Abstract

In the first part of this thesis we review the concept of stochastic Langevin equations. We state a simple example and explain its physical meaning in terms of Brownian motion. We then calculate the mean square displacement and the velocity autocorrelation function by solving this equation. These quantities are related to the diffusion coefficient in terms of the Green-Kuba formula, and will be defined properly. In the second part of the thesis we introduce a deterministic Langevin equation which models Brownian motion in terms of deterministic chaos, as suggested in recent research literature. We solve this equation by deriving a recurrence relation. We review Takagi function techniques of dynamical systems theory and apply them to this model. We also apply the correlation function technique. Finally, we derive, for the first time, an exact formula for the diffusion coefficient as a function of a control parameter for this model.

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Chapter 1

Introduction

The stochastic Langevin equation is the simplest and the most widely known mathematical model for the phenomenon of Brownian motion. It is a first-order differential equation which contains a stochastic term corresponding to a random force. From physics point of view a *deterministic equation* is an equation that governs the motion of a dynamical system and does not contain terms corresponding to random forces. The dynamical system concept is a mathematical formalization for any fixed "rule" which describes the time dependence of an evolved variable in its ambient space. Deterministic models thus produce the same output for a given starting condition. In the picture of classical physics, any macroscopic transport is caused mechanically by microscopic dynamics. The theory of dynamical systems allows a description of the deterministic dynamics of a chaotic system, i.e, the microscopic movements of the particles are taken into account completely [10].

The modern theory of chaotic dynamical systems thus provides an opportunity to "take the microscopic dynamics seriously" in the calculation of macroscopic statistical quantities in the sense that the complete, usually highly non-linear deterministic dynamics of a system can be taken into account. In this sense the motivation arises to replace the randomness in the stochastic Langevin equation by a deterministic chaotic force in order to get back to a microscopic setting [1]. This way we are closer to the statistical phenomenon of Brownian motion in terms of fully deterministic equations of motion.

This thesis consists of five Chapters and is organized as follows.

In Chapter 2, we give a brief historical overview of Brownian motion. One way to model the Brownian motion is via the stochastic Langevin equation.

We present a physical derivation of this equation. Then we calculate the mean square displacement and the autocorrelation function for the Brownian/particle by using this equation.

In Chapter 3, as motivated above, we replace the randomness in the stochastic Langevin equation by a deterministic term. In our case this term is a deterministic chaotic kick force. By making suitable approximations, we then solve this equation by deriving a recurrence relation. Based on this result, we calculate the value for the diffusion coefficient for the kick force using the Green-Kubo formula. The kick force is given by a Bernoulli shift map model. We develop two different techniques to achieve this: the correlation function technique and the Takagi function approach. Both are new results.

Finally, in Chapter 4 we first parametrize our Bernoulli shift model with a control parameter h. We then derive a generalized Takagi function which depends on h. Finally, for the first time again, we derive an exact analytical formula for the diffusion coefficient as a function of the control parameter h.

Chapter 2

Stochastic Langevin Equation

2.1 What is Brownian motion?

Brownian motion is the seemingly random movement of a tracer particle suspended in a fluid.

The phenomenon of Brownian motion was first observed by J. Ingenhousz for coal dust particles on the surface of alcohol. However, it became more widely known only later on by the work of botanist R. Brown in 1827, who reported vigorous irregular motion of small particles originating from pollen floating on water [14]. It was Einstein who first provided a theoretical analysis of the Brownian motion by describing this irregular motion in terms of diffusion processes. Einstein proved that the diffusion constant D is related to its mobility μ by

$$D = \mu k T \tag{2.1}$$

where k is the Boltzmann constant and T is temperature. Equation (2.1) is called *Einstein relation*. It is a good basis of experimental verification that Brownian motion is related to the thermal motion of molecules. Einstein's work led J.B. Perrin to the experimental measurement of the Avogadro number. Brownian motion can give considerable insight into the mechanism responsible for the existence of fluctuations and "dissipation of energy" [16]. This problem is also of great practical interest because of the fact that such fluctuations represent "noise" which can limit the accuracy of physical measurements. The theory of Brownian motion was further developed by P.

Langevin, and many others. Brownian motion is very common. It takes place in electrical circuits, in finance, such as stock market fluctuations, etc.

2.2 The Langevin equation

The time evolution of the position of a Brownian particle is best described using the Langevin equation, an equation which involves a random force representing the effect of thermal fluctuations of the solvent on the particle.

We consider the simple case of a Brownian (tracer) particle in a fluid. The particle is not acted upon by any other force except the one arising from the collisions with molecules in the fluid [15]. The physical model for this should start from the microscopic motion itself. Recall that Newton's second law of motion can be written as

$$m\frac{dv}{dt} = F, \tag{2.2}$$

where m is the mass of the particle, v is the velocity and F is the force acting on the particle from the molecules of the fluid surrounding the Brownian particle. We treat only the one-dimensional case. Langevin suggested that the force F can be written as a sum of two parts, i.e two different forces. The first part is the frictional force (viscous drag) which represents the dynamical friction experienced by the particle and is proportional to the velocity of the particle. This force is

$$F_A = -m\gamma v, \tag{2.3}$$

where $m\gamma$ is the friction coefficient. The second part of the force, F_B, is regarded as random, in the sense that it does not depend on the motion of the particle, i.e its displacement. It is a rapidly fluctuating force which is again due to the impacts of the molecules of the fluid on the particle ([14],[6]). The Gaussian white noise is considered to be a model of this force. This force fulfils certain stochastic conditions, the most important being that the time average is zero, and that the force is δ-correlated [2]. This means that the autocorrelation function is

$$\langle F_B(t)F_B(t')\rangle = C\delta(t-t'), \tag{2.4}$$

where $\delta(t)$ denotes the Dirac delta function (see Appendix), t and t' are different times, $\langle\cdots\rangle$ denotes the expectation value, and C is called the *spectral density.* In physics, the spectral density, is a positive real function of a frequency variable associated with a stationary stochastic process, or a deterministic function of time, which has dimensions of power per Hz, or energy per Hz. It is often called simply the spectrum of the signal. Intuitively, the spectral density captures the frequency content of a stochastic process and helps identify periodicities. In general, by autocorrelation we mean the quantity,

$$\langle A\,(t_1)\,A\,(t_2)\rangle = K_A(t_1,t_2) \tag{2.5}$$

which is a measure of the "statistical correlation between the value of the fluctuating variable A at time $t_1$and its value at time t_2". Moreover, if the force $F_B(t)$ is passed through a filter (by Fourier transforming it), the spectral density is not a function of the angular frequency ω, it is constant for all values of ω. In this case we have *white noise* [6]. Now (2.2) can be written as

