Thesis for the degree of Master of Science

Generalized Ornstein-Uhlenbeck processes

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Abstract

This thesis discusses diffusive motion of particles experiencing random forcing in a viscous medium. It generalizes the standard Ornstein-Uhlenbeck process in one spatial dimension (which is also discussed) for the case when the dependence of the force on the position of the particle cannot be neglected. Expectation values and correlation functions of physical observables (momentum and displacement) are calculated. This is achieved by finding the spectrum of the so-called Fokker-Planck operator describing the time evolution of the probability distribution of momentum. Numerical experiments are performed confirming the analytical results obtained. The case of two spatial dimensions is briefly discussed and numerical results for this case are presented.

Contents

Chapter 1

Introduction

This thesis addresses the problem of describing the dynamics of particles moving in a viscous medium. This problems has recently been intensively investigated. Examples are passive tracers in turbulent flows [1] and inertial particles in turbulent flows [2, 3, 4, 5]. Early works go back to Einstein [6] and Smoluchowski [7] in the theory of Brownian motion showing among other results diffusive motion of particles. Subsequently Ornstein and Uhlenbeck [8] considered the equation of motion of a particle of mass m,

$$m\frac{du}{dt} = -ku + f(t). \tag{1.1}$$

Here, $f(t)$ represents a randomly fluctuating force, u is the velocity of the particle and k is the friction coefficient. Ornstein and Uhlenbeck obtained results for the mean square values of the displacement of the particle, $\langle x^2(t)\rangle$, and the velocity $\langle u^2(t)\rangle$, as well as the probability distribution of the velocity.

In this thesis this problem is generalized by considering the equation of motion,

$$m\frac{du}{dt} = -ku + f(x,t), \tag{1.2}$$

where the force $f(x,t)$ depends not only on time, but also on the position of a particle (as is generally the case).

Properties of particles moving according to (1.2) have been studied intensively in the past. In particular, the evolution of distribution of many particles moving in a turbulent flow that can be approximated by (1.2) is of major interest. Surprisingly, for non-interacting particles, it appeared that (1.2) exhibits a phase transition between two regimes: in the first one particles seem to move completely independently as one might expect for diffusive motion; in the second one particles tend to cluster together and, in the end, explore the same trajectory. Deutsch [9] described this phenomenon and gave theoretical statements and numerical simulations showing an existence of a phase transition. In [10, 11] the Lyapunov exponent - the rate

of exponential convergence (divergence) of nearby trajectories - was explicitly calculated as a function of a dimensionless parameter characterizing the model (1.2) both for one-dimensional and two-dimensional cases. The Lyapunov exponent for the three-dimensional case was calculated in [5] and [12], which is most important for physical applications. Sigurgeirsson and Stuart [16] investigated model (1.2) incorporating collisions between particles.

The aim of this thesis is to calculate the mean square values of the momentum and the displacement, $\langle p^2(t)\rangle$, $\langle x^2(t)\rangle$ respectively, as well as the correlation function of the momentum $\langle p(t)p(t+\Delta t)\rangle$ in equilibrium for particles moving according to (1.2). This is achieved by finding a spectrum of the corresponding operator of the Fokker-Planck equation that describes the evolution of the probability distribution of momentum. The spectrum is used to write the propagator that defines correlation functions. This is done assuming motion in the limit of small damping and large forcing. This makes it possible to simplify the Fokker-Planck equation. This problem has been investigated in [15], and the results obtained there are generalized. There are also asymptotic scaling results available in [13] and [14] for the case of undamped motion ($k = 0$), for an arbitrary dimension both for classical and quantum particles.

This report is organized in the following way. The second chapter describes the model and introduces all parameters. It also describes the method used for the numerical simulation of random force field $f(x,t)$. Chapter 3 is dedicated to the standard Ornstein-Uhlenbeck process. Chapter 4 introduces the Fokker-Planck equation for model (1.2) and the corresponding operator, its spectral decomposition, and correlation functions that can be determined using eigenvalues and eigenfunctions. Chapter 5 presents the results for momentum and spatial diffusion for the generalized Ornstein-Uhlenbeck process compared with numerical results. Chapter 6 gives a brief discussion for the case of two spatial dimensions. Conclusions are summarized in chapter 7.

Chapter 2

The model

Consider a particle with mass m, position x and momentum p moving in an one-dimensional random force field $f(x,t)$ characterized by damping rate γ. The equation of motion is

$$\begin{aligned} \frac{dx}{dt} &= \frac{p}{m}, \\ \frac{dp}{dt} &= -\gamma p + f(x,t). \end{aligned} \tag{2.1}$$

Note that the original Ornstein-Uhlenbeck equation (1.1) is written in terms of a friction coefficient k. It is related to γ as follows: $k = \gamma m$.

The following assumptions concerning $f(x,t)$ are made. First, the mean value of the force $f(x,t)$ over an ensemble of realizations for any x and t is assumed to vanish, that is,

$$\langle f(x,t) \rangle = 0. \tag{2.2}$$

Angular brackets denote the mean value throughout the report.

Furthermore, it is assumed that correlations between values of $f(x,t)$ for different x_1, t_1 and x_2, t_2 decay fast with increasing $|x_2 - x_1|$ and $|t_2 - t_1|$ with scaling factors, ξ and τ respectively. The correlation function of the force can be written as follows,

$$\langle f(x_1,t_1) f(x_2,t_2) \rangle = c(x_1 - x_2, t_1 - t_2). \tag{2.3}$$

In the numerical simulations, the following form of the correlation function is used,

$$\begin{aligned} c(x,t) &= \langle f(x_1,t_1) f(x_1 + x, t_1 + t) \rangle \\ &= \sigma^2 \exp\left(-\frac{x^2}{2\xi^2}\right) \exp\left(-\frac{|t|}{\tau}\right), \end{aligned} \tag{2.4}$$

where σ is the typical strength of the force. A random field having such properties is referred as a generic random field and, accordingly, this case is called the generic case. Another possibility is to generate a force field as

$$f(x,t) = \frac{\partial \psi(x,t)}{\partial x}, \tag{2.5}$$

where $\psi(x,t)$ is a generic random field as described above. This case is referred as the gradient case. Note that for this case the typical strength of the force is σ/ξ. Later it will be shown how the form of the correlation function for the gradient case can be calculated.

2.1 Random-field generation

Numerical methods for creating random fields are usually based on spectral or Fourier decomposition of a random function similar to the case of a non-random function. In order to verify the analytical results discussed in chapter 5, it is important to have a method for simulating the random force in (1.2) that is fast and memory efficient.

2.1.1 Spectral decomposition of a random function

Here, spectral decomposition of a random function of one variable is briefly described. It is assumed that

$$\begin{aligned} \langle f(x) \rangle &= 0, \\ \langle f(x_1) f(x_1 + x) \rangle &= c(x). \end{aligned} \tag{2.6}$$

An extension to the case of more than one variable is straightforward.

The spectral decomposition of a periodic random function $f(x)$ with a period L looks as follows,

$$f(x) = \sum_{k \in \mathbb{K}} f_k \exp(\mathrm{i}kx), \tag{2.7}$$

where $\mathbb{K}$ is the set of the form $\frac{2\pi}{L}n$ and $n = 0, \pm 1, \pm 2, \ldots$ The coefficients f_k are complex numbers, but in order for $f(x)$ to be real one has to choose f_0 to be a real number and $f_{-k} = f_k^*$, where the asterisk denotes complex-conjugation. The f_k's are chosen to be independent random numbers with particular properties, and from the first condition of (2.6) it clearly follows that $\langle f_k \rangle = 0$. The second condition implies that the variance of any f_k must be equal to the value of a required spectral density $s(k)$, which is, simply, the Fourier transform of a correlation function,

$$\begin{aligned} s(k) &= \frac{1}{L} \int_{-\infty}^{\infty} c(x) \exp\left(\mathrm{i}kx\right) dx, \\ c(x) &= \frac{L}{2\pi} \int_{-\infty}^{\infty} s(k) \exp\left(\mathrm{i}kx\right) dk. \end{aligned} \tag{2.8}$$

This implies that the variance of $f(x)$ is equal to the sum of variances of all f_k's, that is,

$$\langle f^2(x)\rangle = c(0) = \sum_{k\in\mathbb{K}} \langle |f_k|^2\rangle. \tag{2.9}$$

These statements might be enough to start generating a random function. However, computational problems arises. The time necessary for computing the sum (2.7) grows quickly with a number of terms N and the dimension d, namely as N^d, that is exponentially with the dimension. Note also that upon increasing the period L, one has to increase the number of terms to reliably approximate the indefinite sum (2.7). If a random field depends on discrete variables it is possible to apply fast Fourier transforms (FFT) to compute (2.7). This might be useful for the present problem. FFT is a very powerful technique that makes it possible to reduce the growth of the computing time from N^d to $N^{d-n}\log N^n$, where n is the number of discrete variables, but it can be crucially exacting for memory resources, if the number of discrete steps is very large (and this is the case).

Sigurgeirsson and Stuart [16] described a method for generating a spatial random field evolving in time that is also based on spectral decomposition. They showed that it is possible to use a differential equation to generate $f_k(t)$ to simulate the desired time correlation function while at a given time t the coefficients $f_k(t)$ determine the desired spatial correlation function. Sigurgeirsson *et al.* [17] referred to this approach as synthetic turbulence.

