{i\omega t} \mathcal{Q}(x,t) = \lim_{\gamma \to \infty} \frac{1}{-i\omega + \varepsilon} \frac{\gamma}{1 + \gamma R(x_1,\omega + i\varepsilon)} T(x'_0, x'_1, \omega) \tag{4.30}$$

$$= \frac{1}{-i\omega + \varepsilon} \frac{T(x'_0, x'_1, \omega)}{R(x_1, \omega + i\varepsilon)}$$
(4.31)

where I made use of time-translational invariance to write the Fourier-transform in one frequency

only. This then leads to the central result

$$\mathcal{Q}(x,t) = \int d\omega \, e^{-i\omega t} \frac{T\left(x'_0, x'_1, \omega\right)}{(-i\omega)R\left(x'_1, \omega\right)} \tag{4.32}$$

where I have tacitly taken the limit $\varepsilon \to 0$.

4.4 Extreme value distributions from Q(x,t)

The trace function contains the distribution and moment-generating function of three extreme events which are introduced as follows.

4.4.1 First-passage times

The first-passage time (FPT) τ_{x_0,x_1} is the first time it takes a stochastic process to reach a prescribed target x_1 given it is initialised at x_0 and is defined as

$$\tau_{x_0, x_1} = \inf_{t>0} \left\{ t | x_t = x_1, x_0 = x_0 \right\} .$$
(4.33)

Its probability distribution, $\mathbb{P}_{\text{FPT}}(\tau_{x_0,x_1})$, is linked to the trace function via

$$\mathbb{P}_{\text{FPT}}(\tau_{x_0,x_1} = t) = \partial_t \mathcal{Q}(x_1,t) .$$
(4.34)

and its characteristic function $\chi_{\rm FPT}$

$$\chi_{\rm FPT}(\omega) = \left\langle e^{-i\omega\tau_{x_0,x_1}} \right\rangle = i\omega \int dt \, e^{-i\omega t} \mathcal{Q}(x_1,t). \tag{4.35}$$

From Eq. (4.32), the characteristic function immediately follows as

$$\chi_{\rm FPT}(\omega) = \frac{T\left(x_0', x_1'; \omega\right)}{R\left(x_1'; \omega\right)} \tag{4.36}$$

which is the classic result obtained by Darling and Siegert in 1951 [215, 52].

4.4.2 Running Maximum

The running maximum of a stochastic process, \hat{x}_t , is the largest value the process attained up to time t,

$$\hat{x}_t = \sup_{t' < t} x_{t'} \ . \tag{4.37}$$

Its probability distribution, $\mathbb{P}_{Max}(\hat{x}_t)$, is given by

$$\mathbb{P}_{\text{Max}}(\hat{x}_t = x_1) = -\partial_{x_1} \mathcal{Q}(x_1, t), \qquad (4.38)$$

and its characteristic function by

$$\chi_{\text{Max}}(\omega) = \left\langle e^{ik\hat{x}} \right\rangle = -ik \int \mathrm{d}x \, e^{ikx_1'} \mathcal{Q}(x_1', t) \tag{4.39}$$

4.4.3 Mean volume explored

The mean volume explored, $\langle \text{Vol} \rangle_t$, is the average difference between maximum and minimum $(\check{x}_t = \inf_{t' < t} x_{t'})$ of the stochastic process up to time t and describes the mean volume explored by the process. It is defined as

$$\langle \text{Vol} \rangle_t = \hat{x}_t - \check{x}_t \tag{4.40}$$

and is given by the space-integral of the trace function,

$$\langle \operatorname{Vol} \rangle_t = \int \mathrm{d}x_1' \, \mathcal{Q}(x_1', t) \;.$$

$$(4.41)$$

4.5 External Driving Noise

As a further generalisation, the field-theoretic framework is capable of perturbatively describing stochastic processes which are additionally driven by some self-correlated (*i.e.* non-white) noise, y_t , thus extending the Langevin Eq. (4.1) to

$$\dot{x}_t = -V'(x_t) + \xi_t + gy_t \tag{4.42}$$

where y_t is assumed to be stationary noise with zero mean, and g is a coupling constant meant to be small.²

I here assume that together with the externally driven Langevin Eq. (4.42) a further Langevin Equation describes y_t via

$$\dot{y}_t = -F(y_t) + \eta_t \tag{4.43}$$

where $F(y_t)$ is a smooth force-field with an expansion of the form

$$F(y) = F_1 y + F_2 y^2 + \cdots$$
 (4.44)

where I assume $F_{n\geq 2} \ll F_1$ (*i.e.* y_t lies perturbatively close to an Ornstein-Uhlenbeck process), and η is a white Gaussian noise with correlator

$$\langle \eta_{t_1} \eta_{t_2} \rangle = 2D_y \delta(t_1 - t_2) \tag{4.45}$$

with D_y denoting the driving noise diffusivity. In this case, the corresponding Doi-Peliti field

²In the sense that $gy_t \ll \xi_t$. Of course, we could have absobred the "smallness" into y_t . For clarity, however, I choose to think of y_t and ξ_t as being both of $\mathcal{O}(1)$, whilst g is explicitly the parameter of perturbation.

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theory follows the previous steps but the forward operator is shifted to

$$\mathcal{L} \mapsto \mathcal{L} + gy_t \partial_x \varphi(x, t) \tag{4.46}$$

where the added driving term is the translation of the additional noise gy_t into the Fokker-Planck picture (see Chp. 3). The shifted random walker action therefore now depends on a particular realisation of y_t ,

$$\mathcal{S}_{\varphi}[y_t] = \iint \mathrm{d}x \, \mathrm{d}t \, \widetilde{\varphi}(\partial_t - \mathcal{L} - gy_t \partial_x)\varphi \tag{4.47}$$

which needs to be averaged over all realisations of y_t with the correct path measure of y_t . The Martin-Siggia-Rose Jansen-De Dominicis response field formalism [162, 55, 121, 231] constructs this average by introducing an auxiliary field \tilde{y}_t

$$\langle \bullet[y] \rangle_y = \left\langle \int \mathcal{D}[y(t)](\bullet[y(t)]) \delta\left(\dot{y}_t + F(y_t) - \eta_t\right) \right\rangle_\eta \tag{4.48}$$

$$= \int \mathcal{D}[y(t)] \bullet [y(t)] \left\langle \int \mathcal{D}[\tilde{y}_t] \exp\left(-\int \mathrm{d}t \, \tilde{y}_t \left(\partial_t y_t + F(y_t) - \eta_t\right)\right) \right\rangle_{\eta}.$$
 (4.49)

Through this construction the average over a random y_t has been pushed forward to an average over η which is simpler to handle since it is white noise. The average in η is performed as a Gaussian path integral over its probability measure

$$\mathcal{P}_{\eta}[\eta(t)] = \exp\left(-\int \mathrm{d}t' \,\frac{\eta(t')^2}{2D_y}\right) \,, \tag{4.50}$$

which results in

$$\langle \bullet[y] \rangle_y = \iint \mathcal{D}[y] \mathcal{D}[\tilde{y}] \bullet [y] \exp\left(-\mathcal{S}_{RF}[y, \tilde{y}]\right)$$
(4.51)

with the response field action

$$\mathcal{S}_{RF}[y,\tilde{y}] = \int \mathrm{d}t \, \tilde{y}_t \left(\partial_t y_t + F(y_t)\right) - D_y \tilde{y}_t^2. \tag{4.52}$$

Averaging the y_t -dependent action in Eq. (4.47) therefore is equivalent to the y, \tilde{y} -extended field theory

$$\mathcal{P}[\varphi, \tilde{\varphi}, y, \tilde{y}] = \exp\left(-\mathcal{S}_{\varphi}[\varphi, \tilde{\varphi}] + g\mathcal{S}_{g}[\varphi, \tilde{\varphi}, y] - \mathcal{S}_{RF}[y, \tilde{y}]\right)$$
(4.53)

where I introduce the coupling action

$$S_g = \iint \mathrm{d}x \,\mathrm{d}t \,\widetilde{\varphi}(x,t) y_t \partial_x \varphi(x,t). \tag{4.54}$$

The tracing mechanism remains untouched by the external driving and there is no direct coupling between y, \tilde{y} and $\psi, \tilde{\psi}$. The driving noise y does enter, however, into the trace function by affecting the renormalisation in τ (*cf.* (4.28)). The driven and trace-depositing system is

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captured by the six-field theory giving the joint path measure³

$$\mathcal{P}[\varphi, \tilde{\varphi}, \psi, \tilde{\psi}, y, \tilde{y}] = \lim_{\gamma \to \infty} \exp\left(-\mathcal{S}_{\varphi}[\varphi, \tilde{\varphi}] - \mathcal{S}_{\psi}[\psi, \tilde{\psi}] + \gamma \mathcal{S}_{\gamma}[\varphi, \tilde{\varphi}, \psi, \tilde{\psi}] + g \mathcal{S}_{g}[\varphi, \tilde{\varphi}, y] - \mathcal{S}_{RF}[y, \tilde{y}]\right) \quad (4.55)$$

This extended action further adds to the already established propagators (*cf.* Eqs. (4.22), (4.23)) and vertices (*cf.* Eq. (4.26)) the following propagator for y_t (see S_{RF} , Eq. (4.52))

$$\dots = \frac{1}{-i\omega + F_1} \tag{4.56}$$

and vertices (see S_{RF} and S_g , Eqs. (4.52),(4.54))

where the F_n are defined in Eq. (4.44), and the black perpendicular mark in the rightmost diagram represents the gradient term ∂_x applied to the φ field.

I denote by $\langle \bullet \rangle_{\mathcal{S},y}$ the averages taken with respect to the measure in Eq. (4.55). The trace function of the driven system, (*cf.* Eq. (4.42)), then, in analogy to Eq. (4.12), is

$$\mathcal{Q}(x_1', t) = \langle \psi(x, t) \left(1 + \widetilde{\varphi}(x_0, t_0) \right) \rangle_{\mathcal{S}, y}$$
(4.58)

$$= \langle \psi(x,t)\tilde{\varphi}(x_0,t_0)\rangle_{\mathcal{S},y}$$
(4.59)

This average is no longer fully summable, as was the case for the undriven Langevin Eq. (cf. Eq. (4.32)). Instead, the field theory allows for a perturbative treatment in small g. The calculations are cumbersome, since not only the correlators in φ , but also the couplings σ and κ are renormalised by the g-coupling.

In what follows, I briefly illustrate how to compute the trace function to second order in g, assuming $F(y) = -F_1 y$ (*i.e.* y_t becomes an Ornstein-Uhlenbeck Process). To include higher coefficients F_2, F_3, \cdots one would need to renormalise the $\langle y \tilde{y} \rangle$ -propagator in Eq. (4.56). This is conceptually not much more difficult than the other computations presented here and I therefore omit the rather lengthy self-correction induced by non-linear force-fields (*cf.* Eq. (4.44)). To systematically capture the effect of the external driving noise to second order in g (the first order correction vanishes), one needs to compute

$$\langle \varphi \widetilde{\varphi} \rangle_{\mathcal{S};\gamma} = ---+ g^2 D_y - 4 + --- \qquad (4.60)$$

$$= - + g^2 -$$
(4.61)

³This time the probability measure, and therefore all averages, already contains the limit of $\gamma \to \infty$ for better readability.

as well as

$$-\sigma_{R;g} = \frac{1}{r^{r}} + \frac{1}{r^{r}} + \frac{1}{r^{r}} + g^{2} \frac{1}{r^{r}}$$
(4.62)

$$-\kappa_{R;g} = \frac{1}{2^{2} \kappa_{N}} + \frac{1}{2^{2} \kappa_{N}} + g^{2} \frac{1}{2^{2} \kappa_{N}} + g^{2} \frac{1}{2^{2} \kappa_{N}}$$
(4.63)

(4.65)

where the lozenge-shape diagrammatically represents the driving-noise correction to second order (with the g^2 term explicitly taken out). Arranging them delivers the systematic diagrammatic expansion to $\mathcal{O}(g^2)$

$$\mathcal{Q}(x,t) = \lim_{\gamma \to \infty} \cdots + \lim_{\gamma \to \infty} g^2 \left[\gamma \cdots + \gamma^2 \left(\underbrace{\gamma}_{\chi} + \underbrace{\gamma}_{\chi} + \underbrace{\gamma}_{\chi} + \underbrace{\gamma}_{\chi} \right) + \frac{\gamma^3}{\gamma} + \underbrace{\gamma}_{\chi} + \underbrace{\gamma}$$

To calculate the sum, it is useful to re-arrange the diagrams in four distinct terms
$$\mathcal{J}_1, \mathcal{J}_2, \mathcal{J}_3, \mathcal{J}_4$$

$$\mathcal{J}_{1} = \mathbf{\sim} \left(1 + \gamma \mathbf{z}_{\mathcal{I}} + \gamma^{2} \mathbf{z}_{\mathcal{I}} \mathbf{z}_{\mathcal{I}} + \cdots \right) \cdot \mathbf{z}_{\mathcal{I}} \cdot \left(1 + \gamma \mathbf{z}_{\mathcal{I}} + \gamma^{2} \mathbf{z}_{\mathcal{I}} \mathbf{z}_{\mathcal{I}} + \cdots \right) \cdot \mathbf{-}$$
(4.66)

$$\mathcal{J}_2 = \mathbf{v} \left(1 + \gamma \mathbf{z} + \gamma^2 \mathbf{z} \mathbf{z} + \cdots \right) \cdot \mathbf{z} \mathbf{z} \mathbf{z} \cdot \left(1 + \gamma \mathbf{z} + \gamma^2 \mathbf{z} \mathbf{z} \mathbf{z} + \cdots \right) \cdot \mathbf{z}$$
(4.67)

$$\mathcal{J}_{3} = \mathbf{v} \left(1 + \gamma \mathbf{z}_{1} + \gamma^{2} \mathbf{z}_{2} \mathbf{z}_{3} + \cdots \right) \cdot \mathbf{z}_{n} \mathbf{z}_{n}$$

$$\mathcal{J}_{4} = \mathbf{v} \left(1 + \gamma \mathbf{z}_{1} + \gamma^{2} \mathbf{z}_{n} \mathbf{z}_{n} + \cdots \right) \cdot \mathbf{z}_{n} \mathbf{z}_{n} \mathbf{z}_{n}$$

$$(4.68)$$

$$(4.69)$$

I further define the auxiliary functions⁴

 \mathcal{T}_1

$$\mathcal{R}_2 = \bigstar \qquad \qquad \mathcal{R}_1 = \bigstar \qquad (4.74)$$

$$= \overleftarrow{\mathcal{T}_2} = \overleftarrow{\mathcal{T}_2}$$
(4.75)

 4 The notation is intentionally evocative of the one introduced in Chp. 3. I have

$$\mathcal{R}_2 = \int \mathrm{d}\tilde{\omega} R^{(2)} \left(\omega, \tilde{\omega}, -\tilde{\omega}\right) \hat{C}_2(\tilde{\omega}) \tag{4.70}$$

$$\mathcal{T}_2 = \int d\tilde{\omega} T^{(2)}(\omega, \tilde{\omega}, -\tilde{\omega}) \hat{C}_2(\tilde{\omega})$$
(4.71)

$$\mathcal{R}_{1} = \int \mathrm{d}\tilde{\omega}R^{(1)}\left(\omega + \tilde{\omega}, \tilde{\omega}\right)R^{(1)}\left(\omega, -\tilde{\omega}\right)\hat{C}_{2}(\tilde{\omega})$$
(4.72)

$$\mathcal{T}_{1} = \int d\tilde{\omega} T^{(1)} \left(\omega + \tilde{\omega}, \tilde{\omega}\right) R^{(1)} \left(\omega, -\tilde{\omega}\right) \hat{C}_{2}(\tilde{\omega})$$
(4.73)

(cf. Eq. (3.41)).

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Following the same arguments as in App. 4.A, I employ the geometric sum to arrive at

$$\mathcal{K}_1 := \lim_{\gamma \to \infty} \mathcal{J}_1 = \frac{1}{-i\omega + \varepsilon} \frac{\mathcal{R}_2}{\left(R\left(x_1', \omega + i\varepsilon\right)\right)^2}$$
(4.76)

$$\mathcal{K}_2 := \lim_{\gamma \to \infty} \mathcal{J}_2 = \frac{1}{-i\omega + \varepsilon} \frac{\mathcal{K}_1}{\left(R\left(x_1', \omega + i\varepsilon\right)\right)^2}$$
(4.77)

$$\mathcal{K}_3 := \lim_{\gamma \to \infty} \mathcal{J}_3 = \frac{1}{-i\omega + \varepsilon} \frac{\mathcal{T}_2}{R(x_1', \omega + i\varepsilon)}$$
(4.78)

$$\mathcal{K}_4 := \lim_{\gamma \to \infty} \mathcal{J}_4 = \frac{1}{-i\omega + \varepsilon} \frac{\gamma_1}{R(x_1', \omega + i\varepsilon)}$$
(4.79)

Finally, the g^2 correction to the trace function reads (having taken the limit $\varepsilon \to 0$)

$$\mathcal{Q}(x,t) = \int \mathrm{d}\omega e^{-i\omega t} \left(\frac{T\left(x_0', x_1', \omega\right)}{(-i\omega)R\left(x_1', \omega\right)} + g^2\left(\mathcal{K}_1 + \mathcal{K}_2 + \mathcal{K}_3 + \mathcal{K}_4\right) \right).$$
(4.80)

To render this calculation concrete, it thus requires to find the explicit transition and return probability of the process, and to calculate the auxiliary functions defined in Eqs. 4.74 and 4.75.

In Chp. 3, I perform this calculation explicitly for two systems to find $\partial_t Q(x,t)$, the firstpassage time moment generating function (*cf.* Eq. (4.35)). Using the notation in Chp. 3, I identify $(I) = -i\omega \mathcal{K}_1, \cdots, (IV) = -i\omega \mathcal{K}_4$ (*cf.* Eqs. (3.71), (3.73), (3.75), and (3.77)), and Eq. (4.80), modulo a factor of $-i\omega$, with Eq. (3.78). The re-interpretation of the auxiliary function therefore is the second functional derivative of the transition and return probability conditional on y_t evaluated at $y_t \equiv 0$ as introduced earlier in Eq. (3.25).

This result therefore has re-derived the results in Chp. 3 using the technology developed in Chp. 2. This concludes this chapter.

Appendix

4.A Renormalisation of τ

In this appendix, the renormalisation of the coupling τ is computed. To ease computations, I perform the calculation in x, ω variables, *i.e.* in real space and Fourier transformed time. The renormalisation is given by its diagrammatic expansion (*cf.* Eq. (4.28))

which stems from the expansion of the path-integrated average Eq. (4.4) in γ ,

$$\left\langle \psi(x_1',\omega_1)\widetilde{\varphi}(x_0',\omega_0)\right\rangle_{\mathcal{S}} \tag{4.82}$$

$$= \gamma \tau \iint dz \, d\omega' \left\langle \psi(x_1', \omega_1) \widetilde{\psi}(z, \omega') \varphi(z, \omega') \widetilde{\varphi}(x_0', \omega_0) \right\rangle_{\mathcal{S}; \gamma = 0}$$

$$(4.83)$$

$$-\gamma^2 \lambda \sigma \iint \mathrm{d}z_1 \,\mathrm{d}z_2 \,\mathrm{d}\omega_1' \mathrm{d}\omega_2' \mathrm{d}\omega_1'' \mathrm{d}\omega_2'' \tag{4.84}$$

$$\times \left\langle \psi(x_1',\omega_1)\widetilde{\psi}(z_1,-\omega_1'-\omega_1'')\psi(z_1,\omega_1'')\varphi(z_1,\omega_1')\widetilde{\psi}(z_2,\omega_2'')\widetilde{\varphi}(z_2,\omega_2')\varphi(z_2,-\omega_2'-\omega_2'')\widetilde{\varphi}(x_0',\omega_0)\right\rangle_{\mathcal{S};\gamma=0}$$

$$+\cdots$$

Crucially, the averages $\langle \bullet \rangle_{\mathcal{S};\gamma=0}$ are taken over Gaussian random variables since $\gamma = 0$ such that Wick's rule applies [143]. The only non-vanishing Gaussian correlation functions are

$$\langle \varphi(z_1,\omega_1)\widetilde{\varphi}(z_0,\omega_0)\rangle_{\mathcal{S};\gamma=0} = T(z_0,z_1;\omega_1)\,\delta(\omega_0+\omega_1) \tag{4.85}$$

$$= \int d\omega_1 e^{i\omega_1(t-t_0)} T(z_0, z_1; t) \,\delta(\omega_0 + \omega_1)$$
(4.86)

$$\left\langle \psi(z_1,\omega_1)\widetilde{\psi}(z_0,\omega_0)\right\rangle_{\mathcal{S};\gamma=0} = \frac{\delta(z_1-z_0)\delta(\omega_0+\omega_1)}{-i\omega_1+\varepsilon} \tag{4.87}$$

$$= \iint \mathrm{d}\omega_0 \mathrm{d}\omega_1 e^{i\omega_1 t + i\omega_0 t_0} \Theta(t - t_0) \delta(z_1 - z_0) e^{-\varepsilon(t - t_0)}$$
(4.88)

The second correlator intuitively characterises the behaviour of the trace which, once deposited at z_0 at time t_0 , remains there for an infinitely long time, as $\varepsilon \to 0$. Equipped with these correlators and Wick's theorem, the non-vanishing contributions to the averages appearing in

4. Field Theory for Extreme Values in Stochastic Processes

Eq. (4.85) are to first order

$$\gamma \tau \iint dz \, d\omega' \left\langle \psi(x_1', \omega_1) \widetilde{\psi}(z, \omega') \varphi(z, \omega') \widetilde{\varphi}(x_0', \omega_0) \right\rangle_{\mathcal{S}; \gamma = 0}$$

$$= \gamma \tau \iint dz \, d\omega' \frac{\delta(x_1' - z) \delta(\omega_1 + \omega')}{-i\omega_1 + \varepsilon} T(x_0', z, \omega') \delta(\omega' + \omega_0)$$

$$= \gamma \tau \frac{T(x_0', x_1', -\omega_1)}{-i\omega_1 + \varepsilon} \delta(\omega_0 - \omega_1),$$

$$(4.89)$$

and further to second order

$$-\gamma^{2}\lambda\sigma \iint dz_{1} dz_{2} d\omega_{1}^{\prime} d\omega_{2}^{\prime} d\omega_{1}^{\prime \prime} d\omega_{2}^{\prime \prime}$$

$$\times \left\langle \psi(x_{1}^{\prime},\omega_{1})\widetilde{\psi}(z_{1},-\omega_{1}^{\prime}-\omega_{1}^{\prime \prime})\psi(z_{1},\omega_{1}^{\prime \prime})\varphi(z_{1},\omega_{1}^{\prime \prime})\widetilde{\psi}(z_{2},\omega_{2}^{\prime \prime})\widetilde{\varphi}(z_{2},\omega_{2}^{\prime})\varphi(z_{2},-\omega_{2}^{\prime}-\omega_{2}^{\prime \prime})\widetilde{\varphi}(x_{0}^{\prime},\omega_{0})\right\rangle_{\mathcal{S};\gamma=0}$$

$$(4.91)$$

$$(4.92)$$

$$= -\gamma^2 \lambda \sigma \frac{1}{-i\omega_1 + \varepsilon} \int d\omega_2'' \frac{R\left(x_1', x_1', \omega_1 - \omega_2''\right)}{-i\omega_1'' + \varepsilon} T\left(x_0', x_1', \omega_0\right) \delta(\omega_0 + \omega_1)$$
(4.93)

$$= -\gamma^2 \lambda \sigma \frac{R\left(x_1', \omega_1 + i\varepsilon\right)}{-i\omega_1 + \varepsilon} T\left(x_0', x_1', \omega_0\right) \delta(\omega_0 + \omega_1)$$
(4.94)

where in the first equality I used the definition of the return probability to abbreviate

$$\iint dz_1 dz_2 \,\delta(x_1' - z_1) \delta(z_1 - z_2) T(z_1, z_2, \omega) = R(x_1', \omega) \,, \tag{4.95}$$

and in the second equality used Cauchy's residue formula to solve the integral by evaluating the residue of the simple pole at $\omega_2'' = -i\varepsilon$.

Since both correlators in Eq. (4.85) are proportional to $\delta(\omega_0 + \omega_1)$, any higher order expansion term simply factorises into a product over the amputated one-loop bubble diagram (*i.e.* interpreted here as a function of external parameters z_1, ω_1 and z_2, ω_2 , respectively) which by analogous reasoning to the calculation is

$$z_1, \omega_1 \, \, \mathbf{\nabla} \, z_2, \omega_2 = \gamma^2 \lambda \sigma R \, (z_1, \omega_1 + i\varepsilon) \, \delta(\omega_1 + \omega_2) \delta(z_1 - z_2). \tag{4.96}$$

With some casualty, the bubble may be read as the probability of a particle depositing a trace and then return to it, in other words an "ordered" return probability. Likewise the higher order diagrams in Eq. (4.28) may be interpreted as repeated returns to x'_1 .

Returning to Eq. (4.28), the renormalised τ coupling, τ_R , is the effective factor satisfying

$$\left\langle \psi(x_1',\omega_1)\widetilde{\varphi}(x_0',\omega_0)\right\rangle_{\mathcal{S}} = \frac{1}{-i\omega_1 + \varepsilon} \tau_R(\omega_0,\omega_1)T\left(x_0',x_1',-\omega_0\right)$$
(4.97)

and collecting the factors generated by the terms above one obtains

$$\tau_R(\omega_0,\omega_1) = \left[\gamma\tau - \gamma^2\lambda\sigma R\left(x_1',\omega_1 + i\varepsilon\right) + \gamma^3\lambda\sigma\kappa\left(R\left(x_1',\omega_1 + i\varepsilon\right)\right)^2\right]$$
(4.98)

$$-\gamma^4 c \sigma \kappa^2 \left(R \left(x_1', \omega_1 + i\varepsilon \right) \right)^3 + \cdots \right] \delta(\omega_0 + \omega_1)$$
(4.99)

This series can be resummed using the geometric series or, as its known in field-theoretic liter-

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ature, Dyson's equation [4]. Rearranging the sum gives

$$\tau_R(\omega_0,\omega_1) = \left[\gamma\tau + \gamma\frac{c\sigma}{\kappa}\sum_{r=1}^{\infty} \left(-\gamma\kappa R\left(x_1',\omega_1 + i\varepsilon\right)\right)^r\right]\delta(\omega_0 + \omega_1)$$
(4.100)

$$= \left[\gamma\tau + \gamma \frac{c\sigma}{\kappa} \sum_{r=0}^{\infty} \left(-\gamma\kappa R \left(x_{1}^{\prime}, \omega_{1} + i\varepsilon\right)\right)^{r} - \gamma \frac{c\sigma}{\kappa}\right] \delta(\omega_{0} + \omega_{1})$$

$$(4.101)$$

$$= \left[\frac{\lambda\sigma}{\kappa}\frac{\gamma}{1 + \gamma\kappa R\left(x_{1}^{\prime},\omega_{1} + i\varepsilon\right)} + \gamma\left(\underbrace{\tau - \frac{c\sigma}{\kappa}}_{=0}\right)\right]\delta(\omega_{0} + \omega_{1})$$
(4.102)

$$=\frac{\gamma}{1+\gamma R\left(x_{1}^{\prime},\omega_{1}+i\varepsilon\right)}\delta(\omega_{0}+\omega_{1})\tag{4.103}$$

where I made use of the bare values given in Eq. (4.11). This vertex interpolates the physical pictures for $\gamma = 0$, where no deposition takes place ($\tau_R = 0$), and $\gamma \to \infty$, where every newly visited site gets marked immediately by a deposited trace. For $\gamma \to \infty$, the coupling tends to

$$\lim_{\gamma \to 0} \tau_R(\omega_0, \omega_1) = \frac{\delta(\omega_0 + \omega_1)}{R\left(x_1', \omega_1 + i\varepsilon\right)}$$
(4.104)

Part III.

