

Exponentially Distributed Noise:

Correlation Functions and Effects on Non Linear Dynamics

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Abstract

The overdamped Langevin equation is a stochastic differential equation that has applications in several areas of physics; it describes the movement of an overdamped Brownian particle in a force field. In this thesis, two cases of the Langevin equation in linear potentials are studied, their stationary distributions are investigated and the correspondent correlation functions are analytically and theoretically computed. Moreover, the effects of external noise on non linear dynamics are demonstrated by studying the escape rate of particles from a cubic potential under the influence of double exponential distributed noise that is studied in this work and compared to Gaussian distributed noise from an Ornstein-Uhlenbeck process (OU).

To investigate the Langevin equation of interest, its Fokker-Plank representation is used to show its stationary behaviour and it is also used to find analytical expressions of the correlation function. Moreover, analytical approximations for the adiabatic escape rate from a cubic potential with colored noise are investigated. All of these analytical approximations are compared with numerical results.

In this thesis, it is demonstrated that the Langevin equation with positive linear potential has exponential stationary distribution, while the Langevin equation with absolute linear potential has Laplace stationary distribution. Their corresponding correlation functions are investigated and analytically computed and proved to have exponential like behavior. Moreover, the escape rate with colored Laplace stationary process is shown to be higher than that of an OU process due to the fatter tails of the Laplace distribution in comparison with the Gaussian distribution associated with the OU process.

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G. Farah 1 INTRODUCTION

1 Introduction

In the beginning of the twentieth century major works in the field of statistical mechanics from Einstein, Langevin, and Smulochowski led to major development of the theory of Brownian motion paved the way for milestones results such as the Fluctuation-dissipation theorem and the Einstein relation. The theory of Brownian motion became widespread in physics had major applications in Biophysics, Lasers and many other areas in physics. It even inspired the development of the mathematical field of Stochastic Differential Equations (SDE) and Stochastic Processes.(Gardiner 2003 Chapter 1)

One of these discoveries was the Langevin equation which describes the movement of a Browniain particle in a fluid in a force field where its mass is large enough to consider the effects of the fluctuations from the molecules in the fluid as a stochastic force. In the overdamped case of the Langevin equation the friction in the fluid would be large enough so the changes in the velocity of the particle are neglected. These sort of equations have several applications in several areas in physics and other disciplines. One of the most used examples is the Ornstein-Uhlenbeck process (OU) which represents an overdamped Langevin equations in a quadratic potential. The OU process is a Markov-Gaussian process with a stationary Gaussian distribution and has many applications in physics because of the importance of the Normal distribution. (Risken 1989)

However, not everything is Gaussian as there are several cases in physics where an exponential behavior has immersed. For instance increment analysis for tracer motion in biological cells shows an approximately Laplace distributed noise (which is double exponential) instead of a Gaussian one (Otten et al. 2012, Leptos et al. 2009). Moreover, a simple diffusion of an overdamped Brownian particle in a constant gravitational field can be described with an exponentially distributed process (Gardiner 2003 chapter 5). These last two processes can be described either with an overdamped Langevin equation with a positive linear potential and reflecting boundary conditions at the origin yielding an exponential distribution, or with an overdamped Langevin equation with a symmetric linear potential in whole space and natural boundary conditions.

It is also of interest to find the effects of an external colored noises on non linear dynamics. One popular way to study these effects is by examining the escape rate of particles from a potential well represented by a cubic potential under the effects of external colored noise. An escape rate problem of this kind also has uses in several areas of physics, for instance, the firing rate of a noisy quadratic integrate-and-fire neuron can be characterized as an escape rate problem where the Ornstein-Uhlenbeck process represent a noisy input current to the neuron (Burnel and Latham 2003). Therefore, it is of interest to investigate the escape rate from a cubic potential under the colored Laplacian noise mentioned earlier and compare with the escape rate from OU colored noise and see how they act on the system.

This work is structured in the following way; in the first chapter the two Langevin equations with linear potentials are investigated, their Fokker-Plank (FP) representation is introduced and their stationary and general solutions are discussed and simulated. In the second chapter, the correlation functions of the previous processes are analytically computed and simulated, their behavior is examined and a new parameterizations of the Langevin equations in terms of correlation time and stationary variance is presented. In the last chapter, the escape rate from a cubic potential under

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colored Laplace and OU noise is simulated, and the limiting cases for large and small correlation time are analytically approximated and compared with the simulation.

On a side note, it is important to mention that in this work the Langevin equations and the escape rate problem are presented in terms of relative units rather than a specific one because as mentioned and discussed earlier, this kind of problems has several applications in different disciplines with different parameterizations, and there are parameterizations of the escape problem where the units are dimensionless (Vilela and Lindner 2009).

2 Langevin Equation

The overdamped one dimensional Langevin equation describes the movement of a Brownian particle in a fluid under a force field where the friction in the fluid is large enough so the changes in velocities are negligible. The equation takes the form:

$$\gamma \dot{x} = -U'(x) + \sqrt{2D} \, \xi(t)$$

 $\xi(t)$ is White Gaussian noise which is the stochastic term in the Langevin equation: it represent the random forces or fluctuations from the surrounding molecules of the Brownian particle with an intensity D, and U(x) is the potential acting on the particle and γ is the friction coefficient.

The Langevin equation is a stochastic differential equation (SDE) and this form of SDEs has applications in different areas of physics so, in this work, we will consider the case:

$$\dot{x} = -U'(x) + \sqrt{2D} \,\xi(t) \tag{2.1}$$

where $\xi(t)$ is uncorrelated White Gaussian noise with zero mean

$$\langle \xi(t), \xi(t') \rangle = \delta(t - t') \quad \langle \xi(t) \rangle = 0$$
 (2.2)

In this chapter we will study Langevin equation with two different variants of simple linear potentials (see Figure 1), which differ in the form of the potential and the boundary conditions. We will investigate its Fokker-Plank representation and the corresponding general solutions and stationary solutions and simulate it. This kind of equations is not limited to a certain disciplines in physics, but it appears in different areas in physics as mentioned in the introduction, therefore we will present the results dimensionless to assert the generality of the results.

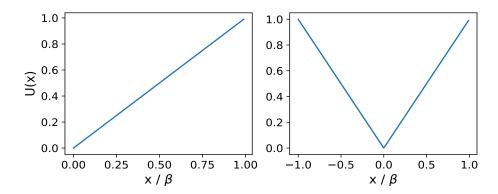


Figure 1: The Potentials we are going to use in this work. The Left panel: $U(x) = \beta x$ for $x \ge 0$. The right panel: $U(x) = \beta |x|$ for $x \in [-\infty, \infty]$ and $\beta > 0$ in both cases

2.1 Langevin equations with Linear Potentials

2.1.1 Langevin equation with linear potential in half space

The first Langevin equation of interest corresponds to (2.1) with linear potential $U(x) = \beta x$ with reflecting boundary conditions at x = 0 and $x \in [0, \infty]$ so we get:

$$\dot{x} = -\beta + \sqrt{2D} \,\xi(t) \tag{2.3}$$

 $\xi(t)$ is uncorrelated white Gaussian noise as in (2.2). The presence of this stochastic term means that the solution of the SDE is not a deterministic path but rather trajectories that have certain probability density function at every point in time (transition probabilities). The Langevin equation can be represented in a Fokker-Plank equation (FP) which is a partial differential equation describing the evolution of the probability density (Risken 1989) The Fokker-Plank representation of the Langevin equation in (2.3) is:

$$\frac{\partial}{\partial t}P(x,t|x',t') = \left(-\beta \frac{\partial}{\partial x} + D \frac{\partial^2}{\partial x^2}\right)P(x,t|x',t') \tag{2.4}$$

The FP equation has the initial condition $P(x,0|x') = \delta(x-x')$ (In this work we will always assume that the process starts at time zero, i.e t'=0, and at point x').

The FP equation (2.4) can be rewritten as a continuity equation of the form $\frac{\partial P(x,t|x')}{\partial t} = -\nabla . j(x,t|x')$, where j is interrupted the probability current.

$$j = (-\beta + D\frac{\partial}{\partial x}) P(x, t|x')$$
(2.5)

The probability current is the probability flux at the boundary S of some region R so it can be used to describe the boundary conditions of the FP equation. In the case of reflective boundary conditions there is zero net flux of probability across the boundaries S of the region R, so we require that the normal \hat{n} on the boundary S to be normal on the probability current i.e:

$$\boldsymbol{n}(\boldsymbol{x}).\boldsymbol{j}(\boldsymbol{x},t,\boldsymbol{x'})=0\;,\;\boldsymbol{x}\in R$$

We have here a one dimensional FP equation, so we can interrupt the condition of the probability current on the reflecting boundary as if the particles cannot penetrate the wall at x = 0, so the flux must vanish at this boundary:

$$(-\beta + D\frac{\partial}{\partial x}) P(x, t|x') = 0 \quad \text{at } x = 0$$
(2.6)

The other boundary condition is a natural boundary that the probability vanishes at infinity:

$$\lim_{x \to \infty} P(x, t | x') = 0$$

2.1.2 Langevin equation with absolute linear potential in whole space

The second Langevin equation of interest corresponds to equation (2.1) with absolute linear potential $U(x) = \beta |x|$, natural boundary conditions at $x = \pm \infty$ and $x \in [-\infty, \infty]$, and initial starting point at x'. So we get:

$$\dot{x} = \begin{cases} -\beta + \sqrt{2D} \,\xi(t) & \text{for } x \ge 0\\ \beta + \sqrt{2D} \,\xi(t) & \text{for } x < 0 \end{cases}$$
 (2.7)

The corresponding FP equation:

$$\frac{\partial P(x,t|x')}{\partial t} = \begin{cases}
(\beta \frac{\partial}{\partial x} + D \frac{\partial^2}{\partial x})P(x,t|x') & \text{for } x \ge 0 \\
(-\beta \frac{\partial}{\partial x} + D \frac{\partial^2}{\partial x})P(x,t|x') & \text{for } x < 0
\end{cases}$$
(2.8)

With initial conditions $P(x,0|x') = \delta(x-x')$ and natural boundary conditions at $\pm \infty$ the transition

probabilities must vanish at the boundaries:

$$\lim_{x \to +\infty} P(x, t|x') = 0 \tag{2.9}$$

Equation (2.8) can also be written as a continuity equation $\frac{\partial P(x,t|x')}{\partial t} = -\nabla \cdot \mathbf{j}$, with j being defined as:

$$j = \begin{cases} (-\beta + D\frac{\partial}{\partial x}) & P(x, t|x') & \text{if } x \ge 0\\ (\beta + D\frac{\partial}{\partial x}) & P(x, t|x') & \text{for } x < 0 \end{cases}$$
 (2.10)

According to the boundary conditions the probabilities should vanish at the boundaries and the probability current, in turn, should also vanish, i.e:

$$j(x,t|x') = 0 \text{ at } x = \pm \infty \tag{2.11}$$

Both SDEs in (2.3) and (2.7) are continuous stochastic processes. Moreover, since they are first order equations and only uncorrelated stochastic noise is present, both equations are determined only by their initial conditions and they have no statistical dependencies on the past; Therefore they are a Markov processes where the value of the process at the next point of time depends only on the value of the process at the current point of time and not on the previous times.(Gardiner 2003)

2.2 Stationary Solution

The stationary solution of the FP equation implies that the transition probability become time independent, i.e $\frac{\partial p}{\partial t} = 0$ so we have that $\nabla \cdot \mathbf{j} = 0$. Since we are working here only with one dimensional SDE $\frac{\partial j}{\partial x} = 0$, so j must be constant in some region R with boundaries (a, b), this suggests the condition for stationary probabilities must be: (Gardiner 2003)

$$j(a) = j(b) = const (2.12)$$

2.2.1 Stationary solution of FP with linear potential in half space

In (2.6) we have shown that j(x, t|x') = 0 at x = 0 and from (2.12) we have now that j = 0, so the stationary solution of (2.4) becomes:

$$(-\beta + D\frac{\partial}{\partial x}) P_0(x) = 0$$
 (2.13)

We can solve this equation for the stationary distribution $P_0(x)$ under the condition of the normalisation of a probability distribution $\int_R dx \, P_0(x) = 1$, we get:

$$P_0(x) = \frac{\beta}{D} e^{-\frac{\beta}{D}x} \tag{2.14}$$

This is an exponential distribution with variance $\sigma^2 = \frac{D^2}{\beta^2}$ and mean $\mu = \frac{\beta}{D}$, the distribution rewritten in terms of the variance:

$$P_0(x) = \frac{1}{\sqrt{\sigma^2}} e^{-\frac{x}{\sqrt{\sigma^2}}}$$
 (2.15)

