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DETERMINISTIC BROWNIAN MOTION

DISSERTATION

Presented to the Graduate Council of the
University of North Texas in Partial
Fulfillment of the Requirements

For the Degree of

DOCTOR OF PHILOSOPHY

By

György Trefán, B.S.

Denton, Texas

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The goal of this thesis is to contribute to the ambitious program of the foundation of developing statistical physics using chaos. We build a deterministic model of Brownian motion and provide a microscopic derivation of the Fokker-Planck equation. Since the Brownian motion of a particle is the result of the competing processes of diffusion and dissipation, we create a model where both diffusion and dissipation originate from the same deterministic mechanism – the deterministic interaction of that particle with its environment.

We show that standard diffusion which is the basis of the Fokker-Planck equation rests on the Central Limit Theorem, and, consequently, on the possibility of deriving it from a deterministic process with a quickly decaying correlation function. The sensitive dependence on initial conditions, one of the defining properties of chaos insures this rapid decay.

We carefully address the problem of deriving dissipation from the interaction of a particle with a fully deterministic nonlinear bath, that we term the booster. We show that the solution of this problem essentially rests on the linear response of a booster to an external perturbation. This raises a long-standing problem concerned with Kubo's Linear Response Theory and the strong criticism against it by van Kampen. Kubo's theory is based on a perturbation treatment of the Liouville equation, which, in turn, is expected to be totally equivalent to a first-order perturbation treatment of single trajectories. Since the boosters are chaotic, and chaos is essential to generate diffusion, the single trajectories are highly unstable and do not respond linearly to weak external perturbation.

We adopt chaotic maps as boosters of a Brownian particle, and therefore address the problem of the response of a chaotic booster to an external perturbation. We notice that a fully chaotic map is characterized by an invariant measure which is a continuous function of the control parameters of the map. Consequently if the external perturbation is made to act on a control parameter of the map, we show that the booster distribution undergoes slight modifications as an effect of the weak external perturbation, thereby leading to a linear response of the mean value of the perturbed variable of the booster. This approach to linear response completely bypasses the criticism of van Kampen.

The joint use of these two phenomena, diffusion and friction stemming from the interaction of the Brownian particle with the same booster, makes the microscopic derivation of a Fokker-Planck equation and Brownian motion, possible.

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CHAPTER 1

INTRODUCTION

Statistical physics addresses the problem of deriving the macroscopic properties of matter from microscopic properties. One of the most difficult problems is that of macroscopic irreversibility versus microscopic reversibility, i.e., how one can derive diffusion, relaxation to equilibrium and other irreversible phenomena from interactions of atoms, molecules or other particles when the interactions are described by the fundamental reversible laws of classical or quantum mechanics.

The first partial solution for the problem of reversibility-irreversibility was proposed by Boltzmann (Boltzmann 1912) who, although he wanted to avoid, made an additional assumption – the assumption of non-decreasing entropy in an isolated physical system, which lead to relaxation and consequently to irreversibility.

Boltzmann's idea – in spite of being decades ahead of the scientific knowledge of his contemporaries – contained the unnecessary assumption on the non-decreasing entropy. This assumption was eliminated by Langevin (Langevin 1908) who assumed an interaction between the system of interest and its environment. In this model the environment acts upon the system with a random force and the system of interest dissipates energy to the environment. The fluctuation and dissipation lead the evolution of the system to equilibrium and consequently irreversibility for arbitrary initial condition.

Although Langevin did not assume entropy in his model he introduced a random force which is a sophisticated way of saying "I do not know the mechanism but I can describe the reality well enough". Although stochastic theories are mathematically refined and elegant, from the point of view of a fundamental physical theory

the introduction of a random force is no better than a purely thermodynamical and therefore phenomenological fluctuation-dissipation theory which was developed earlier by Einstein (Einstein 1905, 1906).

Thus the idea of a stochastic environment had to be replaced with a deterministic environment. Nakijama, Mori and Zwanzig worked out a quantum mechanics-like formalism (Nakijama 1958, Mori 1965, Zwanzig 1960) where they considered a system of interest coupled to the environment which had infinitely many degrees of freedom. They used a projection technique to derive the motion of the system of interest. Their theory has the following, not well established assumptions: the environment of the systems they investigate has an infinite number of degrees of freedom, is described by linear differential equations and the environment is placed initially in thermal equilibrium (statistical assumption) i.e. the energy of the environment follows the Maxwell-Boltzmann distribution from the initial moment of its evolution. These three assumptions are not well justified because one finds relaxation in mesoscopic systems too, although they do not have nearly infinitely many degrees of freedom. Furthermore in a conservative system described by linear differential equations of motion the energy remains confined in the original distribution and does not move from one normal mode to another, thereby preventing the system from relaxing to the equilibrium state in which all modes have the same energy. Finally we want to derive statistical properties from the system dynamics rather than assuming them as an initial condition.

There is a different approach to irreversibility phenomena than the one described and it was proposed by Fermi. Fermi realized that in a conservative system described by linear differential equations of motion one will not find relaxation phenomena. Thus, Fermi, Ulam and Pasta (Fermi et al. 1955) numerically studied a nonlinear system hoping to find relaxation to equilibrium but instead they found a

robust periodicity with soliton solutions and no relaxation. By this attempt Fermi showed that the nonlinearity itself is not sufficient for a conservative physical system to reach equilibrium. The necessary and sufficient condition for a conservative physical system to reach equilibrium is for it to be a mixing system as was proved by Krylov (Krylov 1950). Mixing systems are better known to physicist as a kind of chaotic system thus the idea that the foundation of statistical mechanics for classical systems should rest on chaos (Ford et al. 1963, Arnold et al. 1968, Ehrenfest 1959, Ford 1975) gradually emerged and still has not been universally accepted.

The goal of this thesis is to contribute to the ambitious program of the foundation of statistical physics. We attempt to build up a model of Brownian motion (Brown 1826) which is an important system from the point of view of irreversibility. Since Brownian motion is the result of the competing processes of diffusion and dissipation, we have to create a model where both diffusion and dissipation originate from the same deterministic mechanism – the interaction of a particle with its environment. The particle which interacts with its environment is described by the following differential equations

$$\dot{v} = x, \tag{1.1}$$

and

$$\dot{x} = R(x, -\Delta^2 v(t), \dots). \tag{1.2}$$

Above (1.1) is the Newton equation of motion of the particle since the velocity v of the particle changes according to the force of the environment represented by variable x .

(1.2) is the equation of motion of the environment, where R represents a set of

functions, the term $-\Delta^2 v(t)$ represents the reaction of the particle on the environment (negative feedback) with the reaction coefficient Δ and the dots indicate that the motion of the environment can depend on variables other than x and v .

The differential equations (1.1 – 2) show that when the particle does not react on its environment i.e., $\Delta = 0$, then the environment continuously gives energy to the particle in a random way, thus diffusion with no dissipation takes place. This process is explained in details in Chapter 2, where we use a discrete time representation of (1.1 – 2), for instance the environment is mimicked by a chaotic map. Chaotic maps are deterministic systems so the diffusion we obtain is termed as deterministic diffusion.

When the particle reacts on its environment i.e., v is very large and $\Delta \neq 0$, but weak, then (1.2) immediately yields

$$\langle x(t) \rangle_{eq} = -\chi \Delta^2 \langle v(t) \rangle_{eq} . \quad (1.3)$$

(1.3) shows that in this case the environment rearranges itself in a way that compensates for the action caused in the environment by the Brownian particle. In other words the environment responds to the perturbation, where the average response linearly depends on the velocity, the reaction parameter Δ and coefficient χ , the generalized susceptibility. Thus as we shall show, the reaction of the Brownian particle on its environment is intimately related to Linear Response Theory. We use maps to mimic the dynamics of the environment, so we have to investigate how chaotic maps respond to external perturbations. Linear Response Theory for chaotic maps is the subject of Chapter 3.

The Linear Response Theory for chaotic maps presented in Chapter 3 is the counterpart of Kubo's conventional Linear Response Theory (Kubo 1957). The lat-

ter theory is based on a first-order perturbative treatment of the Liouville equation. Since the evolution of the distribution of chaotic maps is given by the Frobenius operator, the Linear Response Theory for chaotic maps is a first-order perturbation calculation on the Frobenius operator and it recovers Kubo's formula i.e., the susceptibility is related to the equilibrium cross-correlation function of an observable of the unperturbed map and the perturbation variable.

As we mentioned above the conventional theory of Kubo is basically a perturbative treatment of the Liouville equation which is equivalent to the perturbation of single trajectories. Since the trajectories of chaotic systems are unstable, it was thought by van Kampen (van Kampen 1971) that a first-order perturbation treatment is inadequate. Applying Kubo's treatment to maps one faces the same problem as in the case of continuous-time systems i.e., using a first-order perturbation treatment on the Frobenius operator means perturbation of single trajectories. To satisfy the criticisms of van Kampen we adopt a geometrical argument and we build up the Geometrical Linear Response Theory for chaotic maps in Chapter 4.

In Chapter 5 we combine the deterministic diffusion and dissipation, first using a phenomenological dissipation in (1.1 – 2) so that they become the following Langevin equation

$$\dot{v} = x - \gamma v, \quad (1.4)$$

and

$$\dot{x} = R(x, \dots). \quad (1.5)$$

In the above Langevin equation, instead of the stochastic environment (1.5) we use a deterministic, chaotic environment mimicked by the logistic map. The appearance

of phenomenological dissipation is not satisfactory, because a self consistent theory should provide both diffusion and dissipation from the same mechanism, namely the particle-environment interaction as it is given by (1.1 – 2). Thus in the rest of Chapter 5 we realize (1.1 – 2) by a discrete time representation, actually by a 2 dimensional map. The map we present recovers the standard results of the Brownian motion within the framework of a completely deterministic and self consistent model.

CHAPTER 2

DETERMINISTIC DIFFUSION

As we mentioned in the *Introduction* the main goal of this dissertation is to build up a self-contained picture of Brownian motion, without using statistical assumptions, namely from rigorously deterministic equations of motion.

Brownian motion is the result of a dynamical balance between two competing processes, diffusion and dissipation. Therefore, an exhaustive treatment of Brownian motion forces us to investigate both diffusion and friction. In this chapter we focus on diffusion, and, to keep our promise of avoiding statistical assumptions, on deterministic diffusion.

Diffusion, according to traditional wisdom is a genuinely stochastic process, which emerges when a physical variable collects uncorrelated, random actions. There is, however, a wide class of deterministic systems, the chaotic systems, which are reminiscent of random systems in certain aspects. Thus we also expect the appearance of diffusion in certain chaotic systems. This is what we do in this Chapter, namely, we address the problem of diffusion in deterministic, chaotic systems, for the purpose of deriving an analytical expression for the quantity defining the diffusion strength, the so-called diffusion coefficient. For any system under study we shall derive the analytical expression of the corresponding diffusion coefficient.

In understanding diffusion the Central Limit Theorem is of primary importance. Thus we review it in §2.1 and give a physical example of how diffusion emerges when a velocity is coupled to a chaotic environment represented by the logistic map.

In §2.2 we present a less restrictive version of the Central Limit Theorem and

again we give a physical example of how diffusion emerges in the standard map with short correlation time and how one can calculate the diffusion coefficient using the characteristic function technique. In §2.3 we study diffusion for the standard map using a different formalism, i.e., the Zwanzig projection technique.

Diffusion occurs not only in 2-dimensional area preserving maps, but also in 1-dimensional, chaotic maps. This is what we study in §2.4. We derive the diffusion coefficient from dynamical considerations and by using the Frobenius operator to determine the invariant density of the map, i.e., the equilibrium probability density.

§2.1 The Central Limit Theorem

Remark 2.1.1. As we mentioned above the Central Limit Theorem is of paramount importance in understanding diffusion. Therefore first we cite and prove it following the standard procedure (Gnedenko and Khinchin 1962, Bass 1966, Rozanov 1969). Then we give a physical example of deterministic diffusion. In this example the velocity is the collector or integrator variable which is coupled to a chaotic environment. The chaotic environment is represented by the logistic map. In this example we show that the velocity has a Gaussian distribution whose width grows linearly in time.

Proposition 2.1.1. If

- i) we consider the random variables $x_1, x_2, \dots, x_n$
- ii) which are mutually independent,
- iii) have the same mean value $\langle x_j \rangle = 0$, where the symbol $\langle \dots \rangle$ denotes the averaging over an ensemble of realizations

iv) have the same standard deviation $\sqrt{\langle x_j^2 \rangle} = D$,
 v) and have the same ensemble distribution $p(x_j)$ which vanishes quickly as $|x_j| \rightarrow \infty$
 then

the quantity

$$v_n = \frac{1}{\sqrt{n}} \cdot (x_1 + x_2 + \dots + x_n) \quad (2.1.1)$$

• is normally distributed or more precisely the probability that the sum (2.1.1) is less than vD is

$$\lim_{n \rightarrow \infty} P\left(\frac{v_n}{D} \leq v\right) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^v \exp(-t^2/2) dt \quad (2.1.2)$$

Proof. The characteristic function of v_n is defined

$$\begin{aligned} \Phi(v_n) &= \langle \exp(-ikv_n) \rangle = \langle \exp(-ik(x_1 + x_2 + \dots + x_n))/\sqrt{n} \rangle \\ &= \langle \prod_{j=1}^n \exp(-ikx_j/\sqrt{n}) \rangle = \prod_{j=1}^n \langle \exp(-ikx_j/\sqrt{n}) \rangle \\ &= \exp\left(\sum_{j=1}^n A_j(k)\right), \end{aligned} \quad (2.1.3)$$

where

$$A_j(k) = \ln \langle \exp(-ikx_j/\sqrt{n}) \rangle. \quad (2.1.4)$$

Since n is large we expand $A_j(k)$ in Taylor series with respect to k around $k = 0$ and we get

$$A_j(k/\sqrt{n}) \simeq A_j(0) + kA'_j(0) + \frac{k^2}{2}A''_j(0) + \frac{k^3}{n}O(n^{-1/2}). \quad (2.1.5)$$

From the definition (2.1.4) of $A_j(k)$ one sees that $A_j(0) = 0$. The first order term $kA'_j(0)$ vanishes too because

$$\frac{d}{dk}A_j(k)|_{k=0} = \frac{-i}{\sqrt{n}} \langle x_j \rangle = 0. \quad (2.1.6)$$

The second order term $(k^2/2)A''_j(0) = -(k^2/2n)D^2$ because

$$\frac{d^2}{dk^2}A_j(k)|_{k=0} = \frac{i}{\sqrt{n}} \langle x_j \rangle + \frac{i^2}{n} \langle x_j^2 \rangle = -\frac{1}{n} \langle x_j^2 \rangle = -\frac{1}{n}D^2. \quad (2.1.7)$$

So the characteristic function of v_n becomes

$$\langle \exp(-ikv_n) \rangle = \exp\left(-ik^2 \frac{D^2}{n} + O\left(\frac{1}{\sqrt{n}}\right)\right). \quad (2.1.8)$$

Introducing the notation

$$\sigma^2 = \frac{D^2}{n} = \frac{1}{n} \sum_{j=1}^n \langle x_j^2 \rangle \quad (2.1.9)$$

the characteristic function becomes

$$\Phi(v_n) = \exp\left(-\frac{1}{2}k^2\sigma^2 + O\left(\frac{1}{\sqrt{n}}\right)\right). \quad (2.1.10)$$

By neglecting the term $O(1/\sqrt{n})$ one can see the characteristic function is bell-shaped with width $\sigma/\sqrt{2}$. After inverse Fourier transformation of $\Phi(v_n)$ the quantity v_n has a normal distribution according to (2.1.2).

q.e.d.