Fractional Brownian Motion



Untitled, Kay Wiese (2020). Courtesy of Kay Wiese (2020).

Chapter 5

Sampling first-passage times of fractional Brownian Motion using adaptive bisections

Abstract

"We present an algorithm to efficiently sample first-passage times for fractional Brownian motion. To increase the resolution, an initial coarse lattice is successively refined close to the target, by adding exactly sampled midpoints, where the probability that they reach the target is non-negligible. Compared to a path of N equally spaced points, the algorithm achieves the same numerical accuracy $N_{\rm eff}$, while sampling only a small fraction of all points. Though this induces a statistical error, the latter is bounded for each bridge, allowing us to bound the total error rate by a number of our choice, say $P_{\rm error}^{\rm tot} = 10^{-6}$. This leads to significant improvements in both memory and speed. For H = 0.33 and $N_{\text{eff}} = 2^{32}$, we need 5000 times less CPU time and 10000 times less memory than the classical Davies-Harte algorithm. The gain grows for H = 0.25 and $N_{\rm eff} = 2^{42}$ to 3×10^5 for CPU and 10^6 for memory. We estimate our algorithmic complexity as $\mathcal{C}^{\text{ABSec}}(N_{\text{eff}}) = \mathcal{O}\left((\ln N_{\text{eff}})^3\right)$, to be compared to Davies-Harte which has complexity $\mathcal{C}^{\mathrm{DH}}(N) = \mathcal{O}(N \ln N)$. Decreasing $P_{\mathrm{error}}^{\mathrm{tot}}$ results in a small increase in complexity, proportional to $\ln(1/P_{error}^{tot})$. Our current implementation is limited to the values of $N_{\rm eff}$ given above, due to a loss of floating-point precision. Our algorithm can be adapted to other extreme events and arbitrary Gaussian processes. It enables one to numerically validate theoretical predictions that were hitherto inaccessible."

Cited from

B. WALTER AND K. J. WIESE. Sampling first-passage times of fractional brownian motion using adaptive bisections. *Phys. Rev. E* **101**:043312, 2020. arXiv:1908.11634

Overview

In this chapter, I present a near verbatim copy of the peer-reviewed journal article

B. WALTER AND K. J. WIESE. Sampling first-passage times of fractional brownian motion using adaptive bisections. *Phys. Rev. E* **101**:043312, 2020. arXiv:1908.11634 DOI:doi.org/10.1103/PhysRevE.101.043312

This paper introduces a new algorithm which is capable of sampling the first-passage time distribution of fractional Brownian Motion bias-free with a higher numerical accuracy and lower computational costs than any previous comparable sampling algorithm. Why is it needed?

Fractional Brownian Motion is a non-Markovian self-similar process with a first-passage time distribution that is not known in closed form. As is addressed in Chp. 3 and 4, this is typical for non-Markovian processes and calls for powerful perturbative approaches. In order to validate these analytical approximations, one needs to be able to sample the true first-passage time distribution to great accuracy so as to correctly gauge the quality of an approximation. Such an approximation, for the case of a fractional Brownian Motion with linear and non-linear drift, will be developed in the subsequent Chapter 6. In fact, it were the results obtained there which motivated the development of a higher performing algorithm presented here. Simulating fractional Brownian Motion is a fruitful challenge to computational physics and has led to various exact and approximative methods. Since the correlation between increments of fractional Brownian Motion is long-ranged, for an algorithm to produce a great number of such points, as is typically necessary to accurately measure a first-passage event, comes to great cost in both computations and memory.

In principle, the algorithm can also be adapted to sample other extreme events of any stochastic process, provided it is Gaussian, whilst remaining fast and accurate. It will be used to numerically validate the analytical results of the subsequent chapter, Chp. 6, which also was the initial motivation to develop this algorithm.

Statement of Contribution

Kay Wiese and I jointly developed the key ideas of the algorithm. I constructed the logical steps, implemented the algorithm in C, devised and run benchmarks, and wrote the manuscript.

Acknowledgements

I would like to thank Kay Wiese for allowing me to cite our joint work in my thesis. *I have obtained his approval which is shown in App. A.4.* I would like to thank LPTENS and LPENS for their hospitality. Further, I am very grateful for the computing support provided by Marc-Thierry Jaekel and Andy Thomas. Also, I would like to thank Matteo D'Achille for a careful reading of the manuscript.

5. Adaptive Bisections

5.1 Introduction

"Estimating the distribution of first-passage times is a key problem in understanding systems as different as financial markets or biological systems [197, 166], and the dynamics of local reactions [114, 100]. Typically, research focuses on non-Markovian processes and bounded geometries, where first-passage time distributions are difficult to obtain analytically [206, 105, 149, 250] and Chp. 6. Within the class of non-Markovian processes, fractional Brownian Motion (fBm) is of particular interest as it naturally extends standard diffusion to sub- and super-diffusive self-similar processes [160]. Fractional Brownian Motion is a one-parameter family of Gaussian processes, indexed by the Hurst parameter $H \in (0, 1]$. The latter parametrizes the mean-square displacement via

$$\left\langle X_t^2 \right\rangle = 2t^{2H} \,, \tag{5.1}$$

recovering standard Brownian Motion at $H = \frac{1}{2}$. It retains from Brownian motion scale and translational invariance, both in space and time. Due to its correlations, it has peculiar characteristics, as e.g. the recently observed behavior near a reflecting boundary [239, 107]. FBM has long defied an analytic study of its extreme events, except for results in the mathematical literature concerning the tail of these distributions [119, 168, 191, 192].

In order to render the extreme events of this process accessible to an analytical treatment, an ε -expansion around Brownian motion in $\varepsilon = H - \frac{1}{2}$ was proposed [252]. This field theoretic approach was applied to a variety of extreme events, yielding the first-order corrections of several probability distributions [252, 61, 202, 250]. The scaling functions predicted by this perturbative field theory are computationally expensive to verify, since they require a high numerical resolution of the path. Typically this is done by simulating a discretized version of the path over a grid of N equidistant points. Measuring a first-passage time then amounts to finding the first passage of a linear interpolation of these grid points. This approximation, however, can lead to a systematic over-estimation of the first-passage time. As can be seen on Fig. 5.1, a high resolution of the path is necessary in order to find the first-passage event at t = 0.36 instead of the one at t = 0.45 or even t = 0.47 for the coarser grids. To account for this, usually the number of grid points is increased. As the size of fluctuations between gridpoints diminishes as

$$\delta X = N^{-H} , \qquad (5.2)$$

the sub-diffusive regime $(H < \frac{1}{2})$ necessitates an enormous computational effort.

This poses challenges to the numerical validation of high-precision analytical predictions as can be seen for instance in Ref. [250]. There, in order to validate the analytically obtained scaling functions, and to minimize discretisation errors in the sub-diffusive regime, system sizes up to $N = 2^{24}$ are sampled using the standard Davies-Harte algorithm. The implementation used there required a CPU time of 6 seconds per sample. This illustrates that if theories of such high precision are to be tested against simulations, new numerical techniques need to be developed. The present work addresses this problem by designing, implementing, and benchmarking a new algorithm sampling first-passage times of fractional Brownian Motion using several orders of magnitude less CPU time and memory than traditional methods. The general idea is to start from a rather coarse grid (as the red one on Fig. 5.1), and to refine the grid where necessary.

5. Adaptive Bisections



Figure 5.1.: The continuous stochastic path (grey rough line) crosses the barrier (blue horizontal line) for the first time at τ^{∞} (black leftmost square mark). The discretization with N points (red line passing through rightmost square) over-estimates this time as τ^{N} (red rightmost square mark). The numerical estimate is improved to τ^{4N} (green middle square mark) when refining the discretization (green line passing through middle square mark). This systematic error worsens for diminishing values of Hurst parameter H. This figure is accepted for publication as [242]. See App. A.4 for approval of co-authors.

As a testing ground, we simulate and compare to theory the first-passage time of an fBm with drift (*cf.* Chp. 6).

The algorithm proposed here is an adaptive bisection routine that draws on several numerical methods already established in the field of numerical fractional Brownian motion, notably the Davies-Harte algorithm [54], bisection methods [41, 225], and the Random Midpoint Displacement method [88, 173]. It is further closely related to "Exact Algorithms" which have already been established for stochastic differential equations driven by white noise in, *e.g.*, [21] which also address the problem of sampling the first-passage time efficiently and exactly. In difference to [21], we here extend the exact algorithm to processes of the form

$$\mathrm{d}X_t = f'(t)\mathrm{d}t + \mathrm{d}B_t^{(H)} \tag{5.3}$$

where $dB_t^{(H)}$ is a fractional Gaussian noise with Hurst parameter H (see further remarks in Sec. 5.2.4), *i.e.* processes which are, up to an additional deterministic function f(t), a fBm path. The key ideas of this algorithm, however, straightforwardly translate to *all* Gaussian processes provided their correlator is known (see Sec. 5.2.5 for further discussion).

The central, and quite simple, observation is that in order to resolve a first-passage event it is necessary to have a high grid resolution only near the target. This translates into an algorithm that generates a successively refined grid, where refinement takes place only at points close to the target, with the criterion of *closeness* scaling down by 2^{-H} for each bisection. This refinement is stopped after the desired resolution is reached. The sampling method is *exact*, *i.e.* the collection of points is drawn from the ensemble of fBm, a continuous process, with no bias. The only error one can make is that one misses an intermediate point. We have been able to control this error with a failure rate smaller than 10^{-6} per realisation.

While there is a relatively large overhead for the non-homogenous refinement, this is compensated by the use of far less points, leading to a significant increase both in speed and memory efficiency over sampling methods that produce points for the full grid. For H = 0.33 and system size $N = 2^{32}$, our algorithm is 5000 times faster than the Davies-Harte Algorithm (DH), the fastest exact sampler (cf. [69, 49]) if all points are needed. It has computational complexity $\mathcal{O}(N \ln(N))$, which makes it the standard algorithm in most current works, see *e.g.* [106, 149, 132], with system size N ranging from 2^{21} to 2^{24} . Our maximal grid size is limited by the precision of the floating point unit to $N_{\max} \approx 2^{11/H}$.

This paper is organised as follows. In Sec. 5.2, we introduce our adaptive bisection algorithm. First, its higher-level structure is outlined and then each subroutine is detailed. Possible generalisations to other extreme events or other Gaussian processes are discussed at the end of this section. In Sec. 5.3, we present our implementation of the adaptive bisection in C, which is freely available [241]. We benchmark it against an implementation of the Davies-Harte algorithm. We compare error rates, average number of bisections, CPU time and memory. Sec. 5.4 contains a summary of our findings.

5.2 Algorithm

In this section, we introduce the adaptive bisection routine (ABSec). The central aim is to translate the idea of refining the grid "where it matters" into a rigorous routine.

5.2.1 Fractional Brownian Motion and first-passage times

Gaussian processes X_t are stochastic processes for which X_t evaluated at a finite number of points \mathcal{T} in time, has a multivariate Gaussian distribution [192]. They are simple to handle, since their path probability measure can be obtained from their correlation function. The best known Gaussian Process is Brownian Motion which is the only translational invariant Gaussian process with stationary and independent increments.

Fractional Brownian Motion (fBm) generalises Brownian Motion by relaxing the requirement of independent increments, while keeping self-similarity. The latter property means that its path probability measure is invariant under a space-time transformation $t \to ct$, $x \to c^{-H}x$ for c > 0. The parameter H is referred to as *Hurst* exponent. As a Gaussian process, fBm is entirely characterized by its mean $X_0 = \langle X_t \rangle = 0$, and correlation function

$$C(s,t) = \langle X_s X_t \rangle = |s|^{2H} + |t|^{2H} - |t-s|^{2H} , \qquad (5.4)$$

where $H \in (0, 1]$. As a consequence, $\langle (X_t - X_s)^2 \rangle = 2|t - s|^{2H}$, and in particular $\langle X_t^2 \rangle = 2|t|^{2H}$. From the correlation function it follows that on all time scales non-overlapping increments are positively correlated for $H > \frac{1}{2}$ and negatively correlated for $H < \frac{1}{2}$. For $H = \frac{1}{2}$ one recovers Brownian Motion with uncorrelated increments.

The first-passage time (FPT) of a stochastic process is the fist time the process crosses a

5. Adaptive Bisections

threshold m. Since we use $X_0 = 0$, it is defined for m > 0 as

$$\tau_m = \inf_{t>0} \left\{ t | X_t \ge m \right\}.$$
(5.5)

5.2.2 Notation

In simulating a fBm on a computer, one is forced to represent the continuous path by a *discretized path* that takes values on a finite set of points in time, the *grid*. We denote the grid by *ordered* times $\mathcal{T} = \{t_1, t_2, \ldots, t_N\}$, and the corresponding values of the process by $\mathcal{X} = \{X_{t_1}, X_{t_2}, \ldots, X_{t_N}\}$. Together, $(\mathcal{X}, \mathcal{T})$ form the discretized path. Due to self-similarity of the process, we can restrict ourselves to $\mathcal{T} \subset [0, 1]$ with no loss of generality. The intervals between any two successive times $t_i, t_{i+1} \in \mathcal{T}$ are referred to as *bridges* (t_i, t_{i+1}) . Each connected component of $[0, 1] \setminus \mathcal{T}$ is a bridge.

We denote the dyadic lattice on the unit interval by $\Lambda^k = \{i2^{-k}; 0 \leq i \leq 2^k\}$. Our adaptive bisection algorithm sets out from a dyadic lattice Λ^g of relatively low resolution (typically $g \leq 8$ or 10). A fBM path is sampled for every point of the coarse grid Λ^g . If the linear interpolation of this coarse path already surpasses the threshold m at a time $\tau^{(0)}$, or in other words if there is a smallest K such that $X_{K2^{-g}} > m$, then the grid is truncated at $\tau^{(0)}$. (That this truncation does not introduce a bias is shown below.) If this is not the case, i.e. if all points remain below the threshold m, then the full grid is kept. We define the truncation of the grid \mathcal{T} to a certain time $\tau \in [0, 1]$ as

$$\mathcal{T}|_{\tau} := \{ t_i \in \mathcal{T} | t_{i-1} < \tau \}$$

$$(5.6)$$

i.e. the truncation contains all points in time up to time τ plus the next gridpoint of the initial grid Λ^g (cf. section 5.2.3.C). This procedure results in an initial grid $\mathcal{T}^{(0)} \subset \Lambda^g$ containing $|\mathcal{T}^{(0)}| = K$ points, with $K \leq 2^g$. Next, the algorithm performs bisections of this grid in successive iterations $\mathcal{T}^{(0)}, \mathcal{T}^{(1)}, \cdots, \mathcal{T}^{(M)}$, where M is the total number of bisections before the routine terminates. Since each new bisection adds exactly one point to the grid, M also denotes the total number of points added to the initial grid. The final grid $\mathcal{T}^{(M)}$ contains K+M points.

To each bridge (t_1, t_r) between left and right endpoints t_1 and t_r and contained in a grid $\mathcal{T}^{(m)}$, we associate a level ℓ defined by $\ell = -\ln_2(t_r - t_l)$. A bridge is bisected by introducing its midpoint, $t_m = \frac{1}{2}(t_l + t_r) = t_l + 2^{-\ell-1}$ and inserting t_m into the grid $\mathcal{T}^{(m+1)} = \{t_1, ..., t_l, t_m, t_r, ..., t_N\}$. A bridge can be bisected until its level reaches a maximum bisection level L (typically $L \leq 30$ for H = 0.33). Since each iteration only halves an existing interval, all grids are subsets of the maximal dyadic lattice Λ^L ,

$$\Lambda^g \supseteq \mathcal{T}^{(0)} \subset \mathcal{T}^{(1)} \subset \dots \subset \mathcal{T}^{(M)} \subseteq \Lambda^L.$$
(5.7)

Note that for each bridge (t_1, t_r) , there is always one dyadic lattice Λ^n , s.t. t_i and t_{i+1} are neighbouring points in Λ^n ; they are members, but not neighbours in $\Lambda^{n'}$ for n' > n; at least one of them does not exist in $\Lambda^{n'}$ for n' < n.

5.2.3 Definition of the algorithm

The algorithm consists of two phases. In the *first phase*, the initialisation, a coarse grid is generated. In the *second phase*, the adaptive bisection, this grid is successively bisected where necessary. Once the second phase terminates, the first-passage time is calculated using the final grid.

The first phase starts by sampling an initial discretized path $\mathcal{X}^{(0)}$ over a dyadic lattice $\mathcal{T}^{(0)} = \Lambda^g$ with $N = 2^g$ equidistant points, using the *Davies-Harte* algorithm. The latter is the fastest known algorithm to sample an exact fBm path on an equidistant grid in time [69], its execution time scales as $N \ln(N)$, thus only slightly slower than what is needed to generate an uncorrelated sample of the same length N. From this relatively coarse grid, $(\mathcal{X}^{(0)}, \mathcal{T}^{(0)})$, the first-passage time is estimated via linear interpolation as $\tau^{(0)}$.

Subsequently, the grid is truncated by discarding all points behind the first point surpassing m (cf. Eq. (5.6)). That this does not change the measure is explained in section 5.2.3.C. If no such point exists, the full grid is kept. The correlations between the different points X_t at times t stored in the grid are given by the correlation matrix

$$C_{ij}(\mathcal{T}) = C(t_i, t_j) , \qquad t_i, t_j \in \mathcal{T}, 1 \le i, j \le |\mathcal{T}| .$$

$$(5.8)$$

It is a symmetric matrix computed from the correlation function (5.4). It is then inverted to obtain the inverse correlation matrix $C_{ij}^{-1}(\mathcal{T})$. The inversion is optimised by using pre-calculated tabularized matrices. This concludes the *first phase*.

In the second phase, bridges are checked successively until the maximum level is reached. The order in which the bridges of the growing grid are checked is determined by a subroutine whose aim is to find the first-passage event with the least amount of bisections. The check consists in testing whether the midpoint X_{t_m} of the bridge (t_1, t_r) could surpass the threshold m with a probability larger than ε , taken small. If this is the case the bridge is deemed critical and bisected. The bisection consists in generating a midpoint X_{t_m} at time t_m conditional to the pre-existing grid. This computation requires the inverse correlation matrix and is detailed in Sec. 5.2.3.F. Once the midpoint is generated, it is added to the path $(\mathcal{X}, \mathcal{T})$. In a last step the inverse correlation matrix of the new grid, $C^{-1}(\mathcal{T} \cup t_m)$ is stored. Further below, the algorithm is given in pseudocode. The routines in the pseudocode are described in sections 5.2.3.A-5.2.3.G.

5.2.3.A Davies-Harte Algorithm

The Davies-Harte algorithm (DH) is a widely used method to generate fBm samples. It was introduced in [54], is pedagogically described in [69], and has been extended to other Gaussian processes in [49], allowing us to omit an introduction. It generates a sample of fractional Gaussian noise (fGn) $\xi_1, \xi_2, \dots, \xi_N$, the incremental process of fBm $\xi_j = X_{j+1} - X_j, j \in \mathbb{N}$, and then sums the increments to a fBm sample with values $X_{i\delta t} = (\delta t)^H \sum_{j=1}^i \xi_j$. Simulating the increments is more efficient since fGn is a stationary Gaussian process which, for equally sized increments, has a circulant correlation matrix, which can be diagonalised using a fast Fourier transform (FFT). Therefore a fGn sample of N increments can be simulated with computational complexity $\mathcal{O}(N \ln(N))$. The FFT algorithm works optimally when the number of points is a natural power of 2, *i.e.* if the grid is a dyadic lattice.

Algorithm 1: Adaptive bisection

procedure $ABSEC(g, L, m, \varepsilon)$	
$\mathcal{T} \leftarrow \Lambda^g$	
$\mathcal{X} \leftarrow \text{DAVIES_HARTE}(\Lambda^g)$	⊳ 5.2.3.A
$ au \leftarrow ext{FPT_FROM_GRID}(\mathcal{X}, \mathcal{T})$	⊳ 5.2.3.B
$(\mathcal{X},\mathcal{T}) \leftarrow (\mathcal{X},\mathcal{T}) _{ au^{(0)}}$	⊳ 5.2.3.C
$C^{-1} \leftarrow \texttt{CMatrixTable}[au^{(0)}]$	⊳ 5.2.3.D
$(t_{\rm l}, t_{\rm r}) \leftarrow \text{Next Bridge}(\mathcal{T}, 0, \tau^{(0)})$	
while (t_1, t_r) defined do	
if Bridge (t_l, t_r) critical and not yet bisected then	⊳ 5.2.3.E
$C^{-1} \leftarrow \text{Augment } C^{-1}\text{-Matrix}(C^{-1}, t_{\text{m}})$	
$X^* \leftarrow \text{Generate midpoint}(C^{-1}, t_{\text{m}})$	\triangleright 5.2.3.F
$\mathcal{X} \leftarrow \mathcal{X} \cup X^*$	
$\mathcal{T} \leftarrow \mathcal{T} \cup t_{\mathrm{m}}$	
if $X^* > m$ then	
$ au \leftarrow ext{FPT_FROM_GRID}(\mathcal{X}, \mathcal{T})$	
$(t_i, t_{i+1}) \leftarrow \text{Next Bridge}(\mathcal{T}, (t_i, t_{i+1}), \tau)$	⊳ 5.2.3.G
$\mathbf{output}(au)$	

5.2.3.B Estimating the first-passage time

Given a discretized path $(\mathcal{X}, \mathcal{T})$, we use its linear interpolation to give the first-passage time as its first intersection with the threshold (cf. Fig.5.1).

5.2.3.C Truncating the grid

A further optimisation is to discard grid points beyond the first point crossing the threshold (cf. Eq. (5.6)). It is necessary to show that the density of first-passage times conditioned on the full grid equals the distribution conditioned on the truncated grid, *i.e.* that truncating does not change the measure.

The first-passage time distribution (FPTD) $P(\tau)$ can be decomposed into a sum of conditional probabilities for disjoint events. Each term of the sum is the probability that the *i*th point of a grid surpasses *m*, the threshold, for the first time (" $P^{\text{grid}}(X_{t_i} > m \text{ first})$ "), times the FPTD of a fBm conditioned on the event that its discretization on grid \mathcal{T} surpasses *m* at t_i for the first time, *i.e.*

$$P_{\mathcal{T}}(\tau | X_{t_i} > m \text{ first}) = P(\tau | X_t : X_{t_i} > m \text{ and } X_{t_j} < m \forall t_j < t_i)$$
(5.9)

for $t_i, t_i \in \mathcal{T}$. The decomposition thus reads

$$P(\tau) = \sum_{t_i \in \mathcal{T}} P_{\mathcal{T}}(\tau | X_{t_i} > m \text{ first}) P^{\text{grid}}(X_{t_i} > m \text{ first}).$$
(5.10)

By continuity of the process,

$$P_{\mathcal{T}}(\tau > t_i | X_{t_i} > m \text{ first}) = 0, \qquad (5.11)$$

5. Adaptive Bisections

such that the sum in Eq. (5.10) can be truncated to

$$P(\tau) = \sum_{t_{i-1} < \tau} P_{\mathcal{T}}(\tau | X_{t_i} > m \text{ first}) P^{\text{grid}}(X_{t_i} > m \text{ first}).$$
(5.12)

In order to sample $P_{\mathcal{T}}(\tau | X_{t_i} > m \text{ first})$, one would naively sample the entire grid \mathcal{X} over all of \mathcal{T} , but since

$$P_{\mathcal{T}}(\tau|X_{t_i} > m \text{ first}) = P_{\mathcal{T}|_{\tau}}(\tau|X_{t_i} > m \text{ first}),$$
(5.13)

where the restriction is defined in Eq. (5.6), it is sufficient to only regard the smaller grid $\mathcal{T}|_{\tau}$, *i.e.*

$$P(\tau) = \sum_{t_{i-1} < \tau} P_{\mathcal{T}|_{\tau}}(\tau | X_{t_i} > m \text{ first}) P^{\text{grid}}(X_{t_i} > m \text{ first}).$$
(5.14)

Discarding points in the initial stage leads to a smaller correlation matrix to be inverted, which increases performance, and decreases memory.

5.2.3.D Tabulating inverse correlation matrices

The inverse of the correlation matrix (5.8) is necessary to compute the conditional probability of any further midpoint (cf. App. 5.B). Its computation is costly and typically scales with $\mathcal{O}(N^3)$ where $N = 2^g$ is the number of points in $\mathcal{T}^{(0)}$. If the algorithm is run multiple times, this computation slows it down. The initial grid however, is always a dyadic lattice truncated at some point, *i.e.* $\mathcal{T}^{(0)} = \{k2^{-g}; 0 \le k \le K\}$, where $X_{K2^{-g}}$ is the first point to surpass m. Therefore, the initial inverse correlation matrix $C^{-1}(\mathcal{T}^{(0)})$ can take $2^g - 1$ possible values, one for each possible value of K. It is more efficient to pre-calculate all possible inverse correlation matrices in the beginning, and store them in a vector 'CMatrixTable',

$$\mathsf{CMatrixTable}[K] = \left(\left[C(i2^{-g}, j2^{-g}) \right]_{i,j=1}^{K} \right)^{-1} . \tag{5.15}$$

After generating the initial grid and measuring $\tau^{(0)}$, one reads out the appropriate entry of the table at $K = \min \left\{ n \in \mathbb{Z}; n2^{-g} \ge \tau^{(0)} \right\}$.