$$m\frac{dv}{dt} = -m\gamma v + F_B \tag{2.6}$$

In the case of a spherical particle, Eq.(2.6) becomes

$$m\frac{dv}{dt} = -\alpha v + F_B, \tag{2.7}$$

where $\alpha = 6\pi a\eta$ is known as *Stoke's law*. Equation (2.7) is known as the **Langevin equation**. In case of an external force F_C, it can be written as

$$m\frac{dv}{dt} = F_C - \alpha v + F_B \tag{2.8}$$

2.3 Calculation of the mean square displacement

We first define what the mean square displacement (msd) means. It is a measure of the average distance squared a molecule or particle travels. It is defined as

$$msd(t) = \langle x_i(t)^2\rangle = \langle (x_i(t) - x_i(0))^2\rangle \tag{2.9}$$

where $x_i(t) - x_i(0)$ is the distance molecule i travels over some time interval of length t. $\langle\cdots\rangle$ means the ensemble average, which is the statistical average of the quantity inside the brackets at a given time over all systems of the ensemble. If we consider all the molecules in the system then we could write

$$msd(t) = \frac{1}{N}\sum_{i=1}^{N}\langle x_i(t)^2\rangle \tag{2.10}$$

where N is the number of molecules in the system.

In this thesis we only consider a single particle. We wish to proceed by calculating the msd of a Brownian particle at time t. We will employ the Langevin equation in (2.7) to achieve this [16]. Recall that, in Eq.(2.7), we have $v = \frac{dx}{dt} = \dot{x}$. Hence, Eq.(2.7) now becomes

$$m\frac{d\dot{x}}{dt} = -\alpha\dot{x} + F_B \tag{2.11}$$

Multiplying both sides of Eq.(2.11) by x and taking the ensemble average of both sides gives

$$m\langle\frac{d}{dt}(x\dot{x})\rangle - m\langle\dot{x}^2\rangle = -\alpha\langle x\dot{x}\rangle + \langle x\rangle\langle F_B\rangle \tag{2.12}$$

where we have used $x\frac{d\dot{x}}{dt} = \frac{d}{dt}(x\dot{x}) - \dot{x}^2$. Also note that the operations of taking a time derivative and taking an ensemble average commute. The mean value of the fluctuating part F_B always vanishes irrespective of the velocity or position of the particle. So $\langle x\rangle\langle F_B\rangle = 0$. From the equipartition theorem we have $\frac{1}{2}m\langle\dot{x}^2\rangle = \frac{1}{2}kT$. Thus Eq.(2.12) becomes

$$m\frac{d}{dt}\langle x\dot{x}\rangle = kT - \alpha\langle x\dot{x}\rangle \tag{2.13}$$

which is a first-order differential equation and we can solve it for $\langle x\dot{x}\rangle$. We use the integrating factor technique. Letting $y = \langle x\dot{x}\rangle$, Eq.(2.13) becomes

$$\frac{dy}{dt} + \frac{\alpha}{m}y = \frac{kT}{m} \tag{2.14}$$

The solution of Eq.(2.14) is given by

$$ye^{\frac{\alpha}{m}x} = \int \frac{kT}{m}e^{\frac{\alpha}{m}x}dx \tag{2.15}$$

This gives

$$y = Ce^{-\frac{\alpha}{m}x} + \frac{kT}{\alpha} \tag{2.16}$$

where C is a constant of integration. Let $\gamma \equiv \alpha/m$, so that γ^{-1} is a characteristic time constant of the system. Thus we have

$$\langle x\dot{x}\rangle = Ce^{-\gamma t} + \frac{kT}{\alpha} \tag{2.17}$$

Assuming the initial conditions, $x = 0$ at $t = 0$, the above equation implies that $C = -\frac{kT}{\alpha}$. Hence we can write

$$\langle x\dot{x}\rangle = \frac{kT}{\alpha}(1 - e^{-\gamma t}) \tag{2.18}$$

Writing $x\dot{x}$ as $\frac{1}{2}\frac{d}{dt}(x^2)$ in Eq.(2.18) and integrating with respect to time t gives,

$$\frac{1}{2}\int_0^t \frac{d}{dt}\langle x^2\rangle dt' = \int_0^t \frac{kT}{\alpha}dt' - \int_0^t \frac{kT}{\alpha}e^{-\gamma t'}dt' \tag{2.19}$$

which then gives

$$\begin{aligned}\langle x^2\rangle &= \frac{2kT}{\alpha} + \frac{2kT}{\alpha\gamma}\left(e^{-\gamma t} - 1\right) \\ &= \frac{2kT}{\alpha}\left[t - \frac{1}{\gamma}\left(1 - e^{-\gamma t}\right)\right] \end{aligned} \tag{2.20}$$

which is the *mean square displacement* of a Brownian particle at time t.

Depending on the value of t relative to $\frac{1}{\gamma}$, we can consider two limiting cases,

case 1: $t << \gamma^{-1}$. Using Taylor series, we can write $e^{-\gamma t} = 1 - \gamma t + \frac{1}{2}\gamma^2 t^2 - ....$ Then

$$\begin{aligned}\langle x^2\rangle &= \frac{2kT}{\alpha}\left[t - \frac{1}{\gamma}\left(1 - 1 + \gamma t - \frac{1}{2}\gamma^2 t^2 + ...\right)\right] \\ &= \frac{2kT}{\alpha}\left[t - t + \frac{1}{2}\gamma t^2 - ...\right] \\ &= \frac{kT}{m}t^2 \end{aligned} \tag{2.21}$$

where we have used $\gamma \equiv \frac{\alpha}{m}$, and $O(t^3) = 0$.