Remark 2.1.2. In the following *Proposition 2.1.1* we show an example for the application of the Central Limit **Theorem** to a physical system. We consider a model

system where the velocity of a free particle is coupled to a chaotic environment. The chaotic environment acts upon the velocity but the velocity does not react back on the environment. The chaotic environment causes abrupt changes in the velocity i.e., the particle is periodically kicked. The chaotic environment is mimicked by zero centered logistic maps. We note here that the logistic map is one of the most studied map (Ulam and Neumann 1947, May 1976, Feigenbaum 1978, Collet and Eckmann 1980, Eckmann and Ruelle 1985, Schuster 1988).

We now plan to study a model resulting in the diffusion of a variable v , which can be thought of as being the velocity of the Brownian particle. This is the variable under observation. Thus we shall refer to it as the *variable of interest*. The variable x determines the time evolution of the variable of interest, under the form of abrupt changes, or boosts. Thus we shall refer to it as the *booster variable*. Throughout the whole thesis we shall use the term booster to denote a new kind of bath, one that is: deterministic and chaotic, and has only a few degrees of freedom. To keep the booster distinct from conventional baths, which are characterized by infinitely many degrees of freedom, and are in well defined thermodynamical states, as a result of an assumption, rather than of a genuinely microscopic and deterministic dynamics.

Proposition 2.1.1. If

i) we consider a free particle whose velocity is constant for a time but at the end of each time interval the velocity abruptly changes from the value v_n to v_{n+1}

$$v_{n+1} = v_n + x_n, \quad (2.1.11)$$

ii) where the change of the velocity is determined by a sequence of numbers $x_1, x_2, \dots, x_n$ originates from the zero centered logistic map

$$x_{n+1} = 1 - 2x_n^2, \quad (2.1.12)$$

then

- after n iteration the distribution of the variable v_n is

$$p(v_n) = \frac{1}{\sqrt{\pi n}} \exp\left(-\frac{v_n^2}{n}\right). \quad (2.1.13)$$

and

- the variance of the velocity of the kicked particles is linear in time

$$\langle v_n^2 \rangle = n \langle x_j^2 \rangle = n/2. \quad (2.1.14)$$

Proof. As we showed in *Proposition A2.6, Appendix 2* recursive application of the zero centered logistic map (2.1.12) provides a δ -correlated sequence of numbers

$$\langle x_j x_0 \rangle = \langle x_j^2 \rangle \delta_{j,0} \quad (2.1.15)$$

i.e., the numbers $x_1, x_2, \dots, x_n$ are mutually independent. They also have zero mean value

$$\langle x_j \rangle = 0, \quad (2.1.16)$$

and their standard deviation is constant

$$\langle x_j^2 \rangle = 1/2, \quad (2.1.17)$$

and their probability density vanishes as $|x_j| \rightarrow \infty$ i.e.,

$$\lim_{|x_j| \rightarrow \infty} p(x_j) = 0. \quad (2.1.18)$$

Thus they fulfill the requirement of the Central Limit Theorem. In our case the variable of interest v is the collector (integrator) variable. The Central Limit Theorem states about the variable of interest v that it has a Gaussian distribution according to

$$p(v_n) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{v_n^2}{2\sigma^2}\right), \quad (2.1.19)$$

where

$$\sigma^2 = n \langle x_j^2 \rangle. \quad (2.1.20)$$

Substituting (2.1.20) and (2.1.17) into (2.1.19) we obtain

$$p(v_n) = \frac{1}{\sqrt{2\pi n \langle x_j^2 \rangle}} \exp\left(-\frac{v_n^2}{2n \langle x_j^2 \rangle}\right) = \frac{1}{\sqrt{\pi n}} \exp\left(-\frac{v_n^2}{n}\right). \quad (2.1.21)$$

We can calculate the evolution of the variance of the variable of interest from the definition of the second moment i.e., from

$$\langle v_n^2 \rangle = \int_{-\infty}^{\infty} p(v_n) dv_n. \quad (2.1.22)$$

Substituting (2.1.21) into (2.1.22) we end up with (2.1.14).

q.e.d.

Remark 2.1.3. A computer program realized the equations (2.1.11 – 12). In the calculations all variables of interest are initially set to 0 i.e., $v_0 = 0$, and the booster

variable is initially distributed uniformly over the interval $[-1, 1]$. The iterations were executed for 100 steps i.e., $n = 100$ and the final distribution of variable v_{100} was calculated over 50,000 samples. The distribution obtained by the numerical calculations and the one calculated from (2.1.13) are presented in *Figure 2.1.1*.

Figure 2.1.1. The distribution of the velocity v of map (2.1.11 – 12) for 100 iterations. The circles show the results of numerical calculations which are compared to the theoretical results (solid line) given by (2.1.13).

A computer program calculated the diffusion of the velocity based on equations (2.1.11 – 12). In the calculations all variables of interest were initially set to 0 i.e., $v_0 = 0$, and the booster variable was initially distributed uniformly over the interval $[-1, 1]$. The iteration was executed for 1,000 steps i.e., $n = 1,000$, and

the evolution of the variance was calculated over 10,000 samples. The evolution obtained by numerical calculations and the one calculated from equation (2.1.14) are presented in *Figure 2.1.2*.

Figure 2.1.2. The evolution of the variance $\langle v_n^2 \rangle$ of the velocity of map (2.1.11 – 12) for 1,000 iterations. The circles show the results of numerical calculations which are compared to the theoretical results given by (2.1.14).

Definition 2.1.1. In the example above one can see that the individual trajectories of velocity v evolve in a random-like manner, but the average value of the variance of the velocity is proportional to the discrete time n . In this case a *diffusion* of the velocity takes place. The diffusion of the velocity is described by a *diffusion coefficient* D which is defined as follows

$$D = \left\langle \lim_{n \rightarrow \infty} \frac{1}{2n} (v_n - v_0)^2 \right\rangle, \quad (2.1.23)$$

where v_0 is the initial value of variable v and v_n denotes the value of variable v at time n .

Remark 2.1.4. Note that the diffusion is intimately connected to the Central Limit Theorem. Whenever a diffusion process takes place, we can consider the diffusive variable as an accumulation of random or chaotic events with finite correlation time. The variance of the diffusive variable is proportional to the time and its distribution function is Gaussian. On the other side when we find anomalous diffusion i.e., when the evolution of the variance of the diffusive variable is not linear in time, it is an indication that the Central Limit Theorem breaks down for some reasons, for instance the booster variable has infinite correlation time.

§2.2 Deterministic Diffusion in Area Preserving Maps

In this paragraph we first show that there are less restrictive ways than shown in §2.1 of stating and proving the Central Limit Theorem. Then we show how one can derive the diffusion coefficient when the chaotic environment is characterized by a definite, not too long correlation time. Finally we show using the example of the standard map in its chaotic regime how one can derive the diffusion coefficient using the characteristic function technique.

Remark 2.2.1. The way we stated the Central Limit Theorem is too restrictive.

We can use less restrictive assumptions and at the same time we the Central Limit Theorem. We can ease the assumptions on several points.

i) The random numbers x_i -s do not need to have zero mean value. With nonzero mean values we get a “drift” in the variable v , i.e., the mean value of v increases linearly with time. With the deduction of the drift the Central Limit Theorem is easily proved.

ii) The random numbers x_i -s should not necessarily have the same distribution $p(x_j)$. For instance let us consider a sequence of random numbers where the random numbers with odd indices have one distribution $p_1(x_{2j+1})$ with standard deviation $\sqrt{\langle x_{2j+1}^2 \rangle} = D$ and the random numbers with even indices have another distribution $p_2(x_{2j}) \neq p_1(x_{2j+1})$ although their standard deviations is the same $\sqrt{\langle x_{2j+1}^2 \rangle} = \sqrt{\langle x_{2j}^2 \rangle} = D$. The Central Limit Theorem holds true for the random numbers with odd indices and separately for the random numbers with even indices and trivially for their comb-like combinations.

iii) we can ease the assumption of mutual independence and still prove the Central Limit Theorem. We prove this in the following proposition.

Proposition 2.2.1. If the impulse map reads

$$\begin{aligned} v_{n+1} &= v_n + x_n \\ x_{n+1} &= f(x_n), \end{aligned} \tag{2.2.1}$$

where $f(x_n)$ is a map with a dynamics of finite correlation time τ , then

- the variable v is diffusive and
- its diffusion coefficient D is equal to half the product of the variance $\langle x_j^2 \rangle$ and the correlation time τ

$$D = \frac{1}{2} \langle x_j^2 \rangle \tau. \quad (2.2.2)$$

Proof. The diffusion coefficient of variable v is, according to *Definition 2.1.1*,

$$D = \left\langle \lim_{n \rightarrow \infty} \frac{1}{2n} (v_n - v_0)^2 \right\rangle, \quad (2.2.3)$$

where v_0 is the initial value of variable v and v_n is its value after n iteration of the map (2.2.1). The difference $v_n - v_0$ can be written in terms of the difference in consecutive velocities $\Delta v_i = v_i - v_{i-1}$ as $v_n - v_0 = \sum_{i=1}^n \Delta v_i$. So the diffusion coefficient (2.2.3) becomes

$$D = \frac{1}{2} \left\langle \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n \sum_{j=1}^n \Delta v_i \Delta v_j \right\rangle. \quad (2.2.4)$$

We want to reduce the double sum in the expression of the diffusion coefficient so we rewrite it in the form

$$D = \frac{1}{2} \left\langle \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n \sum_{j=1-i}^{n-i} \Delta v_i \Delta v_{i+j} \right\rangle. \quad (2.2.5)$$

The velocities jump Δv_i is caused by the booster, namely $\Delta v_i = x_i$. Thus we can express (2.2.5) in terms of the x_i 's. The booster is chaotic in a way that the variable x has a finite correlation time. Thus we can express the sum over j in (2.2.5) with, Δv_i replaced by x_i , from $n = -\infty$ to $n = \infty$. Thus the diffusion coefficient (2.2.5) takes the form

$$D = \frac{1}{2} \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=1}^n \sum_{j=-\infty}^{\infty} \langle x_i x_{i+j} \rangle. \quad (2.2.6)$$

Since the booster is ergodic the ensemble average over i can be replaced by a single time average

$$D = \frac{1}{2} \sum_{j=-\infty}^{\infty} \langle x_i x_{i+j} \rangle. \quad (2.2.7)$$

Note that the correlation time τ of the booster is defined as

$$\tau = \frac{\sum_{j=-\infty}^{\infty} \langle x_i x_{i+j} \rangle}{\langle x_i x_i \rangle}. \quad (2.2.8)$$

Substituting this expression into (2.2.7) we end up with equation (2.2.2).

q.e.d.

Remark 2.2.2. The impulse maps (2.1.11) and (2.2.1) that we have been dealing with so far were not derived from autonomous systems. The real challenge is to derive diffusion in Hamiltonian systems. Since a 1-dimensional Hamiltonian system often is represented by a 2-dimensional area-preserving map, i.e., by a map whose Jacobian $J = 1$, we investigate the possibility of diffusion in a 2-dimensional area-preserving map. One of the most widely discussed 2-dimensional maps is the standard map

$$\begin{aligned} v_{n+1} &= v_n + K \sin(x_n) \\ x_{n+1} &= x_n + v_{n+1}. \end{aligned} \quad (2.2.9)$$

It was observed that for certain values of the control parameter K the standard map is chaotic (Chirikov 1979). For very large values of the control parameter K the correlation time of variable x is practically unity, i.e., the variable x in its evolution loses memory in a single step. **In this case** diffusion takes place in the variable v and

we can estimate the diffusion coefficient D . Using the result of *Proposition 2.2.1* the diffusion coefficient D of the variable v of the standard map (2.2.9) is

$$D = \frac{1}{2} \langle K^2 \sin(x_n)^2 \rangle = \frac{K^2}{4} \quad (2.2.10)$$

If the control parameter K is large but the variable x is not delta-correlated we need more precise calculations to obtain the diffusion coefficient. The first results in this case were obtained by Rechester and White (Rechester and White 1980), although their method was not completely deterministic. The first completely deterministic derivation of the diffusion coefficient D as the function of the control parameter K was determined by Cary et al. (Cary et al. 1981). Later Cary and Meiss suggested that diffusion takes place in a wide range of deterministic maps and the diffusion coefficient could be calculated in a way similar to that of Rechester and White. Schell et al. (Schell et al. 1982) discussed diffusive dynamics in quite general systems with translational symmetry. Doran and Fishman (Doran and Fishman 1988) showed how diffusion takes place in multidimensional systems. One of the most recent generalizations was presented by Kook and Meiss (Kook and Meiss 1990) who showed how diffusion emerges in symplectic maps.

The case of modest values of the control parameter K , i.e., ($1 < K < 10$) is a subject of intense research (Zisook 1982, Karney 1983, Lichtenberg et al. 1987). In this case long time correlations appear and anomalous diffusion takes place as a result of intermittencies but the phenomena is not well understood.

In *Proposition 2.2.2* we use the characteristic function technique to determine the diffusion coefficient D as the function of the control parameter K in the case of large values of K following the idea of Rechester and White (Rechester and White 1980).

Proposition 2.2.2. If

i) we consider the standard map

$$\begin{aligned} v_{n+1} &= v_n + K \sin(x_n) \\ x_{n+1} &= x_n + v_{n+1} \end{aligned} \quad (2.2.9)$$

ii) in its chaotic case, i.e., control parameter K is large ($K \geq 10$) then

- the variable v shows diffusion
- and its diffusion coefficient is

$$D = \frac{1}{4} K^2 [1 - 2J_2(K) + 2J_3^2(K) - 2J_1^2(K)], \quad (2.2.11)$$

where $J_n(K)$ denotes the n -th order Bessel-function.