2.1.2 Synthetic turbulence

This section describes how a random field of two variables (one in space and one in time) can be generated. The algorithm presented in [16] is adopted with some modifications. The idea is to use spectral decomposition of the form (2.7),

$$f(x,t) = \sum_{k\in\mathbb{K}} f_k(t)\exp(\mathrm{i}kx). \tag{2.10}$$

The distribution of f_k must remain stationary and satisfy the constraint $\langle |f_k(t)|^2\rangle = s(k)$, where $s(k)$ is the Fourier transform of the spatial correlation function. Using the correlation function of the form (2.4) the required spectral density is

$$s(k) = \frac{\sqrt{2\pi}\sigma^2\xi}{L}\exp\left(-\frac{\xi^2\mathrm{k}^2}{2}\right). \tag{2.11}$$

In order to reproduce the desired time correlation function, $f_k(t)$ can be generated dynamically using a differential equation. It can be easily verified that in order to get the time correlation function of the form (2.4) $f_k(t)$ must be solutions of the following differential equation,

$$\frac{df_k}{dt} = -\tau^{-1}f_k + \sqrt{\frac{2s(k)}{\tau}}\frac{d\beta_k}{dt}, \tag{2.12}$$

where β_k is a sequence of standard complex-valued Brownian motions, i.e. $\langle d\beta_k(t)\rangle = 0$, and $\langle d\beta_k(t_1)d\beta_k^*(t_2)\rangle = \delta_{t_1t_2}dt$. In order for $f(x,t)$ to be real one has to choose $\beta_k = \beta_{-k}^*$, $f_k = f_{-k}^*$ and f_0 to be a real number. At $t = 0$, the f_k's must be chosen from a normal distribution $\mathcal{N}[0, s(k)]$, which is a stationary distribution of (2.12).

Unfortunately, there are not many types of correlation functions that can be simulated by this method, and it is not obvious how to construct a differential equation for a given correlation function, whereas for FFT it is necessary to know only a spectral density. The method based on (2.10) and (2.12) is much faster than the one described in section 2.1.1, and it is therefore used to simulate the random force in (2.1).

2.1.3 Time correlation function

It is now possible to calculate the correlation function of the force for the gradient case by writing a spatial derivative of (2.10) as follows,

$$g(x,t) = \frac{\partial f(x,t)}{\partial x} = \mathrm{i}\sum_{k\in\mathbb{K}} k f_k(t)\exp(\mathrm{i}kx). \tag{2.13}$$

The unique solution of (2.12) (assuming $t > 0$) is

$$f_k(t) = f_k(0)\exp\left(-\frac{t}{\tau}\right) + \sqrt{\frac{2s(k)}{\tau}}\int_0^t \exp\left(\frac{z-t}{\tau}\right) d\beta_k(z). \tag{2.14}$$

The time correlation function can be calculated by averaging $g(0,0)g(0,t)$ over an ensemble of realizations,

$$c(t) = \langle g(0,0)g(0,t)\rangle = \sum_{k\in\mathbb{K}}\langle k^2 f_k(0)f_k(t)\rangle. \tag{2.15}$$

Using (2.14) this can be rewritten as follows,

$$c(t) = \sum_{k\in\mathbb{K}} k^2\langle f_k^2(0)\rangle\exp\left(-\frac{t}{\tau}\right) \tag{2.16}$$

$$+ \sum_{k\in\mathbb{K}}\sqrt{\frac{2s(k)}{\tau}}\left\langle\int_0^t \exp\left(\frac{z-t}{\tau}\right) d\beta_k(z)\right\rangle. \tag{2.17}$$

The average value of the term with the integral is 0, since $d\beta_k$ are independent increments in time. Therefore,

$$c(t) = \sum_{k\in\mathbb{K}} k^2\langle f_k(0)^2\rangle\exp\left(-\frac{t}{\tau}\right) \tag{2.18}$$

$$= \sum_{k\in\mathbb{K}} k^2 s(k)\exp\left(-\frac{t}{\tau}\right) = \frac{\sigma^2}{\xi^2}\exp\left(-\frac{t}{\tau}\right).$$

The spatial correlation function $c(x)$ is determined as follows,

$$c(x) = \langle g(0,0)g(x,0)\rangle. \tag{2.19}$$

Using (2.13) this yields,

$$c(x) = \sum_{k\in\mathbb{K}} k^2 s(k)\exp(\mathrm{i}kx) = \frac{\sigma^2(\xi^2 - x^2)}{\xi^4}\exp\left(-\frac{x^2}{2\xi^2}\right). \tag{2.20}$$

Summarizing, the correlation function for the gradient case is

$$c(x,t) = \frac{\sigma^2}{\xi^4}(\xi^2 - x^2)\exp\left(-\frac{x^2}{2\xi^2}\right)\exp\left(-\frac{|t|}{\tau}\right). \tag{2.21}$$

Henceforth $c(x,t)$ is referred as the correlation function and $c(x)$ and $c(t)$ are referred as its spatial and time part respectively.

Chapter 3

The standard Ornstein-Uhlenbeck process

This chapter describes the standard Ornstein-Uhlenbeck process. The material in this chapter is taken from [8] (see also [19]).

The equation of motion considered by Ornstein and Uhlenbeck (in terms of damping rate γ) is

$$\frac{dp}{dt} = -\gamma p + f(t). \tag{3.1}$$

Let $f(t)$ have the following properties:

$$\begin{aligned} \langle f(t) \rangle &= 0, \\ \langle f(t_1) f(t_1 + t) \rangle &= c(t), \end{aligned} \tag{3.2}$$

where $c(t)$ is a function with a sharp maximum at $t = 0$ with correlation length τ [e.g. the time part of the correlation function of the form (2.4)]. The solution of (3.1), that is, the dynamics of the momentum can be calculated by integrating the differential equation (assuming initial condition $p(0) = 0$),

$$p(t) = \mathrm{e}^{-\gamma t} \int_0^t \mathrm{e}^{\gamma s} f(s) ds. \tag{3.3}$$

The variance of the momentum is thus

$$\langle p^2(t) \rangle = \mathrm{e}^{-2\gamma t} \int_0^t ds_1 \int_0^t ds_2 \mathrm{e}^{\gamma(s_1+s_2)} \langle f(s_1) f(s_2) \rangle. \tag{3.4}$$

By changing the variables $s_1 + s_2 = u$, $s_1 - s_2 = v$, (3.4) becomes

$$\langle p^2(t) \rangle = \frac{1}{2} \mathrm{e}^{-2\gamma t} \int_0^{2t} \mathrm{e}^{\gamma u} du \int_{-t}^{t} c(v) dv. \tag{3.5}$$

Since $c(v)$ has a sharp maximum at $v = 0$, it is possible to change the limits of integration of the second integral in (3.5) to $(-\infty; \infty)$ for $t \gg \tau$ to obtain

$$\langle p^2(t) \rangle = \frac{D_0}{\gamma} (1 - \mathrm{e}^{-2\gamma t}) \tag{3.6}$$

with the diffusion constant

$$D_0 = \frac{1}{2}\int_{-\infty}^{\infty} c(t)dt. \tag{3.7}$$

The variance of the displacement is obtained by integrating (3.3) (assuming for the sake of simplicity $x(0) = 0$),

$$x(t) = \frac{1}{m}\int_0^t \mathrm{e}^{-\gamma u}du \int_0^u \mathrm{e}^{\gamma v} f(v)dv, \tag{3.8}$$

or integrating by parts,

$$x(t) = \frac{1}{\gamma m}\left(\int_0^t f(u)du - \mathrm{e}^{-\gamma t}\int_0^t \mathrm{e}^{\gamma u} f(u)du\right). \tag{3.9}$$

By squaring and averaging the variance of the displacement becomes,

$$\begin{aligned}\langle x^2(t)\rangle = &\frac{1}{\gamma^2 m^2}\int_0^t du \int_0^t dv\ \langle f(u)f(v)\rangle \\ &- \frac{2\mathrm{e}^{-\gamma t}}{\gamma^2 m^2}\int_0^t du \int_0^t dv\ \mathrm{e}^{\gamma u}\langle f(u)f(v)\rangle \\ &+ \frac{\mathrm{e}^{-2\gamma t}}{\gamma^2 m^2}\int_0^t du \int_0^t dv\ \mathrm{e}^{\gamma(u+v)}\langle f(u)f(v)\rangle.\end{aligned} \tag{3.10}$$

It is convenient to change variables in the first and the third terms as $a = u + v$ and $b = u - v$, whereas for the second term the change of variables is $a = u$ and $b = u - v$. This gives the following result,

$$\begin{aligned}\langle x^2(t)\rangle\ = &\frac{1}{2\gamma^2 m^2}\int_0^{2t} da\ \int_{-t}^{t} db\ c(b) \\ &- \frac{2\mathrm{e}^{-\gamma t}}{\gamma^2 m^2}\int_0^t da\ \mathrm{e}^{\gamma a}\int_{-t}^{t} db\ c(b) \\ &+ \frac{\mathrm{e}^{-2\gamma t}}{2\gamma^2 m^2}\int_0^{2t} da\ \mathrm{e}^{\gamma a}\int_{-t}^{t} db\ c(b).\end{aligned} \tag{3.11}$$

As before, it is possible to approximate the second integral in all 3 terms as $2D_0$ for $t \gg \tau$ obtaining

$$\langle x(t)^2\rangle = \frac{2D_0}{\gamma^2 m^2}\left[t + \frac{1 - \mathrm{e}^{-2\gamma t}}{2\gamma} - \frac{2(1 - \mathrm{e}^{-\gamma t})}{\gamma}\right]. \tag{3.12}$$

The last expression implies anomalous diffusion at short times,

$$\langle x(t)^2\rangle \sim \frac{2D_0}{3m^2}t^3 \tag{3.13}$$

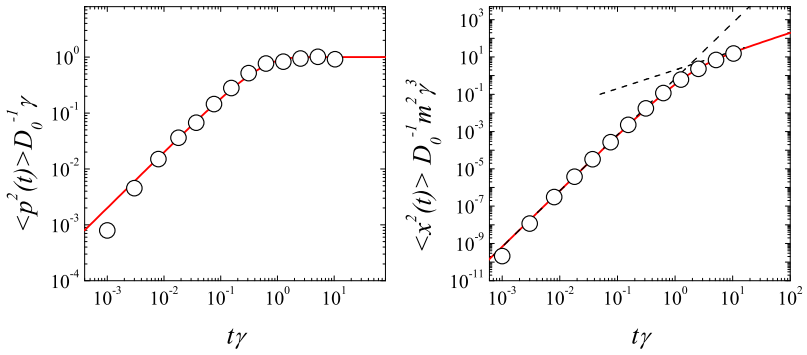

Figure 3.1: Numerical simulations of $\langle p^2(t)\rangle$ and $\langle x^2(t)\rangle$ (circles) for the standard Ornstein-Uhlenbeck process (3.1) compared with the theoretical results (3.6) and (3.12) (red solid lines). For $\langle x^2(t)\rangle$ the limiting behaviours (3.13) and (3.14.) (dashed lines) are shown. The parameters were $\sigma = 1.0$, $\xi = 0.1$, $m = 1.0$, $\gamma = 0.01$, $\tau = 0.1$

and diffusion at long times,

$$\langle x(t)^2\rangle \sim \frac{2D_0}{\gamma^2 m^2} t. \tag{3.14}$$

Numerical simulations for the standard Ornstein-Uhlenbeck process are shown in Fig. 3.1. It should be noticed that the agreement with the theory is reasonable when $t \gg \tau$, as one should expect.