This means that during a short interval of time the particle behaves as though it were a free particle moving with the constant thermal velocity $v = (kT/m)^{1/2}$

case 2: $t >> \gamma^{-1}$. This implies that $e^{-\gamma t} \to 0$. Then Eq.(2.20) becomes,

$$\langle x^2 \rangle = \frac{2kT}{\alpha} t \tag{2.22}$$

This means that the particle exhibits diffusive movements, so that $\langle x^2 \rangle \propto t$. We define the diffusion coefficient D for a tracer particle via the Einstein formula

$$D = \lim_{t\to\infty} \frac{\langle x^2 \rangle}{2t} \tag{2.23}$$

Recalling that $\alpha = 6\pi\eta a$, and using Eq.(2.22), we derive an explicit result for the *msd* of a Brownian particle for $t >> \gamma^{-1}$,

$$\langle x^2 \rangle = \frac{kT}{3\pi\eta a} t \tag{2.24}$$

2.4 Derivation of the velocity autocorrelation function

The velocity autocorrelation function is defined as

$$\langle v(t')v(t'') \rangle = \langle v(0)v(t) \rangle \equiv K_v(t) \tag{2.25}$$

where $t = t'' - t'$. The system is assumed to be in equilibrium state, hence time-translation invariant.
We wish to derive an expression for $\langle v(0)v(t) \rangle$ in terms of t. We start with the Langevin equation (2.7)

$$m\frac{dv}{dt} = -\alpha v + F_B \tag{2.26}$$

Then

$$v(t+\tau) - v(t) = -\gamma v(t)\tau + \frac{1}{m}\int_t^{t+\tau} F_B(t')dt' \tag{2.27}$$

where $\gamma \equiv \alpha/m$ and τ is macroscopically small (but large in a microscopic scale). Next we multiply the last equation by $v(0)$ and take the ensemble average,

$$\langle v(0)v(t+\tau)\rangle - \langle v(0)v(t)\rangle = -\gamma\langle v(0)v(t)\rangle\tau + \frac{1}{m}\langle v(0)\int_t^{t+\tau} F_B(t')dt'\rangle \tag{2.28}$$

The second term on the RHS is zero [16]. This is because $\langle F_B\rangle$ is zero for the reasons explained in section 2.3.

Equation (2.28) now becomes

$$\frac{\langle v(0)v(t+\tau)\rangle - \langle v(0)v(t)\rangle}{\tau} = \frac{d}{ds}\langle v(0)v(t)\rangle = -\gamma\langle v(0)v(t)\rangle \tag{2.29}$$

For $t > 0$, by integration this gives

$$\langle v(0)v(t)\rangle = \langle v^2(0)\rangle e^{-\gamma t} \tag{2.30}$$

Using the equipartition theorem result $\langle \frac{1}{2}v^2(0)\rangle = \frac{1}{2}kT$, the last equation yields

$$\langle v(0)v(t)\rangle = \langle v^2(0)\rangle e^{-\gamma|t|} = \frac{kT}{m}e^{-\gamma|t|} \tag{2.31}$$

for all values of t.

Chapter 3

Deterministic Langevin Equation

In this chapter we wish to replace the randomness (i.e, the stochastic term) in the stochastic Langevin equation by a deterministic chaotic force in order to get back to a microscopic setting [1].

3.1 Langevin equation revisited

In the previous chapter we considered a stochastic Langevin equation. More precisely we considered Eq.(2.7) which contained a random force. We can rewrite this equation in the form

$$\frac{dY}{dt} = -\gamma Y + L(t) \tag{3.1}$$

which is also a linear equation, where we have replaced v by Y, $-\alpha/m$ by γ and F_B/m by $L(t)$. Here $L(t)$ is Gaussian white noise. $\gamma > 0$, which is the same as in (2.6), represents a damping constant.

In [1] a deterministic version of the above stochastic Langevin equation has been proposed. Namely, if the Gaussian white noise as a stochastic term is replaced by a *chaotic* process generated by a *deterministic* chaotic dynamics, one gets a deterministic Langevin equation. These are also called *dynamical systems of Langevin type.*

We consider a one-dimensional particle of unit mass under the influence of a linear damping force that is driven by a rapidly fluctuating chaotic force. As a model, we replace the Gaussian white noise $L(t)$ by a more complicated chaotic process $L_\tau(t)$, which can be considered to be a deterministic chaotic kick force. The velocity $Y(t)$ of the particle obeys

$$\frac{dY}{dt} = -\gamma Y + L_\tau(t) \tag{3.2}$$

At discrete time points $n\tau$, with a fixed τ and integers $n = 0, 1, 2, ...$, the particle gets a kick of strength x_n,

$$L_\tau = \tau^{1/2} \sum_{n=1}^{\infty} x_n \delta\left(t - n\tau\right), \tag{3.3}$$

where again δ is Dirac's delta function, $\tau > 0$ is the time difference between subsequent impulses, and the kick strengths x_n evolve in a deterministic way [2]. So we assume that the kick strength at time $(n+1)\tau$ is a deterministic function of the kick strength at time $n\tau$,

$$x_{n+1} = B(x_n) \tag{3.4}$$

In this thesis the deterministic function will be the Bernoulli shift map in the interval $-1/2 \leqslant x \leqslant 1/2$ (see Section 3.3). The constant factor $\tau^{1/2}$ has been included in Eq.(3.3) for scaling purposes.

3.2 Solving the deterministic Langevin equation

We refer to equation (3.2) as a *deterministic Langevin equation.* We wish to solve this equation, that is, we wish to find $Y(t)$. We use the integrating factor technique with the integrating factor $e^{\gamma t}$. We assume that the impulses start at $t = 0$. Integrating Eq.(3.2) gives

$$e^{\gamma t} Y(t) = \int_0^t L_\tau(t') e^{\gamma t'} dt' + C \tag{3.5}$$

where $C = Y(0)$. Then

$$Y(t) = e^{-\gamma t} Y(0) + \int_0^t L_\tau(t') e^{-\gamma(t-t')} dt' \tag{3.6}$$

For $t >> 0$, the first term on the RHS vanishes. Hence using Eq.(3.3) and the definition of Dirac delta function (see Appendix) we can write

$$\begin{aligned} Y(t) &= \int_0^t L_\tau(t')e^{\gamma(t-t')}dt' \\ &= \tau^{1/2}\int_0^t \sum_{k=1}^{\infty} e^{-\gamma(t-t')}x_k\delta\left(t'-k\tau\right) \\ &= \tau^{1/2}\sum_{k=1}^{n} x_k e^{-\gamma(t-k\tau)} \qquad (3.7) \\ &= e^{-\gamma(t-n\tau)}y_n \qquad (3.8) \end{aligned}$$

where $n\tau < t < (n+1)\tau$, and $n = \lfloor\frac{t}{\tau}\rfloor$, ($\lfloor\rfloor$: floor function).
Using Eqs.(3.7) and (3.8) we can define y_n to be

$$\begin{aligned} y_n &= \tau^{1/2}\sum_{k=1}^{n} x_k e^{-\gamma(t-k\tau)}e^{\gamma(t-n\tau)} \\ &= \tau^{1/2}\sum_{k=1}^{n} x_k e^{-\gamma\tau(n-k)} \qquad (3.9) \end{aligned}$$