Proof. As we showed in *Proposition 2.2.1* the diffusion coefficient D of an impulse map is

$$\begin{aligned} D &= \frac{1}{2} \sum_{l=-\infty}^{\infty} \langle \Delta v_k \Delta v_{k+l} \rangle \\ &= \frac{1}{2} \langle \Delta v_k \Delta v_k \rangle + \frac{1}{2} \sum_{l=1}^{\infty} \langle \Delta v_k \Delta v_{k+l} \rangle + \frac{1}{2} \sum_{l=-\infty}^{-1} \langle \Delta v_k \Delta v_{k+l} \rangle. \end{aligned} \quad (2.2.12)$$

Using the time symmetry of the correlation function the diffusion coefficient becomes

$$D = \frac{1}{2} \left[\langle \Delta v_k \Delta v_k \rangle + 2 \sum_{l=1}^{\infty} \langle \Delta v_k \Delta v_{k+l} \rangle \right]. \quad (2.2.13)$$

The change in the variable v is due to the sine term in the standard map (2.2.9), where $\Delta v_k = K \sin x_k$,

$$D = \frac{K^2}{2} \left[\langle \sin x_k \sin x_k \rangle + 2 \sum_{l=1}^{\infty} \langle \sin x_k \sin x_{k+l} \rangle \right]. \quad (2.2.14)$$

We use exponential representation

$$\sin x_k = \frac{1}{2i} [\exp(ix_k) - \exp(-ix_k)]$$

and the diffusion coefficient D becomes

$$\begin{aligned} D &= \frac{K^2}{4} [\langle \exp(i0x_k) \rangle + \langle \exp(i2x_k) \rangle] \\ &\quad - \frac{K^2}{4} \sum_{l=1}^{\infty} [\langle \exp(ix_k + ix_{k+l}) \rangle + \langle \exp(-ix_k - ix_{k+l}) \rangle] \\ &\quad + \frac{K^2}{4} \sum_{l=1}^{\infty} [\langle \exp(-ix_k + ix_{k+l}) \rangle + \langle \exp(ix_k - ix_{k+l}) \rangle]. \end{aligned} \quad (2.2.15)$$

We can rewrite the diffusion coefficient in terms of the characteristic function since the characteristic function is defined in the following way,

$$\chi_0(m_0) \equiv \langle \exp(im_0 x_k) \rangle \quad (2.2.16.a)$$

$$\chi_0(m_0, m_1) \equiv \langle \exp(im_0 x_k + im_1 x_{k+1}) \rangle \quad (2.2.16.b)$$

$$\chi_0(m_0, m_1, m_2) \equiv \langle \exp(im_0 x_k + im_1 x_{k+1} + im_2 x_{k+2}) \rangle. \quad (2.2.16.c)$$

So the diffusion coefficient becomes

$$\begin{aligned} D &= \frac{K^2}{4} [\chi_0(0) + \chi_0(2)] - \frac{K^2}{4} \sum_{l=1}^{\infty} [\chi_l(1, 0, \dots, 0, 1) + \chi_l(-1, 0, \dots, 0, -1)] \\ &\quad + \frac{K^2}{4} \sum_{l=1}^{\infty} [\chi_l(1, 0, \dots, 0, -1) + \chi_l(-1, 0, \dots, 0, 1)] \\ &= \frac{K^2}{4} \left[\chi_0(0) + \chi_0(2) + 2 \sum_{l=1}^{\infty} (\chi_l(1, 0, \dots, 0, -1) - \chi_l(1, 0, \dots, 0, 1)) \right]. \end{aligned} \quad (2.2.17)$$

Our goal is to simplify the above expression. The way we do is to we derive a recursion relation for the higher order characteristic functions and to calculate the lower order characteristic functions in a straightforward way. Therefore we rewrite the standard map (2.2.1) in a recursive form that depends only on the variable x . It takes the form

$$x_n = 2x_{n-1} - x_{n-2} + K \sin x_{n-1} \quad (2.2.18)$$

The characteristic function is given by the definition in the following form

$$\begin{aligned} \chi(m_0, m_1, \dots, m_k) \equiv \\ \langle \exp(im_0 x_n + \dots + im_{k-3} x_{n+k-3} + im_{k-2} x_{n+k-2} + im_{k-1} x_{n+k-1} + im_k x_{n+k}) \rangle \end{aligned} \quad (2.2.19)$$

Substituting (2.2.18) in the last term of the expression above we get

$$\begin{aligned} \chi(m_0, m_1, \dots, m_k) \equiv \\ < \exp(im_0 x_n + \dots + im_{k-3} x_{n+k-3} + i(m_{k-2} - m_k) x_{n+k-2} \\ + i(m_{k-1} + 2m_k) x_{n+k-1} + im_k K \sin(x_{n+k-1})) > . \end{aligned} \quad (2.2.20)$$

Using the Bessel function identity

$$\exp(iK \sin x) = \sum_{l=-\infty}^{\infty} J_l(K) \exp(ilx) \quad (2.2.21)$$

we end up with the desired recurrence relation of the characteristic functions

$$\begin{aligned} \chi_k(m_0, m_1, \dots, m_k) = \sum_{l=-\infty}^{\infty} J_l(m_k K) \chi_{k-1}(m_0, \dots, m_{k-3}, m_{k-2} - m_k, \\ m_{k-1} + 2m_k + l). \end{aligned} \quad (2.2.22)$$

Now we can evaluate the diffusion coefficient D given by (2.2.17) term by term. The term $\chi_0(0)$ is trivially unity since

$$\chi_0(0) = \langle \exp(i0x_k) \rangle = 1. \quad (2.2.23)$$

The term $\chi_0(2)$ vanishes because

$$\chi_0(2) = \langle \exp(i2x_k) \rangle = \delta_{2,0} = 0. \quad (2.2.24)$$

Now we explicitly write the essential terms of the diffusion coefficient D . Thus (2.2.17) becomes

$$\begin{aligned} D = & \frac{K^2}{4} \left\{ 1 + 2 \sum_{l=5}^{\infty} [\chi_l(1, 0, \dots, 0, -1) - \chi_l(1, 0, \dots, 0, 1)] \right\} \\ & + \frac{K^2}{4} 2 [\chi_4(1, 0, 0, 0, -1) - \chi_4(1, 0, 0, 0, 1) + \chi_3(1, 0, 0, -1) - \chi_3(1, 0, 0, 1)] \\ & + \frac{K^2}{4} 2 [\chi_2(1, 0, -1) - \chi_2(1, 0, 1) + \chi_1(1, -1) - \chi_1(1, 1)]. \end{aligned} \quad (2.2.25)$$

The term $\chi_1(m_0, m_1)$ is calculated from the definition (2.2.16b) by setting $\mathbf{k}=-1$

$$\chi_1(m_0, m_1) = \langle \exp(im_0x_{-1} + im_1x_0) \rangle. \quad (2.2.26)$$

Expressing x_{-1} from the standard map (2.2.9)

$$x_{-1} = x_0 - v_0$$

and substituting back into (2.2.26) we obtain

$$\chi_1(m_0, m_1) = \left(\int_R dv_0 dx_0 \right)^{-1} \int_R dv_0 d\mathbf{x}_0 \exp(i(m_0 + m_1)x_0 - im_0v_0), \quad (2.2.27)$$

where R is an invariant region of the space (x, v) i.e., a region which is mapped onto itself. Evaluating the integral (2.2.27) we get

$$\chi_1(m_0, m_1) = \delta_{m_0, 0} \delta_{m_1, 0}, \quad (2.2.28)$$

from which we conclude that

$$\chi_1(1, 1) = \chi_1(1, -1) = 0. \quad (2.2.29)$$

In the calculation of the terms $\chi_2(m_0, m_1, m_2)$ of the diffusion coefficient (2.2.25) we use the recursion relation (2.2.22). This takes the form

$$\chi_2(m_0, m_1, m_2) = \sum_{l=-\infty}^{\infty} J_l(m_2 K) \chi_1(m_0 - m_2, m_1 + 2m_2 + l). \quad (2.2.30)$$

Substituting (2.2.28) into (2.2.30) we end up with

$$\chi_2(m_0, m_1, m_2) = \delta_{m_0, m_2} J_{-m_1 - 2m_2}(m_2 K), \quad (2.2.31)$$

from where one can see that

$$\chi_2(1, 0, -1) = 0 \quad (2.2.32)$$

and

$$\chi_2(1, 0, 1) = \delta_{1, 1} J_{-2}(K) = J_2(K), \quad (2.2.33)$$

where we used the Bessel function identity

$$J_{-n}(x) = (-1)^n J_n(x). \quad (2.2.34)$$

We calculate the contribution of the term $\chi_3(m_0, m_1, m_2, m_3)$ in a similar way. The recursion relation (2.2.22) reads

$$\chi_3(m_0, m_1, m_2, m_3) = J_{m_3-m_1-2m_0}(m_0 K) J_{m_0-m_2-2m_3}(m_3 K), \quad (2.2.35)$$

from which we get

$$\chi_3(1, 0, 0, 1) = J_{-1}(K) J_{-1}(K) = J_1^2(K) \quad (2.2.36)$$

and

$$\chi_3(1, 0, 0, -1) = J_{-3}(K) J_3(K) = -J_3^2(K) \quad (2.2.37)$$

respectively. Finally the contribution of the terms $\chi_4(m_0, m_1, m_2, m-3, m_4)$ is calculated in a similar manner. We obtain

$$\chi_4(1, 0, 0, 0, 1) = \sum_{l=-\infty}^{\infty} J_l^2(K) J_{2(l+1)}((l+2)K) \quad (2.2.38)$$

and

$$\chi_4(1, 0, 0, 0, -1) = \sum_{l=-\infty}^{\infty} J_l(K) J_{l-4}(K) J_{2(l-2)}((l-2)K) \quad (2.2.39)$$

respectively. Combining equations (2.2.36 – 39) and (2.2.32 – 33) and (2.2.29) with (2.2.25) the diffusion coefficient D becomes

$$\begin{aligned} D = & \frac{1}{4} K^2 [1 - 2J_2(K) + 2J_3^2(K) - 2J_1^2(K)] \\ & + \frac{K^2}{4} 2 \sum_{l=-\infty}^{\infty} [J_l(K) J_{l-4}(K) J_{2(l-2)}((l-2)K) - J_l^2(K) J_{2(l+1)}((l+2)K)] \\ & + \frac{K^2}{4} 2 \sum_{l=5}^{\infty} [\chi_l(1, 0, \dots, 0, -1) - \chi_l(1, 0, \dots, 0, 1)]. \end{aligned} \quad (2.2.40)$$

The Bessel functions for large values of K oscillate in a way that the terms of the infinite sums do not provide a significant contribution to the diffusion coefficient therefore we can neglect those terms and the diffusion coefficient D takes the form (2.2.11).

q.e.d.

Remark 2.2.3. The diffusion coefficient as a function of the control parameter K for the variable v of the standard map is presented in *Figure 2.2.1*. We considered only large values of the control parameter K i.e., $K > 10$. In the figure we can observe the oscillatory behavior of the diffusion coefficient $D(K)$.

§2.3 Deterministic Diffusion in the Standard Map using the Zwanzig Projection Technique

In §2.2 we showed there was a diffusion in the standard map in its chaotic regime. In order to derive the diffusion coefficient D from the dynamics of the map we used the characteristic function technique. There is an alternative way in which one uses the projection operator technique in deriving the diffusion coefficient. In the standard map (2.2.9) we consider variable v to be the variable of interest and variable x the booster variable. We are not interested in the evolution of variable x thus we make a contraction over it. In order to execute the contraction over variable x we need to use the projection operator technique (see *Appendix 1*). This is what we do in this paragraph.

Figure 2.2.1. The diffusion coefficient as a function of the control parameter K for the variable v of the standard map (2.2.9) calculated from (2.2.11) using the characteristic function technique. We considered only large values of the control parameter K i.e., $K > 10$.

Proposition 2.3.1. If

i) we consider the standard map

$$\begin{aligned} v_{n+1} &= v_n + K \sin x_n \\ x_{n+1} &= x_n + v_{n+1} \end{aligned} \tag{2.2.9}$$

ii) in the large control parameter K case ($K > 10$) then

- the variable v shows diffusion
- and its diffusion coefficient is

$$D = \frac{K^2}{4} \left[1 - 2\sqrt{2} \frac{1}{\sqrt{K}} \cos(K - \frac{5}{4}\pi) \right]. \quad (2.3.1)$$

Proof. The proof shown here was suggested by Hasegawa and Shapir (Hasegawa and Shapir 1991) and was worked out in details by Grigolini (Grigolini 1993). The standard map (2.2.9) makes the state (x_n, v_n) of the space (x, v) evolved into the state (x_{n+1}, v_{n+1})

$$(x_n, v_n) \rightarrow (x_{n+1}, v_{n+1}). \quad (2.3.2)$$

If we consider an ensemble of states with the density $\rho(x, v; n)$ they evolve in an ensemble of states with the density $\rho(x, v; n + 1)$

$$\rho(x, v; n) \rightarrow \rho(x, v; n + 1) \quad (2.3.3)$$

or we can write it in a formal way in terms of the evolution operator Π

$$\rho(x, v; n + 1) = \Pi \rho(x, v; n). \quad (2.3.4)$$

We interpret the change in the state (x_n, v_n) to (x_{n+1}, v_{n+1}) as being due to a collision and a free motion. The collision takes place at the beginning of the n th time interval and it is applied for such a short time and with such a strength that we neglect the change in the variable x at the same time. This collision gives a contribution to the evolution of the density $\rho(x, v; n)$ which is described by the evolution operator $\exp(-K \sin x \frac{\partial}{\partial v})$. After the collision a free motion takes place till the beginning of the next time interval while the variable v remains constant. This process gives a contribution to the evolution of the density $\rho(x, v; n)$ described by the operator $\exp(-v \frac{\partial}{\partial x})$. So the complete, one step evolution of the density is given by

$$\rho(x, v; n+1) = \exp\left(-v \frac{\partial}{\partial x}\right) \exp\left(-K \sin x \frac{\partial}{\partial v}\right) \rho(x, v; n). \quad (2.3.5)$$

Now we apply the Zwanzig projection technique (*Appendix 1*) to evaluate the action of the evolution operator upto third order and we use the result to evaluate the diffusion coefficient of the variable v . First we take the double Fourier-transform of the density $\rho(x, v; n+1)$

$$\begin{aligned} \hat{\rho}(k, \omega; n+1) &= \int_0^{2\pi} dx \int_{-\infty}^{\infty} dv \exp(i\omega v) \exp(ikx) \rho(x, v; n+1) \\ &= \int_0^{2\pi} dx \int_{-\infty}^{\infty} dv \exp(i\omega v) \exp(ikx) \exp\left(-v \frac{\partial}{\partial x}\right) \\ &\quad \times \exp\left(-K \sin x \frac{\partial}{\partial v}\right) \rho(x, v; n). \end{aligned} \quad (2.3.6)$$

The differential operator $\exp\left(-v \frac{\partial}{\partial x}\right)$ can be moved to the left by integration by part and we get

$$\begin{aligned} \hat{\rho}(k, \omega; n+1) &= \int_0^{2\pi} dx \int_{-\infty}^{\infty} dv \exp\left(v \frac{\partial}{\partial x}\right) \exp(i\omega v) \exp(ikx) \\ &\quad \times \exp\left(-K \sin x \frac{\partial}{\partial v}\right) \rho(x, v; n) \end{aligned} \quad (2.3.7)$$

Since

$$\begin{aligned} \exp\left(v \frac{\partial}{\partial x}\right) \exp(ikx) &= \left(1 + v \frac{\partial}{\partial x} + \frac{1}{2!} v^2 \frac{\partial^2}{\partial x^2} + \dots\right) \exp(ikx) \\ &= \exp(ikx) \exp(ikv) \end{aligned} \quad (2.3.8)$$

therefore the evolution of the density $\hat{\rho}(k, \omega; n)$ reads

$$\hat{\rho}(k, \omega; n+1) = \int_0^{2\pi} dx \int_{-\infty}^{\infty} dv \exp(i\omega^* v) \exp(ikx) \exp\left(-K \sin x \frac{\partial}{\partial v}\right) \rho(x, v; n), \quad (2.3.9)$$

where the notation $\omega^* = \omega + k$ was introduced. The operator $\exp(-K \sin x \frac{\partial}{\partial v})$ can be put in the front by using integration by part and we get

$$\hat{\rho}(k, \omega; n+1) = \int_0^{2\pi} dx \int_{-\infty}^{\infty} dv \exp\left(K \sin x \frac{\partial}{\partial v}\right) \exp(i\omega^* v) \exp(ikx) \rho(x, v; n). \quad (2.3.10)$$

$$\begin{aligned} \exp\left(K \sin x \frac{\partial}{\partial v}\right) \exp(i\omega^* v) &= \left(1 + K \sin x \frac{\partial}{\partial v} + \frac{1}{2!} (K \sin x)^2 \frac{\partial^2}{\partial v^2} + \dots\right) \\ &\times \exp(i\omega^* v) = \exp(iK\omega^* \sin x) \exp(i\omega v) \end{aligned} \quad (2.3.11)$$

which results for $\hat{\rho}(\omega, k; n+1)$ in

$$\hat{\rho}(k, \omega; n+1) = \int_0^{2\pi} dx \int_{-\infty}^{\infty} dv \exp(i\omega^* v) \exp(ikx) \exp(iK\omega^* \sin x) \rho(x, v; n). \quad (2.3.12)$$