2.2.2 Stationary solution of FP with absolute linear potential in whole space

In a similar way we can find the stationary solution of the process in (2.8). In (2.10) we stated that j(x,t|x')=0 at $x=\pm\infty$ and from the condition (2.12) we get that j=0, so it follows:

$$0 = \begin{cases} (-\beta + D\frac{\partial}{\partial x}) & P_0(x) & \text{if } x \ge 0\\ (\beta + D\frac{\partial}{\partial x}) & P_0(x) & \text{if } x < 0 \end{cases}$$
 (2.16)

We can solve this equation for the stationary distribution $P_0(x)$ under the normalisation $\int_R dx \ p_0(x) = 1$ so we get:

$$P_0(x) = \frac{\beta}{2D} e^{-\frac{\beta|x|}{D}} \tag{2.17}$$

This is a Laplace distribution with mean zero and variance $\sigma^2 = \frac{D^2}{2\beta^2}$ the distribution can be rewritten in terms of the vairance:

$$P_0(x) = \frac{1}{\sqrt{2\sigma^2}} exp(-\frac{\sqrt{2}|x|}{\sqrt{\sigma^2}})$$
 (2.18)

2.3 General Solution of the Fokker Plank Equations

In general it is difficult to find general solutions for the FP equation, but in the case of the FP equation in half space associated with a positive linear potential (equation (2.4)) a general solution exists and was found by Marian Smoluchowski in 1916. For the second FP equation in whole space (2.8), a solution could be found by transforming the FP equation to a Schrödinger equation by reducing the potential to a Schrödinger potential, solve the Schrodinger equation, and then reformulate it as a solution of the FP equation (for a full treatment of the method see Risken 1989)

2.3.1 General Solution of FP equation in half space

A solution to (2.4) was found by using the condition of the probability current explained in (2.6):

$$(-\beta + D\frac{\partial}{\partial x}) P(x, t|x') = 0 \quad \text{at } x = 0$$
(2.19)

And rewriting it as a heat equation by noting that this equation can be transformed to be presented in terms of a new variable $P^*(x,t|x')$

$$P(x,t|x') = \dot{P}^*(x,t|x') \exp\left(-\frac{\beta(x-x')}{2D} - \frac{\beta^2 t}{4D}\right)$$

Where $P^*(x,t|x')$ fulfills the heat equation:

$$\frac{\partial}{\partial t}P^*(x,t|x') = D\frac{\partial^2}{\partial x^2}P^*(x,t|x')$$

After adjusting the boundary conditions of $P^*(x,t|x')$, Smoluchowski got the following solution for the FP equation: (for a detailed solution see Smoluchowski 1916)

$$P(x,t|x') = (4\pi Dt)^{-\frac{1}{2}} \left[\exp(-\frac{(x-x')^2}{4tD}) + \exp(-\frac{-(x+x')^2}{4tD}) \right] \exp(-\frac{\beta(x-x')}{2D} - \frac{\beta^2 t}{4D}) + \frac{\beta}{2D} \exp(\frac{-\beta x}{D}) \operatorname{erfc}(\frac{x+x'-\beta t}{2\sqrt{Dt}})$$

The first term can be written as the sum of two terms (Schulten Lecture Notes Chapter 4) which makes easier to find the correlation function in the next chapter:

$$P_{1}(x,t|x') = (4\pi Dt)^{-\frac{1}{2}} \exp\left(\frac{-(x-x'+\beta t)^{2}}{4tD}\right)$$

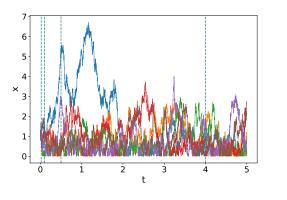
$$P_{2}(x,t|x') = (4\pi Dt)^{-\frac{1}{2}} \exp\left(\frac{\beta x'}{D} - \frac{-(x+x'+\beta t)^{2}}{4tD}\right)$$

$$P_{3}(x,t|x_{0}) = \frac{\beta}{2D} \exp\left(\frac{-\beta x}{D}\right) \operatorname{erfc}\left(\frac{x+x_{0}-\beta t}{2\sqrt{Dt}}\right)$$

$$P(x,t|x') = \sum_{i=1}^{3} P_{i}(x,t|x')$$
(2.20)

Where Exp(x) is the exponential function and erfc(x) is the complementary error function defined as:

$$\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_{x}^{\infty} e^{-\frac{t^{2}}{2}} dt \tag{2.21}$$



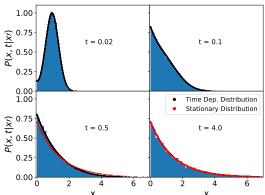


Figure 2: The simulation of 10^4 trajectories of the process in half space according to equation (2.3) for D=4, $\beta=\sqrt{8}$. The variables were chosen so that the process has the same variance ($\sigma^2=2$) and correlation time ($\tau_c=1$) as in Figure (3) (more on that next chapter). The Figure on the left shows 5 trajectories in 5 seconds starting at x'=1. The right panel is for the histogram of the realizations at different times (dashed blue lines on the figure in the left panel) compared with the analytical solution of the FP equation (2.20). First, the term $P_1(x,t|x')$ in equation (2.20) dominates which takes a Gaussian like distribution, but after sufficient time the probability distribution becomes time independent and reaches the stationary limit in (2.14), the can be seen in (2.20) for $t\to\infty$ The first and second term vanish and the third term becomes the stationary distribution ($\lim_{t\to\infty} \operatorname{erfc}(-t)=2$)

2.3.2 General Solution of FP equation in whole space

By transforming the Fokker-Plank equation (2.8) into a Schrödinger equation and using eigenfunction decomposition and perturbation theory and for the detailed steps of the solution of the Schrödinger

equation we arrive at an expression that represents the solution as an integral. We did not arrive to a full solution for the integral but we will present it here because it will help us in the next section to find an analytical expression to the correlation function. (See Risken 1989 p.111 for the detailed steps of the transformation and Cohen-Tannoudji et al. 1977 p. 1360 for the solution of the Schrödinger equation). For a potential of the form: $U(x) = \beta |x|$, its corresponding Schrödinger potential is $U_s(x) = \frac{\beta^2}{4D} - \beta \delta(x)$, the corresponding wave equation is:

$$\Psi(x) = \begin{cases}
\psi_0(x) &= \sqrt{\frac{\beta}{2D}} e^{-\frac{\beta}{2D}|x|} \\
\psi_k^s(x) &= ((4k^2 + ((\frac{\beta}{D})^2)\pi)^{-\frac{1}{2}} (2k\cos(kx) - \frac{\beta}{D}\sin(k|x|)) \\
\psi_k^a(x) &= \pi^{-\frac{1}{2}}\sin kx
\end{cases} (2.22)$$

The first eigenfunction corresponds to the discrete eigenvalue $\lambda_0 = 0$. The other eigenvalues form a continuum $\lambda_k = \frac{\beta^2}{4D} + Dk^2$ and the indices s and a correspond to symmetric and antisymmetric eigenfunctions.

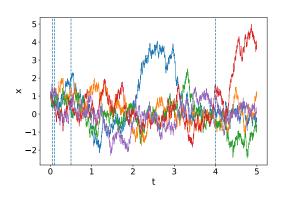
The solution of the FP equation (transition probability) can be found using the potential $\phi(x) = \ln D - \int_{-\infty}^{x} \frac{\beta}{D} dx'$ and then summing over all indices k:

$$P(x,t|x') = e^{\phi(x')/2 - \phi(x)/2} \sum_{k} \psi_k(x)\psi_k(x')e^{-\lambda_k(t)}$$
(2.23)

But in this case the eigenvalues build a continuum, so to find the transition probability we actually have to integrate over all k in equation (2.23) instead of summing, while the discrete term can be added as a single term. We will also assume that the starting time is at zero, i.e t' = 0, so we get:

$$P(x,t|x',0) = e^{-\frac{\beta}{2D}(|x|-|x'|)} \int_{k} \psi_k(x)\psi_k(x')e^{-\lambda_k t} dk$$
 (2.24)

It is still difficult to analytically integrate this expression for the symmetric eigenfunction, but we can make use of it to find the correlation function.



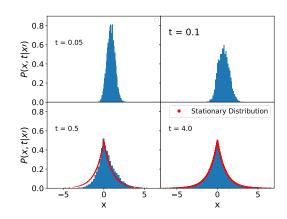


Figure 3: The simulation of 10^4 trajectories of the process in whole space according to equation (2.3) for $D = \frac{5}{2}$, $\beta = \frac{5}{2}$. The variables where chosen so that the processes has the same variance 2 and correlation time 1 as in figure (2) (more on that next chapter).

The Figure on the left shows 5 trajectories in 5 seconds starting at x' = 1. The right figure is for the histogram of the realizations at different times (dashed blue lines on the left figure). No complete solution for the FP equation was presented, but after sufficient time the distribution becomes independent of time and it reaches the stationary Laplace distribution as in (2.17)

2.4 Simulating the SDE

In Figures (2) and (3) we have simulated a large number of realizations of the Langevin equations and compared their histograms we obtained at specific times with the Fokker-Plank equation. To simulate the realizations we have used the standard Euler-Maruyama method (Gardiner 2003 chapter 10). For a SDE of the form:

$$\dot{x} = b(x, t) + \sqrt{2D}\,\xi(t)$$

It can be simulated according to:

$$x_{i+1} = x_i + b(x_i) \Delta t + \sqrt{2D\Delta t} \mathcal{N}(0,1)$$
(2.25)

 Δt is the time step, $i \in (0,...N)$, N is the number of steps in $T = N\Delta t$ where T is the time window of the simulation. b(x,t) is the drift term (the non stochastic term in the SDE) and $\mathcal{N}(0,1)$ are Normal distributed points with zero mean and variance one using x' = 1 as an initial condition.

3 Correlation Function

After we have investigated the Langevin equation with linear potentials and their corresponding FP equations and stationary solutions, now in this chapter we want to find the correlation functions of the stationary processes, simulate them and compare them with exponentially decreasing correlation functions.

3.1 Correlation Function Analytically

The correlation function tells us how two points of the same realization are related, in the case of a stationary stochastic process it depends only on the time lag τ between the two points of the same realization (Risken 1989 chapter 11).

The correlation function is defined as:

$$C(\tau) = \lim_{t \to \infty} (\langle x(t)x(t+\tau)\rangle - \langle x(t)\rangle^2)$$

The correlation function can be computed using the following formulas (Gardiner 2003 p. 64):

$$C(\tau) = \lim_{t \to \infty} \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dx \ x' x (P(x', t; x, t + \tau) - P_0(x) P_0(x'))$$
$$= \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dx \ x' x P_0(x') (P(x, \tau | x') - P_0(x))$$
(3.1)

3.1.1 Correlation function of the Langevin equation in half space

To find an analytical expression of the correlation function of the Langevin equation with linear potential in half space in equation (2.3) we used the formula in (3.1) and inserted the general solutions of the FP equation presented in (2.20) and the stationary solution presented in (2.14): $P_0(x) = \frac{\beta}{D}e^{-\frac{\beta}{D}x}$ The detailed steps of the integration to be found appendix A, and it results:

$$C(\tau) = \left(\frac{D^2}{\beta^2} - \tau D - \frac{\beta^2 \tau^2}{4}\right) \operatorname{erfc}\left(\frac{\beta \tau}{2\sqrt{D\tau}}\right) + \left(\frac{\beta \tau}{2} + \frac{D}{\beta}\right) \sqrt{\frac{D\tau}{\pi}} \ e^{-\frac{\beta^2 \tau}{4D}}$$

This is the correlation function only for positive τ , but it is also plausible to ask how a point in the trajectory is correlated with another point in previous time which results a negative lag time and to take this into account the absolute value of the lag must be taken (it can be analytically found by integrating the formula of the correlation function for negative τ), and the complete correlation function becomes:

$$C(\tau) = \left(-\frac{\beta^2 |\tau|^2}{4} - |\tau|D + \frac{D^2}{\beta^2}\right) \operatorname{erfc}\left(\frac{\beta |\tau|}{2\sqrt{D|\tau|}}\right) + \left(\frac{\beta |\tau|}{2} + \frac{D}{\beta}\right) \sqrt{\frac{D|\tau|}{\pi}} e^{-\frac{\beta^2 |\tau|}{4D}}$$
(3.2)