Then for y_{n+1} we have

$$\begin{aligned} y_{n+1} &= \tau^{1/2}\sum_{k=1}^{n+1} x_k e^{-\gamma\tau(n+1-k)} \\ &= \tau^{1/2}\sum_{k=1}^{n} x_k e^{-\gamma\tau(n+1-k)} + \tau^{1/2}x_{n+1}e^{-\gamma\tau(n+1-n-1)} \\ &= e^{-\gamma\tau}\tau^{1/2}\sum_{k=1}^{n} x_k e^{-\gamma\tau(n-k)} + \tau^{1/2}x_{n+1} \\ &= \lambda y_n + \tau^{1/2}x_{n+1} \qquad (3.10) \end{aligned}$$

where $\lambda = e^{-\gamma\tau}$ is a parameter. The position $Z(t)$ of the particle can be found by integrating $Y(t)$ given by Eq.(3.8),

$$\begin{aligned} Z(t) &= \int_0^t e^{-\gamma(t'-n\tau)} y_n dt' \\ &= \int_0^\tau e^{-\gamma(t'-0\tau)} y_0 dt' + \int_\tau^{2\tau} e^{-\gamma(t'-\tau)} y_1 dt' + \cdots + \int_{n\tau}^t e^{-\gamma(t'-n\tau)} y_n dt' \\ &= \frac{1}{\gamma} \sum_{k=0}^{n-1} y_k \left(1 - e^{-\gamma\tau}\right) + \frac{1 - e^{-\gamma(t-n\tau)}}{\gamma} y_n \end{aligned} \tag{3.11}$$

Let the sum in Eq.(3.11) be z_n. That is, let

$$z_n = \sum_{k=0}^{n-1} y_k \left(1 - e^{-\gamma\tau}\right) \tag{3.12}$$

Then for z_{n+1} we have

$$\begin{aligned} z_{n+1} &= \sum_{k=0}^{n} y_k \left(1 - e^{-\gamma\tau}\right) \\ &= \sum_{k=0}^{n-1} y_k \left(1 - e^{-\gamma\tau}\right) + \frac{1}{\gamma} y_n \left(1 - e^{-\gamma\tau}\right) \\ &= z_n + \kappa y_n \end{aligned} \tag{3.13}$$

where $\kappa = (1 - \lambda)/\gamma$ is also a parameter.

Thus we have established the following *recurrence relation*

$$x_{n+1} = B(x_n) \tag{3.14}$$

$$y_{n+1} = \lambda y_n + \tau^{1/2} x_{n+1} \tag{3.15}$$

$$z_{n+1} = z_n + \kappa y_n \tag{3.16}$$

Equations (3.14)-(3.16) which we have just derived are very important results. They represent *the setup* for the rest of the work in this thesis. Note that the derivation of the above recurrence relation was done independently and is omitted in [1].

3.3 Calculation of the Diffusion Coefficient

In this section we calculate the value for the diffusion coefficient D for the kick force x_n. We do this by using the so-called Green-Kubo formula ([10],[9],[8]) which is given by

$$D = \sum_{k=0}^{\infty} \langle v_k v_0 \rangle - \frac{1}{2} \langle {v_0}^2 \rangle \tag{3.17}$$

where v here is the "velocity" function, which for our map model will be defined precisely, and k is the k-th iterate. A detailed derivation of Green-Kubo formula is shown in [13]. A discrete version of Green-Kubo formula is given in [3].

The Bernoulli shift map on the interval $[-1/2, 1/2]$ is defined by

$$B(x) = \begin{cases} 2x + \frac{1}{2} & -1/2 \leq x < 0 \\ \\ 2x - \frac{1}{2} & 0 \leq x < 1/2 \end{cases} \tag{3.18}$$

The map is shown in Fig.(3.1). We calculate a value for D for the kick force given by this map.

We now return to our recurrence relation that we derived in section 3.4,

$$x_{n+1} = B(x_n) \tag{3.19}$$
$$y_{n+1} = \lambda y_n + \tau^{1/2} x_{n+1} \tag{3.20}$$
$$z_{n+1} = z_n + \kappa y_n \tag{3.21}$$

For simplicity reasons we consider the over-damped case, that is, when $\gamma \gg 0$ for fixed τ. This means $\lambda = e^{-\gamma\tau} \to 0$. In order to compute D by using Eq.(3.17) we need to define a "velocity" function v_n. We define it as $v_n := z_{n+1} - z_n$, which is the difference between two successive positions of the particle, in other words it measures how far a particle travels under one iteration. Using this definition and the above recurrence relation we can write

$$v_n := z_{n+1} - z_n = \kappa y_n \tag{3.22}$$

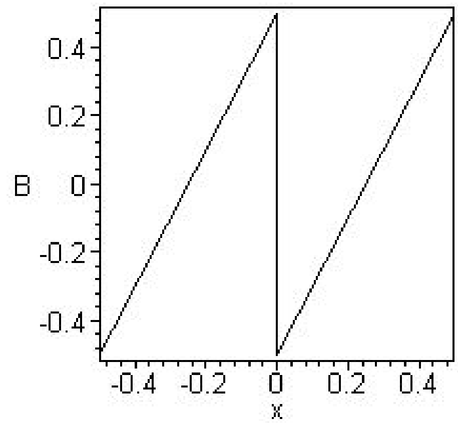

Figure 3.1: The Bernoulli shift map on the interval [-1/2,1/2]

Hence for the velocity function we now have

$$v_n := \tau^{1/2} x_n \tag{3.23}$$

For convenience we let $\tau = 1$ and $\gamma = 1$. Equation (3.17) is equivalent to the equation

$$D = \lim_{n \to \infty} \sum_{k=0}^{n} \int_{-1/2}^{1/2} v(x) v(x_k) dx - \frac{1}{2} \int_{-1/2}^{1/2} v^2(x) dx \tag{3.24}$$

where we have taken $x = x_0$. Note that the integration is performed over the *invariant density* $\rho^*(x)$ and one could show that it is unity for the Bernoulli shift map ([10],[11]).