Using the Bessel function identity

$$\exp(iK\omega^* \sin x) = \sum_{l=-\infty}^{\infty} J_l(K\omega^*) \exp(ilx). \quad (2.2.21)$$

we rewrite the evolution equation of the density (2.3.12) and we obtain

$$\hat{\rho}(k, \omega; n+1) = \sum_{l=-\infty}^{\infty} J_l(K\omega^*) \int_0^{2\pi} dx \int_{-\infty}^{\infty} dv \exp(i\omega^* v) \exp(i(k+l)x) \rho(x, v; n). \quad (2.3.13)$$

Our goal is to express $\hat{\rho}(k, \omega; n+1)$ in terms of the $\hat{\rho}(k, \omega; n)$. Therefore we need to express $\rho(x, v; n)$ from $\hat{\rho}(k, \omega; n)$ by a proper inverse Fourier transformation which is

$$\rho(x, v; n) = \frac{1}{(2\pi)^2} \sum_{k'=-\infty}^{\infty} \int_{-\infty}^{\infty} d\omega' \exp(-iv\omega') \exp(-ixk') \hat{\rho}(k', \omega'; n) \quad (2.3.14)$$

Substituting (2.3.14) into (2.3.13) and using the definition of the δ -function i.e.,

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega' \exp(i\omega'x) \quad (2.3.15a)$$

and

$$\delta_{k',0} = \frac{1}{2\pi} \int_0^{2\pi} dx \exp(ik'x) \quad (2.3.15b)$$

we obtain the evolution of $\hat{\rho}(k, \omega; n)$ in the form of

$$\begin{aligned} \hat{\rho}(k, \omega; n+1) &= \sum_{l=-\infty}^{\infty} J_l(K\omega^*) \int_{-\infty}^{\infty} d\omega' \delta(\omega^* - \omega) \delta_{k+l, k'} \rho(k', \omega'; n) \\ &= \sum_{l=-\infty}^{\infty} J_l(K\omega^*) \rho(k+l, \omega^*; n). \end{aligned} \quad (2.3.16)$$

Since we have the evolution law of the density function $\hat{\rho}(k, \omega; n)$ in the $|k, \omega\rangle$ representation we need to express the evolution operator Π in the same representation.

The scalar product is defined

$$\langle k, \omega | F(x, v) \rangle = \int_0^{2\pi} dx \int_{-\infty}^{\infty} dv \exp(i\omega v) \exp(ikx) F(x, v). \quad (2.3.17)$$

In terms of the scalar product the evolution equation takes the form

$$\hat{\rho}(k, \omega; n+1) = \langle k, \omega | \rho(x, v; n+1) \rangle = \langle k, \omega | \Pi | k', \omega' \rangle. \quad (2.3.18)$$

Comparing (2.3.18) to (2.3.16) we get the form of the evolution operator in the $|k, \omega\rangle$ base

$$\langle k, \omega | \Pi | k', \omega' \rangle = \sum_{l=-\infty}^{\infty} J_l(K\omega^*) \delta_{k+l, k'} \delta(\omega^* - \omega'). \quad (2.3.19)$$

According to our interpretation the standard map (2.2.9) represents a collision (2.3.2) which brings the state (x_n, v_n) into the state (x_{n+1}, v_{n+1}) . The collision can be expressed in the corresponding frequency space as

$$|k, \omega \rangle \rightarrow |k+l, \omega+k \rangle. \quad (2.3.20)$$

In the dynamics given by the map (2.2.9) the variable x is fast. It is assumed to be at equilibrium i.e., it is uniformly distributed over the interval $[0, 2\pi]$ which means that in its corresponding frequency space, the k space, $k=0$ can be chosen. Actually we are interested in the long time behavior of variable v i.e., in its corresponding frequency space, the ω space, the range of $\omega < 1$ is of interest. Thus the projection operator P is defined in the following way

$$P = |0, \omega \rangle \langle 0, \omega| \quad (2.3.21)$$

where $\omega < 1$. The projection operator over the "irrelevant space" is defined as

$$Q = 1 - P, \quad (2.3.22)$$

where 1 is the identity operator i.e.,

$$1|k, \omega \rangle = |k, \omega \rangle. \quad (2.3.23)$$

We apply the projection operators P and Q on the density $\rho(x, v; n+1)$ along with the evolution operator Π so we get

$$\begin{aligned}
P\rho(x, v; n+1) &= P\Pi\rho(x, v; n) = P\Pi 1\rho(x, v; n) \\
&= P\Pi(P+Q)\rho(x, v; n) \\
&= P\Pi P\rho(x, v; n) + P\Pi Q\rho(x, v; n)
\end{aligned} \tag{2.3.24}$$

and

$$Q\rho(x, v; n+1) = Q\Pi P\rho(x, v; n) + Q\Pi Q\rho(x, v; n). \tag{2.3.25}$$

In (2.3.25) we can replace n with $n-1$ and obtain

$$Q\rho(x, v; n) = Q\Pi P\rho(x, v; n-1) + Q\Pi Q\rho(x, v; n-1) \tag{2.3.26}$$

which we substitute into (2.3.24) to get

$$\begin{aligned}
P\rho(x, v; n+1) &= P\Pi P\rho(x, v; n) + P\Pi P Q\Pi P\rho(x, v; n-1) \\
&\quad + P\Pi Q\Pi Q\rho(x, v; n-1).
\end{aligned} \tag{2.3.27}$$

Repeating the procedure we end up with the formal solution

$$\begin{aligned}
P\rho(x, v; n+1) &= P\Pi P\rho(x, v; n) + P\Pi \sum_{k=1}^n (Q\Pi)^k P\rho(x, v; n-k) \\
&\quad + (Q\Pi)^n Q\rho(x, v; 0).
\end{aligned} \tag{2.3.28}$$

The control parameter k is large so we observe a chaotic process. Therefore we can make the nonrestrictive assumption that the variable x initially is equally distributed over the $[0, 2\pi]$ interval. Therefore

$$Q\rho(x, v; n) = 0 \tag{2.3.29}$$

so the equation (2.3.28) becomes

$$P\rho(x, v; n+1) = P\Pi \sum_{k=0}^n (Q\Pi)^k P\rho(x, v; n-k). \quad (2.3.30)$$

We approximate the sum in (2.3.30) up to third order in Π i.e.,

$$\begin{aligned} P\rho(x, v; n+1) &\simeq P\Pi P\rho(x, v; n) + P\Pi Q\Pi P\rho(x, v; n-1) \\ &\quad + P\Pi Q\Pi Q\Pi P\rho(x, v; n-2). \end{aligned} \quad (2.3.31)$$

We can calculate the single terms of the r.h.s of (2.3.31) one by one. From (2.3.19) we get

$$\langle 0, \omega | \Pi | 0, \omega \rangle = J_0(K\omega) \quad (2.3.32a)$$

$$\langle 0, \omega | \Pi Q \Pi | 0, \omega \rangle = 0 \quad (2.3.32b)$$

$$\langle 0, \omega | \Pi Q \Pi Q \Pi | 0, \omega \rangle = \sum_{l \neq 0} J_l^2(K\omega) J_{-2l}(K(\omega + l)). \quad (2.3.32c)$$

Equation (2.3.31) becomes

$$P\rho(x, v; n+1) = P\Pi P\rho(x, v; n) + P\Pi Q\Pi P\rho(x, v; n-2). \quad (2.3.33)$$

We assume that the time evolution from $n-2$ to n is significantly driven by the first order term of (2.3.30) i.e.,

$$P\rho(x, v; n+1) \simeq P\Pi P\rho(x, v; n-2) = J_0^2(K\omega) P\rho(x, v; n-2). \quad (2.3.34)$$

So (2.3.33) becomes

$$P\rho(x, v; n+1) = \left[J_0(K\omega) + \frac{\sum_{l \neq 0} J_{-l}^2(K\omega) J_{-2l}(K(\omega + l))}{J_0^2(K\omega)} \right] P\rho(x, v; n) \quad (2.3.35)$$

which means

$$\hat{\rho}(0, \omega; n+1) = \left[J_0(K\omega) + \frac{\sum_{l \neq 0} J_{-l}^2(K\omega) J_{-2l}(K(\omega + l))}{J_0^2(K\omega)} \right] \hat{\rho}(0, \omega; n). \quad (2.3.36)$$

We can find a good approximation for the diffusion coefficient D based on the following argument. Since $K\omega$ is small we can expand the Bessel-function $J_n(K\omega)$ in an infinite series

$$J_n(K\omega) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(n+k)!} \left(\frac{K\omega}{2} \right)^{n+2k} \quad (2.3.37)$$

and for large arguments $K(\omega + l) \approx Kl$ the Bessel-function is approximated well by a cosine function with decreasing amplitude.

$$J_n(Kl) = \left(\frac{2}{\pi Kl} \right)^{1/2} \left[\cos(Kl - \frac{1}{4}\pi - \frac{1}{2}n\pi) + \dots \right]. \quad (2.3.38)$$

Substituting $n = 0, k = 0, 1$ into (2.3.37) and $n = -2, l = 1$ into (2.3.38) respectively (2.3.36) becomes

$$\hat{\rho}(0, \omega; n+1) = \left[1 - \frac{K^2\omega^2}{4} + \frac{K^2\omega^2}{2} \left(\frac{2}{\pi K} \right)^{1/2} \cos(K - \frac{5}{4}\pi) \right] \hat{\rho}(0, \omega; n). \quad (2.3.39)$$

From (2.3.39) the diffusion coefficient immediately is given

$$D = \frac{K^2}{4} \left[1 - 2\sqrt{2} \frac{1}{\sqrt{K}} \cos(K - \frac{5}{4}\pi) \right] \quad (2.3.1)$$

q.e.d.

Remark 2.3.1. The diffusion coefficient of variable v of the standard map (2.2.9) as a function of K is plotted in *Figure 2.3.1*. We consider only large values of the control parameter K , i.e., $K > 10$. The plotted curve shows the result of the theoretical prediction which is based on equation (2.3.1) (derived from the Zwanzig projection method). Comparing *Figure 2.3.1* to *Figure 2.2.1* we observe that the results on the diffusion coefficient of the standard map obtained by the Zwanzig projection method and the characteristic function method coincide.

§2.4 Deterministic Diffusion in a 1-dimensional map

Remark 2.4.1. As we mentioned in paragraph 2.2 one can observe deterministic diffusion in a Hamiltonian system. There are interesting non-Hamiltonian systems which can be represented by a 1-dimensional map like Rayleigh-Bénard cells (Mauer and Libcheber 1980), anharmonic LRC circuits (Linsay 1981, Testa et al. 1982), Josephson junctions in the presence of microwave field (Hubermann et al. 1980, Cirillo and Pedersen 1982, Jacob and Goldhirsch 1982), chemical reactions (Roux 1983) and certain biological systems (May 1976) and many of them show diffusive behavior. Numerous theoretical and computational efforts attempted to understand the emergence of diffusion of the 1-dimensional maps which describe the systems above (Grossmann and Fujisaka 1982, Geisel and Nierwetberg 1982, Fujisaka and Grossmann 1982, Grossmann and Thomae 1983, Geisel and Nierwetberg 1984, Geisel and Thomae 1984, Fujisaka et al. 1985). In *Proposition 2.4.1* we use the Frobenius

Figure 2.3.1. The diffusion coefficient of variable v of the standard map (2.2.9) as a function of K . We consider only large values of the control parameter K i.e., $K > 10$. The plotted curve shows the result of the theoretical prediction which is based on equation (2.3.1) (derived from the Zwanzig projection method).

operator method to show how to derive deterministic diffusion from a 1-dimensional map. The derivation rests on the idea that the diffusion coefficient is related to the correlation function of the map. The correlation function is a description of the steady state properties of the map, thus the averages that appear in the correlation calculations must be taken over the invariant distribution of the map. Consequently, in order to obtain the correlation function, we need this invariant distribution, i.e., the distribution which does not change under the mapping dynamics. In order to find the invariant distribution we have to find the operator which describes the evolution of the distribution. This operator i.e., the operator which describes the

evolution of a distribution under a certain mapping dynamics is called the Frobenius operator and the fixed point of the Frobenius operator provides the invariant distribution. (For technical details on the Frobenius operator see *Appendix 2*).

Proposition 2.4.1. If

i) the 1-dimensional map reads

$$X_{n+1} = F_a(X_n) \quad (2.4.1)$$

with the control parameter a ;

ii) under the translation $X \rightarrow X + N$ behaves as

$$F_a(X + N) = N + F_a(X), \quad (2.4.2)$$

where N is integer;

iii) is odd i.e., is invariant under the reflection $X \rightarrow -X$

$$F_a(X) = -F_a(-X); \quad (2.4.3)$$

iv) is characterized by $F_a(X)$ with only one maximum and one minimum per cell;

v) is characterized by the control parameter a large enough to map out of the unit cell the points from the neighborhood of the extrema (assumption of chaos);

vi) and $F_a(X)$ is a piecewise linear continuous map with the same slope almost everywhere i.e., in the first cell (interval $[0, 1)$) as follows

$$F_a(X) = \begin{cases} (4a-1)X & \text{for } 0 \leq X < \frac{a}{4a-1} \leq \frac{1}{2}; \\ -(4a-1)(X - \frac{a}{4a-1}) + a & \text{for } \frac{a}{4a-1} \leq X < 1 - \frac{a}{4a-1}; \\ (4a-1)(X-1) + 1 & \text{for } 1 - \frac{a}{4a-1} \leq X < 1; \end{cases} \quad (2.4.4)$$

vii) where a is positive and integer, then

- the variable X is diffusive for almost every initial condition
- and the diffusion constant D is

$$D = \frac{a(a-1)(2a-1)}{3(4a-1)}. \quad (2.4.5)$$

The map for $a = 2$ is plotted in *Figure 2.4.1*.

Figure 2.4.1. The 1-dimensional map (2.4.4) for $a = 2$ which produces diffusion.

Proof. The proof consists of two main parts. In the first part we show examples of nondiffusive trajectories. In the second part we show that the map is chaotic for the control parameter values $a > \frac{1}{2}$ and the trajectories jump back and forth from one to another contiguous cell, thereby leading in the long-time limit to diffusion

with no drift. The diffusion coefficient is related to the correlation function. The correlation function is calculated by averaging over the invariant distribution of the map (2.4.4) whose invariant distribution is obtained by the help of the Frobenius operator.

Nondiffusive, regular trajectories

For initial conditions $X_0 = N$ and $X_0 = 1/2 + N$, where $N = 0, \pm 1, \pm 2 \dots$ the map (2.4.4) provides constant consecutive values because the initial conditions are fixed points of the map.