If $\gamma\tau \ll 1$, the probability distribution $P(p,t)$ of momentum p at time t is determined by a Fokker-Planck equation. Ornstein and Uhlenbeck arrived at the following expression,

$$\frac{\partial P(p,t)}{\partial t} = \frac{\partial}{\partial p}\left(\gamma p P(p,t) + D_0 \frac{\partial P(p,t)}{\partial p}\right), \tag{3.15}$$

where D_0 is the diffusion constant defined above. The solution of this equation can be guessed in the case of particles at rest at $t = 0$, and the distribution of the momentum is

$$P(p,t) = \frac{\gamma^{1/2}}{[2\pi D_0(1-\mathrm{e}^{-2\gamma t})]^{1/2}} \exp\left[-\frac{\gamma p^2}{2D_0(1-\mathrm{e}^{-2\gamma t})}\right], \tag{3.16}$$

which becomes Gaussian for $t \gg \gamma^{-1}$. One can easily calculate $\langle p^2(t)\rangle = \int_{-\infty}^{\infty} p^2 P(p,t)dp$ and, indeed, obtain the result (3.6).

Chapter 4

Spectral decomposition of the Fokker-Planck operator of the generalized Ornstein-Uhlenbeck process

This chapter discusses the spectral decomposition of the Fokker-Planck operator corresponding to (2.1) in the limit of small damping. The Fokker-Planck equation in this case looks as follows [13, 14, 15, 18],

$$\frac{\partial P(p,t)}{\partial t} = \frac{\partial}{\partial p}\left(\gamma p P(p,t) + D(p)\frac{\partial P(p,t)}{\partial p}\right), \tag{4.1}$$

with a diffusion constant that now depends on p,

$$D(p) = \frac{1}{2}\int_{-\infty}^{\infty} c(pt/m,t)\ dt. \tag{4.2}$$

The limits of validity of (4.1) are discussed in [22]. If damping rate γ is small and the force is large particles travel very fast compared with the typical momentum of the model $p_0 = m\xi/\tau$ and the diffusion constant $D(p)$ can be approximated in the limit of $p \gg p_0$.

First, $D(p)$ is calculated for the generic case using the correlation function of the form (2.4),

$$D(p) = \frac{m\sigma^2\xi \exp\left(\frac{m^2\xi^2}{2p^2\tau^2}\right)\operatorname{erfc}\left(\frac{m\xi}{|p|\tau\sqrt{2}}\right)\sqrt{\pi}}{|p|\sqrt{2}}, \tag{4.3}$$

where $\operatorname{erfc}(x)$ is the complementary error function [20]. By denoting $D_1 = \sigma^2\tau$ one has,

$$D(p) = D_1\frac{p_0}{|p|}\exp\left(\frac{p_0^2}{2p^2}\right)\operatorname{erfc}\left(\frac{p_0}{|p|\sqrt{2}}\right). \tag{4.4}$$

Assuming $p \gg p_0$ it is possible to keep only the terms p_0/p of first order and obtain,

$$D(p) \sim D_1 \frac{p_0}{|p|}. \tag{4.5}$$

Now, $D(p)$ for the gradient case can be calculated using the correlation function of the form (2.21),

$$D(p) = \frac{m^2\sigma^2 \left[2|p|\tau - m\xi \exp\left(\frac{m^2\xi^2}{2p^2\tau^2}\right) \operatorname{erfc}\left(\frac{m\xi}{p\tau\sqrt{2}}\right)\sqrt{2\pi}\right]}{2|p|^3\tau^2} \tag{4.6}$$

and denoting $D_2 = \sigma^2\tau/\xi^2$ one obtains,

$$D(p) = D_2\frac{p_0^2}{p^2} - D_2\frac{p_0^3}{|p|^3}\exp\left(\frac{p_0^2}{2p^2}\right)\operatorname{erfc}\left(\frac{p_0}{|p|\sqrt{2}}\right)\sqrt{\frac{\pi}{2}}. \tag{4.7}$$

Assuming $p \gg p_0$ it is possible to keep only the terms p_0/p of second order and obtain,

$$D(p) \sim D_2\left(\frac{p_0}{p}\right)^2. \tag{4.8}$$

It is argued [15] that for any differentiable force (e.g. time correlation function of the Gaussian form) one obtains either $D(p) \sim p^{-1}$ (the generic case) or $D(p) \sim p^{-3}$ (the gradient case). Indeed, the correlation function (2.4) is not differentiable at $t = 0$. This gives rise to $D(p) \sim p^{-2}$ for the gradient case. To generalize, one may assume that the diffusion constant behaves as

$$D(p) = D_\zeta \left|\frac{p_0}{p}\right|^\zeta. \tag{4.9}$$

Values of ζ different from 1,2 or 3 arise for correlation functions of algebraic form.

The Fokker-Planck equation for the generic case with the diffusion constant approximated for large p looks as follows,

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial p}\left(\gamma p P + D_1\frac{p_0}{|p|}\frac{\partial P}{\partial p}\right). \tag{4.10}$$

Assuming that at $t = 0$ all particles are at rest initial condition is $P(p, 0) = \delta(p)$. The solution of (4.10) can be guessed then,

$$P(p,t) = \frac{1}{2\Gamma(4/3)}\,\frac{\gamma^{1/3}}{[3p_0D_1(1-\mathrm{e}^{-3\gamma t})]^{1/3}}\exp\left[-\frac{\gamma|p|^3}{3p_0D_1(1-\mathrm{e}^{-3\gamma t})}\right]. \tag{4.11}$$

Using this probability distribution it is possible to calculate the variance of the momentum,

$$\langle p^2(t)\rangle = \int_{-\infty}^{\infty} p^2 P(p,t)dp = \left(\frac{p_0D_1}{\gamma}\right)^{2/3}\frac{1}{3^{1/3}\Gamma(4/3)}(1-\mathrm{e}^{-3\gamma t})^{2/3}. \tag{4.12}$$

This reproduces the result obtained in [15].

Similarly for the gradient case one obtains the Fokker-Planck equation with the approximated diffusion constant,

$$\frac{\partial P}{\partial t} = \frac{\partial}{\partial p}\left(\gamma p P + D_2 \left(\frac{p_0}{p}\right)^2 \frac{\partial P}{\partial p}\right). \tag{4.13}$$

The probability distribution function for the gradient case is,

$$P(p,t) = \frac{1}{2\Gamma(5/4)} \frac{\gamma^{1/4}}{[4p_0^2 D_2(1-\mathrm{e}^{-4\gamma t})]^{1/4}} \exp\left[-\frac{\gamma p^4}{4p_0^2 D_2(1-\mathrm{e}^{-4\gamma t})}\right] \tag{4.14}$$

and the variance of the momentum,

$$\langle p^2(t)\rangle = \left(\frac{p_0^2 D_2}{\gamma}\right)^{1/2} \frac{2\Gamma(3/4)}{\Gamma(1/4)} (1-\mathrm{e}^{-4\gamma t})^{1/2}. \tag{4.15}$$

4.1 Eigenvalues and eigenfunctions

It has been shown above how the probability distribution of momentum can be obtained using the Fokker-Planck equation. However, the general solution for arbitrary initial condition is not found in closed form. Therefore, the following approach is adopted.

It is assumed that the diffusion constant is of the form (4.9) for large p. First, it is convenient to introduce dimensionless variables,

$$t' = \gamma t, \quad z = p \frac{\gamma^{\frac{1}{2+\zeta}}}{p_0^{\frac{\zeta}{2+\zeta}} D_\zeta^{\frac{1}{2+\zeta}}}. \tag{4.16}$$

Then the Fokker-Planck equation (4.1) becomes

$$\frac{\partial P(z,t')}{\partial t'} = \frac{\partial}{\partial z}\left(z P(z,t') + \frac{1}{|z|^\zeta} \frac{\partial P(z,t')}{\partial z}\right) \equiv \hat{F} P, \tag{4.17}$$

which defines the Fokker-Planck operator $\hat{F}$. The stationary distribution of this equation is $P_0(z) \propto \exp[-|z|^{\zeta+2}/(\zeta+2)]$. Therefore, one can write the Hermitian form of the operator $\hat{F}$,

$$\hat{H} = P_0^{-1/2} \hat{F} P_0^{1/2} = \frac{1}{2} - \frac{|z|^{2+\zeta}}{4} + \frac{\partial}{\partial z} \frac{1}{|z|^\zeta} \frac{\partial}{\partial z}, \tag{4.18}$$

which is sometimes referred as the Hamiltonian operator. To begin with, an eigenvalue of $\hat{H}$ os $\lambda_0^+ = 0$, and the corresponding eigenfunction is $\psi_0^+ = \mathcal{C}_0^+ \exp\left(-\frac{|z|^{2+\zeta}}{4+2\zeta}\right)$. It turns out that λ_0^+ is the lowest eigenvalue. The next eigenvalue can be determined by inspection as well (e.g. by putting ζ

to any particular value and generalizing). It is $\lambda_0^- = -1-\zeta$ and the corresponding eigenfunction is $\psi_0^- = \mathcal{C}_0^- z|z|^\zeta \exp\left(-\frac{|z|^{2+\zeta}}{4+2\zeta}\right)$. The eigenfunctions and eigenvalues are labeled by superscripts '+' and '-' to emphasize that eigenfunctions ψ_n^+ are even functions and ψ_n^- are odd functions.