3.1.2 Correlation Function of the Langevin Equation in whole Space

We can use the integral expression of the general solution of FP equation in (2.24) by inserting it in the integration formula of the correlation function (3.1) and changing the order of integration. First we want to integrate the symmetric eigenfunction:

$$\psi_k^s(x) = ((4k^2 + (\frac{\beta}{D})^2)\pi)^{-\frac{1}{2}} (2k\cos kx - \frac{\beta}{D}\sin k|x|)$$
(3.3)

We insert this in equation (2.24) and then we insert the whole expression into equation (3.1), so we get:

$$\begin{split} C^{s}(\tau) &= \int_{-\infty}^{\infty} dx' x' \int_{-\infty}^{\infty} dx x P(X, \tau | x') P_{0}(x') - (\int_{-\infty}^{\infty} x P_{0}(x) dx)^{2} \\ &= \int_{-\infty}^{\infty} dx' x' \int_{-\infty}^{\infty} dx x \frac{\beta}{2D} e^{-\frac{\beta}{2D}(|x| - |x|') - \frac{\beta}{D}|x|'} \int_{k} dk \frac{(2k \cos kx - \frac{\beta}{D} \sin k |x|) (2k \cos kx' - \frac{\beta}{D} \sin k |x|') e^{-\lambda_{k} t}}{(4k^{2} + (\frac{\beta}{D})^{2})\pi} \\ &= \int_{k} dk \frac{e^{-\lambda_{k} t}}{(4k^{2} + (\frac{\beta}{D})^{2})\pi} \int_{-\infty}^{\infty} dx' x' (2k \cos kx' - \frac{\beta}{D} \sin k |x|') e^{-\frac{\beta}{2D}|x|'} \int_{-\infty}^{\infty} x e^{-\frac{\beta}{2D}(|x|)} (2k \cos kx - \frac{\beta}{D} \sin k |x|) \end{split}$$

We have used Fubini theorem to interchange the order of the integral since the integrand is continuous, also we have used $\int dx \int dx' f(x) f(x') = \int dx f(x) \int dx' f(x')$. This whole integral becomes zero because:

$$I = \int_{-\infty}^{\infty} dx x e^{-\frac{\beta}{2D}(|x|)} (2k\cos kx - \frac{\beta}{D}\sin k|x|)$$

 $\cos(x)$ is an even function, so are $\sin(|x|)$ and $e^{-\frac{\beta}{2D}(|x|)}$ since |x| is even and the function of an even function is even, this makes $(2k\cos kx - |x|)\,e^{-\frac{\beta}{2D}(|x|)}$ even because the subtraction of two even functions is even and the multiplication of two even functions is also even and k is positive. Also since x is an odd function, this makes this whole term odd because the multiplication of odd and even function is odd, and the integration of an odd function on symmetric boundaries is zero, i.e $\int_{-A}^A f_o(x) = 0$, so we get $C^s(\tau) = 0$ We can also easily see that this is also the case for the discrete eigenfunction $\psi_0 = \sqrt{\frac{\beta}{2D}} e^{-\frac{\beta}{2D}|x|}$, if we integrate:

$$C^{0}(\tau) = \int_{-\infty}^{\infty} dx' x' \int_{-\infty}^{\infty} dx x P(X, \tau | x') P_{0}(x') - \left(\int_{-\infty}^{\infty} x P_{0}(x) dx\right)^{2}$$

$$= \int_{-\infty}^{\infty} dx' x' \int_{-\infty}^{\infty} dx x e^{-\frac{\beta}{2D}(|x| - |x|')} \frac{\beta}{2D} e^{-\frac{\beta}{D}|x|'} \sqrt{\frac{\beta}{2D}}$$

$$= \sqrt{\frac{\beta}{2D}} \int_{-\infty}^{\infty} dx' x' e^{-\frac{\beta}{2D}|x|'} \int_{-\infty}^{\infty} dx x e^{-\frac{\beta}{2D}|x|}$$

The function $xe^{-\frac{\beta}{2D}|x|}$ is again odd and it will integrate to zero in the region $[-\infty, \infty]$, so we get $C^0(\tau) = 0$.

Now we are left with the antisymmetric term to integrate and it will be the only component that contributes to this:

$$\begin{split} C^{a}(\tau) &= \int_{-\infty}^{\infty} dx' x' \int_{-\infty}^{\infty} dx x e^{-\frac{\beta}{2D}(|x| - |x|')} \frac{\beta}{2D} e^{-\frac{\beta}{D}|x|'} \int_{k} dk \frac{(\sin kx \sin kx') e^{-\lambda_{k}t}}{\pi} - 0 \\ &= \int_{k} dk \frac{\beta e^{-\lambda_{k}t}}{2D\pi} \int_{-\infty}^{\infty} dx' x' \sin kx' e^{-\frac{\beta}{2D}(|x|')} \int_{-\infty}^{\infty} x e^{-\frac{\beta}{2D}(|x|)} \sin kx \\ &= \int_{k} dk \frac{\beta e^{-\lambda_{k}t}}{2D\pi} (\int_{-\infty}^{\infty} dx' x' \sin kx' e^{-\frac{\beta}{2D}(|x|')})^{2} \\ &= \int_{k} \frac{\beta e^{-\lambda_{k}t}}{2D\pi} (\frac{32\beta D^{3}k}{(\beta^{2} + 4D^{2}k^{2})^{2}})^{2} \\ &= \frac{2\beta^{3}}{\pi D^{3}} \int_{0}^{\infty} dk \frac{k^{2}}{(\frac{\beta^{2}}{4D^{2}} + k^{2})^{4}} e^{-Dt(\frac{\beta^{2}}{4D^{2}} + k^{2})} \\ &= (2\frac{D^{2}}{\beta^{2}} - D\tau + \frac{\beta^{2}\tau^{2}}{2} + \frac{\tau^{3}\beta^{4}}{12D}) \operatorname{erfc}(\frac{\beta\sqrt{\tau}}{2\sqrt{D}}) + (\frac{2D}{\beta} - \frac{2\beta\tau}{3} - \frac{\beta^{3}\tau^{2}}{6D}) \sqrt{\frac{D\tau}{\pi}} e^{\frac{-\beta^{2}\tau}{4D}} \tag{\star} \star \star \end{split}$$

In (\star) we have integrated $\int_{-\infty}^{\infty} dx' x' \sin k x' e^{-\frac{\beta}{2D}(|x|')}$ and inserted the square of it. In $(\star\star)$ we have inserted $\lambda_k = \frac{\beta^2}{4D} + Dk^2$ and rearranged the integrand. In $(\star\star\star)$ we evaluated the integral using Wolfram Mathematica to integrate it, but in general this type of integrals could be recursively solved using the Leibniz rule (differentiating under the integral sign), and since all other components of the wave function do not contribute to the correlation function, we get

$$\begin{split} C(\tau) &= (2\frac{D^2}{\beta^2} - D\tau + \frac{\beta^2 \tau^2}{2} + \frac{\tau^3 \beta^4}{12D}) \operatorname{erfc}(\frac{\beta \sqrt{\tau}}{2\sqrt{D}}) \\ &+ (\frac{2D}{\beta} - \frac{2\beta \tau}{3} - \frac{\beta^3 \tau^2}{6D}) \sqrt{\frac{D\tau}{\pi}} e^{-\frac{\beta^2 \tau}{4D}} \end{split}$$

Like the previous function, we have to replace the parameter τ with its absolute value $|\tau|$ to take negative lag τ into account, so we get:

$$C(\tau) = \left(2\frac{D^2}{\beta^2} - D\tau + \frac{\beta^2 |\tau|^2}{2} + \frac{|\tau|^3 \beta^4}{12D}\right) \operatorname{erfc}\left(\frac{\beta \sqrt{|\tau|}}{2\sqrt{D}}\right) + \left(\frac{2D}{\beta} - \frac{2\beta |\tau|}{3} - \frac{\beta^3 \tau^2}{6D}\right) \sqrt{\frac{D|\tau|}{\pi}} e^{-\frac{\beta^2 |\tau|}{4D}}$$
(3.4)

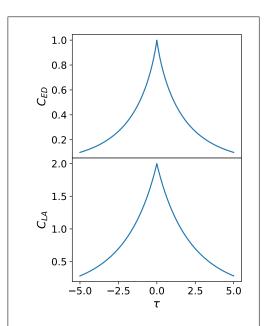


Figure 4: The correlation function of the first process in equation (3.2) (upper panel) and the second process in equation (3.4) for D and β equal 1 (lower panel)

3.2 Properties of the Correlation Function, Finding the Correlation Time, and New Parameters of the Process

In this section we want to investigate several properties of the correlation function: It is even, takes a maximum at the origin $C(\tau) \leq C(0) = \sigma^2$, and it is monotonically decreasing or increasing for positive and negative lags respectively and decaying to zero.

Starting from this section we will refer to the correlation functions in (3.2) and (3.4) as C_{ED} and C_{LA} because they are associated with Laplace and exponential stationary distributions.

3.2.1 Properties of the first correlation function and finding its correlation time

The first correlation function of interest is from (3.2):

$$C_{ED}(\tau) = \left(-\frac{\beta^2 |\tau|^2}{4} - |\tau|D + \frac{D^2}{\beta^2}\right) \operatorname{erfc}\left(\frac{\beta |\tau|}{2\sqrt{D|\tau|}}\right) + \left(\frac{\beta |\tau|}{2} + \frac{D}{\beta}\right) \sqrt{\frac{D|\tau|}{\pi}} e^{-\frac{\beta^2 |\tau|}{4D}}$$

It has the following properties:

- $C_{ED}(0) = \frac{D^2}{\beta^2} = \sigma^2$
- $\lim_{\tau \to \infty} C_{ED}(\tau) = 0$
- ullet It is even function because of the presence of the absolute value of au

Since the correlation function is positive and it is not oscillating a good approximation of the correlation time would be using the formula $\tau_c = \int_0^\infty \frac{C(\tau)}{C(0)} d\tau$ (Lindner lecture notes) so we get:

$$\tau_c = \int_0^\infty \frac{C_{ED}(\tau)}{C_{ED}(0)} d\tau = \frac{2D}{\beta^2}$$
(3.5)

(Last integration was carried out by Wolfram Mathematica). Now we can rewrite the correlation function in terms of the new variables τ_c , σ^2 to get:

$$C_{ED}(\tau) = \left(-\left(\frac{|\tau|}{\tau_{\rm c}}\right)^2 - 2\frac{|\tau|}{\tau_{\rm c}} + 1\right)\sigma^2 \,\operatorname{erfc}\sqrt{\frac{1}{2}\frac{|\tau|}{\tau_{\rm c}}} + \left(1 + \frac{|\tau|}{\tau_{\rm c}}\right)\left(\sqrt{\frac{2}{\pi}\frac{|\tau|}{\tau_{\rm c}}}\right)\sigma^2 e^{-\frac{1}{2}\frac{|\tau|}{\tau_{\rm c}}} \tag{3.6}$$

We will use this form of the correlation function in the rest of this work. We can also use these variables to rewrite the original Langevin equation (2.3):

$$\tau_c \,\dot{x}_{ED} = -2\sigma + \sqrt{4\sigma^2 \tau_c} \,\xi(t) \tag{3.7}$$

The noise intensity of the process is defined as the multiplication of the correlation time and variance because the intensity of the process does not only depend on the variance of the process but also on how long two points of the same realizations are correlated which is characterized by the correlation time (Gardiner 2003, Lindner n.d. Lecture Notes):

$$D_{ED} = \sigma^2 \cdot \tau_c = 2 \frac{D^3}{\beta^4} \tag{3.8}$$

We can parametrize the SDE with the correlation time and noise intensity instead of the correlation time and stationary variance, and we will use this parametrization later in chapter 3:

$$\tau_c \, \dot{x}_{ED} = -2\sqrt{\frac{D_{ED}}{\tau_c}} + \sqrt{4D_{ED}} \, \xi(t)$$
(3.9)

Now we want to show that the correlation function in (3.6) is actually a monotone function, as we have stated before. This can be done by rewriting (3.6) in terms of a new variable $\tau' = \frac{|\tau|}{\tau_c}$ and derive the correlation function in terms of the new variable since τ_c is always positive:

$$C_{ED}(\tau') = (-(|\tau'|)^2 - 2|\tau'| + 1) \sigma^2 \operatorname{erfc} \sqrt{\frac{1}{2}|\tau'|} + (1 + |\tau'|)(\sqrt{\frac{2}{\pi}|\tau'|}) \sigma^2 e^{-\frac{1}{2}|\tau'|}$$

And its derivative:

$$C'(\tau') = 2\sqrt{2} \frac{|\tau'|^{\frac{3}{2}}}{\pi \tau'} e^{-\frac{|\tau|'}{2}} - \frac{2(|\tau'| + \tau'^2)}{\tau'} \operatorname{erfc} \sqrt{\frac{|\tau|'}{2}}$$