3.3.1 Correlation function technique

Here we present a technique for calculating the value for the diffusion coefficient for the kick strength/force given by the Bernoulli shift map $x_{n+1} = B(x_n)$ (see Eq.(3.18)). We use the definition of the two-point position autocorrelation function. The two-point position autocorrelation function is given by

$$C_k = \langle x_k x_0 \rangle \tag{3.25}$$

Then,

$$C_0 = \langle {x_0}^2 \rangle = \int_{-1/2}^{1/2} {x_0}^2 dx_0 = \frac{1}{12} \tag{3.26}$$

We also have that $x_k = B^{(k)}(x_0) = B^{(k)}(x)$, where we have taken $x = x_0$. Then, using Eq.(3.25) we can write

$$\begin{aligned} C_k &= \langle B^{(k)}(x)x \rangle = \int_{-1/2}^{1/2} B^{(k)}(x)xdx & (3.27) \\ &= \int_{-1/2}^{0} B^{(k)}(x)xdx + \int_{0}^{1/2} B^{(k)}(x)xdx \\ &= \int_{-1/2}^{0} B^{(k-1)}(B(x))xdx + \int_{0}^{1/2} B^{(k-1)}(B(x))xdx \\ &= \int_{-1/2}^{0} B^{(k-1)}\left(2x + \frac{1}{2}\right) xdx + \int_{0}^{1/2} B^{(k-1)}\left(2x - \frac{1}{2}\right) xdx & (3.28) \end{aligned}$$

Using the substitutions $u = 2x + \frac{1}{2}$ and $v = 2x - \frac{1}{2}$, and changing the limits of integration accordingly, after some algebra we get

$$\begin{aligned} C_k &= \frac{1}{4}\int_{-1/2}^{1/2} B^{(k-1)}(u)udu + \frac{1}{4}\int_{-1/2}^{1/2} B^{(k-1)}(v)vdv \\ &= \frac{1}{2}\int_{-1/2}^{1/2} B^{(k-1)}(u)udu, & (3.29) \end{aligned}$$

where we have relabelled v with u. Now for C_{k+1} using Eq.(3.27) we can write

$$C_{k+1} = \frac{1}{2}\int_{-1/2}^{1/2} B^{(k)}(u)udu = \frac{1}{2}C_k \tag{3.30}$$

Using this relation we can further write,

$$\begin{aligned} C_k &= \frac{1}{2}C_{k-1} = \left(\frac{1}{2}\right)^k C_0 \\ &= \frac{1}{12}\left(\frac{1}{2}\right)^k \end{aligned} \tag{3.31}$$

Finally, using the Green-Kubo formula (3.17), we get

$$\begin{aligned} D &= \sum_{k=0}^{\infty} C_k - \frac{1}{2}C_0 \\ &= \frac{1}{12}\sum_{k=0}^{\infty}\left(\frac{1}{2}\right)^k - \frac{1}{24} \\ &= \frac{1}{8} \end{aligned} \tag{3.32}$$

We see that the correlation function decays exponentially. This is a new result calculated for the first time by this method. Using different approaches, the two-point correlation function is also evaluated in [5] and [17]. Higher-order correlation functions have been considered in [4] and [5].

3.3.2 Takagi function technique

Here we derive the so-called generalised Takagi function as an alternative technique of calculating a value for the diffusion coefficient for the kick strength $x_{n+1} = B(x_n)$ (see Eq.(3.18))

Following the method outlined in [6], the summation in Eq.(3.24) can be moved inside the integral in order to define a "jump function"

$$J^n(x_0) = \sum_{k=0}^{n} v(x_k) = \sum_{k=0}^{n} x_k, \tag{3.33}$$

where $x_k = B^k(x_0)$. Due to sensitive dependence on initial conditions the function $J^n(x_0)$ will behave very irregularly for large n. Thus in order to calculate D, we need a way to control the function $J^n(x_0)$. We start by deriving a recursion formula for it. We have

$$\begin{aligned} J^n(x_0) &= \sum_{k=0}^{n} v(B^k x_0) \\ &= v(x_0) + \sum_{k=1}^{n} v(B^k x_0) \\ &= v(x_0) + J^{n-1}(B(x_0)) \end{aligned} \tag{3.34}$$

For evaluating the Green-Kubo formula, it is suitable to define a more well-behaved function $T^n(x)$ [10], such that

$$T^n(x) = \int J^n(x)dx \tag{3.35}$$

This will also help us to manipulate $T^n(x)$. Using Eqs.(3.34) and (3.35) we can derive a recursion relation for $T^n(x)$. Hence we can write

$$\begin{aligned} T^n(x) &= \int J^n(x)dx \\ &= \int \left(v(x) + J^{n-1}(B(x))\right) dx \\ &= \int v(x)dx + \int J^{n-1}(B(x))dx \\ &= \int xdx + \frac{1}{2}T^{n-1}(B(x)) \\ &= \frac{x^2}{2} + C + \frac{1}{2}T^{n-1}(B(x)) \end{aligned} \tag{3.36}$$

We define C so that $T^n(x)$ is continuous on the interval $[-1/2, 1/2]$ and $T^n(-1/2) = T^n(1/2) = 0$. In order to be able to use $T^n(x)$, we need a more user friendly recursion relation. Using Eq.(3.23) and Eq.(3.34) we see that $J^n(x)$ is satisfied by

$$J^n(x) = \begin{cases} x + J^{n-1}(2x + \frac{1}{2}) & -1/2 \leq x < 0 \\ \\ x + J^{n-1}(2x - \frac{1}{2}) & 0 \leq x < 1/2 \end{cases} \tag{3.37}$$

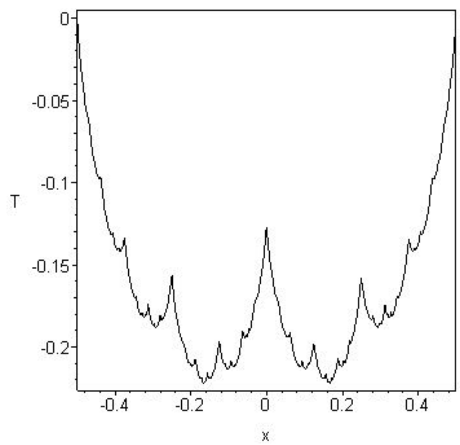

Figure 3.2: *Takagi function.* Note that the function is symmetric about the origin and converges very fast according to Eq.(3.39). Here we have taken n=10, but even for larger values of n, the graph looks the same. It is a continuous but non-differentiable function. This plot was created with Maple 9.5

Integrating the above equation we obtain a recursion relation for $T^n(x)$,

$$T^n(x) = \begin{cases} \frac{x^2}{2} + \frac{1}{2}T^{n-1}(2x + \frac{1}{2}) + C_1 & -1/2 \le x < 0 \\ \\ \frac{x^2}{2} + \frac{1}{2}T^{n-1}(2x - \frac{1}{2}) + C_2 & 0 \le x < 1/2 \end{cases} \tag{3.38}$$