Now, the following operators are introduced,

$$\begin{aligned} \hat{a}^\pm &= \frac{\partial}{\partial z} \pm \frac{z|z|^{-\zeta}}{2}, \\ \hat{A} = \hat{a}^+|z|^{-\zeta}\hat{a}^+, &\quad \hat{A}^+ = \hat{a}^-|z|^{-\zeta}\hat{a}^-, \\ \hat{G} &= \hat{a}^+|z|^{-\zeta}\hat{a}^-. \end{aligned} \tag{4.19}$$

In terms of $\hat{a}^+$ and $\hat{a}^-$ it can be derived that $\hat{H} = \hat{a}^-|z|^{-\zeta}\hat{a}^+$. The following relations hold,

$$[\hat{H}, \hat{A}] = (2+\zeta)\hat{A}, \quad [\hat{H}, \hat{A}^+] = -(2+\zeta)\hat{A}^+, \tag{4.20}$$

where $[\hat{X}, \hat{Y}] = \hat{X}\hat{Y} - \hat{Y}\hat{X}$ is the commutator. Consider, now

$$\hat{H}\hat{A}^+|\psi_n^\pm\rangle - \hat{A}^+\hat{H}|\psi_n^\pm\rangle = -(2+\zeta)\hat{A}^+|\psi_n^\pm\rangle. \tag{4.21}$$

Here eigenfunctions are written using bra-ket or Dirac notation [23]. The definition of the eigenfunction, namely $H|\psi_n^\pm\rangle = \lambda_n|\psi_n^\pm\rangle$, makes it possible to write,

$$\hat{A}^+|\psi_n^\pm\rangle(\lambda_n - 2 - \zeta) = \hat{H}\hat{A}^+|\psi_n^\pm\rangle \tag{4.22}$$

This means that $\hat{A}^+|\psi_n^\pm\rangle$ is also the eigenfunction of $\hat{H}$ with the eigenvalue $\lambda_n - 2 - \zeta$. Together with $\lambda_0^+ = 0$ and $\lambda_0^- = -1-\zeta$ this gives the spectrum of (4.18),

$$\lambda_n^+ = -(2+\zeta)n, \quad \lambda_n^- = -(2+\zeta)n - 1 - \zeta. \tag{4.23}$$

The operators $\hat{A}^+$ and $\hat{A}$ thus act as rasing and lowering operators respectively:

$$\hat{A}^+|\psi_n^\pm\rangle = C_{n+1}^\pm|\psi_{n+1}^\pm\rangle, \quad \hat{A}|\psi_n^\pm\rangle = C_n^\pm|\psi_{n-1}^\pm\rangle. \tag{4.24}$$

To determine the factors $C_n^\pm$ one can use the normalization constraint for the eigenfunctions,

$$\langle\psi_{n+1}^\pm|\psi_{n+1}^\pm\rangle = (C_{n+1}^\pm)^{-2}\langle\psi_n^\pm|\hat{A}\hat{A}^+|\psi_n^\pm\rangle = 1. \tag{4.25}$$

and using the definition of the commutator,

$$1 = (C_{n+1}^\pm)^{-2}\langle\psi_n^\pm|[\hat{A}\hat{A}^+] + \hat{A}^+\hat{A}|\psi_n^\pm\rangle, \tag{4.26}$$

that is,

$$(C_{n+1}^\pm)^2 = (2+\zeta)(-2\lambda_n^\pm + 1) + (C_n^\pm)^2. \tag{4.27}$$

Recursion gives,

$$(C_{n+1}^\pm)^2 = (2+\zeta)\sum_{k=0}^{n}(-2\lambda_k^\pm + 1). \tag{4.28}$$

Evaluation of the sum yields,

$$C_n^\pm = \sqrt{(\zeta+2)n[(\zeta+2)n \mp (\zeta+1)]}. \tag{4.29}$$

4.2 Correlation functions

In this correlation functions of the momentum are obtained using the eigenvalues and eigenfunction of (4.18. The propagator of the Fokker-Planck equation (4.1) can be written in terms of eigenfunctions as follows [15, 19],

$$K(y,z;t') = \sum_{n=0}^{\infty}\sum_{\sigma=\pm} P_0^{-1/2}(y)\psi_n^{\sigma}(y)P_0^{1/2}(z)\psi_n^{\sigma}(z)\exp(\lambda_n^{\sigma}t'). \tag{4.30}$$

The propagator $K(y,z,t')$ satisfies the Fokker-Planck equation (4.1) and can be used to compute correlation functions. In order to find $\langle p^2(t)\rangle$ and $\langle x^2(t)\rangle$ one has to calculate the correlation functions of $z^2(t')$ and $z(t_1')z(t_2')$. For $z^2(t')$ one obtains,

$$\langle z^2(t')\rangle = \int_{-\infty}^{\infty} dz\ z^2 K(0,z;t') = \sum_{n=0}^{\infty}\frac{\psi_n^+(0)}{\psi_0^+(0)}\langle\psi_0^+|z^2|\psi_n^+\rangle\exp(\lambda_n^+t'). \tag{4.31}$$

The required correlation function for $z(t_1')z(t_2')$ is

$$\begin{aligned}\langle z(t_2')z(t_1')\rangle &= \int_{-\infty}^{\infty}dz_1\int_{-\infty}^{\infty}dz_2 z_1 z_2 K(z_1,z2;t_2'-t_1')K(0,z_1;t_1) \\ &= \sum_{n,m}\frac{\psi_m^+(0)}{\psi_0^+(0)}\langle\psi_0^+|z|\psi_n^-\rangle\langle\psi_n^-|z|\psi_m^+\rangle\exp[\lambda_n^-(t_2'-t_1')+\lambda_m^+t_1'].\end{aligned} \tag{4.32}$$

The terms of the sums (4.31) and (4.32) are calculated in the next three sections, namely matrix elements $Y_{0n} = \langle\psi_0^+|z^2|\psi_n^+\rangle$ and $Z_{mn} = \langle\psi_m^+|z|\psi_n^-\rangle$, as well as the ratio of the eigenfunctions $\psi_m^+(0)/\psi_0^+(0)$.

4.2.1 Matrix elements Y_{0n}

Consider $Y_{0n} = \langle\psi_0^+|z^2|\psi_n^+\rangle$. Using (4.24) one can obtain Y_{0n+1} as follows,

$$Y_{0n+1} = \langle\psi_0^+|z^2\hat{A}^+|\psi_n^+\rangle/C_{n+1}^+. \tag{4.33}$$

It is possible to write $z\hat{A}^+$ as $z\hat{G} + z(\hat{A}^+ - G) = z(\hat{H}-\hat{I}) + z(\hat{A}^+ - \hat{G})$, where $\hat{I}$ is the identity operator. Using this (4.33) becomes

$$\begin{aligned}Y_{0n+1}C_{n+1}^+ &= \langle\psi_0^+|z^2(\hat{H}-\hat{I})|\psi_n^+\rangle + \langle\psi_0^+|z^2(\hat{A}^+-\hat{G})|\psi_n^+\rangle \\ &= (\lambda_n^+ - 1)Y_{0n} + \langle\psi_0^+|z^2(\hat{A}^+-\hat{G})|\psi_n^+\rangle,\end{aligned} \tag{4.34}$$

and using $\hat{A}^+ - \hat{G} = -z\hat{a}^-$

$$Y_{0n+1}C_{n+1}^+ = (\lambda_n^+ + 2)Y_{0n}. \tag{4.35}$$

Recursion gives the following,

$$Y_{0n} = Y_{00}\prod_{k=1}^{n}\frac{\lambda_{k-1}^+ + 2}{C_k^+}. \tag{4.36}$$

Taking into account that $Y_{00} = (2+\zeta)^{\frac{2}{2+\zeta}}\Gamma(\frac{3}{2+\zeta})/\Gamma(\frac{1}{2+\zeta})$ evaluation of the product yields the result,

$$Y_{0n} = (-1)^n \frac{(2+\zeta)^{\frac{2}{2+\zeta}}\Gamma(\frac{3}{2+\zeta})\Gamma(n-\frac{2}{2+\zeta})}{\Gamma(-\frac{2}{2+\zeta})\sqrt{\Gamma(n+1)\Gamma(n+\frac{1}{2+a})\Gamma(\frac{1}{2+a})}}. \tag{4.37}$$

4.2.2 Matrix elements Z_{mn}

Now, consider the matrix elements $Z_{mn} = \langle\psi_m^+|\hat{z}|\psi_n^-\rangle$. It is convenient to consider first the following element,

$$J_{mn} = \langle\psi_0^+|\hat{A}^m z(\hat{A}^+)^n|\psi_0^-\rangle. \tag{4.38}$$

The relation between J_{mn} and Z_{mn} is

$$Z_{mn} = \frac{J_{mn}}{\prod\limits_{k=1}^{m} C_k^+ \prod\limits_{k=1}^{n} C_k^-}. \tag{4.39}$$

For $m \leq n$ one has,

$$J_{mn} = \langle\psi_0^+|\hat{A}^m[z,\hat{A}^+](\hat{A}^+)^{n-1}|\psi_0^-\rangle + \langle\psi_0^+|\hat{A}^m\hat{A}^+ z(\hat{A}^+)^{n-1}|\psi_0^-\rangle. \tag{4.40}$$

The following property

$$[z,\hat{A}^+] = -(|z|^{-\zeta}\hat{a}^- + \hat{a}^-|z|^{-\zeta}) \tag{4.41}$$

makes it possible to write

$$\begin{aligned} J_{mn} &= -\langle\psi_0^+|\hat{A}^m|z|^{-\zeta}\hat{a}^-(\hat{A}^+)^{n-1}|\psi_0^-\rangle - \langle\psi_0^+|\hat{A}^m\hat{a}^-|z|^{-\zeta}(\hat{A}^+)^{n-1}|\psi_0^-\rangle \\ &+ \langle\psi_0^+|\hat{A}^m\hat{A}^+ z(\hat{A}^+)^{n-1}|\psi_0^-\rangle = J_{mn}^{(1)} + J_{mn}^{(2)} + J_{mn}^{(3)}. \end{aligned} \tag{4.42}$$

The third terms evaluates to

$$\begin{aligned} J_{mn}^{(3)} &= \langle\psi_0^+|\hat{A}^m\hat{A}^+ z(\hat{A}^+)^{n-1}|\psi_0^-\rangle = (C_m^+)^2\langle\psi_0^+|\hat{A}^{m-1} z(\hat{A}^+)^{n-1}|\psi_0^-\rangle \\ &= (C_m^+)^2 J_{m-1n-1}. \end{aligned} \tag{4.43}$$