5.2.3.E Deciding whether a bridge is critical

Once entering the bisection phase, the algorithm needs to decide whether a particular bridge is *critical*, *i.e.* whether it is suspicious of hiding a "dangereous" excursion crossing the threshold at m (cf. Fig. 5.1). Rather than determining whether *any* point in (t_1, t_r) surpasses the threshold, we focus on the midpoint t_m conditioned on all other points \mathcal{X} , and ask how likely $X_{t_m} > m$. Such an event needs to be avoided with a very low probability ε , the *error tolerance*. The relevant probability,

$$P\left(X_{t_{\rm m}} > m | \mathcal{X}\right) < \varepsilon,\tag{5.16}$$

is too costly to be computed for every bridge in every step of the iteration, as the midpoint is a Gaussian random variable, with its mean and variance determined by every other point in the grid. If we *ignore* all points of the path apart from (t_i, X_{t_i}) and $(t_{i+1}, X_{t_{i+1}})$, a calculation
given in App. 5.A shows that mean and variance would be given by

$$\mu = \frac{1}{2} \left(X_{t_i} + X_{t_{i+1}} \right) \tag{5.17}$$

and

$$\sigma^2 = \left(2^{1-2H} - \frac{1}{2}\right) 2^{-2\ell H} . \tag{5.18}$$

Here ℓ is the level of the bridge of width $\delta t = 2^{-\ell}$. Interestingly, adding to the bridge's endpoints further points *lowers* the variance (cf. Eq. (5.31)) which means that neglecting all but nearest neighbours gives an upper bound on the variance of the midpoint. Further, we conservatively bound the mean by the maximum of both endpoints, $\mu \leq \max(X_{t_i}, X_{t_{i+1}})$. This is a priori not a precise approximation, since far-away grid points are able to "push" the expected midpoint above the bridges' endpoints for values of $H \neq \frac{1}{2}$. As is shown in Sec. 5.3.3, this systematic error can be absorbed by introducing an even smaller error tolerance ε' . Furthermore, it is less relevant in the sub-diffusive regime, where the process is negatively correlated. By giving conservative bounds on mean and variance with quantities that are *local* (*i.e.* do not depend on the remaining grid), we can replace the original criterion (5.16) by a computationally cheaper alternative, namely the local condition

$$P(X_{t_{\rm m}} > m | (X_{t_{\rm l}}, X_{t_{\rm r}})) < \varepsilon'.$$
 (5.19)

This implies that Eq. (5.16) holds for an appropriate choice of ε' , on *average*. This is to be understood as follows. In a simulation, there are *n* decisions of type (5.16) to be taken. The total error is approximately $P_{\text{error}}^{\text{tot}} \approx n\varepsilon$. The parameter ε' is chosen such that the total error rate remains smaller than 10^{-6} , and thus negligible as compared to MC fluctuations. The dependence between ε' and $P_{\text{error}}^{\text{tot}}$ is investigated in Sec. 5.3.3 (cf. Fig. 5.1).

Criterion (5.19) is rephrased, using again ℓ as the level of the bridge, to

$$\Phi\left(\frac{m - \max\left(X_{t_i}, X_{t_{i+1}}\right)}{\left(\sqrt{2^{1-2H} - \frac{1}{2}}\right)2^{-\ell H}}\right) > 1 - \varepsilon'$$
(5.20)

which implies

$$\max\left(X_{t_i}, X_{t_{i+1}}\right) < m - \left(\sqrt{2^{1-2H} - \frac{1}{2}}\right) 2^{-\ell H} \Phi^{-1}(1 - \varepsilon'), \tag{5.21}$$

where we introduced Φ , the cumulative distribution function of the standard normal distribution, and its inverse Φ^{-1} . This is further simplified by defining the *critical strip*

$$c_0 = \left(\sqrt{2^{1-2H} - \frac{1}{2}}\right) \Phi^{-1} \left(1 - \varepsilon'\right) , \qquad (5.22)$$

and the level-corresponding critical strips

$$c_{\ell} = 2^{-\ell H} c_0. \tag{5.23}$$

A bridge (X_{t_1}, X_{t_r}) of level ℓ is deemed critical if either of its endpoints lies above the critical strip corresponding to ℓ , *i.e.*

$$\max(X_{t_i}, X_{t_{i+1}}) > m - c_{\ell} .$$
(5.24)

This makes for a computationally fast decision process, since the critical strip width has to be computed only once. The procedure then checks for a given level of the bridge whether it reaches into the critical strip, in which case it is bisected (cf. Fig. 5.1 for illustration).

5.2.3.F Generating the new midpoint efficiently

If a bridge triggers a bisection, the midpoint is drawn according to its probability distribution, given all points that have been determined previously. If this occurs at, say, the *m*-th iteration, the discretized path is $((X_1, t_1), \dots, (X_N, t_N))$ with $|\mathcal{T}^{(m)}| = |\mathcal{X}^{(m)}| = N = K + m$ where $K \leq 2^g$ is the number of points in the truncated initial grid. Denoting the midpoint to be inserted by (X_{t^*}, t^*) , one needs to find

$$P\left(X_{t^*}|X_1,\cdots,X_N\right).\tag{5.25}$$

The midpoint is again normal distributed with mean $\mu_*(N)$ and variance $\sigma_*(N)$. Let $\mathcal{T}^{(m+1)} = (\mathcal{T}^{(m)}, t^*)$ be the augmented grid, and $C^{-1}(N+1) = C^{-1}(\mathcal{T}^{(m+1)})$ the associated inverse correlation matrix (cf. Eq. (5.8)). Then, as detailed in App. 5.B, the inverse of the variance is given by

$$\sigma_*^{-2}(N) = \left[C^{-1}(N+1)\right]_{N+1,N+1} , \qquad (5.26)$$

and the mean by

$$\mu_*(N) = \sigma_*^2(N) \sum_{i=1}^N \left[C^{-1}(N+1) \right]_{N+1,i} X_{t_i}.$$
(5.27)

Computing the inverse correlation matrix from scratch at every iteration would require a matrix inversion which typically uses $\mathcal{O}(N^3)$ steps. We do this in $\mathcal{O}(N^2)$ steps, by starting from the already calculated inverse correlation matrix of the previous grid $C^{-1}(N) = C^{-1}(\mathcal{T}^{(m)})$. As detailed in App. 5.C, the inverse correlation matrix $C^{-1}(N+1) = C^{-1}(\mathcal{T}^{(m+1)})$ can be constructed as follows. First, generate a vector containing all correlations of the new point with the grid, using Eq. (5.4)

$$\vec{\gamma}(N) = (C(t^*, t_1), C(t^*, t_2), \cdots, C(t^*, t_N))^T.$$
(5.28)

Second, multiply it with the (already constructed) inverse correlation matrix to obtain

$$\vec{g}(N) = C^{-1}(N) \cdot \vec{\gamma}(N)$$
 (5.29)

In terms of $\vec{\gamma}$ and \vec{g} , the mean and variance can be expressed as

$$\mu_*(N) = \vec{X} \cdot \vec{g},\tag{5.30}$$

where we use $\vec{X} = (X_{t_1}, \cdots, X_{t_N})$ for short, and

$$\sigma_*^2(N) = 2 \, (t^*)^{2H} - \vec{\gamma} \cdot \vec{g}. \tag{5.31}$$

Since $\vec{\gamma}^T \vec{g} = \vec{\gamma}^T C^{-1}(N) \vec{\gamma} > 0$, conditioning on more points diminishes the variance of a midpoint. The outer product of \vec{g} defines the matrix

$$G(N) := \vec{g} \otimes \vec{g}^T . \tag{5.32}$$

It is used to build the enlarged inverse correlation matrix

$$C^{-1}(N+1) = \frac{\left(C^{-1}(N) + \sigma^{-2}G(N) \mid -\sigma^{-2}\vec{g}(N)\right)}{-\sigma^{-2}\vec{g}^{T}(N) \mid \sigma^{-2}} , \qquad (5.33)$$

where $\sigma^2 = \sigma_*^2(N)$. In our implementation entries in $\vec{\mu}, \vec{g}, C^{-1}$ etc. are generally not in order of time but in order of their addition to the grid.

5.2.3.G Bridge selection

The task of the bridge-selection routine (cf. Alg. 5.2.3) is to choose the order in which bridges of the successively refined grid are tested, and possibly inserted. Its aim is to find the firstpassage event with the least number of bisections. To this aim, it zooms in into areas where a first-passage time is likely, and zooms out when the possibility of a crossing becomes negligible. In this subsection, we phrase this intuition in more rigorous terms.

Prior to the first call of the routine, the initial grid consists of 2^g bridges of uniform width 2^{-g} . The routine selects the earliest bridge, *i.e.* $(t_1 = 0, t_r = 2^{-g})$, and scans all bridges of the initial grid in ascending order in time until a critical bridge is found (by applying the criticality criterion (5.19)). Once such a bridge is found, the algorithm explores this bridge by successive bisections. After a finite number of bisections the algorithm either has identified a first-passage event to the desired precision, or no crossing was found. In the latter case, the routine then moves on to the next bridge of the initial grid.

In order to illustrate the workings of the bridge-selection routine, it is helpful to consider a bijection between the adaptively bisected grid and a rooted binary tree (cf. Fig. 5.1). Every bridge (t_1, t_r) that is bisected by introducing a point at t_m contains two sub-bridges (t_1, t_m) and (t_m, t_r) . We refer to these bridges as the *left* and *right* children of (t_1, t_r) . Vice versa, every bridge that is not part of the initial bridge (*i.e.* with level $\ell > g$) is the child of another bridge which is referred to as parent of the bridge. The set of all bridges that are contained in a initial bridge of width 2^{-g} is mapped to a rooted binary tree by identifying every node with a bridge, where a node can either have zero or two children depending on whether the bridge has been bisected or not. The root of the tree corresponds to the bridge contained in the initial bridge from where the bisections were spawned off. The generation of a node in the tree corresponds to its level by

generation = $\ell - g + 1$. Therefore, the depth of the tree is limited to generation_{max} = L - g + 1.

The routine stores a representation of this tree internally, together with the information whether a node/bridge has previously been checked for criticality or not. If a bridge is bisected, but its two children have not yet been checked for criticality, the left child is selected. This is because earlier crossings of the threshold render later crossings irrelevant. If a bridge has two children, but the left has already been checked (implying that neither it nor any of its further descendants contains a first-passage event), the right child is selected. If both children of the bridge have already been checked, none of the descendants contains a first-passage event. In that case the parent of the bridge is returned (zooming out). If the routine returns to the root, the bridge of type $(i2^{-g}, (i+1)2^{-g})$ has no parent, and the next such bridge $((i+1)2^{-g}, (i+2)2^{-g})$ is returned. If $i = 2^g - 1$, the routine terminates by returning an empty bridge since the entire grid has been checked. This selection routine implies that in the "worst case", when every point of the initial grid $\mathcal{T}^{(0)}$ lies in the critical strip without ever crossing the threshold m, every single sub-interval will be analysed. This means that in a worst-case scenario up to 2^g search trees (cf. Fig. 5.1) would be generated, each tree containing up to $2^{L-g} - 1$ nodes. This scenario is extremely unlikely

To summarise, the routine is either descending (zooming in) or ascending (zooming out) within the tree, depending on whether the children of a node, if existent, have been visited or not.

The routine takes into account two additional constraints. First, the maximum bisection level L; if a bridge of maximum level L contains a first-passage event, the routine terminates since this estimate has reached the desired resolution. If it contains no crossing, the parent is returned. Second, it takes into account whether a bridge is early enough in time to improve the first-passage estimate. If a bridge at level ℓ records a first-passage event, only its descendants can improve this result.

We give the pseudocode of the routine below. In the implementation we present later (Sec. 5.3.1), the algorithm is implemented slightly differently for performance reasons. The logical steps however are the same and we decided to present them here for pedagogical reasons.

5.2.4 Adding deterministic functions

The adaptive bisection routine can be adapted to further generate first-passage times of stochastic processes of the form

$$Z_t = X_t + f(t), (5.34)$$

where f(t) is a deterministic smooth function, *e.g.* a linear or fractional drift term, and X_t is again a fractional Brownian motion. In its first phase, X_t is generated on a subgrid, and f(t)is added accordingly. The resulting process $Z_t, t \in \mathcal{T}^{(0)}$ is then passed to the bridge-selection routine, where the bridges are checked for criticality using the values of Z_t in the criticality criterion (5.21). Once a bisection is required, the midpoint is generated using the subtracted process $X_t = Z_t - f(t)$, *i.e.* the vector used to generate the midpoint's mean (cf. Eq. (5.27)) is \vec{X} , not \vec{Z} . Then, the generated midpoint X_m is transformed back using $Z_m = X_m + f(t_m)$, and

Algorithm	2 :	Finding	the	\mathbf{next}	bridge	\mathbf{to}	\mathbf{be}	checl	ked
0									

$\mathbf{if} \ (t_{\mathrm{l}},t_{\mathrm{r}}) = 0 \ \mathbf{then}$	ise with first bridge
	ise with first bridge
return $(0, 2^{-g})$ \triangleright Initiali	0
if (t_1, t_r) has no children then	
return parent bridge	
if (t_1, t_r) early enough for τ_m AND level $< L$ then	
if left child not checked then	
return left child	$\triangleright \ {\rm Move \ down \ left}$
${f if}$ left child checked AND right child not checked ${f then}$	
return right child	\triangleright Move down right
\mathbf{if} both children checked \mathbf{then}	
return parent bridge \triangleright	Move up to parent
if level of $(t_1, t_r) = L$ then	
if Bridge crosses threshold then	
return NULL	
else	
return parent bridge	

inserted into the path of Z. Note that even if $f(t) = \mu t$ (linear drift), and contrary to Brownian motion, the iteration can not be performed directly on Z_t .

5.2.5 Further generalisations

The underlying idea of the algorithm – to generate a grid that is fine only where it matters – lends itself to various other non-local observables, in particular extreme events, such as running maxima (minima), positive time (time spent in the region $X_t > 0$), last returns, or the range or span (max $X_t - \min X_t$) of a process.

In each of these examples, one needs to adapt two logical steps in the procedure; (i) the order in which bridges of the grid are iterated, and (ii) the criterion for triggering a bisection. For first-passage times, the order of the bridges is given by the subroutine described above in Sec. 5.2.3.G. The criterion for bisection is determined by the bridge's distance to the threshold. These two choices are particular to first-passage events.

For running maxima, the bridges should be tested in descending order of height, and the bisection-criterion adapted to decide whether the midpoint could surpass the current maximum with a probability larger than ε . If the current maximum changes, the criterion for triggering a bisection also changes. As the maximum can only increase, bridges which were uncritical before do not become critical by a change of the estimate of the maximum.

To find the last return to zero $(t_0 = \sup_{t' < t} \{t' | X_{t'} = 0\})$, the bisection criterion is the same as for first-passage times (with *m* set to zero), but bridges should be iterated over from latest to earliest, choosing the right subinterval first after bisection (cf. Fig. 5.1).

The span of a process at time t is defined as the running maximum minus the running minimum [246, 247, 176, 250, 251]. To find the first time the span reaches one is more delicate. There are two cases, given a discretization. Either span one is reached first when the maximum increases, or the minimum decreases. Suppose that the maximum increases. Then there is



Figure 5.1.: Illustration of the adaptive bisection routine. The grid \mathcal{T} (bottom) contains points in time, here detail shown of initial bridge $t_{\rm l} = i2^{-g}$, $t_{\rm r} = (i+1)2^{-g}$ (labelled bullets) and successively introduced midpoints (bullets on time axis); The path \mathcal{X} (above) samples values at times (dashed lines) which approximate path by linear interpolations (grey and black thick lines). The threshold m (red uppermost horizontal line) is crossed by the path and bisections are generated for every bridge whose endpoints lie in the critical strip corresponding to its level (blue vertical lines underneath). The horizontal arrows on top of the path indicate the bridges in between the grid points. The mapping from bridges to binary tree (top) is indicated with dotted lines. The top node (1) corresponds to the widest bridge $(i2^{-g}, (i+1)2^{-g})$, and children correspond to sub-intervals generated by midpoint. The bridges are explored in order as given by numbers above nodes and chosen by the bridge-selection routine (see text for details). Bridges that are critical (blue filled nodes) are bisected, and their children checked from left to right, until a first-passage event has been identified at maximum bisection level L (red filled node '7'). This event terminates the algorithm. In contrast to Node 1 which belongs to the initial grid $\mathcal{T}^{(0)}$, Nodes 2 to 7 stem from adaptive bisections and contribute to the total count of bisections M. The maximum number of nodes which could theoretically be spawned off this particular sub-interval is $2^{L-g} - 1$. This figure is accepted for publication as [242]. See App. A.4 for approval of co-authors.

a minimum for a smaller time. By refining the grid close to this minimum, the latter may decrease. This in turn shifts down the critical strip for the maximum, and one has to redo all checks for bridges close to the maximum.

The algorithm can be generalized to other Gaussian processes, since the derivations given in Sec. 5.2.3.F and App. 5.B for the insertion of a conditional midpoint apply to *any* Gaussian process. The only point at which we made explicit use of properties for fBm was at the initialisation step, where the Davies-Harte method was employed to generate a path on a coarse dyadic lattice. If one were to study another Gaussian process, one would need to replace the correlation function (5.4), and adapt the routine generating the initial grid.

Once these modifications are made for the new problem, we expect the algorithm to deliver similar improvements in performance and memory.

5.3 Results and Benchmarking

In this section, we compare an implementation of our adaptive bisection method (ABSec) with an implementation of the Davies-Harte (DH) method. Our focus lies on comparing both CPU time and memory usage for a simulation of equal discretization error. We find that for large system sizes, $N_{\text{eff}} \gtrsim 10^{2/H}$, the adaptive bisection routine outperforms the Davies-Harte method both in CPU time and memory. This advantage grows markedly for lower values of H. At H = 0.33, for instance, and a final grid size of $N_{\text{eff}} = 2^{32}$ we need 5000 times less CPU time and 10 000 less memory. At H = 0.25 we find ABSec to be 300.000 times faster and 10⁶ less memory intensive than DH at an effective system size of $N_{\text{eff}} = 2^{42}$.

We then discuss systematic errors and analyse how they depend on the parameters, in order to clarify the payoff between computational cost and numerical accuracy. We conclude with a discussion of our findings.

5.3.1 Implementation in C

We implemented the adaptive biection algorithm in C, using external libraries lapack [5], gsl [91], fftw3 [90], and cblas [24]. The code is published [241] and available under a BSD license. It was compiled using the Clang/LLVM compiler using the -03 flag as only compiler optimisation. The code was executed on an 'Intel(R) Core(TM) i5-7267U CPU 3.10GHz' processor.

As reference, we use an implementation of the Davies-Harte method in C^1 . Compiler settings and hardware are identical to those used for the adaptive bisection algorithm.

In order to compare performance, we used user time and maximum resident set size as measured by the POSIX command getrusage; user time indicates the time the process was executed in user space, and maximum resident set size the amount of RAM held by the process.

5.3.2 Numerical errors and fluctuation resolution

The adaptive bisection algorithm suffers from three errors.

¹B. Walter, K. J. Wiese, https://github.com/benjamin-w/davies-harte-fpt.git

(i) the resolution of the grid itself, determined by the maximum grid size if all bridges were triggered, which we refer to as *horizontal error*. Any discretization of a continuous path suffers from errors that are made when replacing the rough continuous path by the linear interpolation of a grid. Even if the true first-passage time is optimally approximated, the error still depends on the system size N. In that respect, our algorithm does not differ from DH or other exact sampling methods.

(*ii*) the adaptive bisection routine suffers from a probabilistic error, namely false negative results of the criticality check, *i.e.* bridges which do contain an excursion crossing the threshold m, but whose endpoints do not lie in the critical strip (cf. Sec. 5.2.3.E). We refer to these errors as *vertical errors*.

(*iii*) the algorithm suffers from rounding errors of the floating-point unit.

Horizontal errors correspond to the resolution of the process' fluctuations. To contain fluctuations of a fBm between two grid points at distance N^{-1} to the order of δX , one needs to choose $N \sim (\delta X)^{-\frac{1}{H}}$. Horizontal errors are therefore characterised by the effective discretization resolution $N^H \sim (\delta X)^{-1}$ which corresponds to the inverse fluctuation resolution. In order to compare two discretizations of a fBm path for two different values of the Hurst parameter H, comparing N is misleading. Rather, we compare their effective discretization resolutions N^H . Horizontal errors are impossible to measure numerically, since there exists no way to simulate a continuous path. They are however independent of the sampling method used; this implies that the horizontal error of a path generated by DH with system size 2^L and an adaptive bisection routine of maximum bisection level L are *exactly* the same, given no vertical error occurred. For a deeper discussion of discretization errors of the DH algorithm, see [251, Sec.V.E].

Vertical errors are controlled by the error tolerance ε' , of Eqs. (5.21)-(5.22). To study vertical errors systematically, one needs to compare the results with a fully sampled grid using (for instance) DH. This is discussed in the next section.

In the remainder of the section, we run benchmarking experiments that repeat the adaptive bisection routine a large number of times, typically $I = 10^4$. Following the insights of Sec. 5.3.3, we choose an error tolerance that is small enough to neglect errors of the vertical kind (whenever the vertical error rate is much smaller than I^{-1}). In doing so, we can ignore the vertical error such that the numerical discretization error becomes a good common error for both adaptive bisections and DH. This allows us to compare grids sampled with both methods systematically across various values of H and L.

Finally, errors due to the finite precision of the floating-point unit are considered. These arise in the matrix inversion (5.33), where inspection reveals terms of opposite sign. They can be detected by plotting $\sigma_*^2(N)$ as a function of grid resolution. For small grids, $\sigma_*^2(N)$ almost follows a power-law, with little spread. Numerical errors are visible as a net increase of this spread, see Fig. 5.8. To be on the safe side, we choose the maximal L to be 4 less than the point where we first see numerical errors appear.

5.3.3 Error rate depending on ε'

This section addresses the question of vertical errors, *i.e.* bridges that were deemed uncritical by the adaptive bisection routine (cf. Sec. 5.2.3.E), yet contained an excursion that crossed the threshold for the first time. This probability, $P(X_{t_m} > m)$, where X_{t_m} marks the midpoint of



Figure 5.1.: Error rate from phone book test for various values of ε' for H = 0.33. The error rate is almost identical when changing the initial grid size from 2^8 (red square marks) to 2^4 (blue triangle marks) at the same maximum bisection level L = 20. When lowering the maximum bisection level to L = 16, the error rate improves. The relation between error rate and error tolerance decreases approximatively linearly over several orders of magnitude (compare with solid gray line). The total error rate is approximately $10\varepsilon'$ for L = 20 (solid gray line) and about $3\varepsilon'$ for L = 16(dashed gray line). Note that the prefactor is much smaller than the number of points, which can read off from Fig. 5.3. Error rates were averaged over 10^5 to 10^6 iterations. This figure is accepted for publication as [242]. See App. A.4 for approval of co-authors.

a bridge, was bounded using an error tolerance ε' . Therefore, we need to know how ε' controls the error rate. Since we can only measure the error rate when compared to another numerically generated grid, we compare our algorithm to a path generated using the Davies-Harte algorithm of equal precision. The procedure is as follows. In a first step, the Davies-Harte method is used to generate a path on the dyadic lattice Λ^L . For this path, and a threshold m, the first-passage time is calculated using its linear interpolation as detailed in Sec. 5.2.3.B. Then, only times in the subgrid $\Lambda^g \subset \Lambda^L$ are copied into a second path. This path is handed over to a modified adaptive bisection routine (cf. Alg. 5.2.3). The bridges of the grid are successively checked, at each step deciding whether to bisect as discussed in Sec. 5.2.3.E. Once a midpoint needs to be drawn, it is not randomly generated, but taken from the full grid at the same time. The full grid thus serves as a *phone book* for the adaptive bisection algorithm, where points are *looked* up if they lie at points the algorithm would have otherwise generated randomly. The algorithm then outputs its own estimate of the first-passage time. If the first-passage times disagree, this is considered an error. We refer to this check as *phone book test*. This test is iterated 10⁶ times, and the error rate $P_{\text{error}}^{\text{tot}}$ is defined as the ratio between errors and the number of iterations.

The results are shown in Fig. 5.1, where we compare the error-rate for different values of ε' and for three different grids of varying initial grid size, and maximum bisection levels. The plot shows that the total error rate and error tolerance ε' depend on each other linearly, indicating that ε' is a suitable replacement for ε introduced in Eq. (5.16). The plot further shows that



Figure 5.2.: Average number of new midpoints generated at bridge level ℓ , for various values of H (solid, dashed, dash-dotted, and dotted lines) as a function of ℓH . For equal values of ℓH , lower Hurst parameter implies a larger number of average bisections. These numbers are virtually independent of the initial grid size, as is shown for Λ^4 (circle marks) and Λ^8 (triangle marks). This figure is accepted for publication as [242]. See App. A.4 for approval of co-authors.

the error rate remains almost identical when replacing the initial grid Λ^8 by Λ^4 (which contains 16 points only). Further, the error rate improves if the maximum bisection level is lowered. When lowering the effective system size from 2^{20} to 2^{16} , the error rate lowers approximately by a factor of three.

In summary, this plot confirms that the computationally cheap variant (5.19) allows us to control the vertical errors (false negative results of the criticality test).

5.3.4 Average number of bisections

In this section, we investigate how many points are added to the initial grid, and how the additionally inserted midpoints are distributed over the different generations. The number of midpoints generated, M, is the main expense of computational resources, since each point requires promoting an inverse correlation matrix from size n to n + 1 requiring $\mathcal{O}(n^2)$ steps.

Each midpoint that is generated bisects a bridge at level ℓ and creates two sub-bridges at level $\ell + 1$. In order to know how the algorithm spends most of its time, we simulated the adaptive bisection routine 10⁴ times over an initial grid of size Λ^4 or Λ^8 and measured the average distribution of the *M* newly generated midpoints over the different levels. The results are shown in Fig. 5.2.

While the distribution remains virtually unchanged when replacing the initial grid by Λ^8 , its shape changes for different values of Hurst parameter H. For $H > \frac{1}{2}$, the distribution remains flat and even descends for $\ell > 5/H$. For $H = \frac{1}{2}$ it remains constant for $\ell > 8$ (at around 11 midpoints per generation), while for $H < \frac{1}{2}$ (see figure for $H = \frac{1}{3}$ and $H = \frac{1}{4}$), the number of inserted midpoints increases, and tends to be at higher bridges.

Since the number of additionally inserted points M is crucial to the performance of ABSec,



Figure 5.3.: Average number of bisections M as a function of the maximum bisection level L (i.e. $N_{\text{eff}} = 2^L$) for different values of H (diamond, circle, upright and upside down triangle marks). Inset shows M versus LH. As long as $H \ge 0.33$ growth is asymptotically approximately linear in L, corroborating $M \sim \ln(N_{\text{eff}})$. For smaller values of H, either the linear regime is not yet reached, or the growth is stronger. (5000 iterations with initial grid Λ^8 and error tolerance $\varepsilon' = 10^{-9}$). For H = 0.5, extrapolation was used. This figure is accepted for publication as [242]. See App. A.4 for approval of co-authors.

the routine is designed to minimise this number, with a hypothetical minimum of L - g points (when finding the first-passage event with no fault). The hypothetical maximum corresponds to a full bisection of the grid which would require $2^L - 2^g \approx 2^L$ additional points (this occurs when the path does not cross the threshold at all and $\varepsilon' \to 0$). In Fig. 5.3, we show the total number of bisections M for various system sizes L, averaged over 10^4 realisations. The number of additional points ranges from 40 to 1500, where larger system sizes lead to an increase of M. For H = 0.33 and L = 32, the average of additional points is M = 710 which corresponds to 1.6×10^{-7} of the full grid. This means that with that fraction of the full grid only, the algorithm identifies the first-passage time to the same accuracy as DH (up to vertical errors controlled by $\varepsilon' = 10^{-9}$ in this case).

We observe that for values of $H \gtrsim \frac{1}{3}$, the number of bisections grows first sublinearly and then linearly in L. This behaviour changes for values $H \lesssim \frac{1}{4}$, where growth is stronger, and we may not yet be in the asymptotic regime. This is also indicated by the profiles shown in Fig. 5.2, where for lower values of H the distribution ceases to tend to a plateau, but grows for higher levels of bisection ℓ .