Applying the condition $T^n(-1/2) = T^n(1/2) = 0$, we see that $C_1 = C_2 = -\frac{1}{8}$. Then we obtain

$$T^n(x) = \begin{cases} \frac{x^2}{2} - \frac{1}{8} + \frac{1}{2}T^{n-1}(2x + \frac{1}{2}) & -1/2 \le x < 0 \\ \\ \frac{x^2}{2} - \frac{1}{8} + \frac{1}{2}T^{n-1}(2x - \frac{1}{2}) & 0 \le x < 1/2 \end{cases} \tag{3.39}$$

We may call the function $T^n(x)$ as a *generalized Takagi funcion.* It is shown in Fig.(3.2). Letting $n \to \infty$, we assume that $T^n(x)$ converges to some limiting function $T(x)$ [10]. Using the limiting function $T(x)$ we can calculate the diffusion coefficient D. The Green-Kubo formula gives

$$\begin{aligned}
D &= \sum_{k=0}^{\infty}\int_{-1/2}^{1/2} v(x_k)v(x)dx - \frac{1}{2}\int_{-1/2}^{1/2} v^2(x)dx \\
&= \int_{-1/2}^{1/2}\sum_{k=0}^{\infty} v(x_k)v(x)dx - \frac{1}{2}\int_{-1/2}^{1/2} v^2(x)dx \\
&= \int_{-1/2}^{1/2} xJ^n(x)dx - \frac{1}{2}\int_{-1/2}^{1/2} x^2dx \\
&= [xT^n(x)]_{-1/2}^{1/2} - \int_{-1/2}^{1/2} T^n(x)dx - \frac{1}{2}\int_{-1/2}^{1/2} x^2dx \\
&= -\frac{1}{24} - \int_{-1/2}^{1/2} T^n(x)dx \qquad (3.40)
\end{aligned}$$

where the term $[xT^n(x)]_{-1/2}^{1/2}$ vanishes. We now need to compute the second term, where $n \to \infty$. Thus we have

$$\begin{aligned}
\int_{-1/2}^{1/2} T^n(x)dx &= \int_{-1/2}^{0} T^n(x)dx + \int_{0}^{1/2} T^n(x)dx \\
&= \int_{-1/2}^{0} \left(\frac{x^2}{2} - \frac{1}{8} + \frac{1}{2}T^{n-1}(2x+\frac{1}{2})\right) dx \\
&+ \int_{0}^{1/2} \left(\frac{x^2}{2} - \frac{1}{8} + \frac{1}{2}T^{n-1}(2x-\frac{1}{2})\right) dx \\
&= -\frac{1}{12} + \frac{1}{2}\left[\int_{-1/2}^{0} T^{n-1}(2x+\frac{1}{2})dx\right] \\
&+ \frac{1}{2}\left[\int_{0}^{1/2} T^{n-1}(2x-\frac{1}{2})dx\right] \qquad (3.41)
\end{aligned}$$

By assumption, $T^{n-1}(x)$ also converges to the same limiting function $T(x)$. Using the substitutions $2x + \frac{1}{2} = u$ and $2x - \frac{1}{2} = v$ and changing the limits of integration accordingly, one gets

$$\int_{-1/2}^{1/2} T^n(x)dx = -\frac{1}{12} + \frac{1}{4}\left[\int_{-1/2}^{1/2} T^{n-1}(u)du + \int_{-1/2}^{1/2} T^{n-1}(v)dv\right] \qquad (3.42)$$

Relabelling u and v with x, then the above equation is just an equation with one unknown, namely $\int_{-1/2}^{1/2} T^n(x)dx$. After some algebra one gets

$$\int_{-1/2}^{1/2} T^n(x)dx = -\frac{1}{6} \tag{3.43}$$

Finally, for the diffusion coefficient we have

$$\begin{aligned} D &= \frac{1}{6} - \frac{1}{24} \\ &= \frac{1}{8} \end{aligned} \tag{3.44}$$

This is a new result, calculated for the first time by this method. It is identical to the result (3.32).

Chapter 4

Parameter Dependence

In this chapter we consider a parameter dependence of the diffusion coefficient. We introduce a control parameter $h \in [0, 1)$ in the Bernoulli shift map (3.18) that we considered in the previous chapter. We do this in such a way that we lift the left branch by h and lower the right branch of the map by $-h$. Our goal is to derive an analytical expression for the diffusion coefficient in terms of the parameter h.

4.1 Bernoulli shift map with parameter

Let us first redefine the Bernoulli shift map in terms of the parameter h. It is defined as,

$$B_h(x) = \begin{cases} 2x + \frac{1}{2} + h & -1/2 \leq x < 0 \\ \\ 2x - \frac{1}{2} - h & 0 \leq x < 1/2 \end{cases} \tag{4.1}$$

Note that Eq.(3.18) corresponds to the case $h = 0$. After lifting the left branch by h and lowering the right branch by $-h$, Eq.(4.1) becomes,

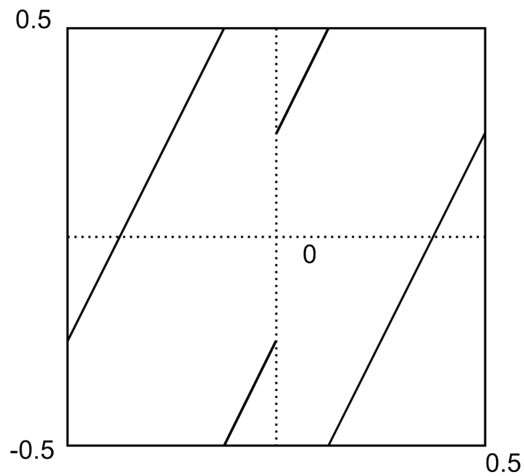

Figure 4.1: *Bernoulli shift map with parameter h.* The horizontal axis is the x axis, whereas the vertical axis is the $\tilde{B}_h(x)$ axis. The graph has four branches for any values of h∈(0,1).

$$\tilde{B}_h(x) = \begin{cases} 2x + \frac{1}{2} + h & -1/2 \le x < -h/2 \\ 2x - \frac{1}{2} + h & -h/2 \le x < 0 \\ 2x + \frac{1}{2} - h & 0 \le x < h/2 \\ 2x - \frac{1}{2} - h & h/2 \le x < 1/2 \end{cases} \tag{4.2}$$

The graph of this map is shown in Fig.(4.1).