Using

$$\begin{aligned} \hat{A}^m|z|^{-\zeta}\hat{a}^-(\hat{A}^+)^{n-1} &= \hat{A}^{m-1}\hat{a}^+|z|^{-\zeta}\hat{a}^+|z|^{-\zeta}\hat{a}^-(\hat{A}^+)^{n-1} \\ &= \hat{A}^{m-1}\hat{a}^+|z|^{-\zeta}\hat{G}(\hat{A}^+)^{n-1}. \end{aligned} \tag{4.44}$$

it follows that

$$\begin{aligned} \langle\psi_0^+|\hat{A}^m|z|^{-\zeta}\hat{a}^-(\hat{A}^+)^{n-1}|\psi_0^-\rangle &= (\lambda_{n-1}^- - 1) \\ &\times \langle\psi_0^+|\hat{A}^{m-1}\hat{a}^+|z|^{-\zeta}(\hat{A}^+)^{n-1}|\psi_0^-\rangle. \end{aligned} \tag{4.45}$$

Using

$$\begin{aligned}\hat{A}^{m-1}\hat{a}^{+}|z|^{-\zeta}(\hat{A}^{+})^{n-1} &= \hat{A}^{m-1}\hat{a}^{+}|z|^{-\zeta}\hat{a}^{-}|z|^{-\zeta}\hat{a}^{-}(\hat{A}^{+})^{n-2} \\ &= \hat{A}^{m-1}\hat{G}|z|^{-\zeta}\hat{a}^{-}(\hat{A}^{+})^{n-2}\end{aligned} \tag{4.46}$$

one obtains the recursion,

$$\begin{aligned}J^{(1)}_{mn} &= (\lambda^{-}_{n-1}-1)(\lambda^{+}_{m-1}-1)J^{(1)}_{m-1n-1} \\ &= (\zeta+2)n[(\zeta+2)m-\zeta-1]J^{(1)}_{m-1n-1}.\end{aligned} \tag{4.47}$$

Now, consider the second term. Using

$$\hat{a}^{-}|z|^{-\zeta}(\hat{A}^{+})^{n-1} = \hat{A}^{+}|z|^{-\zeta}\hat{a}^{-}(\hat{A}^{+})^{n-2} \tag{4.48}$$

it follows,

$$J^{(2)}_{mn} = \frac{(C^{+}_{m})^2}{(\lambda^{-}_{n-1}-1)(\lambda^{+}_{m-1}-1)}J^{(1)}_{mn} = \frac{m}{n}J^{(1)}_{mn}. \tag{4.49}$$

Note that $J^{(3)}_{0n}=0$, $J^{(2)}_{0n}=0$, thus $J^{(3)}_{0n}=J_{0n}$. This gives,

$$J^{(1)}_{mn} = \prod_{k=1}^{m}(\zeta+2)(n-m+k)[(\zeta+2)k-\zeta-1]J_{0n-m} \tag{4.50}$$

and the result is,

$$\begin{aligned}J^{(1)}_{mn} &= (-1)^{n-m}\frac{(2+\zeta)^{-\frac{1+\zeta}{2+\zeta}+m+n}}{\Gamma(\frac{1}{2+\zeta})\Gamma(\frac{\zeta}{2+\zeta})} \\ &\times \frac{\Gamma(\frac{1}{2+\zeta}+m)\Gamma(1+n)\Gamma(\frac{\zeta}{2+\zeta}+n-m)\sqrt{\Gamma(\frac{1}{2+\zeta}+n-m)}}{\Gamma(1+n-m)\sqrt{\Gamma(\frac{3+2\zeta}{2+\zeta}+n-m)}}.\end{aligned} \tag{4.51}$$

Now, it is possible to determine J_{mn} using (4.42), (4.43) and (4.49) with recursion,

$$J_{mn} = (\zeta+2)m[(\zeta+2)m-\zeta-1]J_{m-1n-1} + J^{(1)}_{mn}\left(1+\frac{m}{n}\right). \tag{4.52}$$

Iterating the recursion one obtains,

$$\begin{aligned}J_{mn} &= \sum_{k=0}^{m}\left(\prod_{l=k+1}^{m}(\zeta+2)l[(\zeta+2)l-\zeta-1]\right) \\ &\times\left(1+\frac{k}{n-m+k}J^{(1)}_{k\ n-m+k}\right).\end{aligned} \tag{4.53}$$

Evaluation of the sum gives the following result,

$$J_{mn} = (-1)^{m-n} \frac{(2+\zeta)^{-\frac{\zeta}{2(2+\zeta)}+m+n} \sqrt{\sin(\frac{\pi}{2+\zeta})}}{\Gamma(\frac{\zeta}{2+\zeta})\sqrt{\pi(1+\zeta)}} \times (m+n+1) \frac{\Gamma(\frac{1}{2+\zeta}+m)\Gamma(1+n)\Gamma(\frac{\zeta}{2+\zeta}-m+n)}{\Gamma(2-m+n)}. \tag{4.54}$$

Now, consider J_{mn} for $n < m$,

$$J_{mn} = \langle \psi_0^+ | \hat{A}^{m-1} [z, \hat{A}^+] (\hat{A}^+)^n | \psi_0^- \rangle + \langle \psi_0^+ | \hat{A}^{m-1} \hat{A}^+ z (\hat{A}^+)^n | \psi_0^- \rangle. \tag{4.55}$$

Comparing with (4.40) one can proceed in the same way. It turns out that for $n < m-1$, $J_{mn} = 0$, and for J_{nn+1} one can use (4.54). Finally, one can obtain Z_{mn} using (4.39). For $n \geq m-1$ the result is,

$$Z_{mn} = (-1)^{n-m} \frac{(2+\zeta)^{-\frac{1+\zeta}{2+\zeta}}}{\Gamma(\frac{\zeta}{2+\zeta})} (m+n+1) \times \frac{\Gamma(\frac{\zeta}{2+\zeta}-m+n)\sqrt{\Gamma(n+1)\Gamma(\frac{1}{2+\zeta}+m)}}{\Gamma(2-m+n)\sqrt{\Gamma(\frac{3+2\zeta}{2+\zeta}+n)\Gamma(m+1)}} \tag{4.56}$$

and zero otherwise.

4.2.3 Ratio of the eigenfunctions

In this section, the ratio $\psi_n^+(0)/\psi_0^+(0)$ is calculated (see also [21]). The eigenfunction $\psi_n^+(0)$ is of the form,

$$\psi_n^+ = N_n^+ g_n(z) \exp\left(-\frac{|z|^{2+\zeta}}{4+2\zeta}\right), \tag{4.57}$$

where g_n is a polynomial,

$$g_n(z) = g_n^0 + g_n^1 |z|^{2+\zeta} + \ldots, \tag{4.58}$$

and N_n^+ is a constant,

$$N_n^+ = N_0^+ \prod_{k=0}^{n} C_k^+. \tag{4.59}$$

For $z = 0$ it means that $\psi_n^+(0) = N_n^+ g_n^0$, implying that

$$\psi_{n+1}(0) = \frac{N_{n+1}^+}{N_n^+} \frac{g_{n+1}^0}{g_n^0} \psi_n^+(0). \tag{4.60}$$

The following relation holds [21],

$$g_{n+1}^0 = -(1 + (2+\zeta)n) g_n^0. \tag{4.61}$$

Thus,

$$\psi_{n+1}(0) = \frac{-(1+(2+\zeta)n)}{C^+_{n+1}}\psi^+_n(0) \tag{4.62}$$

or, in other words,

$$\frac{\psi_{n+1}(0)}{\psi_n(0)} = -\sqrt{\frac{1+(2+\zeta)n}{(\zeta+2)(n+1)}}. \tag{4.63}$$

Evaluation of the recursion gives the result,

$$\frac{\psi^+_n(0)}{\psi^+_0(0)} = (-1)^n\sqrt{\frac{\Gamma(n+\frac{1}{2+\zeta})}{\Gamma(n+1)\Gamma(\frac{1}{2+\zeta})}}. \tag{4.64}$$

Chapter 5

Results

In this chapter the results obtained in the section 4.2 are used to analytically characterize momentum and spatial diffusion and the momentum correlation function in equilibrium ($t \gg \gamma^{-1}$). The results are compared with results obtained by numerical integration of (2.1) using a force field generated as described in chapter 1.

5.1 Momentum equilibrium correlation function

Using the propagator $K(y, z; t')$ of the form (4.30) one has,

$$\begin{aligned}\langle z(0)z(t')\rangle &= \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} dy\ zyK(y, z; t')P_0(y) \\ &= \sum_{n=0}^{\infty}[\langle\psi_0^+|z|\psi_n^+\rangle]^2\exp(\lambda_n^- t') = \sum_{n=0}^{\infty} Z_{0n}^2\exp(\lambda_n^- t').\end{aligned} \tag{5.1}$$

This gives for the generic case ($\zeta = 1$),

$$\begin{aligned}\langle p(t)p(t+\Delta t)\rangle_{\text{eq}} = \left(\frac{p_0 D_1}{\gamma}\right)^{2/3} &\frac{\Gamma(4/3)\exp(-2\gamma\Delta t)}{3^{1/3}\Gamma(5/3)} \\ &\times F_{21}(1/3, 1/3, 5/3, \exp(-3\gamma\Delta t)),\end{aligned} \tag{5.2}$$

where F_{21} is a hypergeometric function [20]. For the gradient case ($\zeta = 2$) the sum (5.1) evaluates to the following,

$$\begin{aligned}\langle p(t)p(t+\Delta t)\rangle_{\text{eq}} = \left(\frac{p_0^2 D_2}{\gamma}\right)^{1/2} &\frac{\Gamma(1/4)\exp(-3\gamma\Delta t)}{8\Gamma(7/4)} \\ &\times F_{21}(1/2, 1/2, 7/4, \exp(-4\gamma\Delta t)).\end{aligned} \tag{5.3}$$

Numerical simulations for the equilibrium correlation function are shown in Fig. 5.1. Note that it decays as $\exp(-2\gamma\Delta t)$ for the generic case and $\exp(-3\gamma\Delta t)$ for the gradient case at long times, whereas for the standard Ornstein-Uhlenbeck it decays as $\exp(-\gamma\Delta t)$.