We can see from Figure (5) that the derivative of the correlation function behaves as expected from a monotonically symmetric function, since it is positive and increasing for $\tau' > 0$ and negative and decreasing for $\tau' < 0$, this justify the use of the definition of the correlation time in equation (3.5), and shows that the correlation function itself is symmetric monotone function decreasing for positive τ and increasing for negative τ and has it maximum at $\tau = 0$ for $C(0) = \sigma^2$

3.2.2 Properties of the second correlation function

The properties of the correlation function in equation (3.4) can be done analogously:

$$C_{LA}(\tau) = \left(2\frac{D^2}{\beta^2} - D\tau + \frac{\beta^2 |\tau|^2}{2} + \frac{|\tau|^3 \beta^4}{12D}\right) \operatorname{erfc}(\frac{\beta \sqrt{|\tau|}}{2\sqrt{D}}) + \left(\frac{2D}{\beta} - \frac{2\beta |\tau|}{3} - \frac{\beta^3 \tau^2}{6D}\right) \sqrt{\frac{D|\tau|}{\pi}} e^{-\frac{\beta^2 |\tau|}{4D}}$$

- $C(0) = 2\frac{D^2}{\beta^2} = \sigma^2$
- $\lim_{\tau \to \infty} C_{LA}(\tau) = 0$
- ullet An even function because of the presence of the absolute value of au

We get for the correlation time:

$$\tau_c = \int_0^\infty \frac{C_{LA}(\tau)}{C(0)} d\tau = \frac{5D}{2\beta^2}$$
(3.10)

Reparameterizing the correlation function and the original Langevin equation in terms of the correlation time and the variance of the stationary distribution $(\sigma^2 = 2\frac{D^2}{\beta^2})$ we get:

$$C_{LA}(\tau) = \left(\frac{125}{192} \left(\frac{|\tau|}{\tau_{c}}\right)^{3} + \frac{25}{16} \left(\frac{|\tau|}{\tau_{c}}\right)^{2} - \frac{5}{4} \frac{|\tau|}{\tau_{c}} + 1\right) \sigma^{2} \operatorname{erfc}\left(\sqrt{\frac{5}{8} \frac{|\tau|}{\tau_{c}}}\right) + \left(-\frac{25\sqrt{5}}{96} \left(\frac{|\tau|}{\tau_{c}}\right)^{2} - \frac{5\sqrt{5}}{12} \frac{|\tau|}{\tau_{c}} + \sqrt{\frac{5}{4}}\right) \sqrt{\frac{2}{\pi} \frac{|\tau|}{\tau_{c}}} \sigma^{2} e^{-\frac{5}{8} \frac{|\tau|}{\tau_{c}}}$$

$$(3.11)$$

And the Langevin equation (2.7) becomes:

$$\tau_c \,\dot{x}_{LA} = \begin{cases} -\frac{5\sigma}{2\sqrt{2}} + \sqrt{\frac{5}{2}\sigma_{LA}^2 \tau_c} \,\xi(t) & \text{for } x \ge 0\\ \frac{5\sigma}{2\sqrt{2}} + \sqrt{\frac{5}{2}\sigma_{LA}^2 \tau_c} \,\xi(t) & \text{for } x < 0 \end{cases}$$
(3.12)

 D_{LA} the noise intensity of the process :

$$D_{LA} = \sigma^2 \cdot \tau_c = 5 \frac{D^3}{\beta^4} \tag{3.13}$$

And we can parametrize the SDE with the noise intensity and the correlation time to get:

$$\tau_c \dot{x}_{LA} = \begin{cases} -\frac{5}{2} \sqrt{\frac{D_{LA}}{2\tau_c}} + \sqrt{\frac{5}{2}D_{LA}} \xi(t) & \text{for } x \ge 0\\ \frac{5}{2} \sqrt{\frac{D_{LA}}{2\tau_c}} + \sqrt{\frac{5}{2}D_{LA}} \xi(t) & \text{for } x < 0 \end{cases}$$
(3.14)

Now we can rewrite this function in terms of the new variable $\tau' = \frac{|\tau|}{\tau_0}$

$$C_{LA}(\tau') = (\frac{125}{192}(|\tau'|)^3 + \frac{25}{16}(|\tau'|)^2 - \frac{5}{4}|\tau'| + 1)\sigma^2 \operatorname{erfc}(\sqrt{\frac{5}{8}|\tau'|}) + (-\frac{25\sqrt{5}}{96}(|\tau'|)^2 - \frac{5\sqrt{5}}{12}|\tau'| + \sqrt{\frac{5}{4}})\sqrt{\frac{2}{\pi}|\tau'|}e^{-\frac{5}{8}|\tau'|}$$

And the derivative of it:

$$C'_{LA}(\tau') = (\frac{125}{64}|\tau'|\tau') + \frac{25}{8}(\tau') - \frac{5}{4}sign(\tau'))\sigma^2 \operatorname{erfc}\left(\sqrt{\frac{5}{8}|\tau'|}\right) - (\frac{25}{8}\tau' + \frac{5}{2}sign(\tau'))\sqrt{\frac{5|\tau'|}{8\pi}}\sigma^2 e^{-\frac{5}{8}|\tau'|}$$

Just like the previous process, we can see from Figure (5) the derivative of the correlation function is positive and monotonically increasing for negative τ and negative and monotonically increasing for positive τ , so the correlation function itself is positive everywhere and monotonically decreasing for positive τ and increasing for negative τ , it also has it maximum at $\tau = 0$

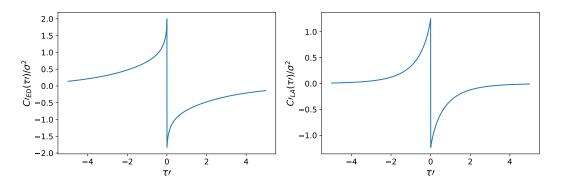


Figure 5: The derivatives of the correlation functions. The left figure is the derivative of the correlation function of the exponentially distributed process in equation (3.15) and to the right is the derivative of the correlation function of the Laplacian distributed process in equation (3.15). We can see that both functions are positive and monotonically increasing for negative τ' and negative and monotonically decreasing for negative τ' and which shows that the both correlation functions are positive, symmetric and absolutely decreasing(increasing) monotone

3.3 Comparing The Correlation Functions

We want to compare the behaviour of both correlation functions with the correlation of an exponentially decreasing correlation associated with the Ornstein-Uhlenbeck process (more on that next chapter). We want also to find the intersection points among all three correlation functions. We will focus solely on correlation for a positive lag τ .

$$C_{OU}(\tau) = \sigma_{OU}^2 e^{-\frac{\tau}{\tau_c}} \tag{3.15}$$

Where σ_{OU}^2 is the variance of the stationary Ornstein-Uhlenbeck process which is Gaussian distributed. We can see in figure (6) that the normed correlation functions of all three function behave in a similar manner, they all intersect in points around $\frac{\tau}{\tau_c} = 0.19$ but not at the same exact point, and both correlation functions do not vary a lot in values from the exponential decreasing function. The exponential correlation C_{OU} falls slower than both correlation functions before the intersection point but after that it shows faster decrease than the other correlation functions, this can be clearly seen in the logarithmic plot of the correlation functions in Figure 7.

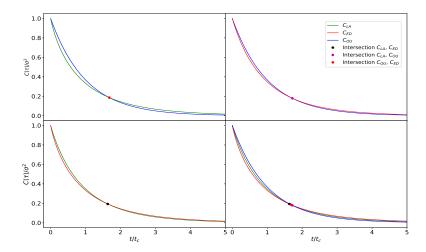


Figure 6: Plots of the three correlation functions against each other with their intersection points at: ($\frac{\tau}{\tau_{\rm c}}=1.68;\,C_{ED,OU}=0.19$), ($\frac{\tau}{\tau_{\rm c}}=1.72;\,C_{OU,LA}=0.18$), ($\frac{\tau}{\tau_{\rm c}}=1.64;\,C_{ED,LA}=0.194$).

3.4 Simulating the Correlation Function

3.4.1 Wiener-Khinchin theorem

The power spectrum of a process describes how the variance of a process is distributed over frequency and it is defined as:

$$S(f) = \lim_{T \to \infty} \frac{\langle x\tilde{x} \rangle}{T}$$
 (3.16)

Where $\tilde{x}(t)$ is the Fourier transform of the time series x(t). the The Wiener-Khinchin theorem states that the power spectrum is the Fourier transform of the correlation function:

$$S(f) = \int_{-\infty}^{\infty} d\tau \, e^{2\pi f \tau} C(\tau)$$
$$C(\tau) = \int_{-\infty}^{\infty} df \, e^{-2\pi f \tau} S(f)$$

This theorem along with the definition of the power spectrum in (3.16) offers a fast and ac-

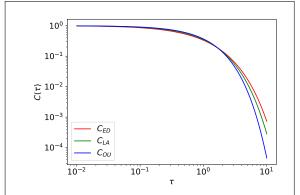


Figure 7: Log Log plot of the normed correlation functions. All functions show an exponential like behavior but C_{OU} shows the fastest drop after the intersection points.

curate numerical way to simulate the correlation function by calculating the Fast Fourier Transform (FFT) of a realization x(t), find the power spectrum according to the formula, and then transform it back (using Inverse Fast Fourier Transform) to get the correlation function. (Gardiner 2003 p.17)

3.4.2 The Simulation

In Figures 8 and 9 we can see the simulation of the correlation functions for several value of the variance and correlation time on a universal curve of the normed correlation function. We can see that the simulations coincide with the theoretical curves deduced in (3.6) and (3.11). We have only

considered the case for a positive lag.

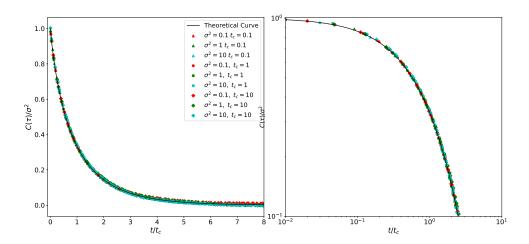


Figure 8: Simulation of the correlation function for the ED process for several values of correlation time and variance in normal and logarithmic scales (right and left panels respectively) compared with the theoretical curve derived in (3.6).

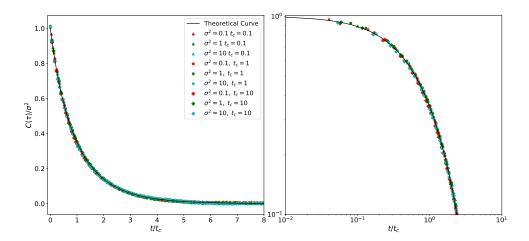


Figure 9: Simulation of the correlation function for the LA process for several values of correlation time and variance in normal and logarithmic scales (right and left panels respectively) compared with the theoretical curve derived in (3.11).

4 Escape Rate over a Potential Barrier

In the Langevin equation we introduced in the first chapter in equation (2.1), we have assumed that the fluctuations in the fluid can be characterized by white Gaussian noise. However, the uncorrelated noise does not represent any real physical system but rather an idealization since it is assumed to be uncorrelated and with infinite variance (Gardiner 2003 chapter 4). So in this chapter, we want to study the effects of correlated colored noise on an overdamped Langevin equation in a cubic potential. We will use the stationary Laplacian distributed noise that has been introduced earlier in section (2.2.2), and we will compare its effects with the more commonly used noise of the Ornstein-Uhlenbeck process which will also be presented in this chapter. Additionally We will study the limiting cases for $\tau_c \to 0$ and $\tau_c \to \infty$. We will present the results in this chapter in relative units.

4.1 The Ornstein-Uhlenbeck Process

Before we proceed to study the effect of the colored noise introduced in on non linear dynamics, we want to briefly introduce the Ornstein-Uhlenbeck Process (OU).