For values of the control parameter a larger than the critical value one can observe regular trajectories. In order to investigate the emergence of the regular trajectories we introduce the concept of the reduced map. The construction of the reduced map from the map (2.4.4) is shown in *Figure 2.4.2*.

Figure 2.4.2. The reduced map of map (2.4.4) for $a = 2$.

For certain values of the control parameter a (e.g. for $a = 1.41144$) the peak of the reduced map can be mapped onto a consecutive peak itself (see *Figure 2.4.3a*). This solution results in a drift with drift velocity $v = 1$ because it takes 1 consecutive step for the trajectory to jump to an equidistant point of the neighboring cell.

Figure 2.4.3a. Drift produced by map (2.4.4). The peak of map (2.4.4) is mapped onto a neighboring peak.

For other values of the control parameter (e.g., for $a = 1 + \sqrt{2}/2$) the local maximum of the map is mapped onto its neighbor local minimum (see *Figure 2.4.3b*). This situation results in a periodic trajectory.

From the examples above we conclude that for particular initial conditions and certain values of the control parameter produce non-diffusional trajectories.

Diffusive trajectories

For most values of the control parameter a we find a diffusively broadening

Figure 2.4.3b. A periodic trajectory produced by map (2.4.4). The peak of map (2.4.4) is mapped into itself eventually.

trajectory. A typical example of a diffusive trajectory is shown in Figure 2.4.4. In order to calculate the diffusion coefficient we rewrite the map (2.4.4) in the form

$$X_{n+1} = X_n + f_a(X_n) = F_a(X_n), \quad (2.4.6)$$

where $f_a(X)$ is a 1-periodic function i.e.,

$$f_a(X + 1) = f_a(X). \quad (2.4.7)$$

It is worthwhile to rewrite the variable X_n with respect to the cell number N_n and the relative position x_n (i.e., inside the cell)

$$X_n = N_n + x_n. \quad (2.4.8)$$

Figure 2.4.4. A diffusive trajectory $(0.017, 0.119, 0.833, -0.169, \dots)$ produced by map (2.4.4) for $a = 2$.

We can rewrite the map (2.4.4) in a way that it represents two kinds of dynamics, one is the jump between the cells and the other one is the dynamics inside a given cell N_n as follows

$$\begin{aligned} N_{n+1} &= N_n + \Delta_a(x_n), \\ x_{n+1} &= g_a(x_n), \end{aligned} \tag{2.4.9}$$

where

$$\Delta_a(x) = [F_a(x)]_{\text{int}} = F_a(x) - g_a(x), \tag{2.4.10}$$

where $[F_a(x)]_{\text{int}}$ denotes the largest integer smaller than $F_a(x)$.

Now we show that the map (2.4.4) does not produce drift. The drift velocity v is defined as the average of the differences in two consecutive positions i.e.,

$$v = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=0}^{n-1} \langle X_{i+1} - X_i \rangle. \quad (2.4.11)$$

Substituting (2.4.6) into (2.4.11) we get

$$v = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=0}^{n-1} \langle f_a(X_i) \rangle = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=0}^{n-1} \langle f_a(x_i) \rangle, \quad (2.4.12)$$

since $f_a(X)$ has the translational symmetry (2.4.7).

From equation (2.4.12) we conclude that one can study the drift of the map (2.4.4) only by using the reduced map of it since the variable $x \in [0, 1)$ and the averaging takes place over the invariant distribution of the reduced map. As we proved in *Appendix 2, Remark A2.2* the reduced form of the map (2.4.4) has a uniform invariant distribution

$$\varrho^*(x) = 1. \quad (2.4.13)$$

Since $f_a(X)$ is an odd, 1-periodic function in its reduced map it has the symmetry

$$f_a(x) = -f_a(1 - x). \quad (2.4.14)$$

Therefore the drift velocity (2.4.12) becomes

$$v = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=0}^{n-1} \int_0^1 f_a(x_i) \varrho^*(x_i) dx_i. \quad (2.4.15)$$

Since $\varrho^*(x) = 1$ we rewrite the drift velocity (2.4.15) in the form of

$$v = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=0}^{n-1} \left[\int_0^{1/2} f_a(x_i) dx_i + \int_{1/2}^1 f_a(y_i) dy_i \right]. \quad (2.4.16)$$

By substituting $y = 1 - x$ and using the symmetry (2.4.14) (2.4.16) becomes

$$v = \lim_{n \rightarrow \infty} \frac{1}{n} \sum_{i=0}^{n-1} \left[\int_0^{1/2} f_a(x_i) dx_i + \int_{1/2}^0 f_a(x_i) dx_i \right] = 0. \quad (2.4.17)$$

We conclude that the map (2.4.4) produces pure diffusion since the drift velocity is $v = 0$.

The diffusion coefficient is calculated from its definition

$$2D = \lim_{n \rightarrow \infty} \frac{1}{n} \left\langle (X_n - \langle X_n \rangle)^2 \right\rangle, \quad (2.4.18)$$

which can be rewritten by using equations (2.4.8) and (2.4.9) in the form of

$$2D = \lim_{n \rightarrow \infty} \frac{1}{n} \left\langle \left(\sum_{i=0}^{n-1} \Delta_a(x_i) - \left\langle \sum_{i=0}^{n-1} \Delta_a(x_i) \right\rangle + x_n - \langle x_n \rangle \right)^2 \right\rangle \quad (2.4.19)$$

Introducing the notation

$$\delta \Delta_a(x_i) = \Delta_a(x_i) - \langle \Delta_a(x_i) \rangle \quad (2.4.20)$$

equation (2.4.19) becomes

$$2D = \lim_{n \rightarrow \infty} \frac{1}{n} \left\langle \sum_{i=0}^n \delta \Delta_a(x_i) \cdot \sum_{j=0}^n \delta \Delta_a(x_j) \right\rangle. \quad (2.4.21)$$

Using the argument that we used in *Proposition 2.2.1* the diffusion coefficient D in (2.4.20) can be expressed in terms of the correlation function

$$2D = \sum_{j=0}^n \langle \delta \Delta_a(x_j) \delta \Delta_a(x_0) \rangle. \quad (2.4.22)$$

Thus we have to calculate the correlation function

$$C(j) = \langle \delta \Delta_a(x_j) \delta \Delta_a(x_0) \rangle. \quad (2.4.23)$$

From the definition (2.4.10) of $\Delta_a(x)$ one can see that for map (2.4.4)

$$\langle \Delta_a(x) \rangle = 0, \quad (2.4.24)$$

therefore

$$\delta \Delta_a(x) = \Delta_a(x), \quad (2.4.25)$$

so the correlation function (2.4.23) can be written in the form of

$$C(j) = \langle \Delta_a(x_j) \Delta_a(x_0) \rangle. \quad (2.4.26)$$

For the sake of simplicity let us assume that the control parameter $a = 2$ and let us calculate the correlation function at "time" $j = 1$

$$C(1) = \langle \Delta_a(x_1) \Delta_a(x_0) \rangle. \quad (2.4.27)$$

From (2.4.4) and (2.4.10) it follows that

$$\Delta_a(x_0) = \begin{cases} 1, & \text{if } x_0 \in \left[\frac{1}{4a-1}, \frac{2a-1}{4a-1} \right] = \left[\frac{1}{7}, \frac{3}{7} \right] \\ -1, & \text{if } x_0 \in \left[\frac{2a}{4a-1}, 1 - \frac{1}{4a-1} \right] = \left[\frac{4}{7}, \frac{6}{7} \right] \\ 0, & \text{otherwise,} \end{cases} \quad (2.4.28)$$

where we notice that the length l_{x_0} of the intervals where $\Delta_a(x_0) \neq 0$ is the same for both intervals $l_{x_0} = \frac{2}{7}$. The application of the reduced map $g(x)$ on the initial x_0 yields x_1

$$x_1 = g(x_0) \quad (2.4.29)$$

and the resulting $\Delta_a(x_1)$ has the following structure. In the interval $\left[\frac{1}{4a-1}, \frac{2a-1}{4a-1} \right] = \left[\frac{1}{7}, \frac{3}{7} \right]$ there are two pieces of intervals where $\Delta_a(x_1) = 1$ and two pieces of intervals

where $\Delta_a(x_1) = -1$. All the four intervals have the same length $l_{x_1} = \frac{4}{49}$. The same is true for the interval $\left[\frac{2a}{4a-1}, 1 - \frac{1}{4a-1}\right] = \left[\frac{4}{7}, \frac{6}{7}\right]$. From this and from the uniform distribution of variable x_0 (See *Appendix 2, Remark A2.2* for proof) we conclude that

$$C(1) = 0. \quad (2.4.30)$$

By similar argument we can prove that

$$C(j) = 0 \text{ for every } j \neq 0. \quad (2.4.31)$$

We can prove by a slightly more complicated argument that for any integer a the correlation function is

$$C(j) = C(0)\delta_{j,0}. \quad (2.4.32)$$

From (2.4.32) and (2.4.22) we see that the diffusion coefficient D for the map (2.4.4) is

$$D = \frac{1}{2}C(0) = \frac{1}{2} \left\langle (\Delta_a(x))^2 \right\rangle. \quad (2.4.33)$$

The variance of $\Delta_a(x)$ can be calculated directly from its definition (2.4.10). From (2.4.10) we see that in the interval $\left[0, \frac{a}{4a-1}\right]$

$$(\Delta_a(x_0))^2 = (n-1)^2, \text{ if } x_0 \in \left[\frac{n-1}{4a-1}, \frac{n}{4a-1}\right]. \quad (2.4.34)$$

Thus

$$\begin{aligned}
\langle (\Delta_a(x_0))^2 \rangle &= \int_0^1 dx_0 (\Delta_a(x_0))^2 \varrho^*(x_0) \\
&= 4 \frac{1}{4a-1} \sum_{n=0}^{a-1} n^2 = \frac{2}{3} \frac{a(a-1)(2a-1)}{4a-1},
\end{aligned} \tag{2.4.35}$$

where we used $\varrho^*(x_0) = 1$ and the symmetry of $(\Delta_a(x_0))^2$ give four contributions, each of them is equal to the contribution of that of the interval $\left[0, \frac{a}{4a-1}\right]$, on the entire interval $[0, 1]$. From (2.4.35) and (2.4.33) the diffusion coefficient D is the one given by (2.4.5).

q.e.d

Remark 2.4.2. In *Proposition 2.4.1* we proved that map (2.4.4) produces $v = 0$ drift velocity. We can prove that the drift velocity is zero for a broader class of maps. Actually maps which satisfy the assumptions *i)–v)* of *Proposition 2.4.1* and the invariant distribution of their reduced map have the symmetry $\varrho^*(x) = \varrho^*(1-x)$, $x \in [0, 1)$ have no drift as well. The proof is identical with the one we used for our case.

Remark 2.4.3. In *Proposition 2.4.1* the assumption of piecewise nonlinearity is not essential since all the topological conjugate maps to the map (2.4.4) show similar behavior to the one we investigated although some of them show drift and diffusion too (Grossmann and Fujisaka 1982, Fujisaka and Grossmann 1982).

Remark 2.4.4. In *Chapter 2.1* we gave an example of diffusion that resulted of the integration of a stochastic variable using the Central Limit Theorem. In *Chapter 2.2–2.4* we showed how diffusion emerges in deterministic systems, where for

the calculations of the diffusion coefficient D we used the characteristic function, the Zwanzig projection approach and the Frobenius operator technique respectively. There are other techniques which derive the diffusion coefficient in chaotic, deterministic systems, e.g., path integral formalism (Jensen and Oberman 1981) but for our further purposes the ones we showed are satisfactory.

CHAPTER 3

LINEAR RESPONSE THEORY FOR MAPS

As we have stressed in *Chapter 1*, the main goal of this thesis is to develop a self-contained and deterministic picture of Brownian motion.

We have also noticed that Brownian motion is the result of the joint action of diffusion and friction. We have also seen that friction implies the solution of the intriguing problem of the linear response of a chaotic system to an external perturbation. Indeed, as pointed out in the *Introduction*, the linear friction, appearing in the standard Fokker-Planck equation, occurs as a consequence of a feedback process, and of the wide time scale separation between system and booster. The system of interest, with a certain velocity v , is perceived by the booster as a field determining the shape of its equilibrium distribution. The rearrangement of the booster is virtually instantaneous compared to the time scale of the variable velocity. On the other hand, the condition of wide time scale separation implies that the perturbation perceived by the booster is weak and that a linear response approach can be adopted. For this reason, the deterministic derivation of friction implies a rigorous treatment of the linear response of a booster to an external perturbation, which is indeed the subject of this chapter.

There are several ways to perturb a chaotic map. The most obvious way is the orbital perturbation which can be applied to maps with unbounded dynamics. The orbital perturbation means the addition of a constant perturbative term to one of the dynamical variables. This is what we study in §3.1 after defining the response in terms of maps dynamics.

The orbital perturbation can not be applied to 1-dimensional chaotic maps

because it can drive the dynamical variable out of the mapping region i.e., the simple orbital perturbation can force the dynamical variable into a region where it is not defined. A map moving beyond its natural range must be perceived as a non-physical result. In order to obtain results that make sense from the point of view of physics, we need to apply dynamical perturbations to 1-dimensional maps. Dynamical perturbations are the ones where the perturbation depends on the actual value of the perturbed variable. Thus in §3.2 we study the actions of dynamical perturbations on 1-dimensional maps, referring ourselves to the illuminating example of the logistic map, and we attempt to build up a Linear Response Theory along the lines established by Kubo (Kubo, 1957) in the case of Hamiltonian system in the continuous time representation. In §3.3 we show a refinement of the theory presented in §3.2. Here we apply a dynamical perturbation on the logistic map and calculate the response by a better than first order perturbation theory. In §3.4 we extend the Linear Response Theory of Kubo for 2-dimensional maps subjected to dynamical perturbations. We calculate the asymptotic and time-dependent susceptibility of Arnold's map. We use in these investigations the Frobenius operator method in order to obtain the evolution of densities associated with the maps of our interest.

Studying chaotic maps in terms of Kubo's Linear Response Theory leads to conceptual difficulties. Since the maps are chaotic, two initially close orbits rapidly diverge from each other. In this way diverge from one another the perturbed and unperturbed orbits starting from the same initial condition, even for small perturbations. Therefore there is no physical justification for the linearisation of individual orbits. Although Kubo's Linear Response Theory essentially linearises the individual orbits (van Kampen 1971) surprisingly it provides correct results for the averages of physical quantities. The probable reason why Kubo's Linear Response Theory works is because the chaotic systems can be associated unambiguously with a proba-

bility density function. This probability density is smooth and it evolves smoothly when it is perturbed. Furthermore the probability density is an analytic function of the perturbation parameter and thus it can be expanded into a Taylor-series with respect to the perturbation parameter. For sufficiently small perturbations it may be approximated by linear functions. For instance the response of an observable may be defined as an average value over a smooth probability density and thus it can be linearized with respect to small enough perturbations which allows the definition of linear response.

§3.1 The Linear Response Theory of van Velsen

In this paragraph we illustrate the ideas of van Velsen (van Velsen 1977) who first addressed the problem of the Linear Response Theory of maps. In this theory a class of area preserving maps is considered, where the perturbation is applied by adding a constant to the r.h.s. of the equation defining the $(n + 1)$ -th value of the variable as a function of the n -th value (orbital perturbation), so as to mimic the procedure of the Linear Response Theory of Kubo. After defining the response, the linear response and the generalized susceptibility for maps, we discuss the Linear Response Theory of van Velsen.