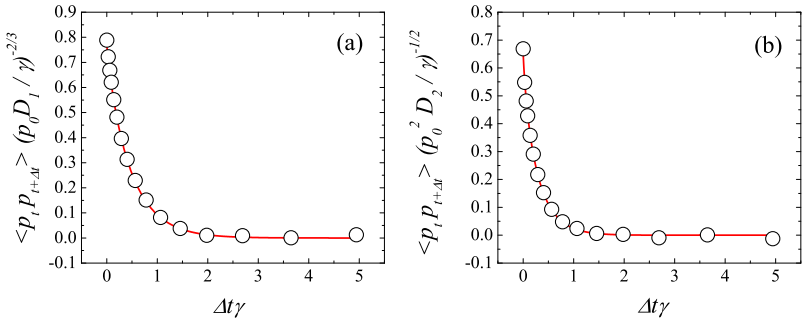

Figure 5.1: Numerical simulations (circles) of (2.1) for the momentum correlation function in equilibrium for the generic (a) and the gradient (b) cases compared with the theoretical results (5.2) and (5.3) (solid lines). The parameters were $\xi = 0.1$, $m = 1.0$, $\gamma = 0.01$, $\tau = 0.1$. For the generic case $\sigma = 35.0$, for the gradient case $\sigma = 20.0$.

5.2 Momentum diffusion

Evaluating the sum in (4.31) one obtains the variance of momentum,

$$\langle p^2(t)\rangle = \left(\frac{p_0^\zeta D_\zeta}{\gamma}\right)^{\frac{2}{2+\zeta}} \frac{(2+\zeta)^{\frac{2}{2+\zeta}}\Gamma(\frac{3}{2+\zeta})}{\Gamma(\frac{1}{2+\zeta})}(1-\mathrm{e}^{-(2+\zeta)\gamma t})^{\frac{2}{2+\zeta}}. \tag{5.4}$$

This reproduces (3.6) for $\zeta = 0$, (4.12) for $\zeta = 1$ and (4.15) for $\zeta = 2$. Numerical simulations for the variance of momentum are presented in Figs. 5.2 and 5.3 for the generic case and in Figs. 5.4 and 5.5 for the gradient case. Note that Figs. 5.3 and 5.5 show simulations for larger damping rate γ, therefore for smaller p, but still fit the theory quite well. At short times, anomalous diffusion of the momentum arises: $\langle p^2(t)\rangle \sim t^{2/3}$ for the generic case and $\langle p^2(t)\rangle \sim t^{1/2}$ for the gradient case. It should be emphasized that results for momentum diffusion in [13], [14] and [15] were obtained assuming the time correlation function of Gaussian form, that is,

$$c(t) = \exp\left(-\frac{t^2}{2\tau^2}\right). \tag{5.5}$$

This gives $\zeta = 1$ for the generic case, thus the result is the same as in [15]. However, for the gradient case the diffusion constant $D(p)$ behaves as p^{-3}, i.e. the case of $\zeta = 3$ arises implying that (5.4) yields anomalous diffusion of the momentum $\langle p^2(t)\rangle \sim t^{2/5}$. This is consistent with a short-time scaling behaviour obtained in [13], [14] and with the analytical expression obtained in [15].

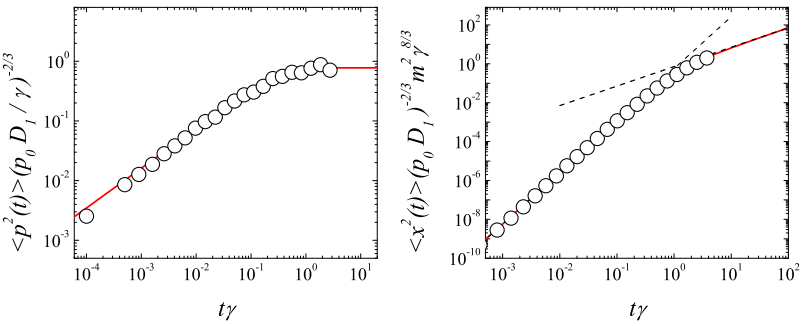

Figure 5.2: Numerical simulations of $\langle p^2(t)\rangle$ and $\langle x^2(t)\rangle$ (circles) of (2.1) for the generic case ($\zeta = 1$) compared with the theoretical results (4.12) and (5.7) (red solid lines). For $\langle x^2(t)\rangle$ the limiting behaviours (5.12) and (5.25) (dashed lines) are shown. The parameters were $\sigma = 20.0$, $\xi = 0.1$, $m = 1.0$, $\gamma = 0.001$, $\tau = 0.1$

5.3 Spatial diffusion

Using the correlation function of momentum of the form (4.32) one can calculate the mean square value of displacement by writing $\langle x^2(t)\rangle$ using the dimensionless variables z and t',

$$\langle x^2(t')\rangle = \frac{1}{m^2\gamma^2}\left(\frac{p_0^\zeta D_\zeta}{\gamma}\right)^{\frac{2}{2+\zeta}} \int_0^{t'} dt_1' \int_0^{t'} dt_2' \langle z(t_1')z(t_2')\rangle. \tag{5.6}$$

Using the fact that $Z_{kl} = 0$ for $l < k-1$ one can write the correlation function of the form (4.32) as follows,

$$\langle x^2(t')\rangle = \frac{1}{m^2}\left(\frac{p_0^\zeta D_\zeta}{\gamma^{3+\zeta}}\right)^{\frac{2}{2+\zeta}} \sum_{k=0}^{\infty}\sum_{l=k-1}^{\infty} \frac{\psi_k^+(0)}{\psi_0^+(0)} Z_{0l} Z_{kl} T_{kl}(t'), \tag{5.7}$$

with

$$T_{kl}(t') = 2\frac{\lambda_k^+(1-\mathrm{e}^{\lambda_l^- t'}) - \lambda_l^-(1-\mathrm{e}^{\lambda_k^+ t'})}{\lambda_l^-\lambda_k^+(\lambda_k^+ - \lambda_l^-)}. \tag{5.8}$$

5.3.1 Long-time diffusion

First, the limit of T_{kl} for $k \to 0$ has to be calculated,

$$T_{0l} = -\frac{2t'}{\lambda_l^-} + \frac{2}{\lambda_l^{-2}}(\mathrm{e}^{\lambda_l^- t'} - 1). \tag{5.9}$$

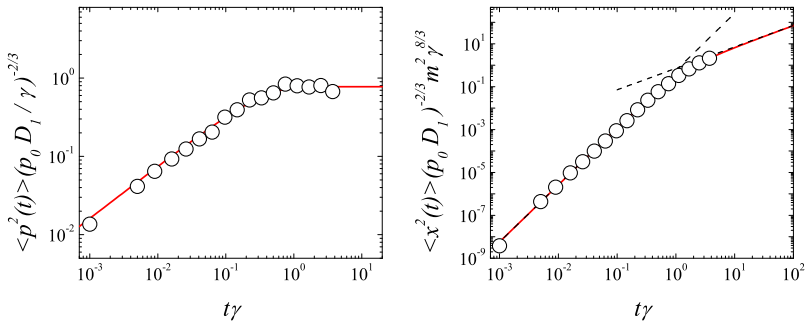

Figure 5.3: Numerical simulations of $\langle p^2(t)\rangle$ and $\langle x^2(t)\rangle$ (circles) of (2.1) for the generic case ($\zeta = 1$) compared with the theoretical results (4.12) and (5.7) (red solid lines). For $\langle x^2(t)\rangle$ the limiting behaviours are shown(5.12) and (5.25) (dashed lines). The parameters were $\sigma = 20.0$, $\xi = 0.1$, $m = 1.0$, $\gamma = 0.01$, $\tau = 0.1$

It is convenient to write the sum (5.7) processing separately the terms with $k = 0$. This gives,

$$\begin{aligned}\langle x^2(t)\rangle &= 2\mathcal{D}_x t \\ &+ \frac{1}{m^2}\left(\frac{p_0^\zeta D_\zeta}{\gamma^{3+\zeta}}\right)^{\frac{2}{2+\zeta}} \sum_{l=0}^{\infty} Z_{0l}^2 \frac{2}{\lambda_l^{-2}}(\mathrm{e}^{\lambda_l^- \gamma t}) \\ &+ \frac{1}{m^2}\left(\frac{p_0^\zeta D_\zeta}{\gamma^{3+\zeta}}\right)^{\frac{2}{2+\zeta}} \sum_{k=1}^{\infty}\sum_{l=k-1}^{\infty} \frac{\psi_k^+(0)}{\psi_0^+(0)} Z_{0l} Z_{kl} T_{kl}(\gamma t),\end{aligned} \tag{5.10}$$

with

$$\begin{aligned}\mathcal{D}_x &= -\frac{1}{m^2}\left(\frac{p_0^{2\zeta} D_\zeta^2}{\gamma^{4+\zeta}}\right)^{\frac{1}{2+\zeta}} \sum_{l=0}^{\infty} \frac{Z_{0l}^2}{\lambda_l^-} \\ &= \frac{1}{m^2}\left(\frac{p_0^{2\zeta} D_\zeta^2}{\gamma^{4+\zeta}}\right)^{\frac{1}{2+\zeta}} \frac{(2+\zeta)^{-\frac{4+3\zeta}{2+\zeta}} \pi F_{32}(\frac{\zeta}{2+\zeta}, \frac{\zeta}{2+\zeta}, \frac{1+\zeta}{2+\zeta}; \frac{3+2\zeta}{2+\zeta}, \frac{3+2\zeta}{2+\zeta}; 1)}{\sin(\frac{\pi}{2+\zeta})\Gamma(\frac{3+2\zeta}{2+\zeta})^2},\end{aligned} \tag{5.11}$$

where F_{32} is a generalized hypergeometric function [20]. At long times, the last two terms in (5.10) approach a constant, and, therefore, diffusion is recovered,

$$\langle x^2(t)\rangle \sim 2\mathcal{D}_x t \tag{5.12}$$

in this limit. Fig. 5.6 shows how $\mathcal{D}_x$ decays with ζ. Note that for $\zeta = 0$ the result (3.14) for the standard Ornstein-Uhlenbeck process is recovered, and for $\zeta = 1$ and $\zeta = 3$ this reproduces the results obtained in [15].