5.3.5 Computing time and complexity estimate

In this section, we analyse how the performance of our algorithm varies with different parameters, and how it compares to DH. In loose terms, we expect the initial grid, generated by DH, to cost $\mathcal{O}(2^g \ln(2^g))$, and each of the *M* bisections to cost k^2 with *k*, the number of gridpoints,



Figure 5.4.: Average user time required to find first-passage time in a grid of effective discretization precision 2^{-LH} . The dashed lines indicate user time for Davies-Harte method, solid lines for the adaptive bisection method. The three different colours indicate H = 0.33, 0.5, 0.67 (bottom, centre, top pairs of lines). Simulations were run 10^4 times for $\varepsilon' = 10^{-9}$ and for two different initial subgrid sizes (Λ^4 circle marks; Λ^8 square marks). For H = 0.33 (top solid blue lines), the effective system sizes range from L = 4 to 32 for Λ^4 , and L = 12 to 28 for Λ^8 . For H = 0.5 (centre solid green lines), L ranges from 4 to 22 for Λ^4 and from L = 12 to 22 for Λ^8 . For H = 0.67(bottom solid red lines), L ranges from 4 to 16 for Λ^4 and 12 to 16 for Λ^8 . This figure is accepted for publication as [242]. See App. A.4 for approval of co-authors.

i.e. costs, or more precisely the algorithmic complexity, should behave as

$$\mathcal{C}^{\text{ABSec}}(g,M) \sim \sum_{k=2^g}^{2^g+M} k^2 \approx \frac{1}{3} (2^g+M)^3 .$$
 (5.35)

It is therefore evident that the majority of the computational cost lies in the bisection phase, and the overall complexity is of order $\mathcal{O}((2^g + M)^3)$. When comparing this to the complexity of generating 2^L gridpoints with DH, which is $\mathcal{O}(2^L \ln(2^L))$, one estimates that ABSec outperforms DH whenever $M^3 \ll 2^L \ln(2^L)$. As is shown below, ABSec outperforms DH for $L \gtrsim 12$ to 16.

We define the performance of the algorithm via its user time, *i.e.* the share of the CPU time the process spends in user space. This means that, depending on the implementation, the total of CPU time ("wall time") might differ. User time is a more robust observable, so we use it as best approximation to the performance of the implementation.

We measure the average user time per generated first-passage time, using either DH or ABSec. To render different Hurst-values and algorithms comparable, we plot the user time versus the inverse of the effective discretization error, which scales as N^H for DH and 2^{LH} for ABSec. It describes how well the fBm-path is resolved numerically, taking into account the fluctuation scaling for different Hurst-parameters.

Since at the beginning of the ABSec procedure inverse correlation matrices are tabulated (cf. section 5.2.3.D), we measured the run time for 10^4 iterations, in order to render the initial overhead irrelevant.

Fig. 5.4 shows the result of the benchmarking. For small effective system sizes, ABSec performs slower than DH, which is due to the relatively complex overhead of bisections. For (effective) system sizes of $N \gtrsim 10^{\frac{2}{H}}$ the ABSec algorithm gains an increasing and significant advantage since its run time only grows sublinearly.

To estimate the performance time, we observe that for values of $H \ge 0.33$, the number of additional gridpoints M grows linearly in the logarithm of the effective system size (cf. Fig. 5.3) throughout the entire observed range. Based on our empirical findings, we propose a linear relation $M \sim L = \ln_2(N_{\text{eff}})$, which implies, cf. Eq. (5.35), an overall computational complexity of

$$\mathcal{C}^{\text{ABSec}}(N_{\text{eff}}) = \mathcal{O}\left(\left(\ln N_{\text{eff}}\right)^3\right) , \qquad H \gtrsim \frac{1}{3} , \qquad (5.36)$$

since eventually $M \gg 2^g$ for N_{eff} large enough (cf. Fig. 5.3 for $H \gtrsim \frac{1}{3}$). This estimate is corroborated by Fig. 5.6, where the scaling of user time with system size agrees with our estimate of $(\ln N_{\text{eff}})^3$ for sufficiently large system sizes. The linear relation between the number of bisections M and the logarithmic system size L, however, does not extend to smaller values of H, where Fig. 5.3 indicates super-linear growth. Still, testing the ABSec routine at H = 0.25for an effective system size of $N_{\text{eff}} = 2^{42}$ gave an average user time of 6.2s and was about 300000 faster than an extrapolation of the user time for DH at the same system size.² This shows that for all practical purposes, ABSec remains a much faster algorithm even at parameters where estimate (5.36) seems to no longer hold.

For H = 0.33, due to memory limitations, DH is unable to generate paths larger than $N = 2^{24}$, where ABSec is already about 40 times faster. Since ABSec is also more memory-efficient (see next section), we can generate grids of size up to 2^{32} for which, if we interpolate the growth of DH³, we find that ABSec is 5500 times faster than DH for these parameters. For $H > \frac{1}{2}$, the advantage is less pronounced, and at a comparable discretization precision, the algorithm is "only" 40-50 times faster at H = 0.67.

Performance also depends on the initial grid size. In Figs. 5.4 and 5.5, we compare run times for two different initial grids, Λ^4 and Λ^8 . For larger initial grid sizes, the algorithm is slower since more points need to be generated initially. An increase in initial grid size leads to a decrease of 15% (for H = 0.33) in the average number of bisections. This is approximately outweighed by the time DH takes to generate a path on Λ^8 (cf. Fig. 5.4).

The run time increases only slowly for a smaller error tolerance. In Fig. 5.5, we show how user time decreases when changing ε' from $\varepsilon' = 10^{-9}$ to $\varepsilon' = 10^{-7}$. For an effective precision of $2^{\frac{32}{3}}$, user time increases by roughly 60 %. Since error rates grow linearly with ε' (see Fig. 5.1), we conclude that for an error rate 100 times lower one only needs to invest 60% more user time.

All together, these observations show that the algorithm behaves in a controlled manner for varying error tolerances and initial grid sizes. Depending on the number of iterations, and the quality of the data desired, choosing g (initial grid size), L (desired precision), and ε' (error tolerance level) accordingly leads to an algorithm that performs up to 5000 times faster than DH at H = 0.33, that was hitherto very hard to access with high precision. The algorithm should be tested more for H = 0.25, where it allows one to reach a precision unimaginable by DH.

²This experiment was run with an initial grid Λ^4 and $\varepsilon' = 10^{-9}$.

³Since DH scales with $N \ln(N)$, we fit with $f(N; a, b, c) = N (a \ln(N) + b) + c$.



Figure 5.5.: User time for ABSec (solid lines) compared to DH (dashed line) for two different initial grid sizes and two different values of error tolerance ε' . For a hundred times higher error tolerance (top semi-transparent pair of lines), user time increase by up to 60%. This figure is accepted for publication as [242]. See App. A.4 for approval of co-authors.



Figure 5.6.: $(t_{\rm user}/{\rm iteration})^{1/3}$ plotted versus effective discretization N^H for various values of H (blue circle marks H = 0.33, green square marks H = 0.5, red diamond marks H = 0.67, cf. Fig. 5.4). They corroborate the estimate of $C^{\rm ABSec} \sim (\ln N_{\rm eff})^3$. Straight lines indicate fits of the form $a \ln(N) + b$ versus $t_{\rm user}^{1/3}$ implying a scaling of $t_{\rm user} \sim a^3 (\ln(N_{\rm eff})^3) + \mathcal{O}((\ln N_{\rm eff})^2)$. This is in agreement with the complexity estimate in Eq. (5.36). The inset shows the ratio between data points and the fit. This figure is accepted for publication as [242]. See App. A.4 for approval of co-authors.



Figure 5.7.: Memory usage for DH (dashed line) and ABSec (solid line) for two different initial subgrid sizes. DH scales linearly in N, while ABSec grows only slowly (see text for estimate). For system of size $N_{\rm eff} = 2^{28}$, ABSec needs only 10^{-2} to 10^{-3} of the memory for DH. For larger systems or smaller H, the advantage of ABSec is even bigger. Measurements were taken after 10^4 iterations. This figure is accepted for publication as [242]. See App. A.4 for approval of co-authors.

5.3.6 Memory requirements

As a final benchmark of our algorithm, we consider memory usage. The latter is defined by the resident set size of the process, as measured by **getrusage**. When using DH, the full grid needs to be saved, and in doing so memory usage scales like N. Fig. 5.7 shows memory usage for both DH and ABSec when performed for different effective discretization precisions and initial grid sizes. It shows that for large system sizes, ABSec gains a growing and significant advantage. To generate a path of 2^{28} lattice points in double precision via DH, one requires 10 GB working memory, whereas ABSec uses between 20 and 80 MB, depending on the initial grid size. This represents an improvement by a factor of 125 to 500. This is due to the fact that only the initial grid which scales as $\mathcal{O}(2^g)$, the additional gridpoints of order $\mathcal{O}(M)$ and a correlation matrix, scaling as $\mathcal{O}(2^g + M)^2$, need to be stored. As implemented, additional memory is needed for the catalogue of inverse correlation matrices (cf. Eq. (5.15)) which occupies memory of order $\mathcal{O}(2^{3g})$, so including the catalogue overall memory space grows like $2^{3g} + (2^g + M)^2$. For N_{eff} large enough, we assume that $2^g \ll M$, such that asymptotically for large effective system sizes the necessary memory grows as order M^2 . For values of $H \gtrsim \frac{1}{3}$, we empirically found that $M \sim \ln(N_{\text{eff}})$, such that in that parameter range we estimate memory to grow as

$$\mathcal{M}^{\text{ABSec}}(N_{\text{eff}}) = \mathcal{O}\left(\left(\ln N_{\text{eff}}\right)^2\right), \qquad H \gtrsim \frac{1}{3}.$$
 (5.37)

This advantage is again due to $M \ll 2^L$, *i.e.* using the fact that the first-passage time can be found to equal precision with much less grid points.



Figure 5.8.: Ratio between sampled variance and no-neighbour-estimate of variance (cf. Eq. (5.18)) of an inserted midpoint X_m versus the level of the bisected bridge. For H = 0.5 (green diamond marks), the ratio equals 1, as BM is Markovian. For $H \neq 0.5$ (red square marks H = 0.67, blue circle lines H = 0.33), the variance fluctuates, as shown by the error bars for one standard deviation. Numerical errors due to a loss of floating point precision become relevant around $L_{\max} \simeq 11/H$. ABSec was used with an initial grid Λ^8 and $\varepsilon' = 10^{-9}$. This figure is accepted for publication as [242]. See App. A.4 for approval of co-authors.

5.3.7 Floating point precision

Currently, our implementation uses the 64-bit double type. Since the variance of a bridge-point is calculated from the subtraction of quantities of $\mathcal{O}(1)$ (cf. Eq. (5.31)) whose difference can be as small as $\mathcal{O}(2^{-LH})$, the subtraction suffers from the finite floating-point precision when L is too large, as is demonstrated in Fig. 5.8 (cf. caption for details). This leads to $L_{\text{max}} \simeq 10.5/H$, or $N_{\text{eff}} \simeq 2 \times 10^{\frac{3}{H}}$.

5.3.8 Discussion

In this section we illuminated several aspects of our algorithm that show how it is capable of generating first-passage times with high numerical precision using several orders of magnitude less CPU time and memory as compared to DH. We chose to compare ABSec to DH because the latter is widely spread in simulating first-passage times of fBm (see *e.g.* [106, 149]), and since it is the fastest known exact generator of fBm. Since our method is also exact (the statistics of the grid generated is bias-free), we think of DH as the natural benchmark. There are related approximative algorithms like the random midpoint displacement algorithm $R_{\ell,r}$ that also inserts midpoints, only taking into account the ℓ left and r right nearest neighbours [173]. This neglects long-range correlations between small increments at t_1, t_2 which even for $t_1 \ll t_2$ are correlated algebraically via $(t_1 - t_2)^{-1} + \mathcal{O}\left((H - \frac{1}{2})^2\right)$ (for $H \neq \frac{1}{2}$). The ABSec algorithm uses the full inverse correlation matrix of all points generated and is therefore closely related to exact procedures like DH.

Supported by our experiments, we are able to control both vertical and horizontal errors at

the scale of inherent errors of a Monte Carlo simulation. In practice, the limiting factors are not systematic errors of the algorithm but floating point imprecisions stemming from the matrix inversion.

The phone-book test used to asses the error rate does not take into account issues of precision when drawing new midpoints, which are copied from a pre-generated grid. Since this is an implementation-dependent grid, we decided to only use the phone-book test since the errors caused in that procedure are the ones inherent to the algorithm itself. An implementation with a higher-precision floating-point unit seems highly desirable.

5.4 Summary

When simulating first-passage times, or any other non-local observable, of fractional Brownian Motion, the large fluctuations for $H < \frac{1}{2}$ require the grid to have a very high resolution for the same quality of data as for $H \ge \frac{1}{2}$. Generating a fine grid is particularly expensive, both in memory and time. The algorithm proposed here refines the grid only where it is likely to impact the first-passage event. To give rigorous notion to that idea, we developed a precise criterion for when and where the grid should be refined. The new mid-points are then sampled exactly. Comparing it to the fastest known exact sampler, the Davies-Harte algorithm, we find that our implementation of the algorithm is 5000 times faster and uses 1000 times less memory when applied to H = 0.33 at $N_{\rm eff} = 2^{32}$, due to the fact that only roughly 0.1% of the full grid is needed to determine the first-passage event. Our algorithm works with a probabilistic approximation, and the error rate can be bounded by 10^{-6} or even 10^{-8} . This should be sufficient for most Monte Carlo experiments and be in the order of numerical (algorithm-independent) errors.

We have successfully used the algorithm to validate the analytic results for the first-passage time in Chp. 6. There we used 2.5 CPU years at precision $N = 2^{28}$. With DH we would have had to reduce the precision to $N = 2^{24}$, which still would have taken 75 CPU years.

Finally, the concepts presented here can be used for other observables and other Gaussian processes. We hope that our algorithm contributes to confirming theoretical predictions on extreme events in Gaussian processes that where hitherto numerically inaccessible at the required precision.

Appendix

5.A Derivation of the critical strip length

In this section we derive the width of the critical strip which was introduced in Sec. 5.2.3.E. The critical strip refers to the distance between a fBm-bridge of size $\delta t = 2^{-\ell}$ and the threshold m, below which the midpoint of the bridge may surpass the threshold with probability larger than ε . We ignore any other grid points beyond the two fixed bridge points. By translational invariance, we set $X_0 = 0$, and $X_{\delta t} = a$ ($a \in \mathbb{R}$). The problem is then equivalently stated as

$$P(X_{\delta t/2}^{\mathrm{B}} > c(\varepsilon)) = \varepsilon, \qquad (5.38)$$

where X_t^{B} is the fBm-bridge process conditioned on $X_0, X_{\delta t}$. Following the derivation in [62], the law of the fBm-bridge is itself a Gaussian process with first and second moment,

$$\left\langle X_t^{\rm B} \right\rangle = \frac{\left\langle X_t \delta(X_{\delta t} - a) \right\rangle}{\left\langle \delta(X_{\delta t} - a) \right\rangle} ,$$
 (5.39)

$$\left\langle X_s^{\rm B} X_t^{\rm B} \right\rangle = \frac{\left\langle X_s X_t \delta(X_{\delta t} - a) \right\rangle}{\left\langle \delta(X_{\delta t} - a) \right\rangle} ,$$
 (5.40)

where on the right-hand-side the averages are over free fBm paths. As shown in Resf. [62], Eqs. (8) and (9), the averages are

$$\left\langle X_t^{\rm B} \right\rangle = a \frac{C(t, \delta t)}{C(\delta t, \delta t)}$$
(5.41)

$$\left\langle X_s^{\rm B} X_t^{\rm B} \right\rangle^{\rm c} = C(s,t) - \frac{C(s,\delta t)C(t,\delta t)}{C(\delta t,\delta t)} , \qquad (5.42)$$

where C(s, t) is the correlation function of Eq. (5.4). Since we are only interested in the midpoint with $s = t = \delta t/2$, this yields

$$\mu = \left\langle X_{\delta t/2}^{\mathrm{B}} \right\rangle = \frac{a}{2} , \qquad (5.43)$$

$$\sigma = \left\langle (X_{\delta t/2}^{\rm B})^2 \right\rangle^{\rm c} = \left(2^{1-2H} - \frac{1}{2} \right) (\delta t)^{2H} \quad . \tag{5.44}$$

This determines the normal distribution of the midpoint and by translational invariance proves the values used in Sec. 5.2.3.E.

5.B How to generate an additional random midpoint

We derive the conditional law of an additional randomly generated midpoint for an arbitrary Gaussian processes as given in Eqs. (5.26)–(5.27). Let $\mathcal{T}^N = t_1, \dots, t_N$ and $\mathcal{X}^N = X_{t_1}, \dots, X_{t_N}$ be given, and denote the point to be inserted by t_{N+1} and $X_{t_{N+1}}$ (the times are not ordered). For ease of notation, we write $X_i = X_{t_i}$. As a Gaussian process, the vector $\vec{X} = (X_1, \dots, X_N, X_{N+1})^T$ is a normal random variable with mean zero and covariance matrix

$$\left\langle \vec{X} \otimes \vec{X} \right\rangle = C(t_i, t_j) =: C(N+1) , \quad 1 \le i, j \le N .$$
 (5.45)

It has a symmetric inverse correlation matrix $C_{i,j}^{-1}$. Its probability law is therefore given by

$$P(\vec{X}) = \frac{\exp\left(-\frac{1}{2}\sum_{i,j=1}^{N+1} X_i C_{i,j}^{-1} X_j\right)}{\sqrt{(2\pi)^{N+1} \det(C)}} .$$
(5.46)

Since X_1, \dots, X_N are fixed, X_{N+1} conditioned on \mathcal{X}^N follows the marginal distribution

$$P(X_{N+1}|\mathcal{X}^N) = \frac{\exp\left(-\frac{1}{2}X_{N+1}^2C_{N+1,N+1}^{-1} - \sum_{j=1}^N X_jC_{N+1,j}^{-1}X_{N+1}\right)}{\sqrt{2\pi/C_{N+1,N+1}^{-1}}} .$$
 (5.47)

Note that the normalizing factor in Eq. (5.46) has cancelled, since Eq. (5.47) is a conditional average. This is a Gaussian distribution

$$P(X_{N+1}|\mathcal{X}^N) = \frac{\exp\left(-\frac{\sigma^2}{2}\left(X_{N+1} - \mu\right)^2\right)}{\sqrt{2\pi}\sigma} , \qquad (5.48)$$

with variance

$$\sigma^2 = \frac{1}{C_{N+1,N+1}^{-1}} , \qquad (5.49)$$

and mean

$$\mu = -\sum_{j=1}^{N} X_j \frac{C_{N+1,j}^{-1}}{C_{N+1,N+1}^{-1}}.$$
(5.50)

The mean can be seen as an average of the X_j with weight $C_{N+1,j}^{-1}/C_{N+1,N+1}^{-1}$.

5.C Derivation of the enlarged correlation matrix

In this section, we derive the algorithm to promote inverse correlation matrices as given in Eqs. (5.28)–(5.33). Assuming that C(N) and $C^{-1}(N)$ are known, the aim is to find C(N + 1) and $C^{-1}(N+1)$ in as little as possible computational steps. The starting point is the observation that C(N + 1) contains C(N) as block matrix and is only augmented by a row and identical

column,

$$C(N+1) = \frac{\begin{pmatrix} C(N) & \vec{\gamma} \\ \vec{\gamma}^T & \langle X_{N+1}^2 \rangle \end{pmatrix}}{\vec{\gamma}^T & \langle X_{N+1}^2 \rangle}$$
(5.51)

where $\vec{\gamma}$ is defined in Eq. (5.28) and $\langle X_{N+1}^2 \rangle = 2t_{N+1}^{2H}$ in the case of fBm, but is intentionally left general. For the more difficult part, the inversion, we assume that the inverse correlation matrix is of the form

$$C^{-1}(N+1) = \frac{\left(\begin{array}{c|c} A(N) & \vec{b} \\ \hline \vec{b}^T & c \end{array}\right)$$
(5.52)

for some arbitrary (symmetric) matrix A, vector \vec{b} and number c. Multiplying matrices (5.51) and (5.52) results in

$$CC^{-1} = \left(\begin{array}{c|c} C(N)A(N) + \gamma \otimes \vec{b}^T & C(N)\vec{b} + c\vec{\gamma} \\ \hline (C(N)\vec{b} + c\vec{\gamma})^T & \vec{b}^T\vec{\gamma} + c\left\langle X_{N+1}^2 \right\rangle \\ \vdots \\ \mathbf{1}_{N+1} , \end{array} \right)$$
(5.53)

such that one obtains the system of equations

$$C(N) \cdot A(N) + \vec{\gamma} \otimes \vec{b}^T = \mathbf{1}_N , \qquad (5.54)$$

$$C(N) \cdot \vec{b} + c\vec{\gamma} = \vec{0} , \qquad (5.55)$$

$$\vec{b} \cdot \gamma + c \left\langle X_{N+1}^2 \right\rangle = 1 \ . \tag{5.56}$$

This is solved by

$$A(N) = C^{-1}(N) + \frac{C^{-1}(N) \cdot \vec{\gamma} \otimes \vec{\gamma}^T \cdot C^{-1}(N)}{\left\langle X_{N+1}^2 \right\rangle - \vec{\gamma} \cdot C^{-1}(N) \cdot \vec{\gamma}} , \qquad (5.57)$$

$$\vec{b} = -\frac{C^{-1}(N) \cdot \vec{\gamma}}{\left\langle X_{N+1}^2 \right\rangle - \vec{\gamma} \cdot C^{-1}(N) \cdot \vec{\gamma}} , \qquad (5.58)$$

$$c = \frac{1}{\left\langle X_{N+1}^2 \right\rangle - \vec{\gamma} \cdot C^{-1}(N) \cdot \vec{\gamma}}$$
(5.59)

Defining \vec{g} as in Eq. (5.29) and σ^2 as in Eq. (5.31), one arrives at the inverse matrix (5.33)."

Chapter 6

Extreme Events for Fractional Brownian Motion with Drift: Theory and Numerical Validation

Abstract

"We study the first-passage time, the distribution of the maximum, and the absorption probability of fractional Brownian motion of Hurst parameter H with both a linear and a non-linear drift. The latter appears naturally when applying non-linear variable transformations. Via a perturbative expansion in $\varepsilon = H - 1/2$, we give the first-order corrections to the classical result for Brownian motion analytically. Using a recently introduced adaptive bisection algorithm, which is much more efficient than the standard Davies-Harte algorithm, we test our predictions for the first-passage time on grids of effective sizes up to $N_{\rm eff} = 2^{28} \approx 2.7 \times 10^8$ points. The agreement between theory and simulations is excellent, and by far exceeds in precision what can be obtained by scaling alone."

Cited from

M. ARUTKIN, B. WALTER, AND K. J. WIESE. Extreme events for fractional Brownian motion with drift: Theory and numerical validation, 2019. Submitted to Phys. Rev. E, arXiv:1908.10801

Overview

In this chapter, I present a near verbatim copy of a preprint that is currently undergoing review

M. ARUTKIN, B. WALTER, AND K. J. WIESE. Extreme events for fractional Brownian motion with drift: Theory and numerical validation, 2019. Submitted to Phys. Rev. E, arXiv:1908.10801

This chapter addresses the first-passage time problem of fractional Brownian Motion by means of a perturbative field theory. The key difference to the approach chosen in Chps. 3 and 4 is that fractional Brownian Motion has increments which are long-ranged correlated. Therefore, one cannot simply decompose it into a Markovian process and a driving noise as has been done in the previous part II.

This Chapter sheds light on the connection between field theory and Gaussian processes. The field-theory associated to Gaussian processes is bilinear. It does not feature any higher-order vertices like the field theories in previous chapters. Instead, the perturbation takes place in the inverse correlation function which features in the bilinear action. For a fractional Brownian Motion this action is not integrable in closed form. But again, perturbative field theory gives us a way of approximating it systematically, and to compute a host of observables of such paths. The expansion takes place around the action of (fully integrable) Brownian Motion. Another interpretation of the field-theoretic technique here, is that the averages which are supposed to be taken over the ensemble of fractional Brownian Motion are first calculated for simple Brownian Motion, which induces a "sampling error", and then later "fixed" by the corrected action which accounts for this sampling error.

Further, this Chapter illustrates an application of the algorithm presented in Chp. 5.

Statement of Contribution

When I joined the project, most of the analytics had already been done by Maxence Arutkin and Kay Wiese (with exception of the absorption probability, Sec. 6.2.13), so I did not do any of the analytic work. Instead, I wrote, ran, and evaluated the numerics (cf. Sec. 6.3) employing the algorithm introduced in Chp. 5. Kay Wiese wrote the initial draft, which he and I discussed in great detail. After the first round of review, I contributed in clarifying the presentation of the results.

Acknowledgements

I would like to thank Maxence Arutkin and Kay Wiese for kindly allowing me to cite our joint work as part of my thesis. *I have obtained their approval which is shown in App. A.5.*

I would like to thank LPTENS and LPENS for their hospitality. The work has benefited from fruitful discussions with J.P. Bouchaud, F. Gorokhovik, and G. Pruessner. I also would like to thank M.T. Jaekel and A. Thomas for computing support.

6.1 Introduction

"Understanding the extreme-value statistics of random processes is important in a variety of contexts. Examples are records [154], e.g. in climate change [248], equivalent to depinning [74], in quantitative trading [199], or for earthquakes [214]. While much is known for Markov processes, and especially for Brownian motion [197, 109, 86, 85, 26, 20, 251], much less is known for correlated, i.e. non-Markovian processes, of which fractional Brownian motion (fBm) is the simplest scale-free version [174, 222, 218, 160, 135, 69, 70, 8].

FBm is important as it successfully models a variety of natural processes [58]: a tagged particle in single-file diffusion (H = 0.25) [133, 203], the integrated current in diffusive transport (H = 0.25) [204], polymer translocation through a narrow pore $(H \simeq 0.4)$ [258, 75, 177], anomalous diffusion [27], values of the log return of a stock $(H \simeq 0.6 \text{ to } 0.8)$ [187, 50, 22, 222], hydrology $(H \simeq 0.72 \text{ to } 0.87)$ [161], a tagged monomer in a polymer (H = 0.25) [110], solar flare activity $(H \simeq 0.57 \text{ to } 0.86)$ [169], the price of electricity in a liberated market $(H \simeq 0.41)$ [216], telecommunication networks $(H \simeq 0.78 \text{ to } 0.86)$ [172], telomeres inside the nucleus of human cells $(H \simeq 0.18 \text{ to } 0.35)$ [32], or diffusion inside crowded fluids $(H \simeq 0.4)$ [82].

Recently, first-passage times of fractional Brownian Motion have been investigated [122, 123, 105, 63, 59, 61]. Due to the non-Markovian nature of the process, translating these results to a fBM with drift is far from trivial, and even properly estimating the drift for H < 1/2 is a challenge [83]. To our knowledge, no analytical result for a fBm with drift are known. It is this gap we intend to fill here.