Definition 3.1.1. Let us consider a map $f_a(x)$ with control parameter a $f_a(x) : [0, 1] \mapsto [0, 1]$. Let us apply an external perturbation P . The dynamics of the map, due to the external perturbation P changes from

$$x_{n+1} = f_a(x_n) \tag{3.1.1}$$

into

$$x_{n+1}(P) = f_a(x_n, P). \quad (3.1.2)$$

The *response of the map* to the external perturbation P is a function of P , denoted by $R(P)$ which is the difference of the perturbed and unperturbed averages i.e.,

$$R(P) = \langle x_n(P) \rangle - \langle x_n(0) \rangle, \quad (3.1.3)$$

where $\langle \dots \rangle$ denotes averaging over an ensemble which is associated with an analytic distribution function. Consequently note that *Definition 3.1.1* is a statistical definition of the response.

Definition 3.1.1. If the $R(P)$ function is linear i.e.,

$$R(P) = \chi P, \quad (3.1.4)$$

then the map produces a *linear response* to the external perturbation P and the coefficient χ is called the *generalized susceptibility* of the map.

Definition 3.1.2. Even if the response of the individual orbits of the map to the external perturbation is not linear we can define a linear response. Since the *perturbation P is small* for physiscal systems the *linear response* is defined as

$$\chi = \left. \frac{dR(P)}{dP} \right|_{P=0}. \quad (3.1.5)$$

Note that in *Definition 3.1.2* we assume that the response $R(P)$ which is an average quantity is a differentiable function of the perturbation P .

Remark 3.1.1. From physical point of view it is very important to investigate how Hamiltonian systems respond to external perturbations. Since Hamiltonian systems are associated with area preserving maps, it is of real interest to investigate the response of area preserving maps to an external perturbation P . If we consider a map M

$$\begin{aligned} v_{n+1} &= F(v_n, x_n) \\ x_{n+1} &= G(v_n, x_n) \end{aligned} \tag{3.1.6}$$

where F and G are analytic functions then, as Birkhoff showed (Birkhoff 1922), in a neighborhood of an elliptic fixed point the mapping M can be brought into the normal form

$$\begin{aligned} v_{n+1} &= v_n \cos(\gamma_0 + \gamma_1(v_n^2 + x_n^2)) + x_n \sin(\gamma_0 + \gamma_1(v_n^2 + x_n^2)) + Q_4 \\ x_{n+1} &= -v_n \sin(\gamma_0 + \gamma_1(v_n^2 + x_n^2)) + x_n \cos(\gamma_0 + \gamma_1(v_n^2 + x_n^2)) + R_4 \end{aligned} \tag{3.1.7}$$

by means of an area preserving (nonlinear) transformation. Here γ_0 and γ_1 are constants, while Q_4 and R_4 are power series in x_n and y_n that begin with terms of order four and are convergent in a neighborhood of $(v, x) = (0, 0)$.

Van Velsen showed (van Velsen 1977) that the map (3.1.7) can be rewritten in the following area preserving form

$$\begin{aligned} v_{n+1} &= v_n + f(x_n) \\ x_{n+1} &= x_n + g(v_{n+1}), \end{aligned} \tag{3.1.8}$$

where $f(x) = \sum_{i=1}^{\infty} \alpha_i x^i$ and $g(v) = \sum_{i=1}^{\infty} \beta_i v^i$ and $\gamma_1 = \gamma_1(\alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2, \beta_3)$. The map (3.1.8) is more suitable for computer calculations than the previous ones. The perturbation P is added in the following way to the map (3.1.8) (orbital perturbation)

$$\begin{aligned}
v_{n+1} &= v_n + f(x_n) + P \\
x_{n+1} &= x_n + g(v_{n+1}),
\end{aligned}
\tag{3.1.9}$$

where P is a constant external force. In the following proposition we show an example of how one can calculate the response of a map in a particular case.

Proposition 3.1.1. If

i) we consider the mapping

$$\begin{aligned}
v_{n+1} &= v_n + f(x_n) + P \\
x_{n+1} &= x_n + g(v_{n+1}),
\end{aligned}
\tag{3.1.10}$$

ii) where f and g are 1-periodic functions (the periods can be assumed to be equal to unity without loss of generality),

iii) when both f and g have zero means

iv) and the initial distributions of v and x are symmetric with respect to $(0, 0)$

then

• the response $R_n(P)$ is

$$R_n(P) = \begin{cases} nP, & \text{for variable } v \\ 0 & \text{for variable } x. \end{cases}
\tag{3.1.11}$$

Proof. The response $R_n(P)$ is defined according to *Definition 3.1.1*

$$R_n(P) = \langle z_n(P) \rangle - \langle z_n(0) \rangle,
\tag{3.1.12}$$

where $\langle z_n(P) \rangle$ denotes the average of z -s over an ensemble

$$\langle z_n(P) \rangle = \frac{1}{N} \sum_{i=1}^N M^n z^{(i)},
\tag{3.1.13}$$

where $z^{(i)} = (v^{(i)}, x^{(i)})$, $i = 1, \dots, N$ and M^n denotes n applications of the map (3.1.10) on a given initial condition (v, x) . We claim that after n application the map takes the form

$$\begin{aligned} v_{n+1} - v &= nP + \Phi_n(v, x|P) \\ x_n - x &= \Psi_n(v, x|P), \end{aligned} \tag{3.1.14}$$

where Φ_n and Ψ_n are periodic functions with period unity in v, x and P .

We prove the claim above by induction. Comparing the claim to the map (3.1.10) we see that the formula (3.1.14) is true for $n = 1$ and

$$\Phi_1(v, x|P) = f(x) \tag{3.1.15}$$

and

$$\Psi_1(v, x|P) = g(v + f(x)). \tag{3.1.16}$$

Now we suppose (inductive assumption) that if (3.1.14) is true for some $n \geq 1$ then it is also true for some $n + 1$ as well. From (3.1.10) and our inductive assumption we have

$$v_{n+1} = v_n + f(x_n) + P = v + nP + \Phi_n(v, x|P) + f(x + \Psi_n(v, x|P)) + P. \tag{3.1.17}$$

Thus

$$\Phi_{n+1}(v, x|P) = \Phi_n(v, x|P) + f(x + \Psi_n(v, x|P)) \tag{3.1.18}$$

has the required properties, e.g. periodicity. Similarly one shows

$$\Psi_{n+1}(v, x|P) = \Psi_n(v, x|P) + g(v + (n+1)P + \Phi_{n+1}(v, x|P)). \quad (3.1.19)$$

Thus we have proved our claim. The important consequence of this result is as follows. Since the map (3.1.10) can be written in the form of (3.1.14) we can calculate the response of map (3.1.10) using the form (3.1.14) i.e.,

$$\begin{aligned} \langle v_n \rangle &= \langle v \rangle + \langle nP \rangle + \langle \Phi_n(v, x|P) \rangle \\ \langle x_n \rangle &= \langle x \rangle + \langle \Psi_n(v, x|P) \rangle. \end{aligned} \quad (3.1.20)$$

When f and g both have period unity a natural choice for an ensemble would be the unit cell $U_1 = \{(x, y) : x \in [-\frac{1}{2}, \frac{1}{2}], y \in [-\frac{1}{2}, \frac{1}{2}]\}$. For symmetric initial conditions the only nonvanishing term in (3.1.20) is $\langle nP \rangle$. Thus the response is given by (3.1.11).

q.e.d.

Remark 3.1.2. The *Proposition 3.1.1* was checked by numerical calculations (van Velsen 1977). Van Velsen used the map

$$\begin{aligned} v_{n+1} &= v_n + 2 \sin 2\pi x_n + P \\ x_{n+1} &= x_n + 3 \sin 2\pi v_{n+1}. \end{aligned} \quad (3.1.21)$$

He found that the response is linear in P and proportional to the “time” n in the way formula (3.1.11) predicts.

§3.2 The Linear Response Theory of Kubo for 1-dimensional maps

Remark 3.2.1. The *Linear Response Theory of Geisel et al.* (Geisel et al. 1984).

In the previous paragraph we considered a case of perturbation when the orbit of a 2-dimensional map was perturbed. If we perturb a 1-dimensional map $f : [0, 1] \mapsto [0, 1]$ then, due to the perturbation the map can map out itself from the interval $[0, 1]$ (Heldstab et al 1983, Geisel et al. 1984). Thus we have to consider perturbations which keep the process being mapped in the interval $[0, 1]$. For these kinds of perturbations Geisel et al. (Geisel et al. 1984) developed a Linear Response Theory which is the counterpart of the Linear Response Theory of Kubo that is worked out in detail in *Appendix 3*.

Let us consider an unperturbed map $f(x)$ with the dynamics

$$x_{n+1} = f(x_n) \quad (3.2.1)$$

and the perturbed one with the dynamics

$$x_{n+1} = f'(x_n, n), \quad (3.2.2)$$

where the perturbed map $f'(x)$ is related to the unperturbed one by addition of the perturbation $\Delta f(x)$

$$f'(x, n) = f(x) + \Delta f(x, n). \quad (3.2.3)$$

Since the trajectories of $f(x)$ and $f'(x)$ are expected to diverge we formulate the response in terms of invariant densities. When we calculate the densities we have to use the corresponding Frobenius operators $\hat{P}$ and $\hat{P}'_n$

$$\hat{P}'_n = \hat{P} + \Delta \hat{P}_n, \quad (3.2.4)$$

where $\hat{P}'_n$ governs the evolution of the density $\varrho'(x)$ of the perturbed map and $\hat{P}$ governs the evolution of the density $\varrho(x)$ of the unperturbed map respectively. The

perturbed density $\varrho'(x)$ evolves according to

$$\varrho'_{n+1}(x) = \hat{P}'_n \varrho'_n(x). \quad (3.2.5)$$

The Frobenius operator for any observable $B(x)$ acts as

$$\int_0^1 B(x) \hat{P}'_n \varrho'_n(x) dx = \int_0^1 B(f'(x, n)) \varrho'_n(x) dx. \quad (3.2.6)$$

Thus the integral Kernel of the Frobenius operator $\hat{P}'_n$ reads (see *Appendix, Remark A2.4* and *Definition A2.7*).

$$\hat{P}'_n(x, y, n) = \delta(x - f'(y, n)). \quad (3.2.7)$$

The unperturbed distribution function $\varrho_n(x)$ is evolved by the time independent Frobenius operator $\hat{P}$.

$$\varrho_{n+1}(x) = \hat{P} \varrho_n(x) \quad (3.2.8)$$

with kernel

$$\hat{P}(x, y) = \delta(x - f(y)). \quad (3.2.9)$$

The time evolution of the distribution function ϱ'_n may be expressed by the propagator $\hat{R}'(n|s)$ in the form

$$\varrho'_n = \hat{R}'(n|s) \varrho'_s, \quad n \geq 1 \quad (3.2.10)$$

where $\hat{R}'(n|s)$ is given by the time-ordered product

$$\begin{aligned} \hat{R}'(n|s) &= \hat{P}'(n) \hat{P}'(n-1) \dots \hat{P}'(s+1), \quad n > s \\ \hat{R}'(n|n) &= 1. \end{aligned} \quad (3.2.11)$$

From this representation we note that $\hat{R}'(n|s)$ satisfies the equation

$$\hat{R}'(n|n_0) = \hat{R}'(n|s)\hat{R}'(s|n_0) \quad (3.2.12)$$

The time independent Frobenius operator $\hat{P}$ of the process generates the unperturbed propagator

$$\hat{R}(n|s) = \hat{P}^{n-s} \quad (3.2.13)$$

with kernel

$$\hat{R}(x, n|y, s) = \delta(x - f^{n-s}(y)). \quad (3.2.14)$$

Because of the decomposition (3.2.4) of the perturbed Frobenius operator $\hat{P}'$ the propagator satisfies the following equation

$$\hat{R}'(n|n_0) = \hat{R}(n|n_0) + \sum_{s=n_0+1}^n \hat{R}(n|s)\Delta\hat{P}(s)\hat{R}'(s-1|n_0), \quad (3.2.15)$$

where we assumed that the propagator $\hat{R}(n|n_0)$ is switched on at time $n = n_0$. To first order in the perturbation the perturbed propagator in the last term may be replaced by the unperturbed one i.e., $\hat{R}'(s-1|n_0) \rightarrow \hat{R}(s-1|n_0)$. Then (3.2.15) yields for the perturbed distribution

$$\varrho'_n(x) = \varrho_n(x) + \sum_{s=n_0+1}^n \hat{R}(n|s)\Delta\hat{P}(s)\varrho_{s-1}(x). \quad (3.2.16)$$

According to (3.2.7) and (3.2.9) the kernel of $\Delta\hat{P}(s)$ is to first order in h_s given by

$$\hat{P}(x, y; s) = -\frac{d}{dx}\delta(x - f(y))h_s, \quad (3.2.17)$$

where h_s is the external perturbation with the causality condition ($h_s = 0$ for $s < 0$). Applying the result of (3.2.17) on the distribution $\varrho_{s-1}(x)$ and using (3.2.8), we have

$$\Delta \hat{P}(s) \varrho_{s-1}(x) = -\frac{d}{dx} \varrho_s(x) h_s \quad (3.2.18)$$

and therefore

$$\varrho'_n(x) = \varrho_n(x) - \sum_{s=n_0+1}^n \int_0^1 \hat{R}(x, n|y, s) \frac{d}{dy} \varrho_s(y) dy h_s. \quad (3.2.19)$$

According to definition (3.1.3) from the perturbed distribution $\varrho'_n(x)$ and the unperturbed distribution $\varrho_n(x)$ we can calculate the response in an arbitrary observable $B(x)$,

$$\langle \Delta B_n \rangle = \langle B(x) \rangle_{\varrho'_n(x)} - \langle B(x) \rangle_{\varrho_n(x)} = \int_0^1 B(x) [\varrho'_n(x) - \varrho_n(x)] dx \quad (3.2.20)$$

to an external perturbation h_s is given in terms of the above generalized susceptibility $\chi_{n,s}$ by

$$\langle \Delta B_n \rangle = \sum_{s=n_0+1}^{\infty} \chi_{n,s} h_s. \quad (3.2.21)$$

Substituting into (3.2.20) and comparing the result to (3.2.21) and assuming a perturbation $h_s = \Theta(s)$ we obtain for the generalized susceptibility

$$\begin{aligned} \chi_{n,s} &= - \int_0^1 \int_0^1 B(x) \hat{R}(x, n|y, s) \frac{d}{dy} [\varrho_s(y)] dx dy \Theta(n-s) \quad \text{for } n \neq s \\ \chi_{n,n} &= 1, \end{aligned} \quad (3.2.22)$$

where $\Theta(n-s)$ is the step function (0 for $n < s$ and 1 for $n \geq s$). Using the definition (3.2.19) of the unperturbed propagator $\hat{R}(n|s)$ (3.2.22) yields

$$\chi_{n,s} = - \int_0^1 \int_0^1 B(x_n(x_0)) \left[\frac{d}{dy} \right] \varrho_0(y) dx_0 dy \Theta(n) \quad (3.2.23)$$

where we denoted the initial condition $s = 0$ and $x = x_s = x_0$ and the propagator acted upon the initial condition x_0 in the usual way

$$\int_0^1 B(x_0) \hat{P}^n \varrho^*(x_0) dx_0 = \int_0^1 B(x_n(x_0)) \varrho^*(x_0) dx_0, \quad (3.2.24)$$

where we used the assumption that the system initially is in a state which would be in equilibrium in the absence of perturbation i.e., $\varrho'_0(x) = \varrho^*(x)$, where $\varrho^*(x)$ denotes the equilibrium distribution of the non-perturbed system. We assume that the external perturbation $\Delta f(x, n)$ couples to the variable A . The generalized susceptibility is according to (3.2.24) and (3.2.18)

$$\chi_n = \int_0^1 \int_0^1 dx_0 dy B(x_n(x_0)) \left(-\frac{d}{dx_0} \right) \delta(x_0 - f(y)) A(y) \varrho^*(y) \quad \text{for } n \geq 0. \quad (3.2.25)$$

The formula (3.2.25) is the discrete counterpart of Kubo's Linear Response formula (A3.4) in *Appendix 3*. Note that in the derivation of (3.2.25) we used essentially the same assumptions as those used in the derivation of (A3.4). For instance in the definition of susceptibility (3.2.21) we assumed that the summation with respect to the discrete time n and the integration with respect to the chaotic variable x are interchangeable. We used a first-order perturbation theory in substituting the perturbed propagator with the unperturbed one. Furthermore the chaoticity assumption assures the existence of a smooth invariant distribution function.