The OU process corresponds to the overdamped Langeving equation in (2.1) with a quadratic potential: $U(x) = \frac{\beta x^2}{2}$, so it becomes:

$$\dot{x} = -\beta x + \sqrt{2D}\,\xi(t) \tag{4.1}$$

Where $\xi(t)$ is the white noise introduced in (2.2), and the corresponding FP equation is:

$$\frac{\partial}{\partial t}P(x,t|x') = \left(-\beta \frac{\partial}{\partial x}x + D\frac{\partial^2}{\partial x^2}\right)P(x,t|x')$$

The natural boundary conditions and initial conditions at x' are: $\lim_{x\to\pm\infty} P(x,t|x')=0$ and $P(x,0)=\delta(x-x')$ The general solution of the FP equation:

$$P(x,t|x') = \frac{1}{\sqrt{2\pi \langle \Delta x^2(t) \rangle}} e^{-\frac{(x-\langle x(t) \rangle)^2}{2\langle \Delta x^2(t) \rangle}}$$

Where $\langle x(t) \rangle = x'e^{-\beta t}$ and $\langle \Delta x^2(t) \rangle = \frac{D}{\beta}(1 - e^{-2\beta t})$ are the time dependent mean and variance respectively. The FP representation has a Gaussian distributed stationary solution for long times:

$$P_0(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}} \tag{4.2}$$

With the stationary variance $\sigma^2 = \frac{D}{\beta}$ And as mentioned in the last chapter, the correlation function of the Ornstein-Uhlenbeck process is exponential:

$$C_{OU}(\tau) = \frac{D}{\beta} e^{-\beta|\tau|}$$

With the same techniques used in the last chapter, the correlation time can be found to be $\tau_c = \frac{D}{\beta}$ and the correlation function becomes:

$$C_{OU}(\tau) = \sigma^2 e^{-\frac{|\tau|}{\tau_c}} \tag{4.3}$$

Therefore the Langevin equation can be rewritten in terms of the correlation time and variance:

$$\tau_c \dot{x}_{OU} = -x_{OU} + \sqrt{2\sigma^2 \tau_c} \xi(t) \tag{4.4}$$

And the quantity $\sigma^2 \tau_c$ is again the noise intensity of the process D_{OU} . We can also parametrize this SDE with the noise intensity and the correlation time of the process:

$$\tau_c \dot{x}_{OU} = -x_{OU} + \sqrt{2D_{OU}}\xi(t) \tag{4.5}$$

The full derivation of the Ornstein-Uhlenbeck process can be found in (Risken 1989), the Ornstein-Uhlenbeck process was used by Langevin in his original work to derive the Einstein relation. It is a Markov Gaussian process because it is a first order equation with uncorrelated stochastic noise and its values determined only by its initial conditions with no dependency on the past. (Gardiner 2003)

4.2 Description of the Problem

We want to consider a Langevin equation with colored noise instead of the white noise introduced in (2.1), i.e:

$$\dot{x} = -U'(x) + \eta(t) \tag{4.6}$$

Where $\eta(t)$ is the colored noise, -U'(x) is the force acting on the particle. The colored noise we are considering is either OU noise or LA noise, we will not consider the case of ED process since it takes only positive values, and the potential we will use in this case is a cubic potential of the form:

$$U(x) = -\frac{x^3}{3} + \beta x \tag{4.7}$$

Where β is a positive constant that characterizes the deepness of the well in the potential. We can see in the figure of the potential (??) that it has a local minima at $x_- = -\sqrt{\beta}$ and a local maxima at $x_+ = \sqrt{\beta}$ and the deepness of the well is $\Delta U = 2\,U(\sqrt{\beta})$. We can ask now how long it takes particles in the local minimum of the potential or to the left of it, to overcome the barrier and reach the local maximum or points on the right of it under the influence of colored noise η . The time the particles take to overcome the barrier is called passage time and by simulating a large number of realizations of the colored noise in a time window we can measure the passage times of particles escaping the potential well, and then find their escape rate which defined as the inverse of the mean of the passage times, i.e $r = \frac{1}{\langle T \rangle}$

In equations (4.4), (4.5), (3.12) and (3.8) we have defined the OU and LA processes in terms of the variance and correlation time or equivalently in terms of noise intensity and correla-

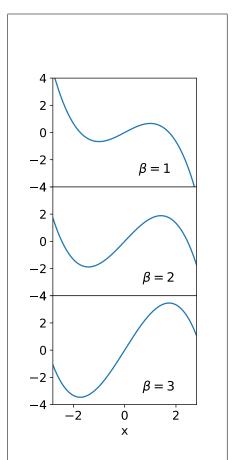


Figure 10: Three cases of the potential for different values of the constant β .

tion time. We will use both definitions to simulate the escape rate for constant stationary variance or constant noise intensity and we will study how the effects on this system vary. Therefore the whole problem can be characterised as the following:

$$\dot{x} = x^2 - \beta + \eta \tag{4.8}$$

$$\eta := \begin{cases}
\tau_c \,\dot{\eta}_{OU} = -\eta_{OU} + \sqrt{2\sigma^2 \,\tau_c} \xi(t) \\
\tau_c \,\dot{\eta}_{LA} = \begin{cases}
-\frac{5}{2} \sqrt{\frac{\sigma^2}{2}} + \sqrt{\frac{5}{2}\sigma^2 \,\tau_c} \,\xi(t) & \text{for } x \ge 0 \\
\frac{5}{2} \sqrt{\frac{\sigma^2}{2}} + \sqrt{\frac{5}{2}\sigma^2 \,\tau_c} \,\xi(t) & \text{for } x < 0
\end{cases} \tag{4.9}$$

We will use η for either OU or LA noise correlated according to (3.15) and (3.11):

$$\begin{split} \langle \eta_{OU}(\tau), \eta_{OU}(0) \rangle &= \sigma^2 e^{-\frac{|\tau|}{\tau_c}} \\ \langle \eta_{LA}(\tau), \eta_{LA}(0) \rangle &= (\frac{125}{192} (\frac{|\tau|}{\tau_c})^3 + \frac{25}{16} (\frac{|\tau|}{\tau_c})^2 - \frac{5}{4} \frac{|\tau|}{\tau_c} + 1) \ \sigma^2 \operatorname{erfc} \left(\sqrt{\frac{5}{8} \frac{|\tau|}{\tau_c}} \right) \\ &+ (-\frac{25\sqrt{5}}{96} (\frac{|\tau|}{\tau_c})^2 - \frac{5\sqrt{5}}{12} \frac{|\tau|}{\tau_c} + \sqrt{\frac{5}{4}} \right) \sqrt{\frac{2}{\pi} \frac{|\tau|}{\tau_c}} \ \sigma^2 \ e^{-\frac{5}{8} \frac{|\tau|}{\tau_c}} \end{split}$$

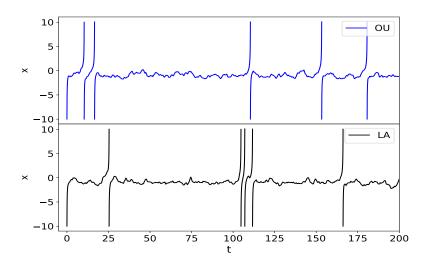


Figure 11: Trajectories of the Langevin equation in equation (4.8) with OU colored noise (upper panel) and LA colored noise (lower panel) with a time step $\Delta t = 10^{-3}$ and starting and end parameters $x_{\pm} = \pm 10$, $\sigma^2 = 1$ and $\tau_c = 2$

4.3 Escape Rate with long correlation time

There are two limiting cases we would like to consider to approximate analytically the escape rate and compare it with the results from the simulation. The first case we would like to consider is for long correlation time and the next case will be discussed in section 3.2.3. In this case we can consider the adiabatic approximation which is similar in concept with the Born-Oppenheimer approximation of multielectron systems in quantum mechanics. If the correlation time is infinite, the process will have infinite correlation which means it will have a constant value equal to the start value of the process which is a stationary OU or LA in our case so the starting point is drawn form a Gaussian or Laplace distribution. Moreover, if the correlation time is very long compared to the time window of the simulation and in regards of the escape problem, if it is large enough in comparison with the

time needed to escape from the potential well characterised by the constant β , we can actually make this assumption that the input noise is constant and we could solve the Langevin equation (4.8) for a constant input noise η_{const} : (see Figure 12), (Moreno-Bote and Parga 2010 and Gardiner 2003 chapter 6):

$$\frac{dx}{dt} = x^2 - \beta + \eta$$

$$dt = \frac{dx}{x^2 - \beta + \eta}$$
(4.10)

$$\int_{0}^{T} dt = \int_{x_{-}}^{x_{+}} dx \frac{1}{x^{2} - \beta + \eta}$$

$$T(\eta) = \frac{Arctan(\frac{x_{+}}{\eta - \beta}) - Arctan(\frac{x_{-}}{\eta - \beta})}{\sqrt{\eta - \beta}})$$
(4.11)

In the last equation the variables x_- and x_+ are the starting point and end point of the particles in the potential, and as mentioned before they should start at the local minima of the potential $x_- = -\sqrt{|\beta|}$ or at smaller values and end at the local maximum $x_+ = \sqrt{|\beta|}$, but we can also set them at $\pm \infty$ because this will help us later to find an analytical expression for the escape rate for large correlation times:

$$r(\eta) = \frac{1}{T} = \frac{\sqrt{\eta - \beta}}{\pi} \tag{4.12}$$

This expression has a solution only for $\eta \geq \beta$ and we call it $\eta_{critical}$ and it is the smallest value for which the particles start escaping the potential well with constant value of the noise.

The last expression for the escape rate is for constant input noise, but this does not mean it is equivalent to the rate for long correlation noise because the value of the constant η depends on the random staring point taken from the stationary distribution and it does not take into account the values under the critical value of the noise. Therefore the escape rate for long correlation time can be obtained by averaging expression (4.12) with the stationary probability distribution of the respective process, in our case we are interested in either Laplace distribution as in (2.18) associated with the LA process or Gaussian distribution as in (4.2) associated with OU process from $\eta_{critical}$ (Moreno-Bote and Parga 2010) i.e:

$$r = \int_{\beta}^{\infty} d\eta \, P_0(\eta) r(\eta) \tag{4.13}$$

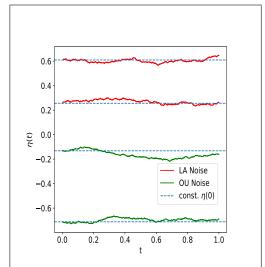


Figure 12: Example of stationary OU and LA noise for $\tau_c=100$ and $\sigma^2=0.1$ for t=1 compared with their initial starting value $\eta(0)$ which is either Laplace or Gaussian distributed.

For the first case of Laplcian noise we insert (4.12) and (2.18) in (4.13):

$$r_{LA} = \frac{1}{\sqrt{2\sigma^2 \pi}} \int_{\beta}^{\infty} d\eta \, e^{-\frac{\sqrt{2}|\eta|}{\sqrt{\sigma^2}}} \sqrt{\eta - \beta} \tag{4.14}$$

$$= \frac{(\sigma^2)^{\frac{1}{4}}}{4\sqrt{\sqrt{2}\pi}} e^{-\beta\sqrt{\frac{2}{\sigma^2}}}$$
 (4.15)

$$\Leftrightarrow \frac{D^{\frac{1}{4}}}{4\sqrt{\sqrt{2\tau_c}\pi}}e^{-\beta\sqrt{\frac{2\tau_c}{D}}} \tag{4.16}$$

For the other case of OU noise with stationary Gaussian distribution in (4.2), this expression can be expressed analytically only with multiple Bessel functions, so we will avoid that and keep the expression as integral and evaluate it numerically:

$$r_{OU} = \frac{1}{\sqrt{2\sigma^2 \pi}\pi} \int_{\beta}^{\infty} d\eta \, e^{-\frac{\eta^2}{2\sigma^2}} \sqrt{\eta - \beta} \tag{4.17}$$

$$\Leftrightarrow \frac{\sqrt{\tau_c}}{\sqrt{2D\pi}\pi} \int_{\beta}^{\infty} d\eta \, e^{-\frac{\eta^2 \tau_c}{2D}} \sqrt{\eta - \beta}$$
 (4.18)

In equations (3.16) and (3.18) we have used the definition of Noise Intensity $D = \tau_c$. σ^2 which we mentioned in section (2.2), and will use these expressions later to compare it with results from the simulation.

It is also of interest to find the values of the variance for which the escape rate is equal for LA and OU noise, and for which values the escape rate of the OU noise is higher than the LA noise and vice versa: This can be obtained by numerically solving the last two expressions in equation (3.17) and (3.15) for some integer values of the constant β

β	σ^2
1	0.57
2	2.3
3	5.16

Table 1: The variance where the Langevin equation has the same escape rate for colored OU and LA process for some values of the constant β . For values of the variance smaller than the listed in the table the escape rate under LA noise is higher than that of OU noise, while for larger values of the variance the escape rate under OU noise will be higher.