4.2 Takagi Function with parameter

In this section we derive a generalized Takagi function with parameter h. We start by defining the velocity function for the map (4.2). Again we define it as

$$v_h(x) := x \qquad -1/2 \le x \le 1/2 \tag{4.3}$$

Using Eq.(4.2) and Eq.(4.3) we see that for the parameter dependent jump function $J_h^n(x)$ we can write,

$$J_h^n(x) = \begin{cases} x + J_h^{n-1}(2x + \frac{1}{2} + h) & -1/2 \leq x < -h/2 \\ x + J_h^{n-1}(2x - \frac{1}{2} + h) & -h/2 \leq x < 0 \\ x + J_h^{n-1}(2x + \frac{1}{2} - h) & 0 \leq x < h/2 \\ x + J_h^{n-1}(2x - \frac{1}{2} - h) & h/2 \leq x \leq 1/2 \end{cases} \tag{4.4}$$

Integrating the above equation gives the parameter dependent Takagi function in terms of constants of integration,

$$T_h^n(x) = \begin{cases} \frac{x^2}{2} + \frac{1}{2}T_h^{n-1}(2x + \frac{1}{2} + h) + c_1 & -1/2 \leq x < -h/2 \\ \frac{x^2}{2} + \frac{1}{2}T_h^{n-1}(2x - \frac{1}{2} + h) + c_2 & -h/2 \leq x < 0 \\ \frac{x^2}{2} + \frac{1}{2}T_h^{n-1}(2x + \frac{1}{2} - h) + c_3 & 0 \leq x < h/2 \\ \frac{x^2}{2} + \frac{1}{2}T_h^{n-1}(2x - \frac{1}{2} - h) + c_4 & h/2 \leq x \leq 1/2 \end{cases} \tag{4.5}$$

In order to compute the constants of integration, we use the condition that $T_h^n(-1/2) = T_h^n(1/2) = 0$ and the fact that the Takagi function above is continuous. Again, we assume that $T_h^n(x)$ and $T_h^{n-1}(x)$ converge to the same limiting function $T_h^\infty(x)$ as $n \to \infty$. For simplicity let this limiting function be just $T_h(x)$. Applying the above conditions gives the following relations:

1. $T_h(-\frac{1}{2}) = \frac{1}{8} + \frac{1}{2}T_h(h - \frac{1}{2}) + c_1 = 0$
2. $T_h(-\frac{h}{2}) = \frac{h^2}{8} + c_1$
3. $T_h(-\frac{h}{2}) = \frac{h^2}{8} + c_2$
4. $T_h(0) = \frac{1}{2}T_h(h - \frac{1}{2}) + c_2$
5. $T_h(0) = \frac{1}{2}T_h(\frac{1}{2} - h) + c_3$
6. $T_h(\frac{h}{2}) = \frac{h^2}{8} + c_3$

7. $T_h(\frac{h}{2}) = \frac{h^2}{8} + c_4$

8. $T_h(\frac{1}{2}) = \frac{1}{8} + \frac{1}{2}T_h(\frac{1}{2} - h) + c_4 = 0$

After some easy algebra we find that

$$c_1 = c_2 = c_3 = c_4 = -\frac{1}{8} - \frac{1}{2}T_h\left(\frac{1}{2} - h\right) \tag{4.6}$$

Note that $T_h(\frac{1}{2} - h)$, by assumption, is a limiting function of $T_h^{n-1}(\frac{1}{2} - h)$ as $n \to \infty$, and the same applies to $T_h(h - \frac{1}{2})$. Substituting the values of the constants in Eq.(4.5), then the Takagi function becomes,

$$T_h(x) = \begin{cases} \frac{x^2}{2} + \frac{1}{2}T_h(2x + \frac{1}{2} + h) - \frac{1}{8} - \frac{1}{2}T_h(\frac{1}{2} - h) & -1/2 \leq x < -h/2 \\ \frac{x^2}{2} + \frac{1}{2}T_h(2x - \frac{1}{2} + h) - \frac{1}{8} - \frac{1}{2}T_h(\frac{1}{2} - h) & -h/2 \leq x < 0 \\ \frac{x^2}{2} + \frac{1}{2}T_h(2x + \frac{1}{2} - h) - \frac{1}{8} - \frac{1}{2}T_h(\frac{1}{2} - h) & 0 \leq x < h/2 \\ \frac{x^2}{2} + \frac{1}{2}T_h(2x - \frac{1}{2} - h) - \frac{1}{8} - \frac{1}{2}T_h(\frac{1}{2} - h) & h/2 \leq x \leq 1/2 \end{cases} \tag{4.7}$$

4.3 Diffusion Coefficient $D(h)$

Having derived the parameter dependent Takagi function, we can proceed to derive an analytical expression for the diffusion coefficient as a function of the parameter h. One could show that the invariant density for the map (4.2) is unity for all $0 \leq h \leq 1$. This is related to the fact that the invariant density for the Bernoulli shift map ($x_{n+1} = 2x \pmod 1$) is unity which is recovered for $h = 0$ and $h = 1$. Also this is based on the fact that in (4.2) there exist full branches, in the sense that after lifting and lowering by h and $-h$, respectively, we don't loose any part of the two branches or we don't create new ones (see Fig.4.1). This will greatly simplify our calculation of the diffusion coefficient in using the Green-Kubo formula (3.17). Thus we can write,

$$\begin{aligned}
D(h) &= \int_{-1/2}^{1/2} v_h(x) J_h^n(x) dx - \frac{1}{2}\int_{-1/2}^{1/2} v_h^2(x) dx \\
&= \int_{-1/2}^{1/2} x J_h^n(x) dx - \frac{1}{2}\int_{-1/2}^{1/2} x^2 dx \\
&= [x T_h^n(x)]_{-1/2}^{1/2} - \int_{-1/2}^{1/2} T_h^n(x) dx - \frac{1}{2}\int_{-1/2}^{1/2} x^2 dx \\
&= -\int_{-1/2}^{1/2} T_h^n(x) dx - \frac{1}{24} \qquad (4.8)
\end{aligned}$$

where the term $[xT_h^n(x)]_{-1/2}^{1/2}$ vanishes. Our next task is to evaluate $\int_{-1/2}^{1/2} T_h^n(x)dx$. It can be written as,

$$\begin{aligned}
\int_{-1/2}^{1/2} T_h^n(x) dx &= \int_{-1/2}^{-h/2} T_h^n(x) dx + \int_{-h/2}^{0} T_h^n(x) dx \\
&+ \int_{0}^{h/2} T_h^n(x) dx + \int_{h/2}^{1/2} T_h^n(x) dx \qquad (4.9)
\end{aligned}$$