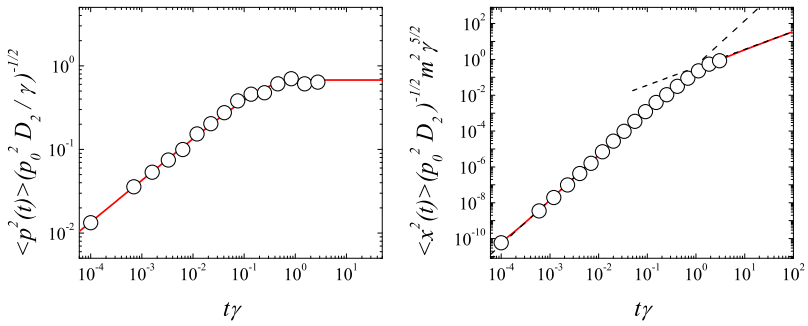

Figure 5.4: Numerical simulations of $\langle p^2(t)\rangle$ and $\langle x^2(t)\rangle$ (circles) of (2.1) for the gradient case ($\zeta = 2$) compared with the theoretical results (4.15) and (5.7) (red solid lines). For $\langle x^2(t)\rangle$ the limiting behaviours (5.12) and (5.26) (dashed lines) are shown. The parameters were $\sigma = 20.0$, $\xi = 0.1$, $m = 1.0$, $\gamma = 0.001$, $\tau = 0.1$

5.3.2 Short-time anomalous diffusion

Consider the limit of short times. Let for $l \geq k - 1$

$$A_{kl} = \frac{\psi_k^+(0)}{\psi_0^+(0)} Z_{0l} Z_{kl} \tag{5.13}$$

and zero otherwise. Apart from the dimensional pre-factor one needs to calculate

$$S(t') = \sum_{kl} A_{kl} T_{kl}(t') = \int_0^\infty dl \int_0^l dk\ T(k,l;t') A(k,l). \tag{5.14}$$

At short times, the behavior of the sum (5.7) is determined by large values of k and l. In this limit, A_{kl} looks as follows,

$$A_{kl} \sim \frac{(2+\zeta)^{-\frac{2+2\zeta}{2+\zeta}} k^{-\frac{1+\zeta}{2+\zeta}} l^{-\frac{3+\zeta}{2+\zeta}} (l-k)^{-\frac{4+\zeta}{2+\zeta}} (l+k)}{\Gamma(\frac{\zeta}{2+\zeta})^2}. \tag{5.15}$$

Note that A_{kl}, as it is given in (5.15), diverges in a non-integrable way as $k \to l$. Using the sum rule

$$\sum_{k=0}^{l+1} A_{kl} = 0. \tag{5.16}$$

one can write,

$$S(t') = \int_0^\infty dl \int_0^l dk \left[T(k,l;t') - \lim_{k\to l} T(k,l;t') \right] A(k,l). \tag{5.17}$$

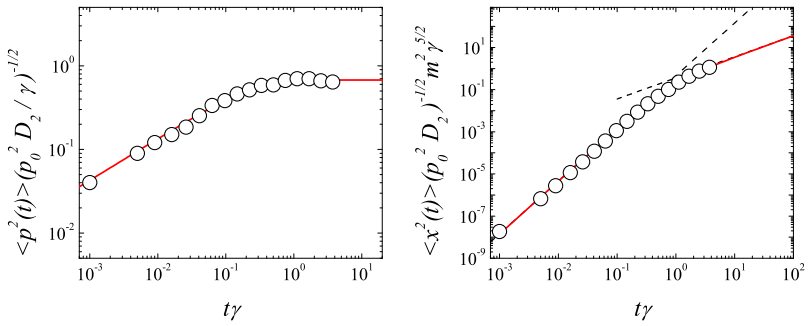

Figure 5.5: Numerical simulations of $\langle p^2(t)\rangle$ and $\langle x^2(t)\rangle$ (circles) of (2.1) for the gradient case ($\zeta = 2$) compared with the theoretical results (4.15) and (5.7) (red solid lines). For $\langle x^2(t)\rangle$ the limiting behaviours (5.12) and (5.26) (dashed lines) are shown. The parameters were $\sigma = 20.0$, $\xi = 0.1$, $m = 1.0$, $\gamma = 0.01$, $\tau = 0.1$

and thus reduce the divergence to the one that can be integrated.

$T(k, l; t')$ in the limit of large k and l looks as follows,

$$T(k,l;t') = 2\frac{l[1-\exp(-(\zeta+2)kt')] - k[1-\exp(-(2+\zeta)lt')]}{(2+\zeta)^2 kl(l-k)}. \tag{5.18}$$

It is convenient to change the variables as $x = (2+\zeta)lt'$, $xy = (2+\zeta)kt'$. Then the inverse transformation is $k = xy/[(2+\zeta)t']$ and $l = x/[(2+\zeta)t']$ implying that the Jacobian of the transformation is $J = x/[(2+\zeta)^2 t'^2]$. Using the new variables $T(k, l, t')$ becomes

$$T(x,y;t') = 2\frac{t'^2}{x}\left[\frac{a(xy)-a(x)}{1-y}\right], \tag{5.19}$$

where $a(x) = [1-\exp(-x)]/x$. It is now possible to find the limit of $T(k, l; t)$,

$$\lim_{k\to l} T(k,l;t) = \lim_{y\to 1} T(x,y;t) = 2\frac{t^2}{x}\lim_{y\to 1}\left[\frac{a(xy)-a(x)}{1-y}\right] \tag{5.20}$$

and using l'Hospital's rule,

$$\lim_{y\to 1} T(x,y;t) = -2\frac{t^2}{x}\left[\frac{\partial}{\partial y}a(xy)\right]\Bigg|_{y=1} = -2\frac{t^2}{x}xa'(x). \tag{5.21}$$

One obtains

$$T(k,l;t') - \lim_{k\to l} T(k,l;t') = 2\frac{t'^2}{x}\left[\frac{a(xy)-a(x)}{1-y} + xa'(x)\right]. \tag{5.22}$$

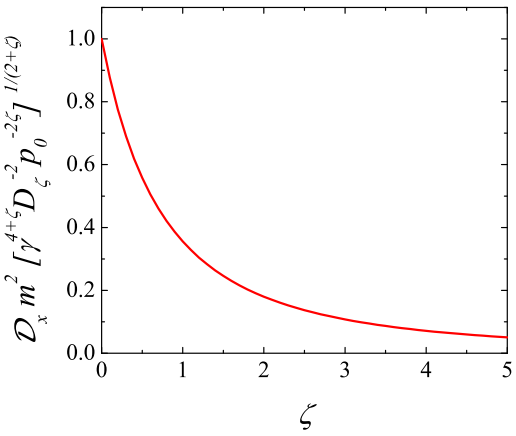

Figure 5.6: Diffusion constant as a function of ζ

Using (5.15), (5.17) and (5.22) to simplify $S(t)$ one can write,

$$\begin{aligned}\langle x^2(t)\rangle &= \frac{1}{m^2}\left(\frac{p_0^{\zeta} D_{\zeta}}{\gamma^{3+\zeta}}\right)^{\frac{2}{2+\zeta}} S(t) \qquad (5.23)\\ &= \frac{2(2+\zeta)^{-\frac{2\zeta}{2+\zeta}}}{\Gamma(\frac{\zeta}{2+\zeta})^2}(p_0^{\zeta} D_{\zeta})^{\frac{2}{2+\zeta}} m^{-2} t^{\frac{6+2\zeta}{2+\zeta}} \int_0^{\infty} dx\, x^{-\frac{2\zeta+6}{2+\zeta}}\\ &\times \int_0^1 dy \left[\frac{a(xy)-a(x)}{1-y} + x a'(x)\right] y^{-\frac{1+\zeta}{2+\zeta}} (1-y)^{-\frac{4+\zeta}{2+\zeta}} (1+y).\end{aligned}$$

This implies for the generic case $\langle x^2(t)\rangle \sim t^{8/3}$ and for the gradient case $\langle x^2(t)\rangle \sim t^{5/2}$, thus anomalous spatial diffusion at short times is discovered. For the case of $\zeta = 3$, (5.23) reproduces results obtained in [13], [14] and [15], that is $\langle x^2(t)\rangle \sim t^{12/5}$.

Consider the following function,

$$\begin{aligned}I(\zeta) &= \frac{2(2+\zeta)^{-\frac{2\zeta}{2+\zeta}}}{\Gamma(\frac{\zeta}{2+\zeta})^2} \int_0^{\infty} dx\, x^{-\frac{2\zeta+6}{2+\zeta}} \qquad (5.24)\\ &\times \int_0^1 dy \left[\frac{a(xy)-a(x)}{1-y} + x a'(x)\right] y^{-\frac{1+\zeta}{2+\zeta}} (1-y)^{-\frac{4+\zeta}{2+\zeta}} (1+y).\end{aligned}$$

Numerical evaluation of (5.24) as a function of ζ is shown in Fig. 5.7. It can be seen that for small values ζ it approaches 0 whereas for $\zeta = 0$ it should reproduce the result for the standard Ornstein-Uhlenbeck process, that is 2/3. Reliable results for small values of ζ are not recovered, however other

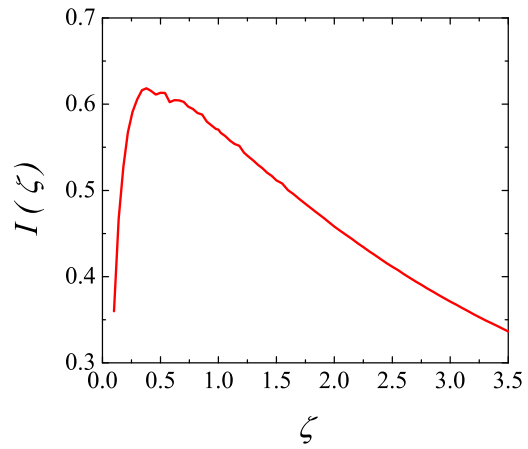

Figure 5.7: Numerical evaluation of the integral (5.24) as a function of ζ (solid line)

values are quite precise. Using the numerical values for $I(\zeta)$ one can rewrite (5.23) for the generic case,

$$\langle x^2(t)\rangle = 0.5705 \times (p_0 D_1)^{2/3} m^{-2} t^{8/3} \tag{5.25}$$

and for the gradient case,

$$\langle x^2(t)\rangle = 0.4580 \times (p_0^2 D_2)^{1/2} m^{-2} t^{5/2}. \tag{5.26}$$

These results agree with the numerical simulations quite well (Figs. 5.2-5.5).