4.3.1 Case Study for $\sigma^2 = 0.5$, $\beta = 1$ and $t_c \to \infty$

In the last section we have seen that the adiabatic escape rate under OU noise is faster than the LA noise for certain values of the variance. This behavior can be best explained by studying a case of the escape rate for infinite correlation time, so we chose an example for $\beta = 1$ and $\sigma^2 = 0.5$

We can find the adiabatic escape rate from the analytical expressions introduced in (4.14) and (4.17):

$$r_{OU} \approx 0.0128 \tag{4.19}$$

$$r_{LA} \approx 0.0135 \tag{4.20}$$

The LA noise has a faster escape rate for $\sigma^2 = 0.5$ and this agrees with the values in Table (1). This is due to the fat tails of the exponential distribution. Although, in our case for $\sigma^2 = 0.5$ there is

a higher probability of drawing points larger than $\eta_{critical} = 1$ from a Gaussian distribution than a Laplace distribution (see Figure (13)): So despite the higher probability of the OU noise, the LA noise causes to a faster escape rate due the fat tails of the Laplace distribution because mean it can reach higher points in the noise which in turn contribute to a faster escape rate.

This can also be seen in (Figure 14) where we plotted the integrand in equations (4.14) and (4.17). It can be seen in the figure there are higher values near the $\eta_{critical}$ for the Gaussian distribution, but the Laplace distribution reaches higher values for η .

For even smaller values of the variance the probability with of the Laplace distribution will be higher than the Gaussian distribution and the escape rate will be much faster for the LA noise. This will be clear in the simulation in the next section.

$$\int_{1}^{\infty} P0_{LA} \approx 0.068$$

$$\int_{1}^{\infty} P0_{OU} \approx 0.079$$

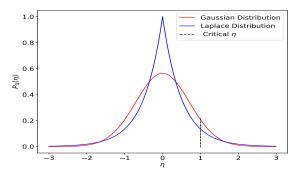


Figure 13: Comparing the Laplace and Normal distributions for $\sigma^2 = 0.5$, we can see that at $\eta_{critical} = 1$ and slightly higher values the Gaussian distribution is higher, but it for lager η values it decays faster than the Laplace distribution because of the fatter tales of the Laplace distribution.

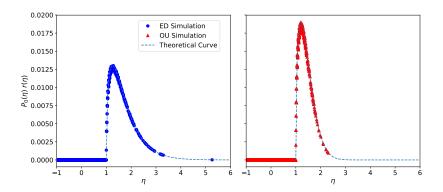


Figure 14: The integrand in equation (4.13) with Laplace distribution in equation (2.18) (left panel) and Gaussian distribution in equation (4.2) (right panel) compared with 5000 simulated points for $\sigma^2 = 0.5$. The Gaussian distributed escape rate has a higher peak around $\eta_{critical} = 1$ because of the higher probability for points to be drawn near it for $\sigma^2 = 0.5$ but it decay fast, while the Laplace distribution has a smaller peak around $\eta = 1$ but it decays slower than the Gaussian distribution because of the fat tails and that is the reason behind the faster escape rate.

4.4 Escape Rate with Short Correlation Time

The other case we want to examine is for vanishing correlation time $\tau_c \to 0$. In this limit the colored noise process becomes a white noise process (Gradiner 2003 chapter 6). So the Langevin equation in equation (4.8) for colored noise become the Langevin equation (2.1) introduced in chapter 1, with the cubic potential in (4.7):

$$\dot{x} = x^2 - \beta + \sqrt{2D}\xi(t) \tag{4.21}$$

Where D here is the noise intensity of the colored noise.

The escape rate with white noise has been treated in literature and several analytical approximations and simulations exist, see for example (H.A.Kramers 1940, Lindner et al. 2003).

The passage times of an arbitrary potential is given by the equation (Gardiner 2003 p. 136, and Linder et al. 2003 Appendix):

$$\langle T(x_{-} \to x_{+}) = \frac{1}{D} \int_{x_{-}}^{x_{+}} dx \, e^{\frac{U(x)}{D}} \int_{-\infty}^{x} dy e^{-\frac{U(y)}{D}}$$
 (4.22)

This integration can be calculated numerically for the starting and endpoints $x\pm$ and the infinite integration boundary can be replaced by sufficiently large finite values that do not change the result of the integration. The escape rate is given by $r=\frac{1}{\langle T\rangle}$. In the simulation when we go for very short correlation times (ca. 10^{-2} or smaller) the effects of the colored noise will be indistinguishable from the white noise process.

4.5 The Simulation

In the simulation we will focus on the case for $\beta = 1$. We have simulated the colored noise for both cases of OU and LA colored noises for a fixed variance and fixed noise intensity so we will use both parameterizations of the OU and LA processes defined in (4.4), (4.5), (3.12) and (3.14) respectively. To simulate the Langevin equation with colored noise numerically, we have used the Runge-Kutta methods (Milshtein and Tret'yakov 1994):

$$x_{i+1} = x_i + dt(x_i^2 - 1 + \eta(t)_i)$$
(4.23)

 η is simulated simultaneously with the same time step according to (2.25). $\eta(0)$ is either Gaussian or Laplace distributed for the OU and LA case respectively in order to ensure we consider the stationary process and $x(0) = x_-$. We simulate the Langevin equation in a time window $T = N\Delta t$ with $i \in (0,...N)$. To find the escape rate we have to measure the passage times when x reaches x_+ and reset it to x_- without resetting the external stochastic noise, and we repeat the simulation multiple times for several time windows to calculate the escape rate according to $r = \frac{1}{\langle T \rangle}$. (Moreno-Bote and Parga 2010, Milshtein and Tret'yakov 1994)

4.5.1 Simulating the escape rate for a fixed input variance

In Figure (15), we simulated the escape rate with constant external variance in three cases for $\sigma^2 = 0.2, 0.5, 1.$

We can see in the Figure that for $\sigma^2 = 0.2$, the escape rate under LA noise is almost 3 times higher than that of OU noise and that is due to the fat tails of the Laplace distribution which will allow the process to reach higher values which in turn will result un a higher number of escapes.

The case $\sigma^2 = 0.5$ has been studied in section 3.3.1, and the simulation coincide with the theoretically expected behavior.

For the case $\sigma^2 = 1$ the escape rate under OU noise exceeds that of the LA noise because of the higher probability of the Gaussian distribution than the Laplace distribution for values around the critical escape value which exceeds the effects of the fatter tails of the Laplace distribution. We can also see that for very small correlation time the escape rate is higher under the LA noise and that is because the noise intensity is small and fluctuating rapidly but the fat tails of the Laplace distribution makes the LA noise reach higher values which results in a higher number of escapes. This behavior explains why even for small correlation times the escape rate is higher for LA noise for $\sigma^2 = 0.2, 0.5$, it will also explain why the escape rate is higher under LA noise with small noise (see the next chapter and Figure (16)). On the other hand when the correlation time gets higher the escape rate the noise intensity gets larger, the fluctuations become less often and the higher probabilities of the Gaussian distribution around $\eta_{critical}$ dominates and causes the higher escape rate of the OU noise as expected analytically from Table 1. This also will explain in the next chapter why the escape rate under OU noise is higher for high noise intensities as shown in Figure (16).

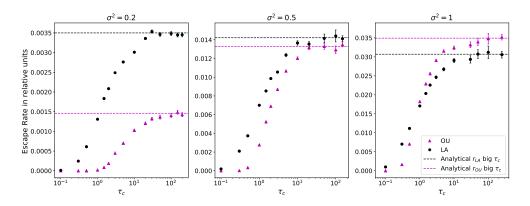


Figure 15: Escape rate with constant input variance for OU and LA external noise for starting and end values $x_{\pm} = \pm 10$ according to (4.23) as a function of the correlation time in relative units, using a time step $\Delta t = 10^{-3}$. The dashed lines correspond to numerically integrating equation (4.13) for the start and end values $x_{\pm} = \pm 10$. We can see that the results coincide with the values in Table 1. Also note that the scales of the escape rate are different for each case.

4.5.2 Simulating the Escape Rate for a Fixed Noise Intensity

In Figure (16) we have simulated the escape rate with a constant noise intensity by using the parameterizations for the LA and OU noise in (3.14) and (4.5) respectively for values of the noise intensity D = 0.5, 1, 5, 10. We compared them with the theoretical approximations for long correlation time in (3.16) and (3.18) and for vanishing correlation time discussed in section 3.3. We can see in Figure 16 that for all cases (except for LA noise with D = 0.5 for small τ_c), the escape rate is decreasing, and that is explained from the definition $D = \sigma^2 \tau_c$ because, for increasing correlation time the input variance is getting smaller so the effects will just decrease from the starting point

For the case D = 0.5 we can see that we had to go for smaller values to reach the case of white noise because ,for weak noise, the LA noise will still have effects on the system due to the fat tails and it will also be higher than the effects of the OU noise as we have explained in the last section. We can also see that it rapidly becomes zero before the analytical long correlation time approximation coincide with many points.

In the other cases for D=1,5,10 the behavior is similar, the OU noise is higher due to the behavior of the associated stationary Gaussian distribution as explained at the end of the last chapter, and long correlation time limits coincide with more points as the noise intensity increases since it will take more time for the variance from the definition of the noise intensity to become small enough so no escapes occurs.

It is also important to note that in the case for long correlation time, we have used the analytical approximations from equations (4.14) and (4.17) where we have used the assumptions that $x_{\pm} = \pm \infty$ to get to these expressions, while in the simulation we have used that $x_{\pm} = \pm 10$ but our choice of these start and endpoints is large enough so we do not see a large deviation from the case of $x_{\pm} = \pm \infty$.

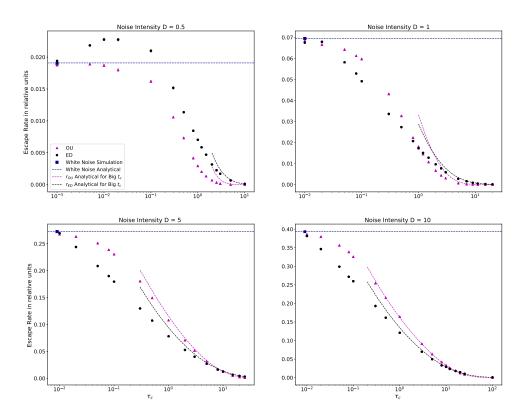


Figure 16: Escape rate with constant input noise intensity for OU and LA external noise for starting and end values $x_{\pm} = \pm 10$ according to (4.23) as a function of the correlation time in relative units using a time step $\Delta t = 10^{-3}$ except for the points smaller than $\tau_c < 10^{-2}$ in the case D = 0.5 where we have used $\Delta t = 10^{-4}, 10^{-5}$. The escape rate for long correlation times agrees with the analytical values in (4.16) and (4.18) (dashed magenta and black lines). The expression in (4.16) was integrated numerically. Also the escape rate for small correlation time limit agrees with the white noise process as discussed in section (4.3) (dashed blue line). It also agrees with simulation (blue square) which was not placed in the figure at $\tau_c = 0$ but rather at a near point so it can be clearly compared with the other two cases. The error bars in this case are very small they cannot be seen on the figures.

5 Summary and Outlook

In the second chapter we presented the Langevin equations with Linear pontetials in equations (2.7) and (2.3). We have seen that these equations have a stationary exponential and Laplace distributions respectively.

In the third chapter, we have investigated the correlation functions of these two processes and have seen that they can be represented in terms of complementary error functions and exponential functions multiplied by a polynomial. We have also shown that despite the complexity of the expressions of the correlation function, they actually behave in a similar manner to an exponential correlation, and they do not deviate in the results. Using the analytical expressions of the correlation functions we were also able to find the correlation time of both processes and reparametrize the Langevin equations and correlation functions in terms of them.

In the last chapter, we have simulated the escape rate of particles from a potential barrier under the influence of Orsntein-Uhlenbeck (OU) and Laplace (LA) external noise, and compared the results with analytical approximations in the case of large and small correlation time. For the case of large correlation time we have found analytical expression for the case of Laplace noise, while for the OU process we had to present it in term of an integral and integrate it numerically; For the case of vanishing correlation time, we have argued that the colored noise process becomes white noise and compared that with the simulation.

In the escape rate problem we have seen that for a small input variance or a small input noise intensity, the escape rate of the LA noise is higher than that of an OU process due to the fat tails of the Laplace distribution, while for higher values of the variance the escape rate under OU noise is higher due to the fatter body of the Normal distribution.