Evaluating each of the four integrals separately, where we use Eq.(4.7), gives

$$\begin{aligned}
\int_{-1/2}^{-h/2} T_h^n(x) dx &= -\frac{h^3}{48} - \frac{1}{24} + \frac{h}{16} + \frac{h}{4} T\left(h - \frac{1}{2}\right) - \frac{1}{4} T\left(h - \frac{1}{2}\right) \\
&+ \frac{1}{2}\int_{-1/2}^{-h/2} T(2x + \frac{1}{2} + h) dx \\
&= \frac{-h^3}{48} - \frac{1}{24} + \frac{h}{16} + \frac{h}{4} T(h - \frac{1}{2}) \\
&- \frac{1}{4} T\left(h - \frac{1}{2}\right) + \frac{1}{4}\int_{-1/2+h}^{1/2} T(u) du \qquad (4.10)
\end{aligned}$$

where we have used the substitution $u = 2x + \frac{1}{2} + h$ and changed the limits of integration accordingly. We do the same with other three integrals. For the second integral we get,

$$\int_{-h/2}^{0} T_h^n(x)dx = -\frac{h^3}{48} - \frac{h}{16} - \frac{h}{4}T\left(h - \frac{1}{2}\right) + \frac{1}{4}\int_{-1/2}^{-1/2+h} T(v)dv \quad (4.11)$$

where we have used the substitution $v = 2x - \frac{1}{2} + h$. For the third and the fourth integral we use the substitutions $w = 2x + \frac{1}{2} - h$ and $z = 2x - \frac{1}{2} - h$, respectively. Thus we get,

$$\int_{0}^{h/2} T_h^n(x)dx = \frac{h^3}{48} - \frac{h}{16} - \frac{h}{4}T\left(h - \frac{1}{2}\right) + \frac{1}{4}\int_{1/2-h}^{1/2} T(w)dw \quad (4.12)$$

and

$$\int_{h/2}^{1/2} T_h^n(x)dx = -\frac{h^3}{48} - \frac{1}{24} + \frac{h}{16} - \frac{1}{4}T\left(h - \frac{1}{2}\right) + \frac{h}{4}T\left(h - \frac{1}{2}\right) + \frac{1}{4}\int_{-1/2}^{1/2-h} T(z)dz \quad (4.13)$$

Substituting Eqs.(4.10), (4.11), (4.12) and (4.13) in Eq.(4.9) gives,

$$\begin{aligned}\int_{-1/2}^{1/2} T_h(x)dx &= \frac{1}{4}\left[\int_{-1/2}^{-1/2+h} T(v)dv + \int_{-1/2+h}^{1/2} T(u)du\right] \\ &+ \frac{1}{4}\left[\int_{-1/2}^{1/2-h} T(z)dz + \int_{1/2-h}^{1/2} T(w)dw\right] \\ &- \frac{1}{12} - \frac{1}{2}T\left(h - \frac{1}{2}\right) \\ &= \frac{1}{2}\int_{-1/2}^{1/2} T_h(x)dx - \frac{1}{12} - \frac{1}{2}T\left(h - \frac{1}{2}\right) \quad (4.14)\end{aligned}$$

Finally, this gives

$$\int_{-1/2}^{1/2} T_h^n(x)dx = -\frac{1}{6} - T_h^{n-1}\left(h - \frac{1}{2}\right) \quad (4.15)$$

where $n \to \infty$. Substituting this into Eq.(4.8) we obtain the analytical expression for $D(h)$,

$$
\begin{aligned}
D(h) &= -\left(-\frac{1}{6} - T_h^{n-1}\left(h - \frac{1}{2}\right)\right) - \frac{1}{24} \\
&= \frac{1}{8} + T_h^{n-1}\left(h - \frac{1}{2}\right)
\end{aligned}
\tag{4.16}
$$

Deriving, for the first time, this exact, analytical formula for the diffusion coefficient in terms of a control parameter was the main goal of this thesis.

Using the above formula and Eq.(4.7) we see that when $h = 0$ and $h = 1$, $D(0) = D(1) = \frac{1}{8}$, which means that for these values of h our previous result $D = \frac{1}{8}$ from Chapter 3 is recovered. A very surprising result is when $h = \frac{1}{2}$. This gives $D\left(\frac{1}{2}\right) = 0$. This simply means that at this value of h there is no diffusion!

Chapter 5

Conclusion and outlook

In this thesis the stochastic Langevin equation has been studied first. This equation was solved by calculating the mean square displacement (msd) and deriving the autocorrelation velocity function for a Brownian particle. Depending on the value of time t, two different explicit expressions for the msd were derived. Then we made a transition to a deterministic Langevin equation. This was done by replacing the randomness in the stochastic Langevin equation by a deterministic chaotic force. For the over-damped case, this equation was solved by deriving a recurrence relation. This setup enabled us to calculate, for the first time, a value for the diffusion coefficient D for the deterministic Langevin dynamics where the Bernoulli shift map on the interval [-1/2,1/2] generates the kicks . Two different techniques were used: the Takagi function technique and the correlation function technique. They both gave the same result. This result does not represent a simple random walk, because the correlation function decays exponentially. Finally, we derived a parameter dependent Takagi function with parameter h. This helped us to derive, again for the first time, an exact formula for the diffusion coefficient as a function of the control parameter h.

For further study, one could plot $D(h)$ in order to see more closely how the diffusion coefficient varies with h in the interval [0,1]. In addition, one could explain, numerically or analytically, the result $D\left(\frac{1}{2}\right) = 0$ obtained in section 4.3. This is a very surprising result and does not seem to have a trivial explanation.

APPENDIX

Dirac delta function

The Dirac delta function is a very convenient "function". More exactly it is the limiting case of a family of functions [16]. It has the property of singling out a particular value of a function $f(t)$ at a value $t = t_0$. The function is characterised by the following properties

$$\delta(t - t_0) = \begin{cases} 0 & t \neq t_0 \\ \infty & t = t_0 \end{cases} \tag{1}$$

in such a way that, for any $\epsilon > 0$,

$$\int_{t_0+\epsilon}^{t_0-\epsilon} \delta(t - t_0) dt = 1 \tag{2}$$

which means that the function $\delta(t - t_0)$ has a very sharp peak at $t = t_0$, but the area under the peak is unity. Given any smooth function $f(t)$, one has

$$\int_p^q f(t)\delta(t - t_0)dt = f(t_0) \int_p^q \delta(t - t_0) \tag{3}$$

since $\delta(t - t_0) \neq 0$ only when $t = t_0$, and there $f(t) = f(t_0)$. Hence

$$\int_p^q f(t)\delta(t - t_0)dt = \begin{cases} f(t_0) & if \quad p < t_0 < q \\ 0 & otherwise \end{cases} \tag{4}$$

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