As is discussed later, apart from a *linear drift*, a *non-linear drift* may appear as well, leading us to consider the process,

$$z_t := x_t + \mu t + \nu t^{2H} . (6.1)$$

Here x_t is a standard fractional Brownian motion (fBm) with mean and variance

$$\langle x_t \rangle = x_0 = 0 , \qquad (6.2)$$

$$\langle x_{t_1} x_{t_2} \rangle = |t_1|^{2H} + |t_2|^{2H} - |t_1 - t_2|^{2H} .$$
 (6.3)

The parameter H is the Hurst parameter. Since fBm is a Gaussian process, the above equations uniquely and completely specify it. Taking a derivative w.r.t. both t_1 and t_2 shows that the increments of the process are correlated,

$$\langle \dot{x}_{t_1} \dot{x}_{t_2} \rangle = 2H(2H-1)|t_1 - t_2|^{2H-2}$$
 (6.4)

Correlations are positive for H > 1/2, and negative for H < 1/2. The case H = 1/2 corresponds to Brownian motion, with uncorrelated increments.

The parameters μ and ν are the strength of linear and non-linear drift. While linear drift is a canonical choice, non-linear drift appears as a consequence of non-linear variable transformations. As an example, consider the process

$$y_t := e^{z_t} avertee ave$$

Р	probability
$P = \partial_x \mathbf{P}$	probability density in x
$\mathbb{P} = \partial_t \mathbf{P}$	probability density in t
$\mathcal{P} = \partial_y \mathbf{P}$	probability density in y

Table 6.1.: Notations used for probabilities and their various densities.

The exponential transformation appears quite often, be it in the Black-Scholes theory of the stock market where the logarithm of the portfolio price is treated as a random walk [23, 50, 28], be it in non-linear surface growth of the Kardar-Parisi-Zhang universality class [128, 249, 120], where the transformation is known as the Cole-Hopf transformation [118, 43], or in the evaluation of the Pickands constant [57, 60, 56, 115, 167, 119, 189, 190]. Like any non-linear transform, this generates an effective drift known from Itô-calculus. Computing the average of y_t gives

$$\langle y_t \rangle = \langle e^{z_t} \rangle = \exp\left(\langle z_t \rangle + \frac{1}{2} \left[\left\langle z_t^2 \right\rangle - \left\langle z_t \right\rangle^2 \right] \right)$$

= $\exp\left(\mu t + \left[\nu + 1\right] t^{2H}\right).$ (6.6)

Thus even if initially there is no nonlinear drift, it is generated by non-linear transformations. For this reason, we include it into our model.

While for Brownian motion, equivalent to $H = \frac{1}{2}$, many results can be obtained analytically [197, 109, 86, 85, 26, 20, 251], for fBm much less is known. Recently, some of us developed a framework [252] for a systematic expansion in

$$\varepsilon := H - \frac{1}{2} . \tag{6.7}$$

It has since successfully been applied to obtain the distribution of the maximum and minimum of an fBm [61, 63], to fBm bridges [62], evaluation of the Pickands constant [60], the 2-sided exit problem [250] and the generalization of the three classical arcsine laws [202]. It is also known that the fractal dimension of the record set of an fBm is $d_{\rm f} = H$ [17].

This chapter is organized into four sections, the introduction, theory in section 6.2, and numerics in section 6.3, followed by conclusions in section 6.4.

6.2 Theory

In this section, we find the probability distribution of first-passage times and running maxima of fractional Brownian motion with linear and non-linear drift by way of a perturbation expansion around simple Brownian motion. The key result of this section is the scaling function (6.89) which together with the auxiliary functions defined in Eqs. (6.92), (6.99) and (6.103) gives the distribution of first-passage times. The majority of this section is devoted to deriving these results.

6.2.1 Scaling dimensions

Before developing the perturbation theory, we consider the scaling dimensions involved. This will be useful for later discussion of the scaling functions. For fractional Brownian motion as defined in Eq. (6.1), there are four dimension-full quantities, x, t, μ , and ν . Scaling functions will thus depend on three scaling variables, which we now identify. We start with the terms without drift:

$$x \sim t^H \iff t \sim x^{\frac{1}{H}}$$
, (6.8)

where the tilde means "same scaling dimension". Thus (without drift), any observable $\mathfrak{O}(x,t)$ can be written as

$$\mathfrak{O}(x,t) = x^{\dim_x(\mathfrak{O})} f_{\mathfrak{O}}(y) , \qquad y := \frac{x}{\sqrt{2}t^H} .$$
(6.9)

The variable y is dimension free. In presence of a linear drift, one has

$$x \sim \mu t \iff \mu \sim \frac{x}{t} \sim x^{1-\frac{1}{H}} \sim t^{H-1}$$
 (6.10)

Thus the combination $u = \mu x^{\frac{1}{H}-1}$ is dimension free, as is $\tilde{u} := u^{\frac{H}{1-H}} = \mu^{\frac{H}{1-H}} x$. For non-linear drift, we have

$$x \sim \nu t^{2H} \iff \nu \sim \frac{x}{t^{2H}} \sim \frac{1}{x} \sim \frac{1}{t^H}$$
 (6.11)

Another scaling variable therefore is $v = \nu x$. In conclusion, any observable \mathcal{O} can, in generalization of Eq. (6.9), be written as

$$\mathfrak{O}(x,t,\mu,\nu) = x^{\dim_x(\mathfrak{O})} f_{\mathfrak{O}}(y,u,v) , \qquad (6.12)$$

$$y = \frac{x}{\sqrt{2}t^H} , \qquad (6.13)$$

$$u = \mu x^{\frac{1}{H}-1}, \quad \text{or} \quad \tilde{u} = \mu^{\frac{H}{1-H}} x , \qquad (6.14)$$

$$v = \nu x . (6.15)$$

6.2.2 The first-passage time

The central result of our work is a perturbative expression of the first-passage-time density of fBM with linear and nonlinear drift as introduced in Eq. (6.1). The first-passage time t_{FP} is defined as

$$t_{\mathrm{FP}}(m) := \inf_{t>0} \{t, z_t \le 0 | z_{t=0} = m\} \quad , \tag{6.16}$$

where m is the starting point of the process z_t , and m > 0. The first-passage-time density for Brownian motion with (linear) drift, see e.g. [197], and rederived below in Eq. (6.30), is

$$\mathbb{P}_0(t_{\mathrm{F}P}(m) = t) = \frac{m}{2\sqrt{\pi}t^{3/2}} e^{-\frac{1}{2}\left(\frac{m}{\sqrt{2t}} + \frac{\mu}{2}\sqrt{2t}\right)^2} .$$
(6.17)

This density in time is most naturally expressed in terms of the scaling variable y introduced in Eq. (6.9), and which for Brownian motion (H = 1/2) reads

$$y = \frac{m}{\sqrt{2t}} \bigg|_{t=t_{\mathrm{F}P}(m)} \,. \tag{6.18}$$

For Brownian Motion, and the probability distribution of y takes the simple form

$$\mathcal{P}_0(y;\mu) = \sqrt{\frac{2}{\pi}} e^{-\mathcal{F}_0(y;\mu)} , \qquad (6.19)$$

$$\mathcal{F}_0(y;\mu) = \frac{1}{2} \left(y + \frac{\mu}{2} \frac{m}{y} \right)^2 .$$
 (6.20)

Note that the measure is dt in Eq. (6.17) (density in time), whereas in Eq. (6.19) it is dy (density in y). To avoid confusion, we use distinct symbols for probabilities **P**, densities \mathbb{P} in time t, densities \mathcal{P} in y, and densities P in space x, independent of the actual choice of variables. This is summarized in table 6.1.

We introduced the scaling function \mathcal{F}_0 . Below we compute its corrections to first order in ε , leading to a correction of the first-passage density in y,

$$\mathcal{P}(y;\mu,\nu) = \frac{y^{\frac{1}{H}-2}}{\sqrt{2\pi}} e^{-\mathcal{F}_0(y;\mu,\nu) - \varepsilon\delta\mathcal{F}(y;\mu,\nu)} + \mathcal{O}(\varepsilon^2) .$$
(6.21)

The result is given in Eqs. (6.88)-(6.89). Two comments are in order: (i) the exponential resummation is chosen for better convergence for larger ε , as discussed in [250], section IV.C; (ii) the distribution of first-passage times is related to the distribution of maxima.

Readers wishing to skip ahead will find the function $\delta \mathcal{F}$ evaluated using path-integral methods, described in section 6.2.5. For the explicit result, see section 6.2.12. A confirmation by numerical simulations is shown in section 6.3.2.

6.2.3 Summary of calculations to be done

In order to calculate the first-passage-time distribution, we consider the process $z_t > 0$ in the presence of an absorbing boundary condition at z = 0 and restrict ourselves to $z_t > 0$. The transition probability density of the process z_t to pass from $z_0 > 0$ to $z_1 > 0$ in time t, without being absorbed at z = 0 is denoted $P^{\mu,\nu}_+(z_0, z_1; t)$. The probability density of first-passage times $\mathbb{P}(t_{\mathrm{FP}}(m) = t)$ can then be obtained as

$$\mathbb{P}(t_{\mathrm{F}P}(m) = t) = \partial_{z_1} P^{\mu,\nu}_+(m, z_1, t) \big|_{z_1 = 0}.$$
(6.22)

This relation holds since the derivative on the right-hand-side picks out those trajectories which assume $z_t = 0$ at time t for the first time. The general strategy of this work is to compute $\partial_{z_1} P^{\mu,\nu}_+(m, z_1, t)|_{z_1=0}$ and its perturbative corrections using path-integral methods. In the subsequent section 6.2.4, we discuss the reference point of our expansion, simple Brownian motion. In section 6.2.5, we introduce a perturbative expansion around Brownian motion, based on a path-integral formalism. This yields a diagrammatic expansion (section 6.2.6), with three diagrams, listed in section 6.2.7, evaluated in sections 6.2.8 to 6.2.10, and regrouped in section 6.2.11. The final result is given in section 6.2.12. Contrary to the drift-free case, not all processes are absorbed, as is discussed in section 6.2.13. Relations between the different probability densities are discussed in section 6.2.14, followed by an analysis of the tail of these distributions in section 6.2.15. Numerical checks are presented in section 6.3, followed by conclusions in section 6.4.

6.2.4 Simple Brownian Motion: First-passage time and absorption probability

The perturbation theory is an expansion around simple Brownian Motion. This base point is considered here. By setting $H = \frac{1}{2}$ and $\nu = 0$ in Eq. (6.1), we obtain simple Brownian Motion with drift. For this process, we compute *(i)* the positive transition probability and *(ii)* the absorption probability.

The transition probability of simple Brownian Motion P^{μ}_{+} (to alleviate our notations, we do not put an index 0 to indicate Brownian motion, since P_{+} is not used for fBm), the probability to pass from z_0 to z_1 within time t without crossing the line $z \equiv 0$, satisfies the associated Fokker-Planck equation

$$\partial_t P^{\mu}_+(z_0, z_1, t) = \partial^2_{z_1} P^{\mu}_+(z_0, z_1, t) - \mu \partial_{z_1} P^{\mu}_+(z_0, z_1, t) .$$
(6.23)

with appropriate absorbing boundary condition at $z \equiv 0$. Its solution is given by the mirrorcharge solution

$$P_{+}^{\mu}(z_{0}, z_{1}, t) = \frac{1}{\sqrt{4\pi t}} \left(e^{-(z_{1}-z_{0})^{2}/4t} - e^{-(z_{1}+z_{0})^{2}/4t} \right) e^{\frac{\mu}{2}(z_{1}-z_{0}) - \frac{\mu^{2}t}{4}} , \qquad (6.24)$$

which for $z_0, z_1 > 0$ satisfies the initial condition

$$P^{\mu}_{+}(z_0, z_1, t = 0^+) = \delta(z_0 - z_1) . \qquad (6.25)$$

It is useful to consider its Laplace-transformed version. We define the Laplace transform of a function f(t), with $t \ge 0$ as

$$\tilde{f}(s) := \mathcal{L}_{t \to s} \left[f(t) \right] = \int_0^\infty \mathrm{d}t \, e^{-st} f(t) \;. \tag{6.26}$$

This yields

$$\tilde{P}^{\mu}_{+}(z_0, z_1, s) = e^{\frac{\mu}{2}(z_1 - z_0)} \tilde{P}_{+}\left(z_0, z_1, s + \frac{\mu^2}{4}\right) , \qquad (6.27)$$

where the drift-free propagator reads

$$\tilde{P}_{+}(z_0, z_1, s) = \frac{e^{-\sqrt{s}(z_0 - z_1)} - e^{-\sqrt{s}(z_0 + z_1)}}{2\sqrt{s}} .$$
(6.28)

The Laplace transform $\tilde{\mathbb{P}}(m, s)$ of the first-passage-time probability density, following Eq. (6.22), equals the probability to go close to the boundary, and there being absorbed for the first time,

$$\tilde{\mathbb{P}}(m,s) := \int_0^\infty dt \, e^{-st} \mathbb{P}(t_{\mathrm{F}P}(m) = t) = \partial_{z_1} \tilde{P}^{\mu}_+(m, z_1, s) \Big|_{z_1 = 0} = e^{-\frac{\mu}{2}m} e^{-m\sqrt{s + \mu^2/4}} .$$
(6.29)

Its inverse Laplace transform is the first-passage-time probability density

$$\mathbb{P}(t_{\mathrm{F}P}(m)=t) = e^{-\frac{\mu}{2}m - \frac{\mu^2}{4}t} \frac{me^{-\frac{m^2}{4t}}}{2\sqrt{\pi}t^{3/2}}, \qquad (6.30)$$

confirming the result in Eq. (6.17). The total (time integrated) absorption probability is

$$\begin{aligned} \mathbf{P}_{abs}(m) &= \tilde{\mathbb{P}}(m, s = 0) \\ &= e^{-\frac{\mu}{2}m} e^{-\frac{|\mu|}{2}m} = \begin{cases} e^{-\mu m} &, \quad \mu > 0 \\ 1 &, \quad \mu \le 0 \end{cases} \end{aligned}$$
(6.31)

In what follows, we present perturbative corrections of these results for $\varepsilon \neq 0$.

6.2.5 The path-integral of a fBm with drift

The technology developed in [252, 63, 250] uses a path-integral to describe fBM. Since z_t is Gaussian, its path-probability measure on a finite interval [0, T] is

$$\mathbf{P}[z_t] = \exp\left(-\mathcal{S}[z_t;\mu,\nu]\right) , \qquad (6.32)$$

where $S[z_t; \mu, \nu]$ is an action quadratic in z_t . Without drift ($\mu = \nu = 0$), the action for a fBM to order ε is [252, 63, 250]

$$\mathcal{S}[z_t; \mu = \nu = 0] = \int_0^T \mathrm{d}t \, \frac{\dot{z}_t^2}{4D_\varepsilon} - \frac{\varepsilon}{2} \int_\tau^T \mathrm{d}t_2 \int_0^{t_2 - \tau} \mathrm{d}t_1 \frac{\dot{z}_{t_1} \dot{z}_{t_2}}{|t_1 - t_2|} \,. \tag{6.33}$$

The action consists of a local part, corresponding to simple Brownian motion, and a non-local part, proportional to ε . The idea behind the perturbative expansion is that Brownian motion (as given by the first term) samples the whole phase space of fBm, albeit with the wrong probability measure. Our perturbation theory corrects this, by weighing each path with the second term in Eq. (6.33). This implies that the absorbing boundary conditions at the origin are properly taken into account, and that observables as the absorption current, which are given by local operators, remain valid. For regularity, a short-distance cutoff $|t_1 - t_2| > \tau$ is introduced in the last integral, which is reflected in the diffusion constant [63]

$$D_{\varepsilon} = 2H\tau^{2H-1} = (1+2\varepsilon)\tau^{2\varepsilon} = (e\tau)^{2\varepsilon} + \mathcal{O}(\varepsilon^2) .$$
(6.34)

Inserting the definition (6.1), we arrive after some algebra at the action for an arbitrary drift

$$S[z_{t}] = \int_{0}^{T} dt \frac{\dot{z}_{t}^{2}}{4D_{\varepsilon}} + \int_{0}^{T} dt \frac{\varepsilon}{2} \dot{z}_{t} \left[(\mu + \nu) \ln \left(\frac{t(T-t)}{\tau^{2}} \right) - 2\nu \ln \left(\frac{t}{\tau} \right) \right] - \frac{\varepsilon}{2} \int_{\tau}^{T} dt_{2} \int_{0}^{t_{2}-\tau} dt_{1} \frac{\dot{z}_{t_{1}} \dot{z}_{t_{2}}}{|t_{1} - t_{2}|} - \frac{z_{T} - z_{0}}{2} \left[\frac{\mu}{D_{\varepsilon}} + \nu \right] + \frac{T}{4} (\mu + \nu)^{2} + \frac{T}{2} \varepsilon \left(\nu^{2} - \mu^{2} \right) \ln(T) + \mathcal{O}(\varepsilon^{2}) .$$
(6.35)

Some checks are in order. In absence of absorbing boundaries, the exact free propagator reads

$$P^{\mu,\nu}(0,z,T) = \frac{1}{2\sqrt{\pi}T^{H}}e^{-\frac{(z-\mu T-\nu T^{2H})^{2}}{4T^{2H}}}$$
$$= \frac{1}{2\sqrt{\pi}T^{H}}\exp\left(-\frac{z^{2}}{4T^{2H}} + \frac{z}{2}\left[\nu+\mu T^{-2\varepsilon}\right] - \frac{T}{4}\left[\nu T^{\varepsilon}+\mu T^{-\varepsilon}\right]^{2}\right). \quad (6.36)$$

Since the above formalism has variables \dot{z} only, the term $\sim z^2$ is given by the drift-free perturbation theory. We can further check that if we replace in the action $\dot{z}(t)$ by its "classical trajectory", i.e. $\dot{z}(t) \rightarrow [z(T) - z(0)]/T$, then both the normalization and the drift term agree with the exact propagator.

Let us specify Eq. (6.35) to the two cases of interest: For a fBm with *linear drift* as given in Eq. (6.1) with $\nu = 0$, we have

$$S_{\nu=0}[z_t] = \int_0^T dt \, \frac{\dot{z}_t^2}{4D_{\varepsilon}} - \frac{\mu}{2D_{\varepsilon}} (z_T - z_0) + \frac{T^{1-2\varepsilon}}{4} \mu^2 \\ - \frac{\varepsilon}{2} \int_{\tau}^T dt_2 \int_0^{t_2 - \tau} dt_1 \frac{\dot{z}_{t_1} \dot{z}_{t_2}}{|t_1 - t_2|} + \frac{\varepsilon \mu}{2} \int_0^T dt \, \dot{z}_t \ln\left(\frac{[T-t]t}{\tau^2}\right) + \mathcal{O}(\varepsilon^2) \,. \quad (6.37)$$

For a fBm with non-linear drift as given in Eq. (6.1) with $\mu = 0$, we have

$$S_{\mu=0}[z] = \int_{0}^{T} \mathrm{d}t \, \frac{\dot{z}_{t}^{2}}{4D_{\varepsilon}} - \frac{\nu}{2}(z_{T} - z_{0}) + \frac{T^{1+2\varepsilon}}{4}\nu^{2} \\ -\frac{\varepsilon}{2} \int_{\tau}^{T} \mathrm{d}t_{2} \int_{0}^{t_{2}-\tau} \mathrm{d}t_{1} \frac{\dot{z}_{t_{1}}\dot{z}_{t_{2}}}{|t_{1} - t_{2}|} + \frac{\varepsilon\nu}{2} \int_{0}^{T} \mathrm{d}t \, \dot{z}_{t} \ln\left(\frac{T-t}{t}\right) + \mathcal{O}(\varepsilon^{2}) \,.$$
(6.38)

Note the appearance of the diffusion constant in the "bias" (Girsanov) term $z_T - z_0$ for a linear drift, and its absence for a non-linear drift.

To simplify the notation, we introduce

$$S_0[z_t] = \int_0^T \mathrm{d}t \, \frac{\dot{z}_t^2}{4} \tag{6.39}$$

as a shorthand for the Brownian action around which perturbation theory expands. The drift (Girsanov) term is e^{-S_d} , with

$$\mathcal{S}_{\mathrm{d}}[z] = \frac{z_0 - z_T}{2} \left(\frac{\mu}{D_{\varepsilon}} + \nu\right) + \frac{T}{4} \left(\mu T^{-\varepsilon} + \nu T^{\varepsilon}\right)^2 \ . \tag{6.40}$$

Further, define

$$\alpha := \mu - \nu, \qquad \beta := \mu + \nu, \qquad (6.41)$$

$$\mu = \frac{\alpha + \beta}{2}, \qquad \nu = \frac{\beta - \alpha}{2}. \tag{6.42}$$



Figure 6.1.: Graphical representation of the path-integral for diagram $\mathbb{G}_1(m, t)$ (left, expectation of \mathcal{S}_1 , Eq. (6.52)), $\mathbb{G}_{\alpha}(m, t)$ (middle, expectation of \mathcal{S}_{α} , Eq. (6.53)), and $\mathbb{G}_{\beta}(m, t)$ (right, expectation of \mathcal{S}_{β} , Eq. (6.54)). The wiggly line in the first diagram represents the interaction proportional to $1/(t_2 - t_1)$. The red lines in the second and third diagram contain a log of the corresponding time difference, $\ln(t/T)$ for the first, and $\ln((T - t)/T)$ for the second. This figure has been submitted for publication to Phys. Rev. E. See App. A.5 for approval of co-authors.

This simplifies the drift terms in the action to

$$\mathcal{S}_{\alpha}[z_t] := \frac{1}{2} \int_0^T \mathrm{d}t \, \dot{z}_t \ln\left(\frac{t}{\tau}\right) \,, \tag{6.43}$$

$$\mathcal{S}_{\beta}[z_t] := \frac{1}{2} \int_0^T \mathrm{d}t \, \dot{z}_t \ln\left(\frac{T-t}{\tau}\right) \,. \tag{6.44}$$

Finally, the drift-independent perturbative correction containing the non-local interaction reads

$$S_1[z_t] = \frac{1}{2} \int_{\tau}^{T} \mathrm{d}t_2 \int_{0}^{t_2 - \tau} \mathrm{d}t_1 \frac{\dot{z}_{t_1} \dot{z}_{t_2}}{|t_1 - t_2|} .$$
(6.45)

In these notations, the action to order ε reads

$$\mathcal{S}[z_t; \mu, \nu] = \frac{\mathcal{S}_0}{D_{\varepsilon}} + \mathcal{S}_d - \varepsilon \left(\mathcal{S}_1 - \alpha \mathcal{S}_\alpha - \beta \mathcal{S}_\beta \right).$$
(6.46)

Perturbation theory takes place in the three interaction-terms proportional to ε , plus an additional contribution due to D_{ε} . The bare result Eq. (6.27) of transition probabilities of fBM will thus be corrected by three different terms corresponding to the three interaction terms S_{α}, S_{β} and S_1 , plus a correction from D_{ε} . The (diagrammatic) rules for computing these corrections are outlined in the next section.

6.2.6 Diagrammatic expansion

The central aim of this work is to calculate the first-passage-time density. This is done by taking the derivative of the survival transition density at its endpoint (cf. Eq. (6.22)). The latter is obtained perturbatively by evaluating a path-integral over the action defined previously.

$$\mathbb{P}^{\mu,\nu}(m,t) := \partial_{z_1}|_{z_1=0} P^{\mu,\nu}_{+,\varepsilon}(m,z_1,t)
\equiv \lim_{z_1\to 0} \frac{1}{z_1} P^{\mu,\nu}_{+,\varepsilon}(m,z_1,t) .$$
(6.47)

Here we introduced $P^{\mu,\nu}_{+,\varepsilon}(m,z_1,t)$

$$P_{+,\varepsilon}^{\mu,\nu}(m,z_1,t) := \int_{z_0=m}^{z_t=z_1} \mathcal{D}[z_t]\Theta(z_t) \exp\left(-\mathcal{S}\right) , \qquad (6.48)$$

the probability of a path z_t to pass from m to z_1 within time t without being absorbed at z = 0(cf. Eq. (6.24)). At first order in ε , this path integral has four perturbative contributions: The three diagrams induced by S_1 , S_α , and S_β , as well as the change in the diffusion constant D_{ε} . The simplest way of doing these calculations is to calculate with D = 1, and finally correct for $D_{\varepsilon} \neq 1$ by writing the FPT density in time of z_t as

$$\mathbb{P}^{\mu,\nu}(m,t) = \mathbb{G}^{\mu,\nu}(m,tD_{\varepsilon}) \tag{6.49}$$

where we introduce the auxiliary probability density

$$\mathbb{G}^{\mu,\nu}(m,t) = \frac{\partial}{\partial z_1} \Big|_{z_1=0} \int_{z_0=m}^{z_t=z_1} \mathcal{D}[z_t] \Theta(z_t) e^{-\mathcal{S}^0 - \mathcal{S}_d + \varepsilon(\mathcal{S}_1 - \alpha \mathcal{S}_\alpha - \beta \mathcal{S}_\beta)} + \mathcal{O}(\varepsilon^2) .$$

We now use the perturbation expansion established in Ref. [252, 61, 62, 63]; we refer to [63, 59] for a detailed introduction, and only briefly summarise the method.

The function $\mathbb{G}^{\mu,\nu}(m,t)$ introduced above has the perturbative expansion

$$\mathbb{G}^{\mu,\nu}(m,t) = e^{-\mathcal{S}_{d}} \left[\mathbb{G}_{0}(m,t) + \varepsilon \, \delta \mathbb{G}(m,t) \right] \tag{6.50}$$

where

$$\delta \mathbb{G}(m,t) = \partial_{z_1} \Big|_{z_1=0} \int_{z_0=m}^{z_t=z_1} \mathcal{D}[z_t] \Theta(z_t) \left(\mathcal{S}_1 - \alpha \mathcal{S}_\alpha - \beta \mathcal{S}_\beta\right) e^{-S_0} \\ \stackrel{!}{=} \mathbb{G}_1(m,t) - \alpha \mathbb{G}_\alpha(m,t) - \beta \mathbb{G}_\beta(m,t) + \mathcal{O}(\varepsilon) .$$
(6.51)

The three auxiliary functions are defined as

$$\mathbb{G}_{1}(m,t) := \partial_{z_{1}}\Big|_{z_{1}=0} \int_{z_{0}=m}^{z_{t}=z_{1}} \mathcal{D}[z_{t}]\Theta(z_{t})\mathcal{S}_{1}e^{-S_{0}} , \qquad (6.52)$$

$$\mathbb{G}_{\alpha}(m,t) := \partial_{z_1} \Big|_{z_1=0} \int_{z_0=m}^{z_t=z_1} \mathcal{D}[z_t] \Theta(z_t) \mathcal{S}_{\alpha} e^{-S_0} , \qquad (6.53)$$

$$\mathbb{G}_{\beta}(m,t) := \partial_{z_1} \Big|_{z_1=0} \int_{z_0=m}^{z_t=z_1} \mathcal{D}[z_t] \Theta(z_t) \mathcal{S}_{\beta} e^{-S_0} .$$
(6.54)

As the term S_d only depends on the initial and final point, as well as the time T, we were able to take it out. Each of the perturbations S_1 , S_{α} , and S_{β} , defined in Eqs. (6.43)-(6.45) has to be evaluated inserted into the path integral with absorbing boundaries at z = 0.

Let us summarize the rules of this perturbative expansion, explained in detail in Ref. [63]. The first step is to perform a Laplace transform, from the time variable t to the Laplace conjugate s. This transform has two advantages: First of all, it eliminates integrals over the intermediate times. Second, the propagator (6.27)-(6.28) is exponential in the space variables, thus the latter can be integrated over.