In the following proposition we show by an example how the Linear Response Theory above works for the perturbed logistic map.

Proposition 3.2.1. If

i) the unperturbed map is the logistic map $f(x) : [-1, 1] \mapsto [-1, 1]$

$$f(x) = 1 - 2x^2 \quad (3.2.26)$$

ii) the perturbation $\Delta f(x, n)$

$$\Delta f(x, n) = \kappa A(x) \Theta(n), \quad (3.2.27)$$

iii) where

$$A(x) = 2(x^2 - x^4) \quad -\frac{3}{4} < \kappa < 1, \quad (3.2.28)$$

iv) and the perturbation parameter κ is small then

• the generalized susceptibility χ_n of the system

$$\chi_n = \frac{\kappa}{2} \langle B(x_n(x_0)) x_0 \rangle \quad n = 1, 2, \dots \quad (3.2.29)$$

where x_0 is the initial value of x and $B(x)$ is a physical quantity whose response is of interest.

Proof. The generalized susceptibility of the system is to be calculated from its definition (3.2.25). Using the property of the δ -function (for example in ref. Messiah 1961)

$$\delta[f(y)] = \sum_i \frac{1}{|f'(y_i)|} \delta(y - y_i) \quad (3.2.30)$$

with $f(y_i) = 0$ and $f'(y_i) \neq 0$ the generalized susceptibility χ_n (3.2.24) after integration with respect to y becomes

$$\chi_n = -\kappa \int_{-1}^1 dx_0 B(x_n(x_0)) \frac{d}{dx_0} \sum_i \frac{A(y_i(x_0)) \varrho^*(y_i(x_0))}{|f'(y_i(x_0))|}, \quad (3.2.31)$$

where $y_i(x)$ denotes the roots of equation

$$x = f(y) = 1 - 2y^2, \quad (3.2.32)$$

i.e.,

$$y_{1,2} = \pm \sqrt{\frac{1-x}{2}}. \quad (3.2.33)$$

Substituting (3.2.33) and (3.2.28) into (3.2.31) and using the invariant distribution $\varrho^*(x)$ of the unperturbed logistic map (3.2.26) ($\varrho^*(x)$ is given by *Remark A2.9, Appendix 2*)

$$\varrho^*(x) = \frac{1}{\pi \sqrt{1-x^2}} \quad (3.2.34)$$

the generalized susceptibility χ_n is

$$\begin{aligned} \chi_n &= -\kappa \int_{-1}^1 dx_0 B(x_n(x_0)) \frac{d}{dx_0} \frac{1}{\pi} \sqrt{\left(\frac{1-x_0}{2}\right) \left(1 - \frac{1-x_0}{2}\right)} \\ &= \frac{\kappa}{2} \int_{-1}^1 dx_0 B(x_n(x_0)) x_0 \frac{1}{\pi \sqrt{1-x_0^2}}. \end{aligned} \quad (3.2.35)$$

Identifying the invariant distribution (3.2.34) of the unperturbed logistic map (3.2.26) in (3.2.35) we can rewrite the generalized susceptibility as a cross correlation function between the observable B and initial condition x_0

$$\begin{aligned} \chi_n &= \frac{\kappa}{2} \int_{-1}^1 dx_0 B(x_n(x_0)) x_0 \varrho^*(x_0) \\ &= \frac{\kappa}{2} \langle B(x_n(x_0)) x_0 \rangle. \end{aligned} \quad (3.2.36)$$

q.e.d.

Remark 3.2.2. If we consider the assumptions of the *Proposition 3.2.1* and the physical quantity whose response we are interested in is the variable x itself then the response is given as

$$\chi_n = \frac{\kappa}{2} \langle x_n x_0 \rangle \quad (3.2.37)$$

As we proved in *Proposition A2.6, Appendix 2* the logistic map (3.2.35) is δ -correlated so the generalized susceptibility χ_n is a 1-step vanishing function of "time" n

$$\chi_n = \kappa \frac{\langle x_0^2 \rangle}{2} \delta_{n,0}. \quad (3.2.38)$$

Remark 3.2.3. The Linear Response Theory of Grossmann (Grossmann 1984).

The Linear Response Theory of Geisel et al. (see above) can be refined as was shown by Grossmann (Grossmann 1984). It is because the Linear Response Theory of Geisel et al., following Kubo's idea developed for continuous systems, is a first-order perturbation theory. The first-order perturbation was introduced when we assumed that in (3.2.15) the perturbed propagator $\hat{R}'(s-1|n_0)$ can be replaced by the unperturbed propagator $\hat{R}(s-1|n_0)$. If we do not use this assumption and we keep the perturbed propagator and we use for the initial distribution an estimate better than that for the equilibrium distribution ϱ^* of the unperturbed map, then we can get a more precise result for the generalized susceptibility χ_n i.e., (3.2.25) becomes

$$\chi_n = \int_0^1 \int_0^1 dx_0 dy B(x_n(x_0)) \left(-\frac{d}{dx_0} \right) \delta(x - f(y)) A(y) \varrho_\kappa^*(y) \quad \text{for } n \geq 0 \quad (3.2.39)$$

where $\varrho_\kappa^*(y)$ is the above mentioned better estimate for the equilibrium distribution of the perturbed map. In the following *Proposition 3.2.2* we show how this method works for the logistic map and its dynamical perturbation of *Proposition 3.2.1*.

Proposition 3.2.2. If

i) the unperturbed map is the logistic map $f(x) : [-1, 1] \mapsto [-1, 1]$

$$f(x) = 1 - 2x^2, \quad (3.2.26)$$

ii) and the perturbation $\Delta f(x, n)$

$$\Delta f(x, n) = \kappa A(x) \Theta(n), \quad (3.2.27)$$

iii) where

$$A(x) = 2(x^2 - x^4) \quad -\frac{3}{4} < \kappa < 1, \quad (3.2.28)$$

iv) the perturbation parameter κ is small,

v) and we use the theory of Grossmann then

• the generalized susceptibility χ_n of the system is

$$\chi_n = \frac{3\kappa}{2} \langle B(x_n(x_0) \delta x_0^2) \rangle, \quad n = 1, 2, \dots \quad (3.2.40)$$

where δx_0^2 denotes $x_0^2 - \langle x_0^2 \rangle$, with $\langle x_0^2 \rangle = 1/2$.

Proof. The proof consist of the evaluation of (3.2.39). In order to evaluate the

expression (3.2.39) we need a good estimate for the perturbed equilibrium $\varrho_\kappa^*(x)$. As Györgyi et al. showed (Györgyi et al. 1984) a good estimate for $\varrho_\kappa^*(x)$ is

$$\varrho_\kappa^*(x) = \varrho^*(x) \left[1 + \frac{\kappa}{2}x + \frac{3\kappa^2}{8}(1+x-2x^2) + O(h^3) \right], \quad (3.2.41)$$

where $\varrho^*(x)$ is the equilibrium distribution (3.2.34) of the unperturbed logistic map (3.2.26).

Using the (3.2.30) property of the δ -function the generalized susceptibility (3.2.39) becomes

$$\chi_n = -\kappa \int_{-1}^1 dx_0 B(x_n(x_0)) \frac{d}{dx_0} \sum_i \frac{A(y_i(x_0)) \varrho_\kappa^*(y_i(x_0))}{|f'_\kappa(y_i(x_0))|}, \quad (3.2.42)$$

where $y_i(x)$ denotes the roots of the equation

$$x_0 = f_\kappa(y) = 1 - 2y^2 + 2\kappa(y^2 - y^4), \quad (3.2.43)$$

i.e.,

$$y_{1,2} = \pm \sqrt{\frac{1-\kappa}{2\kappa}} \sqrt{-1 + \sqrt{1 + \frac{2\kappa(1-x_0)}{(1-\kappa)^2}}}. \quad (3.2.44)$$

Substituting (3.2.41), (3.2.44) and (3.2.27) into (3.2.42) and doing some lengthy but straightforward algebra we find that (3.2.42) becomes

$$\chi_n = -\kappa \int_{-1}^1 dx_0 B(x_n(x_0)) \left[\frac{x_0}{2} \varrho^*(x_0) + \frac{3\kappa}{2} \varrho^*(x_0) \delta x_0^2 \right], \quad (3.2.45)$$

where $\varrho^*(x_0)$ is the equilibrium distribution (3.2.34) of the unperturbed map and

$$\delta x_0^2 = x_0^2 - \langle x_0^2 \rangle. \quad (3.2.46)$$

After the integration with respect to x_0 we end up with (3.2.40) for the generalized susceptibility.

q.e.d.

§3.3 The Linear Response Theory of Kubo for 2-dimensional area preserving maps

Remark 3.3.1. The Linear Response Theory of Breyman et al. (Breyman et al. 1992).

In §3.1 we investigated how certain 2-dimensional area preserving maps respond to a constant external perturbation. In §3.2 we were interested in the response of the logistic map to a dynamical perturbation i.e., the perturbation depended on the actual state of the logistic map itself. The dynamical perturbations are of paramount importance because in an interaction between a system of interest and its environment (or booster) the booster is subjected to a dynamical perturbation originating with the system of interest. In this paragraph we consider Arnold's map (Arnold 1968) subjected to dynamical perturbation. First we calculate the response at very long times, then the time dependent linear response following the procedure as worked out by Breyman et al. (Breyman et al. 1992).

Proposition 3.3.1. If

i) the map $f(x) : [0, 1] \times [0, 1] \mapsto [0, 1] \times [0, 1]$

$$\begin{aligned} x_{n+1} &= x_n + y_n \mod 1 \\ y_{n+1} &= 2y_n \mod 1 \end{aligned} \tag{3.3.1}$$

ii) is subjected to an additive perturbation $ah(x)$ so it yields the map $f_a(x) :$

$$[0, 1] \times [0, 1] \mapsto [0, 1] \times [0, 1]$$

$$\begin{aligned} x_{n+1} &= x_n + y_n + ah(x) \mod 1 \\ y_{n+1} &= 2y_n \mod 1, \end{aligned} \tag{3.3.2}$$

iii) where a is the perturbation parameter, and

$$h(x) = \begin{cases} x, & \text{for } 0 \leq x < \frac{1}{2} \\ 1 - x, & \text{for } \frac{1}{2} \leq x < 1, \end{cases} \tag{3.3.3}$$

then

- the asymptotic response i.e., the response for very long times is

$$\langle \delta(x) \rangle = \frac{a}{4} \tag{3.3.4}$$

and

$$\langle \delta(y) \rangle = 0 \tag{3.3.5}$$

respectively.

Proof. The central idea of the proof is that if we can determine the invariant densities of the cat map (3.3.1 – 2) then we can calculate any steady state averages of an observable by averaging over the invariant distributions. Therefore our goal is to determine the invariant distributions of the unperturbed and the perturbed maps (3.3.1 – 2). We calculate the invariant distribution by finding it as the fixed point of the Frobenius operator. The proof consist of two parts. In the first part we calculate the invariant distributions of the unperturbed and the perturbed maps $\varrho^*(x, y)$ and $\varrho'^*(x, y)$, respectively. In the second part, knowing $\varrho^*(x, y)$ and $\varrho'^*(x, y)$, the response of an observable is calculated from its definition. The formalism we use in this proof is similar to the one we used in *Remark 3.2.1*.

Arnold's cat map (3.3.1) is chaotic (see Tabor 1989 for proof). The perturbation (3.3.2) preserves its chaoticity. (Actually one can show that both the perturbed and the unperturbed maps are mixing systems, Lasota et al. 1985). The consequence of the chaoticity or more precisely of the mixing property is that both the perturbed and unperturbed systems have a unique invariant distribution $\varrho'^*(x, y)$ and $\varrho^*(x, y)$, respectively.

The invariant distribution of the unperturbed and perturbed maps. We claim that the invariant distribution $\varrho^*(x, y)$ of Arnold's cat map is

$$\varrho^*(x, y) = 1. \quad (3.3.6)$$

We have to show that the Frobenius operator of the unperturbed map $\hat{P}(x, y)$ acts upon $\varrho^*(x, y)$ in the following way

$$\hat{P}\varrho^*(x, y) = \hat{P}1 = \varrho^*(x, y) = 1. \quad (3.3.7)$$

The Frobenius operator $\hat{P}$ is given by *Definition A2.29* that we apply on the density $\varrho^*(x, y) = 1$, so (A2.9) is

$$\hat{P}1 = \frac{\partial^2}{\partial x \partial y} \int \int_{f^{-1}([a, x] \times [b, y])} 1 ds dy \quad (3.3.8)$$

The integral (3.3.8) has a geometrical interpretation. It is a volume element whose height is unity and the base is the area of the preimage of the rectangle $[a, x] \times [b, y]$. The map (3.3.1) is area preserving therefore the rectangle $[a, x] \times [b, y]$ and its preimage $f^{-1}([a, x] \times [b, y])$ have the same area so

$$\begin{aligned} \int \int_{[a, x] \times [b, y]} 1 ds dt &= \int \int_{f^{-1}([a, x] \times [b, y])} 1 ds dt = (x - a)(y - b) \\ &= xy - ax - by + ab. \end{aligned} \quad (3.3.9)$$

Substituting (3.3.9) into (3.3.8) we obtain

$$\hat{P}1 = \frac{\partial^2}{\partial x \partial y}(xy - ax - by + ab) = 1. \quad (3.3.10)$$

Thus we showed that the invariant distribution $\varrho^*(x, y) = 1$ is invariant under the action of the Frobenius operator $\hat{P}$ of the unperturbed map.