A Appendix: Integrating the Correlation Function

A.1 Integration of the first correlation function

(We want to find the correlation function corresponding to the following Lavengin equation)

$$\dot{x} = -\beta + \sqrt{2D}\xi(t)$$

Which in turns obeys the following Fokker Plank equation:

$$\frac{\partial p}{\partial t} = \beta \frac{\partial p}{\partial x} + D \frac{\partial p^2}{\partial x}$$

The solution of the equation (according to Smoluchowski):

$$p(x,t|x_0,0) = (4\pi Dt)^{-\frac{1}{2}} \left(Exp\left[-\frac{(x-x_0+\beta t)^2}{4tD}\right]\right)$$
(A.1)

$$+Exp[\frac{\beta x_0}{D} - \frac{(x+x_0+\beta t)^2}{4tD}])$$
 (A.2)

$$+\frac{\beta}{2D}Exp\left[-\frac{\beta x}{D}\right]\operatorname{erfc}\left(\frac{x+x_0-\beta t}{2\sqrt{Dt}}\right) \tag{A.3}$$

And the stationary process is:

$$p_0(x) = \frac{\beta}{D} exp(-\frac{\beta x}{D})$$

We will integrate each term seperately, using the formula

$$C(\tau) = \int_0^\infty dx_0 \int_0^\infty x_0 x P_0(x_0) (P(X, \tau | x_0) - P_0(x)) dx$$

We can see that the last term of this integration is just the square of the expected value of the stationary process, i.e:

$$-\int_0^\infty dx_0 \int_0^\infty x_0 x P_0(x_0) P_0(x) dx = -\frac{D^2}{\beta^2}$$
(A.4)

A.2 Integrating the First Term

Now let's proceed with the integration of:

$$\int_0^\infty dx_0 \int_0^\infty dx \, x_0 \, x \, P_0(x_0) \, P(X, \tau | x_0) \tag{A.5}$$

Let us start with the integration of the first term:

$$p_1(x,t|x_0) = (4\pi Dt)^{-\frac{1}{2}} Exp\left[-\frac{(x-x_0+\beta t)^2}{4tD}\right]$$

We integrate according to equation A.5, first we start to integrate in x:

$$I_1 = \int_0^\infty dx \, x \, P(X, \tau | x_0) = A \int_0^\infty dx \, x \, Exp(-\frac{(x - x_0 + \beta t)^2}{4tD})$$
 (A.6)

With $A = (4\pi Dt)^{-\frac{1}{2}}$ Integrate by substitution:

$$z = x - x_0 + \beta t \rightarrow x = z + x_0 - \beta t$$

Insert in I_1

:

$$I_1 = A \int_{-x_0 + \beta t}^{\infty} dz \left(z + x_0 - \beta t \right) Exp\left(-\frac{z^2}{4tD} \right)$$

First term:

$$I_{11} = \int_{-x_0 + \beta t}^{\infty} dz \, z \, Exp(-\frac{z^2}{4tD})$$

$$I_{11} = \left[-\frac{1}{2\frac{1}{4tD}} e^{\frac{-z^2}{4tD}} \right]_{-x_0 + \beta t}^{\infty} = 2tDe^{-\frac{-(x_0 + \beta t)^2}{4tD}}$$

(This could be integrated also by substitution or partial, but I just wrote the results since it is straightforward) Second Term:

$$I_{12} = \int_{-x_0 + \beta t}^{\infty} dz (x_0 - \beta t) Exp(-\frac{z^2}{4tD})$$

By substitution: $u = \frac{z}{2\sqrt{tD}} du = \frac{dz}{2\sqrt{dt}}$

$$I_{12} = \int_{\frac{-x_0 + \beta t}{2\sqrt{D}}}^{\infty} du \, 2\sqrt{tD} (x_0 - \beta t) \, e^{-u^2}$$

$$I_{12} = \sqrt{tD\pi}(x_0 - \beta t)\operatorname{erfc}(\frac{-x_0 + \beta t}{2\sqrt{dt}})$$

Now we insert I_{11} and I_{12} in I_{11} to get:

$$I_{1} = A \left(2tD e^{-\frac{(x_{0} + \beta t)^{2}}{4tD}} + \sqrt{tD\pi} \left(x_{0} - \beta t\right) \operatorname{erfc}\left(\frac{-x_{0} + \beta t}{2\sqrt{dt}}\right)$$
(A.7)

Now we have to integrate equation (A.7) in x_0 according to equation 2, i.e:

$$I_2 = \int_0^\infty dx_0 \, x_0 \, P_0(x_0) \, I_1$$

$$I_2 = A \frac{\beta}{D} \int_0^\infty dx_0 \, x_0 \, exp(-\frac{\beta x_0}{D}) \left(2tD \, e^{-\frac{-(x_0 + \beta t)^2}{4tD}} + \sqrt{tD\pi} \left(x_0 - \beta t\right) \, \text{erfc}(\frac{-x_0 + \beta t}{2\sqrt{dt}}) \right)$$

Take the first term:

$$I_{21} = A_1 \int_0^\infty dx_0 \, x_0 \, e^{\left(-\frac{\beta x_0}{D}\right)} \, e^{-\frac{-(x_0 + \beta t)^2}{4tD}}$$

Where $A_1 = \frac{\beta}{D} (4\pi Dt)^{-\frac{1}{2}} 2tD$ And the second term:

$$I_{22} = A_2 \int_0^\infty dx_0 \, x_0 \, (x_0 - \beta t) \, e^{\left(-\frac{\beta x_0}{D}\right)} \, \operatorname{erfc}\left(\frac{-x_0 + \beta t}{2\sqrt{dt}}\right)$$

Where $A2 = \frac{\beta}{D} \sqrt{tD\pi} \, (4\pi dt)^{-\frac{1}{2}} = \frac{\beta}{2D}$ We start integrating the first term:

$$I_{21} = A_1 \int_0^\infty dx_0 \, x_0 \, e^{\left(-\frac{\beta x_0}{D}\right)} \, e^{-\frac{-(x_0 + \beta t)^2}{4tD}}$$

$$= A_1 \int_0^\infty dx_0 \, x_0 \, e^{-\frac{-(x_0 - \beta t)^2}{4tD}}$$

(This is the same integration as I_1 and the result is the same as (A.7)

$$I_{21} = A_1 \left(2tD e^{-\frac{(\beta t)^2}{4tD}} - \beta t \sqrt{\pi t D} \operatorname{erfc}\left(\frac{\beta \sqrt{t}}{2D}\right)\right)$$
(A.8)

Now we have to integrate I_{22}

$$I_{22} = A_2 \int_0^\infty dx_0 \, x_0 \, (x_0 - \beta t) \, e^{(-\frac{\beta x_0}{D})} \, \operatorname{erfc}(\frac{-x_0 + \beta t}{2\sqrt{dt}})$$

This should be taken into two parts, namely:

$$I_{221} = -A_2 \, \beta t \int_0^\infty dx_0 \, x_0 \, e^{\left(-\frac{\beta x_0}{D}\right)} \, \operatorname{erfc}\left(\frac{-x_0 + \beta t}{2\sqrt{dt}}\right)$$

$$I_{222} = A_2 \int_0^\infty dx_0 \, x_0^2 \, e^{\left(-\frac{\beta x_0}{D}\right)} \, \operatorname{erfc}\left(\frac{-x_0 + \beta t}{2\sqrt{dt}}\right)$$

Where $I_{22} = I_{221} + I_{222}$

We start integrating the first term:

$$I_{221} = -A_2 \, \beta t \int_0^\infty dx_0 \, x_0 \, e^{\left(-\frac{\beta x_0}{D}\right)} \, \operatorname{erfc}\left(\frac{-x_0 + \beta t}{2\sqrt{dt}}\right)$$

This can be integrated by parts:

$$U = \operatorname{erfc}(\frac{-x_0 + \beta t}{2\sqrt{dt}}), \ dU = \frac{1}{\sqrt{\pi Dt}}e^{-(\frac{(-x_0 + \beta t)^2}{4Dt})}$$

$$dV = x_0 e^{-\frac{\beta x_0}{D}}, \ \ V = -\frac{D^2}{\beta^2} e^{-\frac{\beta x_0}{D}} (\frac{\beta x_0}{D} + 1)$$

Integrate according to : $UV - \int V \, dU$

$$UV = \frac{D^2}{\beta^2} \left[\operatorname{erfc}\left(\frac{-x_0 + \beta t}{2\sqrt{dt}}\right) \left(e^{-\frac{\beta x_0}{D}} \left(\frac{\beta x_0}{D} + 1\right)\right) \right]_0^{\infty}$$
$$= 0 + \frac{D^2}{\beta^2} \operatorname{erfc}\left(\frac{\beta t}{2\sqrt{tD}}\right)$$
$$= \frac{D^2}{\beta^2} \operatorname{erfc}\left(\frac{\beta t}{2\sqrt{tD}}\right)$$

considering the other constant factor

$$= (-A_2\beta t) \frac{D^2}{\beta^2} \operatorname{erfc}(\frac{\beta t}{2\sqrt{tD}})$$

$$= -\frac{Dt}{2} \operatorname{erfc}(\frac{\beta t}{2\sqrt{tD}})$$
(A.9a)

Now we want to integrate

$$-\int V dU = \int_{0}^{\infty} dx_{0} \frac{1}{\sqrt{\pi D t}} \frac{D^{2}}{\beta^{2}} e^{-\frac{(-x_{0}+\beta t)^{2}}{4Dt}} e^{-\frac{\beta x_{0}}{D}} (\frac{\beta x_{0}}{D} + 1)$$

$$= A_{21} \int_{0}^{\infty} dx_{0} x_{0} e^{-\frac{(x_{0}+\beta t)^{2}}{4tD}} (\frac{\beta x_{0}}{D} + 1)$$

$$= A_{21} \int_{0}^{\infty} dx_{0} \frac{\beta x_{0}^{2}}{D} e^{-\frac{(x_{0}+\beta t)^{2}}{4tD}} + x_{0} e^{-\frac{(x_{0}+\beta t)^{2}}{4tD}}$$
where $A_{21} = -A_{2} \beta t \frac{1}{\sqrt{\pi D t}} \frac{D^{2}}{\beta^{2}} = -\sqrt{\frac{Dt}{4\pi}}$

$$= (-\frac{tD}{2} + \frac{\beta^{2} t^{2}}{2}) \operatorname{erfc}(\frac{\beta t}{2\sqrt{tD}}) - \frac{BDt}{\sqrt{\pi D t}} e^{-\frac{\beta^{2} t}{4D}}$$
(A.9b)

If we add the equations (A.8) (A.9a) (A.7) 6b we get:

$$I = -\left(\frac{\beta^2 t^2}{2} + tD\right) \operatorname{erfc}\left(\frac{\beta\sqrt{t}}{2\sqrt{D}}\right) + \left(\sqrt{\frac{Dt}{\pi}}\beta t\right) e^{-\frac{\beta^2 t}{4D}}$$
(A.10)

We have only one term left to integrate and add to I to finish the first integration, namely:

$$I_{222} = A_2 \int_0^\infty dx_0 \, x_0^2 \, e^{\left(-\frac{\beta x_0}{D}\right)} \, \operatorname{erfc}\left(\frac{-x_0 + \beta t}{2\sqrt{dt}}\right)$$

This term can also be integrated by partial integration by taking:

$$U = \operatorname{erfc}(\frac{-x_0 + \beta t}{2\sqrt{dt}}), \ dU = \frac{1}{\sqrt{\pi Dt}}e^{-(\frac{(-x_0 + \beta t)^2}{4Dt})}$$

$$dV = x_0^2 e^{-\frac{\beta x_0}{D}}, \ V = -\frac{D}{\beta^3} e^{-\frac{\beta x_0}{D}} (2D^2 + 2D\beta + \beta^2 x_0^2)$$

Integrate according to : $UV - \int V dU$ We will write down directly the result of the integration since we use the same steps as before:

$$I_{222} = \left(\frac{2D^2}{\beta^2} + \frac{\beta^2 t^2}{2}\right) \operatorname{erfc}\left(\frac{-x_0 + \beta t}{2\sqrt{dt}}\right) + \left(2\frac{D^2}{\beta^2}\sqrt{\frac{t}{D\pi}} - \sqrt{\frac{t}{D\pi}}D\beta t\right)e^{-\frac{\beta x_0}{D}}$$
(A.11)

Now if we add (A.11), (A.10) we get:

$$I = (-tD + 2\frac{D^2}{\beta^2})\operatorname{erfc}(\frac{-x_0 + \beta t}{2\sqrt{dt}}) + (\frac{2D}{\beta}\sqrt{\frac{Dt}{\pi}})e^{-\frac{\beta x_0}{D}}$$
(A.12)

which is the final answer of the first integral

A.3 The Second Integral

$$p_2(x,t|x_0,0) = (4\pi Dt)^{-\frac{1}{2}} Exp\left[\frac{\beta x_0}{D} - \frac{(x+x_0+\beta t)^2}{4tD}\right]$$