The next step is to eliminate the denominator in Eq. (6.45), using a Schwinger parametrization (Eq. (31) of [63]),

$$\frac{1}{t_2 - t_1} = \int_{y>0} e^{-y(t_2 - t_1)} . \tag{6.55}$$

The variable y on the r.h.s. of Eq. (6.55) can be interpreted as a shift in the Laplace variable s associated to the time difference $t_2 - t_1$, i.e.

$$s \to s + y \tag{6.56}$$

for all propagators between times t_1 and time t_2 . For an example see the first diagram in Eq. (6.64) below.

The integral over times necessitates a cutoff τ at small times, which can be replaced by a cutoff Λ for large y (Eq. (A3) of [63]). Their relation is

$$\int_{0}^{T} \mathrm{d}t \int_{0}^{\Lambda} e^{-yt} \mathrm{d}y = \ln(T\Lambda) + \gamma_{\mathrm{E}} + \mathcal{O}(e^{-T\Lambda})$$
$$\stackrel{!}{=} \ln\left(\frac{T}{\tau}\right) = \int_{\tau}^{T} \frac{1}{t} \,\mathrm{d}t \;. \tag{6.57}$$

This implies the choice

$$\Lambda = e^{-\gamma_{\rm E}}/\tau \ . \tag{6.58}$$

Finally, while the insertion of the position z_t at time t with 0 < t < T leads to a factor of z in the corresponding propagators,

$$\langle z_t \rangle_{z_0=a, z_T=b} = \int_z P_+(a, z, t) z P_+(z, b, T-t) ,$$
 (6.59)

the insertion of \dot{z}_t yields a derivative (Eq. (A1) of [63])

$$\langle \dot{z}_t \rangle_{z_0 = a, z_T = b} = 2 \int_z P_+(a, z, t) \partial_z P_+(z, b, T - t)$$
 (6.60)

Here $P_+(a, b, T)$ is the Brownian transition density introduced in Eq. (6.24) in the absence of drift $(\mu = 0)$.

6.2.7 Diagrams to be evaluated

The three auxiliary functions introduced in Eqs. (6.52)-(6.54) have a diagrammatic representation presented in Fig. 6.1. They give to first order in ε for \mathbb{G} ,

$$\mathbb{G}^{\mu,\nu}(m,T) := \exp\left(-\frac{m}{2}\left(\frac{\mu}{D_{\varepsilon}} + \nu\right) - \frac{T}{4}\left(\mu T^{-\varepsilon} + \nu T^{\varepsilon}\right)^{2}\right) \\
\times \left\{\mathbb{G}_{0}(m,T) + \varepsilon \left[\mathbb{G}_{1}(m,T) - \alpha \mathbb{G}_{\alpha}(m,T) - \beta \mathbb{G}_{\beta}(m,T)\right]\right\}. \quad (6.61)$$

The zeroth order contribution $\mathbb{G}_0(m,t)$ follows from Eqs. (6.29) and (6.30),

$$\mathbb{G}_0(m,t) = \frac{me^{-\frac{m^2}{4t}}}{2\sqrt{\pi}t^{3/2}} \tag{6.62}$$

$$\tilde{\mathbb{G}}_0(m,s) = e^{-m\sqrt{s}} . \tag{6.63}$$

6.2.8 Order ε , first diagram \mathbb{G}_1

The Laplace transform of the first diagram is obtained from the insertion of S_1 (without drift), as represented by the first diagram of figure 6.1, using the Brownian propagators found in Eq. (6.27). (The global factor of $2 = 2^2/2$ comes from a factor of 2 for each insertion of \dot{x} , and the 1/2 from the action.)

$$\begin{split} \tilde{\mathbb{G}}_{1}(m,s) & (6.64) \\ &= \lim_{x_{0} \to 0} \frac{2}{x_{0}} \int_{0}^{\Lambda} \mathrm{d}y \int_{x_{1} > 0} \int_{x_{2>0}} \tilde{P}_{+}(m,x_{1},s) \partial_{x_{1}} \tilde{P}_{+}(x_{1},x_{2},s+y) \partial_{x_{2}} \tilde{P}_{+}(x_{2},x_{0},s) \\ &= 2 \int_{0}^{\Lambda} \mathrm{d}y \frac{\sqrt{s} \left(e^{-m\sqrt{s}} \left(my - 2\sqrt{s+y} \right) + 2\sqrt{s+y} e^{-m\sqrt{s+y}} \right)}{2y^{2}} \\ &= e^{m\sqrt{s}} \left(m\sqrt{s} + 1 \right) \mathrm{Ei} \left(-2m\sqrt{s} \right) + e^{-m\sqrt{s}} \left[m\sqrt{s} \left(\ln \left(\frac{m}{2\sqrt{s\tau}} \right) - 1 \right) - \ln \left(2m\sqrt{s} \right) - \gamma_{\mathrm{E}} \right] \,, \end{split}$$

where we introduced the exponential integral function $\operatorname{Ei}(z) = -\int_{-z}^{\infty} dt \, \frac{e^{-z}}{z}$, and used Eq. (6.58) to eleminate Λ . For the inverse Laplace transform we find using appendix C of Ref. [62]

$$\mathbb{G}_{1}(m,t) = \mathbb{G}_{0}(m,t) \left[\mathcal{I}\left(\frac{m}{\sqrt{2t}}\right) + 2\left(\frac{m^{2}}{4t} - 1\right) \ln\left(\frac{m^{2}}{\tau}\right) + \ln\left(\frac{t}{\tau}\right) + \frac{(\gamma_{\mathrm{E}} - 1)m^{2}}{2t} - 2\gamma_{\mathrm{E}} - 1 \right]. \quad (6.65)$$

The special function \mathcal{I} appearing in this expression was introduced in Ref. [252], Eq. (B53)

$$\mathcal{I}(z) = \frac{z^4}{6} {}_2F_2\left(1, 1; \frac{5}{2}, 3; \frac{z^2}{2}\right) + \pi(1 - z^2) \operatorname{erfi}\left(\frac{z}{\sqrt{2}}\right) - 3z^2 + \sqrt{2\pi}e^{\frac{z^2}{2}}z + 2 , \quad (6.66)$$

where $\operatorname{erfi}(z)$ is the imaginary error function. Using the definition (6.58) of Λ , Eq. (6.65) and introducing the variable

$$z := \frac{m}{\sqrt{2t}} , \qquad (6.67)$$

 $\mathbb{G}_0(m,t)$ and $\mathbb{G}_1(m,t)$ can be written more compactly as

$$t\mathbb{G}_0(m,t) = \frac{e^{-\frac{z^2}{2}}z}{\sqrt{2\pi}}, \qquad (6.68)$$

$$\mathbb{G}_1(m,t) = \mathbb{G}_0(m,t) \left\{ \mathcal{I}(z) - \ln\left(\frac{4tz^4}{\tau}\right) + z^2 \left[\ln\left(\frac{2tz^2}{\tau}\right) + \gamma_{\rm E} - 1\right] - 2\gamma_{\rm E} - 1 \right\} . (6.69)$$

Note that there is a global prefactor of 1/t, and a logarithmic dependence on t and τ for \mathbb{G}_1 .

6.2.9 Order ε , second diagram \mathbb{G}_{α}

To study perturbations with S_{α} defined in Eq. (6.43), we represent the logarithm as

$$\ln\left(\frac{t}{\tau}\right) = \int_0^\infty \frac{\mathrm{d}y}{y} \left[e^{-\tau y} - e^{-ty}\right] \,. \tag{6.70}$$

This yields for the insertion of \mathcal{S}_{α}

$$\tilde{\mathbb{G}}_{\alpha}(m,s) = \lim_{x_{0}\to 0} \frac{1}{x_{0}} \int_{0}^{\Lambda} \frac{dy}{y} \int_{x_{1}>0} \left[\tilde{P}_{+}(m,x_{1},s)e^{-\tau y} - \tilde{P}_{+}(m,x_{1},s+y) \right] \partial_{x_{1}} \tilde{P}_{+}(x_{1},x_{0},s)
= \int_{0}^{\Lambda/s} dy \left[\frac{e^{-m\sqrt{s}}}{\sqrt{s}y^{2}} - \frac{e^{-m\sqrt{s}\sqrt{y+1}}}{\sqrt{s}y^{2}} - \frac{me^{-m\sqrt{s}-s\tau y}}{2y} \right]
= \frac{1}{4} m e^{-m\sqrt{s}} \left[2e^{2m\sqrt{s}} \operatorname{Ei}\left(-2m\sqrt{s}\right) + \ln\left(\frac{4s\tau^{2}}{m^{2}}\right) + 2 \right] + \mathcal{O}(\Lambda^{-1}) .$$
(6.71)

We checked that the y integrand is convergent, at least as $1/y^2$ for large y, and has a finite limit for $y \to 0$; thus neither x_0 nor Λ are necessary as UV cutoffs, and the y-integral is finite. The τ -dependence stems from the $\ln(t/\tau)$ of the perturbation term.

Doing the inverse Laplace transform using appendix C of [62], we get with z defined in Eq. (6.67)

$$\sqrt{t}\mathbb{G}_{\alpha}(m,t) = \frac{e^{-\frac{z^2}{2}}z^2\left[\mathcal{I}(z)-2\right]}{2\sqrt{\pi}(1-z^2)} + \frac{z\operatorname{erfc}(\frac{z}{\sqrt{2}})}{\sqrt{2}\left(z^2-1\right)} - \frac{e^{-\frac{z^2}{2}}z^2\left[\ln\left(\frac{2tz^2}{\tau}\right) + \gamma_{\rm E} - 1\right]}{2\sqrt{\pi}} , \qquad (6.72)$$

defining the complementary error function $\operatorname{erfc}(z) = 1 - \operatorname{erf}(z)$. Note that there is no pole at z = 1. Indeed, for $z \to 1$ one obtains

$$\frac{1}{8\sqrt{e\pi}} \left(-{}_{2}F_{2}\left(1,1;\frac{5}{2},3;\frac{1}{2}\right) - 4{}_{2}F_{2}\left(1,1;\frac{3}{2},2;\frac{1}{2}\right) + 2\sqrt{2e\pi} \left(\operatorname{erfc}\left(\frac{1}{\sqrt{2}}\right) - 3\right) + 4\pi\operatorname{erfi}\left(\frac{1}{\sqrt{2}}\right) - 4\ln\left(\frac{2t}{\tau}\right) - 4\gamma_{\mathrm{E}} + 22\right) .$$

$$(6.73)$$

6.2.10 Order ε , third diagram \mathbb{G}_{β}

Using again the integral representation (6.70), the third diagram for the insertion of S_{β} is read off from Fig. 6.1 as

$$\begin{split} \tilde{\mathbb{G}}_{\beta}(m,s) &= \lim_{x_{0} \to 0} \frac{1}{x_{0}} \int_{0}^{\Lambda} \frac{dy}{y} \int_{x_{1} > 0} \tilde{P}_{+}(m,x_{1},s) \,\partial_{x_{1}} \Big[\tilde{P}_{+}(x_{1},x_{0},s) e^{-\tau y} - \tilde{P}_{+}(x_{1},x_{0},s+y) \Big] \\ &= \int_{0}^{\infty} dy \left[\frac{\sqrt{y+1}e^{-m\sqrt{s}}}{\sqrt{sy^{2}}} - \frac{\sqrt{y+1}e^{-m\sqrt{s}\sqrt{y+1}}}{\sqrt{sy^{2}}} - \frac{me^{-m\sqrt{s}-s\tau y}}{2y} \right] \\ &= \frac{e^{-m\sqrt{s}} \left(m\sqrt{s} \Big[2 - \ln\left(\frac{m^{2}}{4s\tau^{2}}\right) \Big] + \ln\left(4m^{2}s\right) + 2\gamma_{\mathrm{E}}\right)}{4\sqrt{s}} - \frac{e^{m\sqrt{s}} \left(m\sqrt{s}+1\right) \mathrm{Ei}\left(-2m\sqrt{s}\right)}{2\sqrt{s}} (6.74) \end{split}$$

We checked that the y integrand is convergent, as it decays at least as $1/y^{3/2}$ for large y, and has a finite limit for $y \to 0$, thus no UV cutoff is necessary, and the y-integral is finite.

Doing the inverse Laplace transform using appendix C of Ref. [62], we get with z defined in Eq. (6.67)

$$\sqrt{t} \mathbb{G}_{\beta}(m,t) = \frac{e^{-\frac{z^2}{2}} [\mathcal{I}(z) - 2]}{2\sqrt{\pi} (1 - z^2)} + \frac{z \operatorname{erfc}(\frac{z}{\sqrt{2}})}{\sqrt{2} (z^2 - 1)} + \frac{e^{-\frac{z^2}{2}} z^2 \left[1 - \ln(\frac{t}{\tau})\right]}{2\sqrt{\pi}} .$$
(6.75)

6.2.11 Combinations

In the drift-free case the result for $\mathbb{G}_0(z)$ is given in Eq. (6.68), while $\mathbb{G}_1(z)$ is given in Eq. (6.69). Let us now turn to the corrections for drift. While \mathbb{G}_{α} and \mathbb{G}_{β} are the appropriate functions for the calculations, we finally need the corrections for linear drift μ and non-linear drift ν . Demanding that

$$\alpha \mathbb{G}_{\alpha} + \beta \mathbb{G}_{\beta} \stackrel{!}{=} \mu \mathbb{G}_{\mu} + \nu \mathbb{G}_{\nu} , \qquad (6.76)$$

and using Eqs. (6.41) and (6.42) yields

$$\begin{split} \sqrt{t} \mathbb{G}_{\mu}(m,t) &= \sqrt{t} \left[\mathbb{G}_{\alpha}(m,t) + \mathbb{G}_{\beta}(m,t) \right] \\ &= -\frac{e^{-\frac{z^2}{2}} \left(z^2 + 1 \right) \left[\mathcal{I}(z) - 2 \right]}{2\sqrt{\pi} \left(z^2 - 1 \right)} + \frac{\sqrt{2} z \operatorname{erfc}(\frac{z}{\sqrt{2}})}{z^2 - 1} - \frac{e^{-\frac{z^2}{2}} z^2 \left[\ln\left(\frac{2t^2 z^2}{\tau^2}\right) + \gamma_{\mathrm{E}} - 2 \right]}{2\sqrt{\pi}} \end{split}$$

as well as

$$\begin{aligned}
\sqrt{t} \mathbb{G}_{\nu}(m,t) &= \sqrt{t} \left[\mathbb{G}_{\beta}(m,t) - \mathbb{G}_{\alpha}(m,t) \right] \\
&= \frac{e^{-\frac{z^2}{2}} [\mathcal{I}(z) - 2]}{2\sqrt{\pi}} + \frac{e^{-\frac{z^2}{2}} z^2 \left[\ln(2z^2) + \gamma_{\rm E} \right]}{2\sqrt{\pi}} .
\end{aligned}$$
(6.77)

The perturbative contributions can be grouped together as (cf. Eqs. (6.51) and (6.61))

$$\mathbb{G}(m,t) := \exp\left(-\frac{m}{2}\left[\frac{\mu}{D_{\varepsilon}} + \nu\right] - \frac{t}{4}\left[\mu t^{-\varepsilon} + \nu t^{\varepsilon}\right]^{2}\right) \\
\times \left\{\mathbb{G}_{0}(m,t) + \varepsilon \left[\mathbb{G}_{1}(m,t) - \mu \mathbb{G}_{\mu}(m,t) - \nu \mathbb{G}_{\nu}(m,t)\right]\right\}.$$
(6.78)

This expression is to this order equivalent to

$$\mathbb{G}(m,t) := \exp\left(-\frac{m}{2}\left[\frac{\mu}{D_{\varepsilon}} + \nu\right] - \frac{t}{4}\left[\mu t^{-\varepsilon} + \nu t^{\varepsilon}\right]^{2}\right) \\
\times \mathbb{G}_{0}(m,t) \exp\left(\varepsilon \frac{\mathbb{G}_{1}(m,t) - \mu \mathbb{G}_{\mu}(m,t) - \nu \mathbb{G}_{\nu}(m,t)}{\mathbb{G}_{0}(m,t)}\right) .$$
(6.79)

See [250], Sec. IV.C for a discussion of why it is better to write the perturbative corrections in an exponential form.

6.2.12 Scaling and corrections from the diffusion constant, final result

The natural scaling variable for fBm is not z, but

$$y := \frac{m}{\sqrt{2}t^H} \ . \tag{6.80}$$

This will induce some corrections (cf. Eq.(6.49)). Consider

$$\frac{e^{-\frac{y^2}{2}}y}{\sqrt{2\pi}} = \frac{e^{-\frac{z^2}{2}}z}{\sqrt{2\pi}} \Big[1 + (z^2 - 1)\varepsilon \ln(t) \Big] + \mathcal{O}(\varepsilon^2) \ . \tag{6.81}$$

There is also a correction to the diffusion constant,

$$D_{\varepsilon} \simeq (e\tau)^{2\varepsilon}$$
 . (6.82)

According to Eq. (6.49), this implies that

$$\mathbb{P}(m,t) = \mathbb{G}(m,tD_{\varepsilon}) \\
= \frac{e^{-\frac{y^2}{2}y}}{\sqrt{2\pi}tD_{\varepsilon}}\exp\left(-\frac{m}{2}\left[\frac{\mu}{D_{\varepsilon}}+\nu\right] - \frac{D_{\varepsilon}t}{4}\left[\mu^2(D_{\varepsilon}t)^{-2\varepsilon}+\nu^2(D_{\varepsilon}t)^{2\varepsilon}\right]\right) \\
\times \exp\left(\varepsilon\left[\frac{\mathbb{G}_1(m,t)-\mu\,\mathbb{G}_\mu(m,t)-\nu\,\mathbb{G}_\nu(m,t)}{\mathbb{G}_0(m,t)}-(y^2-1)\ln(t)\right]\right) (6.83)$$

Note that we used the factored form (6.79) to make appear the ratios of \mathbb{G}_1 , \mathbb{G}_{μ} and \mathbb{G}_{ν} with \mathbb{G}_0 , yielding more compact special functions \mathcal{F}_1 , \mathcal{F}_{μ} and \mathcal{F}_{ν} defined below. Regrouping terms yields

$$\mathbb{P}(m,t) = \frac{e^{-\frac{y^2}{2}}y^{\frac{1}{H}-1}}{\sqrt{2\pi}t} \exp\left(-\frac{\mu m^{1-2\varepsilon/H}}{2}y^{2\varepsilon} - \frac{\nu m}{2}y^{\varepsilon} - \frac{t}{4}\left[\mu t^{-\varepsilon} + \nu t^{\varepsilon}\right]^2\right) \\ \times \exp\left(\varepsilon\left[\mathcal{F}_1(y) - \mu m\mathcal{F}_\mu(y) - \nu m\mathcal{F}_\nu(y)\right]\right) .$$
(6.84)

To order ε , this can be rewritten in a more intuitive form as

$$t \mathbb{P}(m,t) = \frac{y^{\frac{1}{H}-1}}{\sqrt{2\pi}} \exp\left(-\frac{y^2}{2}\right)$$

$$\times \exp\left(\varepsilon \left[\mathcal{F}_1(y) + \mathcal{F}_1^0\right] - \mu m^{\frac{1}{H}-1} y^{2\varepsilon} \left[\frac{1}{2} + \varepsilon \mathcal{F}_\mu(y)\right] - \nu m y^{2\varepsilon} \left[\frac{1}{2} + \varepsilon \mathcal{F}_\nu(y)\right] - \frac{m^2}{8y^2} \left[\mu \left(\frac{2y^2}{m^2}\right)^{\frac{\varepsilon}{H}} + \nu\right]^2\right).$$
(6.85)

Note that since our expansion is restricted to the first order in ε , in expressions like

$$\frac{1}{H} - 1 = 1 - 4\varepsilon + \mathcal{O}(\varepsilon^2) , \qquad 1 - \frac{1}{2H} = 2\varepsilon + \mathcal{O}(\varepsilon^2) , \qquad (6.86)$$

we have no means to distinguish between left- and right-hand side. Some choices are given by scaling, as the prefactor of $y^{\frac{1}{H}-1}$, or seem natural, others are educated guesses.

Finally, we wish to rewrite Eq. (6.85) (a density in time) as a density in y, given distance m
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from the absorbing boundary for the starting point. Using that

$$\frac{\mathrm{d}t}{t} = \frac{1}{H} \frac{\mathrm{d}y}{y} , \qquad (6.87)$$

this yields

$$\mathcal{P}(y|m,\mu,\nu) = \mathcal{P}_{>}(y|m,\mu,\nu) + \mathbf{P}_{\text{escape}}(m,\mu,\nu)\delta(y) .$$
(6.88)

The function $\mathcal{P}_{>}(y|m,\mu,\nu)$ is equivalent to Eq. (6.85) after the change in measure (6.87),

$$\mathcal{P}_{>}(y|m,\mu,\nu) = \frac{y^{\frac{1}{H}-2}}{\sqrt{2\pi}H} \exp\left(-\frac{y^{2}}{2} + \varepsilon \left[\mathcal{F}_{1}(y) + \mathcal{F}_{1}^{0}\right] - \mu m^{\frac{1}{H}-1}y^{2\varepsilon} \left[\frac{1}{2} + \varepsilon F_{\mu}(y)\right] - \nu m y^{2\varepsilon} \left[\frac{1}{2} + \varepsilon \mathcal{F}_{\nu}(y)\right] - \frac{m^{2}}{8y^{2}} \left[\mu \left(\frac{2y^{2}}{m^{2}}\right)^{\frac{\varepsilon}{H}} + \nu\right]^{2}\right).$$
(6.89)

Some trajectories escape, which we count as absorption time $t = \infty$, equivalent to y = 0, resulting into the contribution proportional to $\delta(y)$ in Eq. (6.88), with amplitude

$$\mathbf{P}_{escape}(m,\mu,\nu) = 1 - \mathbf{P}_{abs}(m,\mu,\nu) , \qquad (6.90)$$

where

$$\mathbf{P}_{abs}(m,\mu,\nu) := \int_0^\infty \mathrm{d}y \,\mathcal{P}_>(y|m,\mu,\nu) \;. \tag{6.91}$$

It is evaluated in the next section, see Eqs. (6.119)-(6.121).

The three special functions appearing in Eq. (6.84) are defined as follows: First, the drift-free contribution are

$$\mathcal{F}_{1}(y) + \mathcal{F}_{1}^{0} := \frac{\mathbb{G}_{1}(y)}{\mathbb{G}_{0}(y)} - (y^{2} - 1) \Big[\ln(t/\tau) - 1 \Big] + 4 \ln y$$

$$= \mathcal{I}(y) + y^{2} \Big(\ln \Big(2y^{2} \Big) + \gamma_{\mathrm{E}} \Big) - 2 \left(\gamma_{\mathrm{E}} + 1 + \ln 2 \right) .$$

$$(6.92)$$

The conventions are s.t. $\mathcal{F}_1(y)$ agrees with Refs. [252, 63, 61], i.e. $\mathcal{F}_1(0) = 0$. The constant part \mathcal{F}_1^0 is equivalent to a change in normalization, $\mathcal{N} = \exp(-\varepsilon \mathcal{F}_1^0)$, which for the drift-free case was of no interest [252, 63, 61], as there the absorption probability is one, which is not the case with drift. In the chose convention,

$$\mathcal{F}_1(y) = \mathcal{I}(y) + y^2 \left(\ln \left(2y^2 \right) + \gamma_{\rm E} \right) - 2 , \qquad (6.93)$$

$$\mathcal{F}_1(0) = 0 , \qquad (6.94)$$

$$\mathcal{F}_1^0 = -2(\gamma_{\rm E} + \ln 2) . \tag{6.95}$$



Figure 6.2.: Left: The function $\mathcal{F}_1(y)$ (blue, solid), with its asymptotic expansions (red and green dashed). Middle: *i*bid. for $\mathcal{F}_{\mu}(y)$. Right: *i*bid. for $\mathcal{F}_{\nu}(y)$. Numerical measurements are presented on Figs. 6.2, 6.3 and 6.5. This figure has been submitted for publication to Phys. Rev. E. See App. A.5 for approval of co-authors.

Its asymptotic expansions for small and large y are

$$\mathcal{F}_{1}(y) = 2\sqrt{2\pi}y + y^{2}\left(\ln\left(2y^{2}\right) + \gamma_{\mathrm{E}} - 3\right) - \frac{1}{3}\sqrt{2\pi}y^{3} + \frac{y^{4}}{6} - \frac{1}{30}\sqrt{\frac{\pi}{2}}y^{5} + \frac{y^{6}}{90} - \frac{1}{420}\sqrt{\frac{\pi}{2}}y^{7} + \frac{y^{8}}{1260} - \frac{\sqrt{\frac{\pi}{2}}y^{9}}{6048} + \frac{y^{10}}{18900} + \mathcal{O}(y^{11}), \qquad (6.96)$$

$$\mathcal{F}_1(y) = \ln(y^2/2) + 1 - \psi\left(\frac{1}{2}\right) + \frac{1}{2y^2} - \frac{1}{2y^4} + \frac{5}{4y^6} - \frac{21}{4y^8} + \frac{63}{2y^{10}} + \mathcal{O}(y^{-11}) . \quad (6.97)$$

Eq. (6.93) is equivalent to Eqs. (55) in [252], and (56) in [63]. The second function is for the drift proportional to μ ,

$$\mathcal{F}_{\mu}(y) := \frac{\mathbb{G}_{\mu}(m,t)}{m\mathbb{G}_{0}(m,t)} + \partial_{\varepsilon} \Big|_{\varepsilon=0} \left(\frac{m^{4\varepsilon}}{2D_{\varepsilon}y^{2\varepsilon}}\right) .$$
(6.98)

It is evaluated as

$$\mathcal{F}_{\mu}(y) = \frac{(y^2+1)\left[\mathcal{I}(y)-2\right]}{2y^2(1-y^2)} + \frac{\sqrt{2\pi}e^{\frac{y^2}{2}}\operatorname{erfc}\left(\frac{y}{\sqrt{2}}\right)}{y\left(y^2-1\right)} + \frac{1}{2}\left[\ln(2)-\gamma_{\rm E}\right]. \tag{6.99}$$

Its asymptotic expansions are

$$\mathcal{F}_{\mu}(y) = \frac{1}{2} \Big[1 - \gamma_{\rm E} + \ln(2) \Big] + \frac{1}{3} \sqrt{2\pi} y - \frac{y^2}{4} + \frac{1}{15} \sqrt{\frac{\pi}{2}} y^3 - \frac{y^4}{36} + \frac{1}{140} \sqrt{\frac{\pi}{2}} y^5 \\ - \frac{y^6}{360} + \frac{\sqrt{\frac{\pi}{2}} y^7}{1512} - \frac{y^8}{4200} + \frac{\sqrt{\frac{\pi}{2}} y^9}{19008} - \frac{y^{10}}{56700} + \mathcal{O}(y^{11}) , \qquad (6.100)$$

$$\mathcal{F}_{\mu}(y) = \ln(2y) + \frac{\ln(2y^2) + \gamma_{\rm E} - 1}{2y^2} + \frac{3}{4y^4} - \frac{5}{4y^6} + \frac{35}{8y^8} - \frac{189}{8y^{10}} + \mathcal{O}(y^{-11}) \,. \quad (6.101)$$

Note that we added some strangely looking factors into the result (6.89). The factor $m \times m^{-\frac{2\varepsilon}{H}} = m^{\frac{1}{H}-1}$ accounts for the dimension of the diffusion constant, $m/D_{\varepsilon} \sim m\tau^{-2\varepsilon}$, and takes out the term $\ln(m)$ from $\mathcal{F}_{\mu}(y)$. We moved out also a remaining term $\sim \ln y$.