Chapter 6

Motion in two spatial dimensions

This chapter gives a brief discussion for the case of motion in two spatial dimensions. In this case the equation of motion replacing (1.2) is,

$$\frac{d\boldsymbol{p}}{dt} = -\gamma \boldsymbol{p} + \boldsymbol{f}(\boldsymbol{x}, t), \tag{6.1}$$

where $\boldsymbol{p} = (p_x,\ p_y)^T$, $\boldsymbol{x} = (x,\ y)^T$ and $\boldsymbol{f} = (f_x,\ f_y)^T$ are two-dimensional vectors (superscript T denotes transposition). One can consider several possibilities of how the random force field $\boldsymbol{f}$ can be generated (see e.g. [11]). One possibility is a potential field,

$$\boldsymbol{f}(\boldsymbol{x}, t) = \begin{pmatrix} \partial_x \phi(\boldsymbol{x}, t) \\ \partial_y \phi(\boldsymbol{x}, t) \end{pmatrix} \tag{6.2}$$

where ϕ is a generic random field described in chapter 2. Another possibility is a solenoidal (or rotational) field that looks as follows,

$$\boldsymbol{f}(\boldsymbol{x}, t) = \begin{pmatrix} \partial_y \phi(\boldsymbol{x}, t) \\ -\partial_x \phi(\boldsymbol{x}, t) \end{pmatrix} \tag{6.3}$$

To generalize, one can also consider a combination of a potential and a solenoidal field,

$$\boldsymbol{f}(\boldsymbol{x}, t) = \alpha \begin{pmatrix} \partial_x \psi(\boldsymbol{x}, t) \\ \partial_y \psi(\boldsymbol{x}, t) \end{pmatrix} + \beta \begin{pmatrix} \partial_y \phi(\boldsymbol{x}, t) \\ -\partial_x \phi(\boldsymbol{x}, t) \end{pmatrix}, \tag{6.4}$$

where ψ and ϕ are independent generic random field having identical statistical properties, and α and β are real numbers.

The Fokker-Planck equation for the two-dimensional case is derived analogously to the one-dimensional case. One obtains,

$$\frac{\partial P(\boldsymbol{p}, t)}{\partial t} = \nabla_{\boldsymbol{p}}^T \left(\gamma \boldsymbol{p} P + \mathbf{D}(\boldsymbol{p}) \nabla_{\boldsymbol{p}} P \right), \tag{6.5}$$

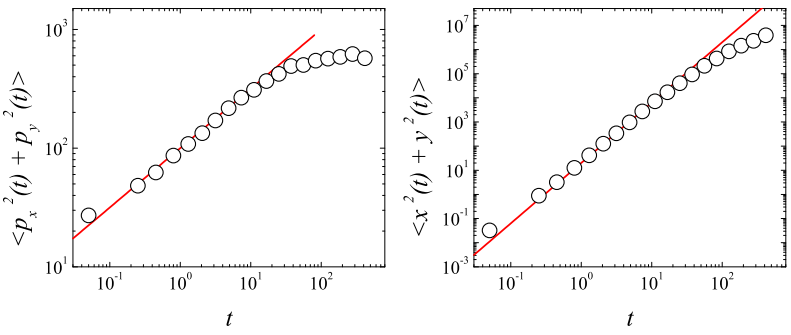

Figure 6.1: Numerical simulations (circles) for two-dimensional generalized Ornstein-Uhlenbeck process for the case of potential force field. Red lines show slope 1/2 for the momentum and 5/2 for the displacement

where $\nabla_{\boldsymbol{p}}$ denotes a gradient with respect to $\boldsymbol{p}$ and $\mathbf{D}(\boldsymbol{p})$ is a diffusion matrix. It is defined as follows [19],

$$\mathbf{D}(\boldsymbol{p}) = \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix}, \tag{6.6}$$

with

$$\begin{aligned} D_{11} &= \frac{1}{2}\int_{-\infty}^{\infty} c_{xx}(\boldsymbol{p}t/m, t)\ dt, \\ D_{12} = D_{21} &= \frac{1}{2}\int_{-\infty}^{\infty} c_{xy}(\boldsymbol{p}t/m, t)\ dt, \\ D_{22} &= \frac{1}{2}\int_{-\infty}^{\infty} c_{yy}(\boldsymbol{p}t/m, t)\ dt, \end{aligned} \tag{6.7}$$

where c_{xx}, c_{xy} and c_{yy} are correlation functions of components of $\boldsymbol{f}$, that is

$$\begin{aligned} c_{xx}(x, y, t) &= \langle f_x(x_1, y_1, t_1) f_x(x_1 + x, y_1 + y, t_1 + t)\rangle, \\ c_{xy}(x, y, t) &= \langle f_x(x_1, y_1, t_1) f_y(x_1 + x, y_1 + y, t_1 + t)\rangle, \\ c_{yy}(x, y, t) &= \langle f_y(x_1, y_1, t_1) f_y(x_1 + x, y_1 + y, t_1 + t)\rangle. \end{aligned} \tag{6.8}$$

It is convenient to transform $\boldsymbol{p}$ to polar coordinates as follows,

$$\begin{aligned} p_x &= p\cos\theta, \\ p_y &= p\sin\theta. \end{aligned} \tag{6.9}$$

As before, the case of large forcing and small damping is considered, that

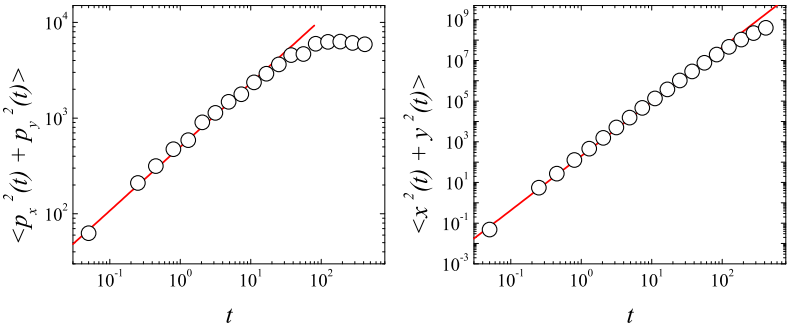

Figure 6.2: Numerical simulations (circles) for two-dimensional generalized Ornstein-Uhlenbeck process for the case of solenoidal force field. Red lines show slope 2/3 for the momentum and 8/3 for the displacement

is $|\boldsymbol{p}| \gg p_0$. In this limit the diffusion matrix in polar coordinates is

$$\mathbf{D}(\boldsymbol{p}) = \frac{D_2 p_0}{p} \begin{pmatrix} \sin^2\theta & -\cos\theta\sin\theta \\ -\cos\theta\sin\theta & \cos^2\theta \end{pmatrix} \tag{6.10}$$

for the potential force field, and

$$\mathbf{D}(\boldsymbol{p}) = \frac{D_2 p_0}{p} \begin{pmatrix} \cos^2\theta & \cos\theta\sin\theta \\ \cos\theta\sin\theta & \sin^2\theta \end{pmatrix} \tag{6.11}$$

for the solenoidal one. Here, D_2 is the same as it was defined in chapter 4.

It is, however, not obvious that an approximation of the diffusion matrix should be carried out before it is used in the Fokker-Planck equation. In fact, the diffusion matrices in the case of the Gaussian time correlation function are equal to those obtained above. This would imply the same result for both types of correlation function. Numerical results performed for the correlation function of the form (2.4) are consistent with short-time scaling behaviours obtained in [13] ($\langle|\boldsymbol{p}|^2\rangle \sim t^{1/2}$) for the Gaussian time correlation function and potential force field (Fig. 6.1). Yet, it is believed that the results obtained in [13] for multi-dimensional cases are not correct and one should refer to [14] where the result is $\langle|\boldsymbol{p}|^2\rangle \sim t^{2/5}$. For the solenoidal force field numerical simulations give $\langle|\boldsymbol{p}|^2\rangle \sim t^{2/3}$ (Fig. 6.2)

Chapter 7

Conclusions and future work

The most important property of the generalized Ornstein-Uhlenbeck process may be the fact that the spectrum of the corresponding Fokker-Planck operator consists of two rows of eigenvalues λ_n^+ and λ_n^- that are evenly spaced in each row, and the rows are staggered with respect to each other. Such a spectrum was called as staggered ladder spectrum in [15]. Using the spectral decomposition of the Fokker-Planck operator, correlations and fluctuations of observables in generalized Ornstein-Uhlenbeck process could be calculated analytically. It is found that the momentum variance exhibits anomalous diffusion at short times and grows until particles accelerate to a certain level, but then saturates in equilibrium. The mean square value of the displacement also exhibits anomalous spatial diffusion at short times, however, at long times an expected result, that is, ordinary diffusion, is confirmed. The spectral decomposition approach makes it possible to determine in a very clear way many other quantities that are related to momentum of a particle. Among such quantities, the correlation function of the momentum in equilibrium has been calculated; it decays exponentially for long time but faster than $\exp(-\gamma t)$ as in the standard Ornstein-Uhlenbeck process. The Fokker-Planck equation also gives the probability distribution of the momentum as a function of time, which turns out to be non-Maxwellian in equilibrium for the generalized Ornstein-Uhlenbeck process, unlike Gaussian distribution for the standard one. The theory has been successfully verified by numerical experiments.

In chapter 6, it has been shown that numerical results for the case of motion in two spatial dimensions are not consistent with the analytical ones obtained in [14]. The reason for this inconsistence could be the difference in time correlation functions, however the diffusion matrices approximated for the case of large p turn out to be the same for both types of correlation function. Thus a careful investigation of motion in two spatial dimensions is the next question to address.

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