We want to integrate $p_2(x, t|x_0)$ using equation (A.5):

$$I = \int_0^\infty dx_0 \int_0^\infty dx \, x_0 \, x \, P_0(x_0) \, P(X, \tau | x_0)$$

$$= (4\pi Dt)^{-\frac{1}{2}} \frac{\beta}{D} \int_0^\infty dx_0 \int_0^\infty dx \, x_0 \, x \, e^{-\frac{(x+x_0+\beta t)^2}{4tD}}$$

First we integrate in x direction:
$$I_1 = A_1 \int_0^\infty dx \ x \ e^{-\frac{(x+x_0+\beta t)^2}{4tD}} A_1 = \frac{\beta}{D} (4\pi Dt)^{-\frac{1}{2}}$$

This is the same integration that we have done in (A.6) just with different sign, so we will write directly the results:

$$I_{1} = \frac{\beta t}{\sqrt{\pi D t}} e^{-(\frac{x_{0} + \beta t}{2\sqrt{D t}})^{2}} - A_{1}(x_{0} + \beta t) \operatorname{erfc}(\frac{x_{0} + \beta t}{2\sqrt{D t}})$$
(A.13)

Now we have to integrate equation (A.13) in x_0 , the first term:

$$I_{21} = \frac{\beta t}{\sqrt{\pi D t}} \int_0^\infty dx_0 \, x_0 e^{-(\frac{x_0 + \beta t}{2\sqrt{D t}})^2}$$

$$= \frac{2\beta D t^2}{\sqrt{\pi D t}} e^{-\frac{\beta^2 t}{4D}} - \beta^2 t^2 \operatorname{erfc}(\frac{\beta \sqrt{t}}{2D})$$
(A.14)

(We used the same method to integrate as (A.6)) now we have to integrate:

$$I_{22} = -A_1 \int_0^\infty dx_0 \, x_0(x_0 + \beta t) \operatorname{erfc}(\frac{x_0 + \beta t}{2\sqrt{Dt}})$$
(A.15)

We integrate the first term

$$I_{221} = -A_1 \beta t \int_0^\infty dx_0 \, x_0 \, \text{erfc}(\frac{x_0 + \beta t}{2\sqrt{Dt}})$$

We integrate by parts:

$$U = \operatorname{erfc}(\frac{-x_0 + \beta t}{2\sqrt{dt}}), \quad dU = \frac{1}{\sqrt{\pi Dt}} e^{-(\frac{(-x_0 + \beta t)^2}{4Dt})}$$
$$dV = x_0, \ V = \frac{x_0^2}{2}$$

Integrate according to : $UV - \int V \, dU$

$$UV = 0$$

$$-\int V dU = A_1 \frac{\beta t}{2\sqrt{\pi D t}} \int_0^\infty x_0^2 e^{-(\frac{(-x_0 + \beta t)^2}{4Dt})}$$

$$= \frac{\beta^3 t^3}{2\sqrt{\pi D t}} e^{-\frac{\beta^2 t}{4D}} - (\frac{\beta^2 t^2}{2} + \frac{\beta^4 t^3}{4D}) \operatorname{erfc}(\frac{\beta t}{\sqrt{D t}})$$
(A.16)

Now with the last term:

$$I_{22} = -A_1 \int_0^\infty dx_0 \, x_0^2 \operatorname{erfc}(\frac{x_0 + \beta t}{2\sqrt{Dt}})$$

We integrate by parts:

$$U = \operatorname{erfc}(\frac{-x_0 + \beta t}{2\sqrt{dt}}), \quad dU = \frac{1}{\sqrt{\pi Dt}} e^{-(\frac{(-x_0 + \beta t)^2}{4Dt})}$$
$$dV = x_0^2, \ V = \frac{x_0^3}{3}$$

Integrate according to : $UV - \int V \, dU$

$$UV = 0$$

$$-\int V dU = \frac{A_1}{3\sqrt{\pi Dt}} \int_0^\infty x_0^3 e^{-(\frac{(-x_0 + \beta t)^2}{4Dt})}$$

$$= -\left(\frac{\beta^3 t^3}{3\sqrt{\pi D t}} + \frac{4\beta t^2 D}{\sqrt{\pi D t}}\right) e^{-\frac{\beta^2 t}{4D}} + \left(\beta^2 t^2 + \frac{\beta^4 t^3}{6D}\right) \operatorname{erfc}(\frac{\beta t}{\sqrt{D t}})$$
(A.17)

The complete integration is the sum of equations: (A.17) + (A.16) + (A.14) so we get:

$$I = \left(\frac{\beta^3 t^3}{6\sqrt{\pi D t}} + \frac{2\beta t^2 D}{3\sqrt{\pi D t}}\right) e^{-\frac{\beta^2 t}{4D}} - \left(\frac{\beta^2 t^2}{2} + \frac{\beta^4 t^3}{12D}\right) \operatorname{erfc}\left(\frac{\beta t}{\sqrt{D t}}\right)$$
(A.18)

A.4 Third Term

$$p_3(x,t|x_0,0) = \frac{\beta}{2D} Exp\left[-\frac{\beta x}{D}\right] \operatorname{erfc}\left(\frac{x+x_0-\beta t}{2\sqrt{Dt}}\right)$$

We want to integrate $p_3(x, t|x_0)$ using equation (A.5):

$$I = \int_0^\infty dx_0 \int_0^\infty dx \, x_0 \, x \, P_0(x_0) \, P(X, \tau | x_0)$$

$$= \frac{\beta^2}{2D^2} \int_0^\infty dx_0 \int_0^\infty dx \, x_0 \, x \, e^{-\frac{\beta x}{D}} e^{-\frac{\beta x_0}{D}} \operatorname{erfc}(\frac{x + x_0 - \beta t}{2\sqrt{Dt}})$$

First we integrate in x direction: $I_1 = A_1 \int_0^\infty dx \ x \ e^{-\frac{\beta x}{D}} \operatorname{erfc}(\frac{x + x_0 - \beta t}{2\sqrt{Dt}}) A_1 = \frac{\beta^2}{2D^2} e^{-\frac{\beta x_0}{D}}$

We will write down the result of this integration, since we have done in detail almost the same integral in (A.9b)

$$I_1 = \frac{1}{2}e^{-\frac{\beta x_0}{D}}\operatorname{erfc}(\frac{x_0 - \beta t}{2\sqrt{Dt}}) \tag{A.19}$$

$$I_2 = \left(-\frac{1}{2} + \frac{\beta(x_0 + \beta t)}{2D}\right) \operatorname{erfc}\left(\frac{x_0 + \beta t}{2\sqrt{Dt}}\right)$$
(A.20)

$$I_3 = -\frac{\beta}{D} \sqrt{\frac{Dt}{\pi}} e^{-\left(\frac{x_0 + \beta t}{2\sqrt{Dt}}\right)^2} \tag{A.21}$$

We start by integrating I_1 (A.19), it is important to note here, that this term is different from the other terms we had because of the minus sign.

$$I_1 = \frac{1}{2} \int_0^\infty dx_0 \ x_0 \ e^{-\frac{\beta x_0}{D}} \operatorname{erfc}(\frac{x_0 - \beta t}{2\sqrt{Dt}})$$

We integrate by parts:

$$U = \operatorname{erfc}(\frac{x_0 - \beta t}{2\sqrt{dt}}), \ dU = -\frac{1}{\sqrt{\pi Dt}}e^{-(\frac{(x_0 - \beta t)^2}{4Dt})}$$

$$dV = \frac{x_0}{2}e^{-\frac{\beta x_0}{D}}, \ V = -\frac{D^2}{2\beta^2}e^{-\frac{\beta x_0}{D}}(\frac{\beta x_0}{D} + 1)$$

Integrate according to : $UV - \int V dU$

$$UV = \frac{D^2}{2\beta^2} \operatorname{erfc}(-\frac{\beta t}{2\sqrt{Dt}})$$

$$= \frac{D^2}{2\beta^2} (2 - \operatorname{erfc}(\frac{\beta t}{2\sqrt{Dt}}))$$

$$= \frac{D^2}{\beta^2} - \frac{D^2}{2\beta^2} \operatorname{erfc}(\frac{\beta t}{2\sqrt{Dt}})$$
(A.22)

We used the identity $\operatorname{erfc}(-x) = 2 - \operatorname{erfc}(x)$, and it is important to notice that the first term can be

subtracted from (A.4), continue the integration:

$$-\int V dU = -\frac{D^2}{2\beta^2} \frac{1}{\sqrt{\pi D t}} \int_0^\infty x_0 e^{-(\frac{(x_0 - \beta t)^2}{4Dt})} e^{-\frac{\beta x_0}{D}} (\frac{\beta x_0}{D} + 1)$$

$$= -\frac{D^2 t}{\beta \sqrt{\pi D t}} e^{-\frac{\beta^2 t}{4D}} - (\frac{D^2}{2\beta^2} - \frac{Dt}{2}) \operatorname{erfc}(\frac{\beta t}{\sqrt{D t}})$$
(A.23)

Now we integrate the second term (A.20):

$$I_{2} = \int_{0}^{\infty} dx_{0} \ x_{0} \ (-\frac{1}{2} + \frac{\beta(x_{0} + \beta t)}{2D}) \operatorname{erfc}(\frac{x_{0} + \beta t}{2\sqrt{Dt}})$$

We have integrated a similar term in (A.15), so we will just write down the results;

$$I_{2} = \left(-\sqrt{\frac{Dt}{\pi}} \frac{\beta^{3} t^{2}}{6D} + \sqrt{\frac{Dt}{\pi}} \frac{11\beta t}{6}\right) e^{-\frac{\beta^{2} t}{4D}} + \left(\frac{\beta^{4} t^{3}}{12D} - \frac{1}{2}\beta^{2} t^{2} - \frac{Dt}{2} - \frac{\beta^{2} t^{2}}{4}\right) \operatorname{erfc}\left(\frac{x_{0} + \beta t}{2\sqrt{Dt}}\right)$$
(A.24)

Now with the last integration I_3 (A.22)

$$I_{3} = -\frac{\beta}{D} \sqrt{\frac{Dt}{\pi}} \int_{0}^{\infty} dx_{0} \ x_{0} e^{-(\frac{x_{0} + \beta t}{2\sqrt{Dt}})^{2}}$$

$$I_{3} = (-2\beta t \sqrt{\frac{Dt}{\pi}}) e^{-\frac{\beta^{2} t}{4D}} + (\beta^{2} t^{2}) \operatorname{erfc}(\frac{x_{0} + \beta t}{2\sqrt{Dt}})$$
(A.25)

The complete integration is the sum of (A.22) (A.23) (A.25) (A.24)

$$\begin{split} I &= (-\frac{D^2}{\beta^2} + \frac{\beta^2 t^2}{4} + \frac{t^3 \beta^4}{12D}) \operatorname{erfc}(\frac{x_0 + \beta t}{2\sqrt{Dt}}) \\ &+ (-\frac{t^2 \beta D}{6\sqrt{\pi Dt}} - \frac{\beta^3 t^2}{6D} \sqrt{\frac{Dt}{\pi}} - \frac{D^2 t}{\beta \sqrt{\pi Dt}}) e^{-\frac{\beta^2 t}{4D}} \\ &+ \frac{D^2}{\beta^2} \end{split} \tag{A.26}$$

A.5 The final Integration

The final answer of the integration is the sum of the terms (A.4) (A.12) (A.18)(A.26)

$$I = \left(-TD + \frac{D^2}{\beta^2} - \frac{\beta^2 t^2}{4}\right) \operatorname{erfc}\left(\frac{\beta t}{2\sqrt{Dt}}\right) + \left(\frac{\beta t}{2} + \frac{D}{\beta}\right) \sqrt{\frac{Dt}{\pi}} e^{-\frac{\beta^2 t}{4D}}$$
(A.27)

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Eidesstattliche Erklärung

Hiermit erkläre ich an Eides statt, dass ich die vorliegende Abschlussarbeit selbstständig angefertigt habe und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt habe. Die den benutzten Quellen wortlich oder inhaltlich entnommenen Stellen (Abbildungen, direkte oder indirekte Zitate) habe ich unter Benennung des Autors / der Autorin und der Fundstelle als solche kenntlich gemacht. Mir ist bekannt, dass die wortliche oder nahezu wortliche Wiedergabe von fremden Texten oder Textpassagen ohne Quellenangabe als Tauschungsversuch gewertet wird. Ich erkläre weiterhin, dass die vorliegende Arbeit noch nicht im Rahmen eines anderen Prufungsverfahrens eingereicht wurde.

George Farah Berlin, January 17, 2020