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The third function is for the drift proportional to ν ,

$$\mathcal{F}_{\nu}(y) := \frac{\mathbb{G}_{\nu}(y)}{\mathbb{G}_0(y)m} - \ln(y) .$$
(6.102)

It is evaluated as

$$\mathcal{F}_{\nu}(y) = \frac{\mathcal{I}(y) - 2}{2y^2} + \frac{\ln(2) + \gamma_{\rm E}}{2} . \tag{6.103}$$

Its asymptotic expansions read

$$\mathcal{F}_{\nu}(y) = \frac{\sqrt{2\pi}}{y} + \frac{-3 + \gamma_{\rm E} + \ln(2)}{2} - \frac{1}{3}\sqrt{\frac{\pi}{2}}y + \frac{y^2}{12} - \frac{1}{60}\sqrt{\frac{\pi}{2}}y^3 + \frac{y^4}{180} - \frac{1}{840}\sqrt{\frac{\pi}{2}}y^5 + \frac{y^6}{2520} - \frac{\sqrt{\frac{\pi}{2}}y^7}{12096} + \frac{y^8}{37800} - \frac{\sqrt{\frac{\pi}{2}}y^9}{190080} + \frac{y^{10}}{623700} + \mathcal{O}(y^{11})$$

$$\mathcal{F}_{\nu}(y) = -\ln(y) + \frac{2\ln(y) + \gamma_{\rm E} + 1 + \ln(2)}{2y^2} + \frac{1}{4y^4} - \frac{1}{4y^6} + \frac{5}{8y^8} - \frac{21}{8y^{10}} + \mathcal{O}(y^{-11})$$
(6.105)

Using Eq. (6.89) for small y, there is a problem when $\varepsilon \nu < 0$, since then the combination (second-to-last term in the exponential)

$$-\varepsilon\nu my^{2\varepsilon} \left[\frac{1}{2} + \varepsilon \mathcal{F}_{\nu}(y)\right] \xrightarrow{y \to 0} -\varepsilon\nu m\sqrt{2\pi}y^{2\varepsilon-1} \approx -2\nu\sqrt{\pi}t^{H}.$$
(6.106)

diverges (at least for $\frac{1}{4} < H < \frac{1}{2}$), which is amplified since it appears inside the exponential. We propose to use the following Padé variant, which seems to work well numerically,

$$\left[\frac{1}{2} + \varepsilon \mathcal{F}_{\nu}(y)\right] \xrightarrow{\varepsilon < 0, \, \nu > 0} \frac{1}{2 - 4\varepsilon \mathcal{F}_{\nu}(y)} . \tag{6.107}$$

While $\mathcal{F}_{\nu}(y)$ diverges for small y, this is at leading order nothing but a normalization factor depending on νt^{H} .

All three functions $\mathcal{F}_1(y)$, $\mathcal{F}_{\mu}(y)$ and $\mathcal{F}_{\nu}(y)$ are measured in section 6.3, see figures 6.2, 6.3, and 6.5.

6.2.13 Absorption probability

From Eq. (6.61), we obtain, $\mathbf{P}_{\mathrm abs}(m,\alpha,\beta)$

$$\begin{aligned} \mathbf{P}_{abs}(m,\alpha,\beta) &= \int_{0}^{\infty} \mathrm{d}t \, \mathbb{G}(m,tD_{\varepsilon}) \\ &= \int_{0}^{\infty} \mathrm{d}t \, \exp\left(-\frac{m}{2} \left[\frac{\mu}{D_{\varepsilon}} + \nu\right] - \frac{t}{4} \left[\mu t^{-\varepsilon} + \nu t^{\varepsilon}\right]^{2}\right) \mathbb{G}_{0}(m,tD_{\varepsilon}) \\ &\quad + \varepsilon \int_{0}^{\infty} \mathrm{d}t \, \exp\left(-\frac{m}{2}\beta - \frac{t}{4}\beta^{2}\right) \times \left[\mathbb{G}_{1}(m,t) - \alpha \, \mathbb{G}_{\alpha}(m,t) - \beta \mathbb{G}_{\beta}(m,t)\right] + \dots \\ &= \exp\left(-\frac{m}{2} \left[\frac{\mu}{D_{\varepsilon}} + \nu\right]\right) \\ &\quad \times \left\{\int_{0}^{\infty} \mathrm{d}t \, \exp\left(-\frac{t}{4} \left[\mu t^{-\varepsilon} + \nu t^{\varepsilon}\right]^{2}\right) \mathbb{G}_{0}(m,tD_{\varepsilon}) \\ &\quad + \varepsilon \left[\tilde{\mathbb{G}}_{1}(m,s) - \alpha \, \tilde{\mathbb{G}}_{\alpha}(m,s) - \beta \tilde{\mathbb{G}}_{\beta}(m,s)\right]\Big|_{\sqrt{s} = |\beta|/2}\right\} + \dots \end{aligned}$$
(6.108)

Here $\tilde{\mathbb{G}}_1(m,s)$ is given by Eq. (6.64), $\tilde{\mathbb{G}}_{\alpha}(m,s)$ by Eq. (6.71), and $\tilde{\mathbb{G}}_{\beta}(m,s)$ by Eq. (6.74). We still need the integral

$$\int_{0}^{\infty} \mathrm{d}t \, \exp\left(-\frac{t}{4} \left[\mu t^{-\varepsilon} + \nu t^{\varepsilon}\right]^{2}\right) \mathbb{G}_{0}(m, tD_{\varepsilon}) = e^{-|\beta|m/(2\sqrt{D}_{\varepsilon})} + \frac{\alpha\beta}{2} \varepsilon \,\mathbb{G}_{3}(m, \beta) , (6.109)$$
$$\mathbb{G}_{3}(m, \beta) = \int_{0}^{\infty} \mathrm{d}t \, e^{-\frac{\beta^{2}t}{4}} t \ln(t) \mathbb{G}_{0}(m, t) . \quad (6.110)$$

The last expression can be calculated as

$$\begin{split} \mathbb{G}_{3}(m,\beta) &:= \int_{0}^{\infty} \mathrm{d}t \, e^{-\frac{\beta^{2}t}{4}} t \ln(t) \mathbb{G}_{0}(m,t) \\ &= \left. \partial_{\kappa} \right|_{\kappa=0} \int_{0}^{\infty} \mathrm{d}t \, e^{-\frac{\beta^{2}t}{4}} t^{1+\kappa} \mathbb{G}_{0}(m,t) \\ &= \left. \partial_{\kappa} \right|_{\kappa=0} \frac{|\beta|^{-\kappa-\frac{1}{2}} m^{\kappa+\frac{3}{2}} K_{\kappa-\frac{1}{2}} \left(\frac{m|\beta|}{2}\right)}{\sqrt{\pi}} \\ &= \left. -\frac{m^{3/2} \partial_{\kappa} \right|_{\kappa=0} K_{\kappa-\frac{1}{2}} \left(\frac{|\beta|m}{2}\right)}{\sqrt{\pi|\beta|}} + \frac{m e^{-\frac{|\beta|m}{2}} \ln\left(\frac{m}{|\beta|}\right)}{|\beta|} \\ &= \left. -\frac{m e^{\frac{m|\beta|}{2}} \mathrm{Ei}(-m |\beta|)}{|\beta|} + \frac{m e^{-\frac{m|\beta|}{2}} \ln\left(\frac{m}{|\beta|}\right)}{|\beta|} \\ &= \left. -\frac{m}{|\beta|} [-2 \ln(|\beta|) - \gamma_{\mathrm{E}}] + \frac{1}{2} m^{2} [-2 \ln(m) - \gamma_{\mathrm{E}} + 2)] + \mathcal{O}(m^{3}) \,, \quad (6.111) \end{split}$$

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where $K_n(z)$ denotes the modified Bessel function of the second kind. With the above formulas, Eq. (6.108) is rewritten as

$$\mathbf{P}_{abs}(m,\alpha,\beta) = e^{-m(\beta+|\beta|)/2} \left\{ 1 + \varepsilon \, e^{|\beta|m/2} \left[\frac{\alpha\beta}{2} \mathbb{G}_3(m,\beta) + \frac{\alpha+\beta+|\beta|}{2} m(1+\ln\tau) e^{-|\beta|m/2} \right] \\ + \tilde{\mathbb{G}}_1(m,s) - \alpha \tilde{\mathbb{G}}_\alpha(m,s) - \beta \tilde{\mathbb{G}}_\beta(m,s) \right]_{\sqrt{s} = \frac{|\beta|}{2}} + \mathcal{O}(\varepsilon^2) \right\}.$$
(6.112)

We note the exact relations, which can be verified using a computer algebra system,

$$\tilde{\mathbb{G}}_1(m,s) + 2\sqrt{s}\,\tilde{\mathbb{G}}_\beta(m,s) = 0 , \qquad (6.113)$$

$$\mathbb{G}_{3}(m,\beta)|\beta| + 2\tilde{\mathbb{G}}_{\alpha}(m,s) - m(1+\ln\tau)e^{-\frac{m|\beta|}{2}}\Big|_{\sqrt{s}=\frac{|\beta|}{2}} = 0.$$
(6.114)

Let us analyse \mathbf{P}_{abs} separately for $\beta < 0$ and $\beta > 0$, starting with the former. Using both cancelations in Eqs. (6.113) and (6.114), we find

$$\mathbf{P}_{abs}(\alpha,\beta<0) = 1 + \mathcal{O}(\varepsilon^2) \ . \tag{6.115}$$

Thus there is no change in normalisation for a drift towards the absorbing boundary. For $\beta > 0$, we find again with the use of Eqs. (6.113) and (6.114)

$$\mathbf{P}_{abs}(\alpha,\beta>0) = e^{-m\beta} \left\{ 1 + \varepsilon \left[(\alpha+\beta)m(1+\ln\tau) + 2e^{\beta m/2} \left(\tilde{\mathbb{G}}_1(m,s) - \alpha \tilde{\mathbb{G}}_\alpha(m,s) \right)_{\sqrt{s}=\frac{\beta}{2}} \right] + \mathcal{O}(\varepsilon^2) \right\}.$$
(6.116)

For what follows, we note regularity of the combination $\text{Ei}(-x) - \ln(x) - \gamma_{\text{E}}$. We can write Eq. (6.116) as

$$\mathbf{P}_{abs}(m,\alpha,\beta) = e^{-m\beta} \left\{ 1 + \varepsilon \left[(m(\beta - \alpha) + 2) \left(e^{\beta m} \operatorname{Ei}(-m\beta) - \ln(\beta m) - \gamma_{\mathrm{E}} \right) - \alpha m(2\ln(\beta) + \gamma_{\mathrm{E}}) + \beta m(2\ln(m) + \gamma_{\mathrm{E}}) \right] + \mathcal{O}(\varepsilon^{2}) \right\}$$

$$= e^{-m\beta} \left\{ 1 + \varepsilon m \left[2(\beta - \alpha) \ln(\beta) - \gamma_{\mathrm{E}}(\alpha + 3\beta) - 2\beta + 4\beta \ln(m) \right] + \mathcal{O}(\varepsilon^{2}) + \mathcal{O}(m^{2}\varepsilon) \right\}.$$
(6.117)

As the asymptotic expansion in the last line shows, a common resummation is possible; passing to variables μ and ν , it reads

$$\mathbf{P}_{abs}(m,\mu,\nu) = \exp\left(-m^{\frac{1}{H}-1}\mu\left[1+2(1-\gamma_{\rm E})\varepsilon\right] - m^{\frac{1}{H}-1}\nu(\mu+\nu)^{\frac{1}{H}-2}\left[1+2(1-2\gamma_{\rm E})\varepsilon\right]\right) + \mathcal{O}(\varepsilon^{2}) + \mathcal{O}(m^{2}\varepsilon) .$$
(6.118)

This formula represents the leading behavior of $\mathbf{P}_{abs}(m,\mu,\nu)$ for small m; thus terms of order $\mathcal{O}(m^2\varepsilon)$ could be neglected. Note that the (inverse) powers of H were chosen s.t. the resulting

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object is scale invariant. Expanding in ε leads back to Eq. (6.117). One finally arrives at

$$\mathbf{P}_{abs}(m,\mu,\nu) = \exp\left(-m^{\frac{1}{H}-1}\left\{\mu\left[1+2(1-\gamma_{\rm E})\varepsilon\right]+\nu(\mu+\nu)^{\frac{1}{H}-2}\left[1+2(1-2\gamma_{\rm E})\varepsilon\right]\right\}\right.\\ \left.+\varepsilon\left\{2(m\nu+1)\left[e^{m(\mu+\nu)}{\rm Ei}(-m(\mu+\nu))-\ln\left(m(\mu+\nu)\right)-\gamma_{\rm E}\right]\right.\\ \left.-2m(\mu+\nu)\left[\ln\left(m(\mu+\nu)\right)+\gamma_{\rm E}-1\right]\right\}\right) + \mathcal{O}(\varepsilon^{2}) .$$
(6.119)

In order that this formula be invariant under $m \to \lambda m$, $\mu \to \lambda^{1-\frac{1}{H}}\mu$ and $\nu \to \lambda^{-1}\nu$, we can either replace $m\mu$ by $m\mu^{\frac{H}{1-H}}$, or $m^{\frac{1}{H}-1}\mu$. The first version is

$$\mathbf{P}_{abs}^{(a)}(m,\mu,\nu) = \exp\left(-m^{\frac{1}{H}-1}\left\{\mu\left[1+2(1-\gamma_{\rm E})\varepsilon\right]+\nu\left(\mu^{\frac{H}{1-H}}+\nu\right)^{\frac{1}{H}-2}\left[1+2(1-2\gamma_{\rm E})\varepsilon\right]\right\}\right.\\ \left.+\varepsilon\left\{2(m\nu+1)\left[e^{m\left(\mu^{\frac{H}{1-H}}+\nu\right)}{\rm Ei}\left(-m\left(\mu^{\frac{H}{1-H}}+\nu\right)\right)-\ln\left(m\left(\mu^{\frac{H}{1-H}}+\nu\right)\right)-\gamma_{\rm E}\right]\right.\\ \left.-2m\left(\mu^{\frac{H}{1-H}}+\nu\right)\left[\ln\left(m\left(\mu^{\frac{H}{1-H}}+\nu\right)\right)+\gamma_{\rm E}-1\right]\right\}\right)+\mathcal{O}(\varepsilon^{2}). \quad (6.120)$$

The alternative second version is

$$\mathbf{P}_{abs}^{(b)}(m,\mu,\nu) = \exp\left(-m^{\frac{1}{H}-1}\left\{\mu\left[1+2(1-\gamma_{\rm E})\varepsilon\right]+\nu(\mu^{\frac{H}{1-H}}+\nu)^{\frac{1}{H}-2}\left[1+2(1-2\gamma_{\rm E})\varepsilon\right]\right\}\right.\\ \left.+\varepsilon\left\{2(m\nu+1)\left[e^{m^{\frac{1}{H}-1}\mu+m\nu}{\rm Ei}(-m^{\frac{1}{H}-1}\mu-m\nu)-\ln\left(m^{\frac{1}{H}-1}\mu+m\nu\right)-\gamma_{\rm E}\right]\right.\\ \left.-\left(m^{\frac{1}{H}-1}\mu+m\nu\right)\left[\ln\left(m^{\frac{1}{H}-1}\mu+m\nu\right)+\gamma_{\rm E}-1\right]\right\}\right)+\mathcal{O}(\varepsilon^{2}). (6.121)$$

From the appearance of fractal powers of m and ν in Eq. (6.118), we suspect that both power series in $m\mu^{\frac{H}{1-H}}$ and $m^{\frac{1}{H}-1}\mu$ might appear. While numerical simulations could decide which version is a better approximation, only higher-order calculations would be able to settle the question.

6.2.14 Relation between the full propagator, first-passage times, and the distribution of the maximum

In this section, we demonstrate how the probability densities of three different observables follow from the same scaling function. This shows how our result can be used to find the probability distribution of both running maxima and first-passage times for fBM with linear and non-linear drift.

Let us start with the drift-free case, $\mu = \nu = 0$.

(i) In Ref. [252], we calculated P₊(m, t), the normalised probability density to be at m, given t, when starting at x₀ close to 0 (in [252] this quantity is denoted P₊(x, t) with m = x). This object is the constrained propagator of the process, obtained by solving the Fokker Planck equation with vanishing Dirichlet boundary conditions at the absorbing boundary



Figure 6.3.: Example for the absorption probability as a function of μ at $\nu = 0$ (left), and ν at $\mu = 0$ (right). In all cases m = 0.1. The blue solid line represents the result obtained by a direct numerical integration of Eq. (6.89), and adjusting the overall normalisation at $\mu = \nu = 0$ to 1; this has the advantage that the combination $\mu m^{\frac{1}{H}-1}$ appears naturally. The green dashed curve is the same, without adjustment of normalisation. The red dotted curve (visible only on the left plot) is obtained using Eq. (6.119). The magenta curve is obtained using Eq. (6.120). The cyan curve is from Eq. (6.121), and is identical to the magenta one on the right plot. This figure has been submitted for publication to Phys. Rev. E. See App. A.5 for approval of co-authors.

 $x \equiv 0$, *i.e.* $\mathbb{P}_+(m = 0, t) = 0$. While \mathbb{P}_+ is a density in m, and thus should be denoted P_+ (cf. Tab. 6.1), it is the time derivative of a probability, see Eq. (6.127). This can be seen from its definition,

$$\mathbb{P}_{+}(m,t) := \frac{P_{+}(m,t|x_{0})}{\int_{0}^{\infty} \mathrm{d}m \, P_{+}(m,t|x_{0})} , \qquad (6.122)$$

and the asymptotic expansion at small x_0 , (see e.g. [252], appendix C)

$$\int_0^\infty \mathrm{d}m \, P_+(m,t|x_0) \sim x_0^{\frac{1}{H}-1} \,, \tag{6.123}$$

which implies that $\mathbb{P}_+(m,t)$ has dimension 1/time.

- (ii) Here we consider the probability density to be absorbed at time t when starting at m. This is a first-passage time, with distribution $\mathbb{P}_{\text{first}}(m, t)$.
- (iii) Third, let the process start at 0, and consider the distribution of the max m, given a total time t, $P_{\max}(m, t)$, denoted by $P_H^T(m)$ (with t = T) in Ref. [63].

All three objects have a scaling form depending on the same variable $y = \frac{m}{\sqrt{2t^{H}}}$:

$$\mathbb{P}_{\text{first}}(m,t) = \frac{H}{t} \mathcal{P}_{\text{first}}(y) , \qquad (6.124)$$

$$\mathbb{P}_{+}(m,t) = \frac{H}{t} \mathcal{P}_{+}(y) , \qquad (6.125)$$

$$P_{\max}(m,t) = \frac{1}{\sqrt{2}T^H} \mathcal{P}_{\max}(y) . \qquad (6.126)$$

The factors of H and $\sqrt{2}$ where chosen for later convenience. These objects are related. Denote $\mathbf{P}_{surv}(m,t)$ the probability to start at x = 0, and to survive in presence of an absorbing boundary

at m up to time t. Note that $\mathbf{P}_{surv}(m, t)$ is a probability, whereas $\mathbb{P}_{first}(m, t)$, $\mathbb{P}_{+}(m, t)$, and $P_{max}(m, t)$ are densities, the first two in t, the latter in m. Then

$$\mathbb{P}_{+}(m,t) = \mathbb{P}_{\text{first}}(m,t) = -\partial_t \mathbf{P}_{\text{surv}}(m,t) , \qquad (6.127)$$

$$P_{\max}(m,t) = \partial_m \mathbf{P}_{surv}(m,t) . \tag{6.128}$$

Since $\mathbf{P}_{surv}(m,t)$ is a probability, it is scale free, and scaling implies that

$$\mathbf{P}_{surv}(m,t) = \mathbf{P}_{surv}\left(y = \frac{m}{\sqrt{2}t^H}\right) . \tag{6.129}$$

Putting together Eqs. (6.127), (6.128) and (6.129) proves Eqs. (6.124) to (6.126), with

$$\mathcal{P}_{\text{first}}(y) = \mathcal{P}_{+}(y) = y \mathbf{P}'_{\text{surv}}(y) \tag{6.130}$$

$$\mathcal{P}_{\max}(y) = \mathbf{P}'_{\operatorname{surv}}(y) . \tag{6.131}$$

The scaling functions appearing are *almost* the same, differing by (innocent looking) factors of t and H and a (non-innocent looking) factor of y. However, when changing to the measure in y, all of them become *i*dentical. The survival probability in absence of a drift is given in Eqs. (63)-(64) of Ref. [63].

Let us finally add drift. Then the survival probability $\mathbf{P}_{surv}(y, \tilde{u}, v)$ depends on three variables introduced in Eqs. (6.12)-(6.15), setting there $x \to m$. Since $\tilde{u} = m\mu^{\frac{H}{1-H}}$, and $v = \nu m$ are both constants multiplying m, we can write $\mathbf{P}_{surv}(y, \tilde{u}, v) = \mathbf{P}_{surv}(y, m)$. Using Eqs. (6.127) and (6.128), we find

$$\mathbb{P}_{+}(m,t) = \mathbb{P}_{\text{first}}(m,t) = -\frac{\mathrm{d}}{\mathrm{d}t} \mathbf{P}_{\text{surv}}(y,m)$$
$$= \frac{H}{t} \partial_{y} \mathbf{P}_{\text{surv}}(y,m) , \qquad (6.132)$$

$$P_{\max}(m,t) = \frac{\mathrm{d}}{\mathrm{d}m} \mathbf{P}_{\mathrm{surv}}(y,m)$$
$$= \left[\frac{y}{m}\partial_y + \partial_m\right] \mathbf{P}_{\mathrm{surv}}(y,m) . \qquad (6.133)$$

Passing to the measure in y, we obtain

$$\mathcal{P}_{+}(y,m) = \mathcal{P}_{\text{first}}(y,m) = y\partial_{y}\mathbf{P}_{\text{surv}}(y,m) , \qquad (6.134)$$

$$\mathcal{P}_{\max}(y,m) = \left[\partial_y + \frac{m}{y}\partial_m\right] \mathbf{P}_{surv}(y,m) .$$
(6.135)

This set of equations allows us to express $\mathcal{P}_{\max}(y,m)$ as an integral over $\mathcal{P}_+(y,m) = \mathcal{P}_{\mathrm{first}}(y,m)$.

6.2.15 Tail of the distribution

In this section, we briefly discuss a notable contradiction between the textbook by Piterbarg [192] and our calculations that concerns the tail of the distribution of maxima of a fBm. This clash is, as of now, not resolved and at the time of writing lacks a satisfying answer. We did attempt unsuccessfully to reach out and to discuss this matter with Piterbarg.

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Piterbarg [192] states (section 11.3, page 85) that for a fBm defined on the interval [0,1], with $\langle x_1^2 \rangle = 1$, in the limit of $u \to \infty$,

$$\mathbf{P}(\max_{0 \le t \le 1} x_t > u) \simeq \mathbf{\Psi}(u) \times \begin{cases} 2 & H = 1/2 \\ 1 & H > 1/2 \\ \frac{\mathcal{H}_{2H}}{2H} 2^{\frac{1}{2H}} u^{\frac{1}{H}-2} & H < 1/2 \end{cases}$$
with $\mathbf{\Psi}(u) := \frac{1}{\sqrt{2\pi u}} \exp\left(-\frac{u^2}{2}\right) \simeq \frac{1}{\sqrt{2\pi}} \int_{u}^{\infty} \exp\left(-\frac{x^2}{2}\right) \mathrm{d}x$. (6.136)

$$\int du = \int (u) \int \sqrt{2\pi} u = \int (u) \int \sqrt{2\pi} \int u = \int (u) ($$

The estimate for H < 1/2 seems to contain misprints: We find $\sigma(t) := \sqrt{\langle x_t^2 \rangle} = 1 - H|1 - t|$ (i.e. *H* instead of 2*H*). Rescaling $t - 1 \rightarrow 2^{\frac{1}{2H}}(t - 1)$ gives $\sigma(t) \rightarrow 1 - 2^{\frac{1}{2H}} \cdot H \cdot |1 - t|$, thus

$$\mathbf{P}(\max_{0 \le t \le 1} x_t > u) \simeq \frac{\mathcal{H}_{2H}}{2^{\frac{1}{2H}} H} u^{\frac{1}{H} - 2} \Psi(u) , \quad H < \frac{1}{2}.$$
(6.138)

Using the latter result, taking a derivative w.r.t. u, and passing to the measure in y, one obtains $\mathcal{P}(y) \equiv \mathcal{P}_{>}(y|m, \mu = \nu = 0) \equiv \mathcal{P}_{\max}(y)$ (in terms of our variable y), in the limit of large y,

$$\mathcal{P}(y) \simeq \frac{e^{-\frac{y^2}{2}}}{\sqrt{2\pi}} \times \begin{cases} 2 & H = 1/2 \\ 1 & H > 1/2 \\ \frac{\mathcal{H}_{2H}}{2^{\frac{1}{2H}}H} y^{\frac{1}{H}-2} & H < 1/2 \end{cases}$$
(6.139)

The Pickands constant \mathcal{H}_{2H} has ε -expansion [60]

$$\mathcal{H}_{2H} = 1 - 2\gamma_{\rm E}\varepsilon + \mathcal{O}(\varepsilon)^2 . \qquad (6.140)$$

How is this consistent with Eq. (6.89)? Taylor-expanding the latter for large y yields

$$\mathcal{P}(y) \simeq 2 \frac{e^{-y^2/2}}{\sqrt{2\pi}} \left\{ 1 - \left[1 + \gamma_{\rm E} + 2\ln(y) + \ln(2) \right] \varepsilon + \mathcal{O}(\varepsilon^2) + o(y^0) \right\} \,. \tag{6.141}$$

In Ref. [252] this was interpreted as $\mathcal{P}(y) \sim y^{-2\varepsilon} e^{-y^2/2}$. Eq. (6.139) shows that this interpretation is incorrect. For large y, our expansion is almost the sum of the two contributions in Eq. (6.139) for $H \neq 1/2$,

$$\mathcal{P}(y) \approx \frac{e^{-y^2/2}}{\sqrt{2\pi}} \left[1 + \frac{\mathcal{H}_{2H}}{2^{\frac{1}{2H}}H} y^{\frac{1}{H}-2} + \dots \right]$$

$$\simeq 2 \frac{e^{-y^2/2}}{\sqrt{2\pi}} \left\{ 1 - \left[1 + \gamma_{\rm E} + 2\ln(y) - \ln(2) \right] \varepsilon + \mathcal{O}(\varepsilon^2) + o(y^0) \right\}.$$
(6.142)

Note the difference in sign for the $\ln(2)$ term between Eqs. (6.141) and (6.142), showing that the guess (6.142) slightly underestimates the amplitude for $\varepsilon < 0$.



Figure 6.1.: Left: First-passage time density $\mathcal{P}_{\text{first}}(m,t) = \mathcal{P}(y)$ plotted as a function of y as given in Eq. (6.9). In order to increase the resolution of the plot, we use overlapping bins with binsize 5×10^5 , with y increasing by 10^5 points for each bin; (Averages taken over 2.5×10^7 samples per curve, m = 0.1). For various values of H and μ , numerical simulations are compared to the theory. As can be seen on this plot, and on the **ratio between simulations and theory to the right**, the relative error is about 3% at the extreme points. Note that neglecting $\mathcal{F}_1(y)$ would lead for H = 0.4/0.6 to an error of 15%, and for H = 0.33/0.67 to an error of 25%. This figure has been submitted for publication to Phys. Rev. E. See App. A.5 for approval of co-authors.

6.3 Numerics

6.3.1 Simulation protocol

Fractional Brownian motion can be simulated with the classical Davis-Harte (DH) algorithm [54, 69], whose algorithmic complexity (execution time) scales with system size N as $N \ln N$. Here we use the adaptive bisection algorithm introduced and explained in Chp. 5. For H = 1/3 its measured algorithmic complexity grows as $(\ln N)^3$, making it about 5000 times faster, and 10000 times less memory consuming than DH for an effective grid size of $N = 2^{32}$.

To measure the functions \mathcal{F}_1 , \mathcal{F}_μ and \mathcal{F}_ν , which all depend on y only, we

- (i) generate a (drift free) fBm x_t with $x_0 = 0$, of length N; the latter corresponds to a time T = 1.
- (ii) add the drift terms to yield $z_t = x_t + \mu t + \nu t^{2H}$
- (iii) for given m, find the first time t, s.t. $z_t = m$
- (iv) evaluate $y = \frac{m}{\sqrt{2}t^H}$; add a point to the histogram of y.

This histogram misses values of t > T = 1, i.e. $y < \frac{m}{\sqrt{2}}$.

We checked the procedure for Brownian motion (with $\nu \to 0$), where

$$\mathcal{P}(y|m,\mu) = \sqrt{\frac{2}{\pi}} e^{-\frac{(\mu m + 2y^2)^2}{8y^2}} .$$
(6.143)



Figure 6.2.: Numerical estimate of \mathcal{F}_1 . The black curve is the theoretical estimate (6.93), followed by a number of estimates using Eq. (6.145). Solid lines are for m = 0.1(ca. 2.5×10^7 samples per curve), dashed ones for m = 1 (ca. 5×10^7 samples per curve). The symmetrised estimates (6.146) are in olive/cyan. The latter has minimal deviations from the theory. The inset shows a numerical estimate for $\mathcal{F}_2(y)$, as given by Eqs. (6.147) and (6.148). All curves are consistent, and let appear even the next-to-leading corrections. (Remind that changing the normalization is equivalent to adding a constant to $\mathcal{F}_1(y)$ or $\mathcal{F}_2(y)$). The strong curve-down for small and large y are due to numerical problems. This figure has been submitted for publication to Phys. Rev. E. See App. A.5 for approval of co-authors.

Note that this is a function of y and $m\mu$ only, so that we can write

$$\mathcal{P}(y|m\mu) = \sqrt{\frac{2}{\pi}} e^{-\frac{y^2}{2}} \times e^{-\frac{m\mu}{2}} e^{-\frac{(m\mu)^2}{8y^2}} .$$
(6.144)

For fBm, we measure $\mathcal{P}(y|m,\mu,\nu)$, and then extract \mathcal{F}_1 , \mathcal{F}_μ and \mathcal{F}_ν . Firstly,

$$\mathcal{F}_{1}^{\varepsilon}(y|m) := \frac{1}{\varepsilon} \ln \left(\mathcal{P}(y|m)y^{2-\frac{1}{H}}e^{\frac{y^{2}}{2}} \right) \Big|_{\mu=\nu=0}$$
(6.145)

and $\mathcal{F}_1^{\varepsilon}(y|m) = \mathcal{F}_1(y) + \mathcal{O}(\varepsilon^2)$. The following combination is more precise, since terms even in ε cancel,

$$\mathcal{F}_{1}^{\varepsilon, sym}(y|m) = \frac{1}{2} \Big[\mathcal{F}_{1}^{\varepsilon}(y|m) + \mathcal{F}_{1}^{-\varepsilon}(y|m) \Big] + \mathcal{O}(\varepsilon^{2}) .$$
(6.146)

The second-order correction can be estimated as

$$\mathcal{F}_{2}^{\varepsilon}(y|m) := \frac{1}{\varepsilon} \left[\mathcal{F}_{1}^{\varepsilon}(y|m) - \mathcal{F}_{1}(y|m) \right] + \mathcal{O}(\varepsilon) .$$
(6.147)

Its symmetrised version again suppresses subleading corrections,

$$\mathcal{F}_{2}^{\varepsilon, sym}(y|m) := \frac{1}{2\varepsilon} \Big[\mathcal{F}_{1}^{\varepsilon}(y|m) - \mathcal{F}_{1}^{-\varepsilon}(y|m) \Big] + \mathcal{O}(\varepsilon^{2}) .$$
(6.148)

6. Extreme values of Fractional Brownian Motion

The third order correction can be extracted as

$$\mathcal{F}_{3}^{\varepsilon}(y|m) := \frac{1}{2\varepsilon^{2}} \left[\mathcal{F}_{1}^{\varepsilon}(y|m) + \mathcal{F}_{1}^{-\varepsilon}(y|m) - 2\mathcal{F}_{1}(y|m) \right] + \mathcal{O}(\varepsilon) .$$
(6.149)

For the remaining functions \mathcal{F}_{μ} and \mathcal{F}_{ν} , we can employ similar formulas; we have to decide how to subtract \mathcal{F}_1 , numerically from the simulation, or analytically, i.e. by supplying numerically or analytically the denominator in

$$\mathcal{F}^{\varepsilon}_{\mu}(y|m,\mu) := -\frac{1}{\varepsilon} \left[\ln \left(\frac{\mathcal{P}(y|m,\mu,\nu=0)}{\mathcal{P}(y|m,\mu=\nu=0)} \right) \frac{y^{-2\varepsilon}}{\mu m^{\frac{1}{H}-1}} + \frac{1}{2} + \frac{\mu}{4} \left(\frac{m}{2} \right)^{\frac{1}{H}-1} y^{3-\frac{5}{2H}} \right] (6.150)$$

$$\mathcal{F}_{\nu}^{\varepsilon}(y|m) := -\frac{1}{\varepsilon} \left[\ln \left(\frac{\mathcal{P}(y|m,\mu=0,\nu)}{\mathcal{P}(y|m,\mu=\nu=0)} \right) \frac{y^{-2\varepsilon}}{\nu m} + \frac{1}{2} + \frac{\nu m}{8} y^{-\varepsilon-2} \right].$$
(6.151)

We can also work symmetrically

$$\mathcal{F}^{\varepsilon}_{\mu}(y|m) := -\frac{1}{\varepsilon} \left[\ln \left(\frac{\mathcal{P}(y|m,\mu,\nu=0)}{\mathcal{P}(y|m,-\mu,\nu=0)} \right) \frac{y^{-2\varepsilon}}{2\mu m^{\frac{1}{H}-1}} + \frac{1}{2} \right].$$
(6.152)

$$\mathcal{F}_{\nu}^{\varepsilon}(y|m) := -\frac{1}{\varepsilon} \left[\ln \left(\frac{\mathcal{P}(y|m,\mu=0,\nu)}{\mathcal{P}(y|m,\mu=0,-\nu)} \right) \frac{y^{-2\varepsilon}}{2\nu m} + \frac{1}{2} \right] .$$
(6.153)

Finally, a more precise estimate of the theoretical curves is given by symmetrizing results for the same $|\varepsilon|$, using the analogue of Eq. (6.146).

Below, we measure the three scaling functions \mathcal{F}_1 , \mathcal{F}_μ and \mathcal{F}_ν for H = 0.33, using our recently introduced adaptive-bisection algorithm Chp. 5. The latter starts out with an initial coarse grid of size 2^g , which is then recursively refined up to a final gridsize of 2^{g+G} . It gains its efficiency by only sampling *necessary points*, i.e. those close to the target.

The optimal values of g and G depend on H. We run simulations with the following choices: H = 0.33 (g = 8, G = 18), H = 0.4 (g = 10, G = 14), H = 0.6 (g = 8, G = 8), and H = 0.67(g = 8, G = 6). Thanks to the adaptive bisection algorithm, we can maintain a resolution in x of 10^{-3} , with about 25 million samples at H = 0.33, H = 0.6 and H = 0.67, and twice as much for H = 0.4. As we will see below, this allows us to precisely validate our analytical predictions.

6.3.2 Simulation results

We show simulation results on Figs. 6.1 to 6.5. First, on figure 6.1 (left), we present results for the first-passage probability $\mathcal{P}(y|m,\mu,\nu=0)$, using m = 0.1. The numerical results (in color) are compared to the predictions from Eq. (6.89). One sees that theory and simulations are in good quantitative agreement. This comparison is made more precise by plotting the ratio between simulation and theory on the right of Fig. 6.1.

The function $\mathcal{F}_1(y)$ is extracted on Fig. 6.2. We show simulations for m = 0.1 (colored solid lines), and m = 1 (colored dashed lines). The theoretical result (6.93) agrees with numerical simulations for all H, at both values of m. Using the symmetrized form (6.146) with H = 0.4/0.6 shows a particularly good agreement. It allows us to extract the subleading correction via Eqs. (6.147) and (6.148). This is shown in the inset of Fig. 6.2; again the symmetrized estimate is the most precise. Note that the second-order correction is rather sensitive to the choice of m;



Figure 6.3.: Numerical estimate of \mathcal{F}_{μ} . The black curve is the theoretical result (6.99). The colored curves are obtained using Eq. (6.152) with $\mu = \pm 1$ for H = 0.6and H = 0.67, and $\mu = \pm 3$ for H = 0.33 and H = 0.4. Solid lines are for m = 0.1 (ca. 2.5×10^7 samples per curve), dashed ones for m = 1 (ca. 5×10^7 samples per curve). The symmetrised estimates (6.146) are in olive/cyan. The cyan curve using the equivalent of Eq. (6.146) with H = 0.4/0.6 is our best numerical estimate of $\mathcal{F}_{\mu}(y)$. The inset shows the estimated second-order correction, analogous to Eqs. (6.147)-(6.148). This figure has been submitted for publication to Phys. Rev. E. See App. A.5 for approval of co-authors.

more effort would be needed to estimate it properly. Also note that adding a constant to $\mathcal{F}_1(y)$ is equivalent to an overall change in normalization, thus one should concentrate on the shape of the cuves.

Using the data presented on Fig. 6.1, Fig. 6.3 shows the order- ε correction \mathcal{F}_{μ} extracted via Eq. (6.152). The symmetrized estimate is rather close to the analytical result. The inset estimates the subleading correction. Again, estimates for m = 0.1 (dashed lines) and m = 1 (solid lines) are consistent, and a proper measure of the second-order correction would demand a higher numerical precision.

The results for non-linear drift ν are presented on Fig. 6.4, starting with the probability distribution $\mathcal{P}(y|m)$ (left), followed by the ratio between simulation and theory on the right, using m = 0.1. The agreement is again good. From these data is extracted the function $\mathcal{F}_{\nu}(y)$ defined in Eq. (6.103), see Fig. 6.5. Note that $\mathcal{F}_{\nu}(y)$ is much larger than $\mathcal{F}_{\mu}(y)$ (Fig. 6.3), and diverges for small y. The subleading corrections to $\mathcal{F}_{\nu}(y)$ are not negligible, *seemingly* m-dependent, and estimated as well, allowing us to collapse all measured estimates on the theoretical curve.

In summary, we have measured all scaling functions with good to excellent precision, ensuring that the analytical results are correct.



Figure 6.4.: Left: first-passage-time density plotted with overlapping bins as in Fig. 6.1 for various values of H and non-linear drift ν compared to the theory given in Eq. (6.89). Right: Ratio of simulation and theoretical values. This figure has been submitted for publication to Phys. Rev. E. See App. A.5 for approval of co-authors.

6.4 Conclusion

In this work, we gave analytical results for fractional Brownican motion, both with a linear and a non-linear drift. Thanks to a novel simulation algorithm, we were able to verify the analytical predictions with grid sizes up to $N = 2^{28}$, leading to a precise validation of our results.

Our predictions to first order in H - 1/2 are precise, and many samples of very large systems are needed to see statistically significant deviations. We therefore hope that our formulas will find application in the analysis of data, as e.g. the stock market.

Another interesting question is how a trajectory depends on its history, i.e. prior knowledge of the process. We obtained analytical results also in this case, and will come back with its numerical validation in future work.

Our study can be generalised in other directions, as e.g. making the variance a stochastic process, as in [44] or in the rough-volatility model of Ref. [96], which both use fBm in their modelling."



Figure 6.5.: Left: Numerical estimate of \mathcal{F}_{ν} , using Eq. (6.153). The black curve is the theoretical prediction (6.103). The colored curves are simulation results using Eq. (6.153). Solid lines are for m = 0.1, dashed ones for m = 1. The cyan and olive curves are the symmetrised results using the equivalent of Eq. (6.146) for H = 0.4/0.6 (cyan) and H = 0.33/0.67 (olive). The former one is the best numerical estimate of the theory, and very close to the latter. The inset shows the estimated second-order corrections, analogous to Eqs. (6.147)-(6.148). There seem to be non-negligible corrections of order three. An almost perfect data collapse can be obtained for m = 0.1 as $\mathcal{E}\mathcal{F}^{\varepsilon}_{\nu}(y) \simeq \mathcal{F}_{\nu}(y)\mathcal{E} + (2y^{-2} - 4y^{-1} - 6 + y)\mathcal{E}^2 + (3y - 20)\mathcal{E}^3$, and for m = 1 as $\mathcal{E}\mathcal{F}^{\varepsilon}_{\nu}(y) \simeq \mathcal{F}_{\nu}(y)\mathcal{E} + (y - 1.7)(1.5\mathcal{E}^2 - 6\mathcal{E}^3)$, see right figure. Since extrapolation problems mentioned around Eq. (6.107) become important for small y, this estimate is intended as a fit only, to show that the scatter on the left plot is consistent with higher-order corrections. This figure has been submitted for publication to Phys. Rev. E. See App. A.5 for approval of co-authors.

Chapter 7

Conclusion

Throughout the three parts of this thesis, I have demonstrated various ways in which field theories are capable of systematically studying various observables in stochastic processes.

Chapter 1 hopefully conveyed that branching processes are a fruitful playground for Doi-Peliti field theories. A particularly nice feature is the very visual correspondence between the branching events and the associated Feynman diagrams as introduced in Chp. 1. By translating a non-spatial branching process into a Doi Peliti field theory with only time-dependent fields, many interesting observables such as the avalanche shape are cast into diagrammatic language. The combinatorial problems which one encounters when computing them provide intuition and a deeper understanding of branching processes. A key finding which is made transparent by the diagrammatics is the universality of a variety of observables (such as the moments of active particles, the avalanche shape, or the survival property) near or at the critical point. Now that we established a field-theoretic route to universality in branching process, this enables many new research questions.

What happens if the lifetime of a particle no longer is exponentially distributed, but has a lifetime-dependent extinction rate? Understanding such processes would be useful for the study of ageing cell populations. Another interesting problem are genealogical observables. As of now, the fields introduced in Chp. 1 do not contain any genealogical information concerning the particles.¹

If one is to cast genealogical information into a field theory, this is essentially returning to the problem of memory: how can fields keep track of past events? This is precisely the sort of questions addressed by the tracing mechanisms in Chps. 2 and 4. A possible synthesis of these parts of my thesis is therefore the development of a family-tree preserving Doi Peliti field theory to study the genealogy of branching processes.

In fact, my collaborators have already advanced the research developed in Chp. 1 to another field of study. In [182], they consider branching processes with a periodically oscillating extinction rate which is relevant to the study of neuronal avalanches. A further possible future direction of research would be to combine the branching field theory with the external driving framework introduced in Chp. 4 to study the impact of randomly fluctuating extinction or branching rates with small short-range correlations. The diagrammatic correction should yield

¹An example for genealogical information is the time of death of the last common ancestor of two chosen active particles, or the average generation of alive particles. See [77] for a classic study of genealogy in critical branching processes, and [7] for a more recent summary of results on coalesence.

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a systematic approximation (in the spirit of Chp. 4) with many applications to branching in noisy environments, such as reproductive processes in ecology or epidemiology.

In Chp. 2, I presented our collaborative work on branching random walks. By casting the process into a two-species reaction-diffusion problem, we are able to translate the observable of "number of visited sites" into a field-theoretic observable whose renormalisation group behaviour near the critical point provides the scaling behaviour in time and system size. As I point out in Chp. 4, this is merely one of many applications of what I call the tracing mechanism. In fact, it can be similarly used to calculate the *full distribution* of a variety of extreme values of stochastic processes, among others first-passage times.

I argue that the tracing mechanism is capable of addressing a variety of questions arising in statistical dynamics which I did not cover yet in this thesis but wish to explore in the future. I plan, for instance, on investigating its application to extreme value problems (such as first-passage times and running maxima) of more than one walker, such as studied in, *e.g.*, [134]. Further, field theory is destined to tackle extreme value problems of (weakly) interacting random walkers by way of a perturbative expansion.

I have collected a few questions which I believe to be within reach by some modest development of the tools introduced in Chp. 2 and 4:

- First-passage time distribution of N independent stochastic processes subject to white and active noise (in the sense of Chp. 3).
- Extreme Events (running maxima) of branching Ornstein-Uhlenbeck processes such as those studied in the mathematical branching community (*cf.* [18]).
- The volume explored by a branching random walk whose adiabatically changing extinction rate lets the branching random walker oscillate between the super-critical and the subcritical phase. Numerical evidence from an earlier project suggests that through the "adiabatic pumping" an additional net effective current of visited sites is generated which is related to a Berry phase (which would connect it to the research in [219, 220]).

Chapter 3, which I consider the central chapter of this work, provides a perturbative framework to study the full first-passage time distributions for a certain class of non-Markovian processes relevant to the study of active matter. This result is given by corrections to the Markovian distribution which is assumed to be known and requires the diagonalisation of a second-order differential operator. Albeit the latter poses some restrictions on the practically accessible processes, the range of possible applications of this framework is rather large. For illustration, we demonstrated its usefulness calculating the first-order correction to the firstpassage time distribution of an active thermal Ornstein Uhlenbeck process and active thermal Brownian motion. Further, the framework is easily adapted to deterministic driving such as, for instance, a (small) periodic forcing on a particle otherwise driven by white noise. This opens up the possibility to address questions like

• What is the first-passage time distribution of a periodically driven Ornstein-Uhlenbeck process? Are there stochastic resonances? How does the mean first-passage time depend on the frequency?

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- Extend the framework to potentials whose associated Fokker Planck equation is not fully diagonalisable by introducing a second perturbative expansion in the eigenfunctions. In doing so, one could approach the problem of first-passage time in disordered potentials. A particularly simple case of first-passage time in disordered potentials is already addressed in the main text as a limit case of the theory.
- Finally, I think that the link to experiments is crucial at this stage of the project. In the future, I would very much look forward to discuss possible experimental realisations of such processes, ideally *in vivo*, and develop collaborations.

In the third part, I have presented my joint work with Kay Wiese which is the field-theoretic calculation of the first-passage time distribution of a fractional Brownian Motion with drift(s). My contribution to this project was numerical. I designed an algorithm which is capable of sampling first-passage times of fractional Brownian Motion with a significantly lower demand with regards to computing power and memory. This algorithm is abstract enough to deal with other extreme values and processes. Currently, Alexander Shpilkin is improving and extending it to study the running maxima of fractional Brownian Motion with drift which incidentally is also a future research direction logically following Chp. 6. A further extension of this project is the exact numerical sampling of trajectories of stochastic differential equations (SDE) with fractional driving term, *i.e.* processes defined via

$$dX_t = \mu(X_t, t)dt + \sigma dB^{(H)}(t)$$
(7.1)

where $dB^{(H)}(t)$ is a fractional Gaussian noise (see *e.g.* [111] for a discussion of fractional SDE and their ergodic properties). The exact sampling of general fractional SDE at high numerical precision remains challenging, but for specific observables adaptive bisections may provide a substantial improvement in performance.

Altogether, this thesis develops tools and viewpoints which will certainly foster future research advances. Field theory is a useful tool to study stochastic processes, as is underlined by the range of different processes considered and observables computed in this thesis. From fractional Brownian Motion to branching processes, I have considered a wide area of questions which connect various communities, ranging from active matter to stochastic dynamics and finance, and hopefully will contribute to increasing scientific interdisciplinary exchange in the future.

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Appendix A

Approvals for Citations

The Chapters 1,2, 5 and 6 are near verbatim copies of published journal articles or manuscripts. I have sought my co-authors' approval to do so and have obtained it in each and every case. I have also contacted the journals for permission which has been granted. I have followed their guidelines on how to cite my own work. Chapter 3 and 4 are manuscripts in preparation. Chp. 3 is almost finished, so out of courtesy I have also asked for the approval of my co-authors.

A.1 Approvals for Chapter "Field theory of Branching Processes"

I asked my co-authors via email on 03/03/2020:

Dear Rosalba, Dear Johannes, Dear Gunnar,

I would like to use our jointly published paper "Field-theoretic approach to the universality of branching processes" (2018) as a part of my PhD thesis and cite it as a whole and verbatim. I will inquire APS about copyright separately, but would like to ask you as my co-authors for your approval. I would then publish your responses in my thesis. Thanks a lot!

Best, Benjamin

They responded as follows. Rosalba Garcia Millan

> Dear Ben, Yes, of course! Good luck with the thesis. All the best, Rosalba

Johannes Pausch

Dear Ben,

I'm happy with and support the reproduction of our PRE paper "Field-theoretic approach to the universality of branching processes" (2018) as part of your PhD thesis!

Best wishes, Johannes
Gunnar Pruessner

Of course, I approve.

When you include the paper in your thesis, please make sure that you state your contributions to the work clearly. I suggest you do this in the introduction, when you quote the paper and maybe in some summarising table. I believe Johannes' thesis can serve as a model here.

I would also like to take the opportunity to state clearly that I think that Imperial's rules and regs at the very least discourage such verbatim quotes. I also think most examiners agree that the best way for a student to demonstrate their ability to produce original, meaningful research is by publishing.

Cheers, G

Further, I asked the publishers (APS) for their permission and received following response.

Dear Mr Walter,

In response to your email message of 4 March, we refer you to https://journals. aps.org/copyrightFAQ.html - specifically, the question:

"As the author of an APS-published article, may I include my article or a portion of my article in my thesis or dissertation?

Yes, the author has the right to use the article or a portion of the article in a thesis or dissertation without requesting permission from APS, provided the bibliographic citation and the APS copyright credit line are given on the appropriate pages."

This answer is also true before the article is published. The bibliographic citation can then be "Submitted to Physical Review E" or something similar and there is not yet an "APS copyright credit line."

We hope this adequately responds to your query. Yours sincerely,

Dirk Jan Bukman Managing Editor Physical Review E

A.2 Approvals for Chapter "Branching Random Walks on General Graphs"

I asked my co-authors via email on 03/03/2020:

Dear Ignacio, Saoirse, Rosalba, Nanxin and Gunnar,

I am writing to you to let you all know that I will be using our joint publication "Volume explored by a branching random walk on general graphs (2019)" for my PhD thesis, by citing it as a whole and (nearly) verbatim.

This is covered by the Creative Commons Licence under which the article has been published and that Ignacio kindly pointed out to me (see quote below). As co-authors, I would appreciate if you could briefly respond in writing indicating whether you approve of this. I will then include your responses in the thesis.

Thanks a lot!

Best, Benjamin

A. Approvals for Citations

They responded as follows. Ignacio Bordeu:

> Dear Ben, I am happy for you to reproduce this article in your thesis. All the best, Ignacio

Saoirse Amarteifio

Dear Ben, I am happy for you to reproduce this article in your thesis without restriction. All the best, Saoirse Amarteifio

Rosalba Garcia Millan

Dear Ben, I do approve! Best, Rosalba

Nanxin Wei

Dear Benjamin, Of course. Best wishes for the thesis ;) Cheers, Nanxin

Gunnar Pruessner

Of course, I approve. See my previous email for details. G[unnar]

Further, the publisher, Springer Nature, allows for the inclusion of papers into theses. As is stated¹

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 $^{^{1}}$ In https://www.nature.com/nature-research/reprints-and-permissions/permissions-requests, from 31/03/2020.

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A.3 Approvals for Chapter "Fist passage time distribution of active thermal particles"

The Chapter 3 is not yet published. Nevertheless, since the draft is intended for a joint publication with Guillaume Salbreux and Gunnar Pruessner, I reached out asking

Dear Guillaume, Dear Gunnar,

I plan on using our draft on "first-passage times of active and thermal particles in a potential" in near verbatim citation as a chapter of my thesis.

Could I ask you for your written response indicating whether you approve of this? I will then include your response in the thesis.

Many thanks!

Best, Benjamin

Guillaume Salbreux replied

Dear Benjamin, I approve of course that you are using our draft on 'first-passage times of active and thermal particles in a potential' for your thesis. Best wishes, Guillaume

Gunnar Pruessner replied

Of course.

I wonder, whether you are going to include the email verbatim. And if so, whether I will have the last word?

\end{document} \endinput Cheers, G

Bien joué. But no.

A.4 Approval for Chapter "Adaptive Bisections"

On 03/03/2020, I wrote to Kay Wiese

Dear Kay,

I am writing to you to inform you that I am planning to use our joint manuscript "Sampling first-passage times of fractional Brownian Motion using adaptive bisections (2019)" as part of my PhD thesis, and to cite it as a whole and (essentially) verbatim. In doing so, I will ensure that this quotation is transparently stated as such and that my contribution to the project is clearly defined. I would like to ask you as my co-author for your approval which I would then also cite in my thesis.

Many thanks! Best wishes, Benjamin

He replied

Dear Benjamin, you have my authorization. Yours sincerely Kay Wiese

For the permission by the publisher, the American Physical Society, please confer to the reply of the Managing Editor in Sec. A.1. Since it has been accepted for publication, but not printed, I do not need to cite the "APS credit line", but instead state the submission at the beginning of the text and in every figure.

A.5 Approvals for Chapter "Extreme values of Fractional Brownian Motion"

On 03/03/2020, I wrote to Maxence Arutkin and Kay Wiese

Dear Maxence, Dear Kay,

I am writing to you to inform you that I am planning to use our joint manuscript "Extreme Events for Fractional Brownian Motion with Drift: Theory and Numerical Validation (2019)" as part of my PhD thesis, and to cite it as a whole and (essentially) verbatim. In doing so, I will ensure that this quotation is transparently stated as such and that my contribution to the project is clearly defined. I would like to ask you as my co-authors for your approval which I would then also cite in my thesis.

Many thanks! Best wishes, Benjamin Hello, Yes of course. Best, Maxence Kay responded

Dear Benjamin, you have my authorization. Yours sincerely Kay Wiese

We have submitted the manuscript to Phys. Rev. E where it is currently undergoing review. Following the reply of the managing editor of PRE, I do not need to cite a full credit line, but instead state the submission at the beginning of the main text and in every figure.