The invariant distribution of the perturbed map is calculated along the same line as those adopted above. According to these calculations the invariant distribution of the perturbed map is

$$\varrho'^*(x, y) = \begin{cases} \frac{1}{1+a}, & \text{for } 0 \leq x < \frac{1+a}{2}, \\ \frac{1}{1-a}, & \text{for } \frac{1+a}{2} \leq x < 1. \end{cases} \quad (3.3.11)$$

The response. Now, since we know the perturbed and unperturbed invariant distributions $\varrho^*(x, y)$ and $\varrho'^*(x, y)$ respectively it is straightforward to calculate the responses. The response of the variable x is defined by

$$\langle \delta x \rangle = \langle x \rangle_{\varrho'^*} - \langle x \rangle_{\varrho^*}, \quad (3.3.13)$$

where from (3.3.11) we substitute the invariant distribution $\varrho'^*(x, y)$ so

$$\begin{aligned} \langle x \rangle_{\varrho'^*} &= \int_0^1 dx \int_0^1 dy \varrho'^*(x, y) x = \int_0^{\frac{1+a}{2}} dx \int_0^1 dy \frac{1}{1+a} x \\ &\quad + \int_{\frac{1+a}{2}}^1 dx \int_0^1 dy \frac{1}{1-a} x = \frac{a}{4} + \frac{1}{2}, \end{aligned} \quad (3.3.14)$$

and we use equation (3.3.6) for averaging over the invariant distribution $\varrho^*(x, y)$ of the unperturbed cat map in order to calculate $\langle x \rangle_{\varrho^*}$ so

$$\langle x \rangle_{\varrho^*} = \int_0^1 dx \int_0^1 dy \varrho^*(x, y) x = \int_0^1 dx \int_0^1 dy 1x = \frac{1}{2}. \quad (3.3.15)$$

From (3.3.13), (3.3.14) and (3.3.15) clearly

$$\langle \delta x \rangle = \frac{a}{4}. \quad (3.3.16)$$

Similarly the long time response of y is given by

$$\langle \delta y \rangle = \langle y \rangle_{\varrho'^*} - \langle y \rangle_{\varrho^*}, \quad (3.3.17)$$

where

$$\langle y \rangle_{\varrho'^*} = \int_0^{\frac{1+a}{2}} dx \int_0^1 dy \frac{1}{1+a} x + \int_{\frac{1+a}{2}}^1 dx \int_0^1 dy \frac{1}{1-a} x = \frac{1}{2}, \quad (3.3.18)$$

and

$$\langle y \rangle_{\varrho^*} = \int_0^1 dx \int_0^1 dy 1y = \frac{1}{2}, \quad (3.3.19)$$

where we used the invariant distribution (3.3.11) for ϱ'^* and (3.3.6) for ϱ^* respectively. (3.3.18) and (3.3.19) with (3.3.17) yield for the response in observable y

$$\langle \delta y \rangle = 0. \quad (3.3.20)$$

q.e.d.

Remark 3.3.2. Previously we investigated the asymptotic response of the system due to a perturbation. It is more interesting to know how an observable $B(x, y)$ reaches its asymptotic value in time. In order to do it we assume the system is in unperturbed equilibrium at time $n = 0$. The unperturbed equilibrium is characterized by the invariant distribution of the unperturbed system $\varrho^*(x, y)$. We assume

furthermore that the perturbation $ah(x)$ couples to variable x and it is switched on $n = 0$. Then the system evolves until it reaches its new equilibrium which is characterized by the perturbed invariant distribution $\varrho'^*(x, y)$. The evolution of the perturbed distribution $\varrho'_n(x, y)$ is governed by the perturbed Frobenius operator $\hat{P}'$

$$\varrho'_{n+1}(x, y) = \hat{P}' \varrho'_n(x, y). \quad (3.3.21)$$

The time dependent response $\langle \delta B \rangle_n$ of observable B to a perturbation is defined as the difference between the average of observable B taken over the actual distribution $\varrho'_n(x, y)$ of the perturbed map

$$\langle B \rangle_{\varrho'_n} = \int_0^1 \int_0^1 dx dy B(x, y) \varrho'_n(x, y) \quad (3.3.22)$$

and the average of the observable B taken over the invariant distribution $\varrho^*(x, y)$ of the unperturbed map

$$\langle B \rangle_{\varrho^*} = \int_0^1 \int_0^1 dx dy B(x, y) \varrho^*(x, y) \quad (3.3.23)$$

i.e.,

$$\langle \delta B \rangle_n = \langle B \rangle_{\varrho'_n} - \langle B \rangle_{\varrho^*}. \quad (3.3.24)$$

In the following *Proposition 3.3.2* we show that the response of an observable $B(x, y)$ consist of two parts — a stationary one and a vanishing, time dependent part.

Proposition 3.3.2. If

- i) the map $f(x) : [0, 1] \times [0, 1] \mapsto [0, 1] \times [0, 1]$

$$\begin{aligned}
x_{n+1} &= x_n + y_n \pmod{1} \\
y_{n+1} &= 2y_n \pmod{1}
\end{aligned} \tag{3.3.1}$$

ii) is subjected to an additive perturbation $ah(x)$ so it yields the map $f_a(x) : [0, 1] \times [0, 1] \mapsto [0, 1] \times [0, 1]$

$$\begin{aligned}
x_{n+1} &= x_n + y_n + ah(x) \pmod{1} \\
y_{n+1} &= 2y_n \pmod{1},
\end{aligned} \tag{3.3.2}$$

iii) where a is the perturbation parameter, and

$$h(x) = \begin{cases} x, & \text{for } 0 \leq x < \frac{1}{2} \\ 1 - x, & \text{for } \frac{1}{2} \leq x < 1 \end{cases}, \tag{3.3.3}$$

then

- the response of an observable $B(x, y)$

$$\langle \delta B \rangle_{e_n} = \langle \delta B \rangle_{e'^*} + \langle \delta B \rangle_n, \tag{3.3.25}$$

where $\langle \delta B \rangle_{e'^*}$ is the stationary part and $\langle \delta B \rangle_n$ is the time dependent part with

$$\langle \delta B \rangle_{e'^*} = a \int_0^1 dx \int_0^1 dy B(x, y) \text{sign}(x - \frac{1}{2}) \tag{3.3.26a}$$

$$\langle \delta B \rangle_n = -a \int_0^1 dx \int_0^1 dy B(x, y) \hat{P}^n \text{sign}(x - \frac{1}{2}). \tag{3.3.26b}$$

Proof. To calculate the response, the perturbed Frobenius operator $\hat{P}'$ is approximated to first order in the perturbation parameter a

$$\hat{P}' \simeq \hat{P} + a\hat{P}'^{(1)}, \tag{3.3.27}$$

where $\hat{P}'^{(1)}$ denotes the first order term of the power series expansion of $\hat{P}'$ in a . Therefore for the time-evolution operator for n time steps one finds to first order in a

$$\hat{P}'^n = \hat{P}^n + a \sum_{s=1}^n \hat{P}^{n-s} \hat{P}'^{(1)} \hat{P}^{s-1}, \quad (3.3.28)$$

which is the counterpart of (3.2.15). The time-dependent response of an observable $B(x, y)$ is given by (3.3.24) into which substituting (3.3.28) we get

$$\langle \delta B \rangle_n = a \sum_{s=1}^n \int_0^1 dx \int_0^1 dy B(x, y) \hat{P}^{n-s} \hat{P}'^{(1)} \varrho^*(x, y), \quad (3.3.29)$$

where we used that $\varrho'_0 = \varrho^*$ and $\hat{P}^k \varrho^* = \varrho^*$ i.e., assumptions iv) and v). In order to evaluate the expression $\hat{P}'^{(1)} \varrho^*$ we express the perturbed map as a conjugation of the unperturbed map and we associate a Frobenius operator with the conjugation function. We express the operator $\hat{P}'^{(1)}$ in terms of the new Frobenius operator which allows us to calculate $\hat{P}'^{(1)} \varrho^*$.

We consider that the perturbed map (3.3.2) is related to the unperturbed map (3.3.1) by a conjugation described by a conjugating function g_a (see e.g. *Appendix 2*)

$$f_a = g_a \circ f \circ g_a^{-1}. \quad (3.3.30)$$

According to the conjugation we can build up the Frobenius operator $\hat{P}'$ of the perturbed map f_a

$$\hat{P}' = \hat{P}_a \cdot \hat{P} \cdot \hat{P}_a^{-1}, \quad (3.3.31)$$

where $\hat{P}$ is the Frobenius operator of the unperturbed map and $\hat{P}_a$ is the Frobenius

operator related to the conjugating function g_a . To first order in a the Frobenius operator is given

$$\hat{P}'^{(1)} = \hat{P} + a(\hat{P}_a^{(1)}\hat{P} - \hat{P}\hat{P}_a^{(1)}) + O(a^2). \quad (3.3.32)$$

Comparing (3.3.32) to (3.3.27) and substituting $\hat{P}'^{(1)}$ into (3.3.29) we get for $\langle \delta B \rangle_n$

$$\begin{aligned} \langle \delta B \rangle_n &= a \sum_{s=1}^n \int_0^1 dx \int_0^1 dy B(x, y) \hat{P}^{n-s} (\hat{P}_a^{(1)} \hat{P} - \hat{P} \hat{P}_a^{(1)}) \varrho^*(x, y) \\ &= -a \sum_{s=1}^n \int_0^1 dx \int_0^1 dy B(x, y) \hat{P}^{n-s} (\hat{I} - \hat{P}) \hat{P}_a^{(1)} \varrho^*(x, y), \end{aligned} \quad (3.3.33)$$

where $\hat{I}$ denotes the identity operator. $\hat{P}_a^{(1)} \varrho^*$ can be evaluated from the *Definition A2.6, Appendix 2* which gives

$$\hat{P}_a^{(1)} \varrho^* = -\text{sign}(x - \frac{1}{2}). \quad (3.3.34)$$

Substituting (3.3.34) into (3.3.33) we end up with (3.3.25) and (3.3.26).

q.e.d.

CHAPTER 4

THE GEOMETRICAL LINEAR RESPONSE THEORY FOR MAPS

In this chapter we develop the Geometrical Linear Response Theory for 1 dimensional maps. The reason why we call this method geometrical is because the main idea behind it is derived from a paper (Bianucci et al. 1993a), where the geometrical nature of the method is evident. They (Bianucci et al. 1993a) have faced the problem of the response of a Hamiltonian system to an external perturbation, adopting a method to which the criticism of van Kampen might not apply (van Kampen 1971). These authors noticed that a Hamiltonian system which is chaotic and mixing is expected to be ergodic and therefore to have a microcanonical equilibrium distribution. If the perturbation acts in the form of a field K changing the potential that drives the dynamics of the system without affecting its ergodic properties, then the equilibrium distribution can be expressed as a continuous function of K . This makes it possible to adopt a perturbation expansion of the distribution around $K = 0$, thereby bypassing van Kampen's criticism regarding the impossibility of using perturbation methods within the context of chaotic systems characterized by orbit instabilities. It is evident from the arguments of Bianucci et al. (1993a) that the stability of the distributions is compatible with the instabilities of the trajectories.

Here, we shall adopt this geometrical method to the case of 1 dimensional maps. This has been the subject of a very recent paper (Bianucci et al., 1993b). It has been observed that by a suitable transformation, the conjugation transformation, controlled by a parameter a called the conjugation parameter, the zero-centered tent map is changed into a different map, with the invariant distribution of the tent

map changing into a corresponding transformed, or conjugated, distribution. This is reminiscent of the microcanonical distribution of the Hamiltonian case which upon changes of the field K adopts itself smoothly to the new geometry of the phase space. Here the invariant distribution is a continuous function of the conjugation parameter a , as, in the truly geometrical case, the microcanonical distribution is a continuous function of K . The conjugation transformation can also break the symmetry of the tent map so as to result in a new invariant measure which is no longer symmetric with respect to the center of the map domain. Let us imagine that at $a = a_0$, the map is symmetric, and results in a symmetric invariant distribution. Then the mean value of x will turn out to be a continuous function of a , vanishing at $a = a_0$. Thus the parameter $a - a_0$ plays the role of an external perturbation, and with criteria reminiscent of the geometrical criteria adopted by Bianucci et al. (Bianucci et al. 1993a) it turns out to be easy to evaluate the corresponding susceptibility of the map. All this is illustrated in the following *Proposition 4.1*.

§4. The Geometrical Linear Response Theory for 1 dimensional maps

Proposition 4.1. If

- i) the unperturbed map $f(t) : [-1, 1] \mapsto [-1, 1]$ is the zero centered tent map

$$t_{n+1} = f(t_n) = 1 - 2|t_n| \tag{4.1}$$

(see *Figure 4.1*),

- ii) it is subjected to a conjugation with the conjugation function

$$x = h(t) = \begin{cases} -1 + \sqrt{a^2 - (t+1-a)^2}, & \text{for } -1 \leq t \leq a-1 ; \\ 1 - \sqrt{(2-a)^2 - (t+1-a)^2}, & \text{for } a-1 < t \leq 1 \end{cases} \quad (4.2)$$

with $a \in [0, 2]$ (see *Figure 4.2*),

iii) and the initial values of t are uniformly distributed over the interval $[-1, 1]$ then

- the response $R(a)$ of the map

$$R(a) = \left(\frac{\pi}{2} - 1 \right) (a - 1) \quad (4.3)$$

- and the generalized susceptibility is

$$\chi = \left(\frac{\pi}{2} - 1 \right). \quad (4.4)$$

Proof. The response of the conjugated map is calculated from its definition. Since the unperturbed map is the zero centered tent-map (4.1) and the perturbed map is the conjugated map

$$g_a(x) = h \circ f \circ h^{-1}, \quad (4.5)$$

(see *Figure 4.3*) the response $R(a)$ is given

$$R(a) = \langle x \rangle - \langle t \rangle, \quad (4.6)$$

Figure 4.1. The zero centered tent map (4.1).

where the averaging takes place over the invariant distributions $\varrho^*(x)$ and $\varrho^*(t)$ respectively.

We can use the invariant distributions instead of the time dependent distributions in averaging because we assumed (assumption iii)) that the tent map is initially uniformly distributed over the interval $[-1, 1]$ thus the conjugated map reaches its invariant distribution instantly after the application of the perturbation i.e., conjugation. (In Figure 4.4 the evolution of $\langle x_n \rangle$ is plotted for several values of the perturbation or conjugation parameter a).

The figure shows that $\langle x_n \rangle$ does not depend on time n . This is numerical evidence that the perturbation causes instant response in the variable x). As we showed in

Figure 4.2. The conjugating function (4.2) for some values of the conjugation parameter a , $a = 1.0$ (solid line, unperturbed case), $a = 0.7$ (long dashed line) and $a = 1.3$ (short dashed line).

Proposition A2.1, Appendix 2 the invariant distribution of the tent map is uniform i.e., the invariant distribution $\varrho^*(t)$ of the map (4.1) is

$$\varrho^*(t) = \frac{1}{2}, \quad (4.7)$$

where $t \in [-1, 1]$. Thus

$$\langle t \rangle = \int_{-1}^1 t \varrho^*(t) dt = \int_{-1}^1 t \frac{1}{2} dt = 0, \quad (4.8)$$

that means the response $R(a)$ is the average of x

$$R(a) = \langle x \rangle. \quad (4.9)$$

Figure 4.3. The conjugated map (4.5) for some values of the conjugation parameter a , $a = 1.0$ (solid line, unperturbed case), $a = 0.7$ (long dashed line) and $a = 1.3$ (short dashed line).

In order to calculate $\langle x \rangle$ we explore the fact that x is the conjugate of t therefore, as we proved in *Proposition A2.4, Appendix 2* the invariant density $\varrho^*(x)$ is given in terms of the invariant density of the tent map and the Jacobian of the inverse of the conjugating function $x = h(t)$

$$\varrho_g^*(x) = \varrho_f^*(h^{-1}(x)) \left| \frac{dh^{-1}(x)}{dx} \right|. \quad (4.10)$$

From (4.2)

$$t = h^{-1}(x) = \begin{cases} a - 1 - \sqrt{a^2 - (x + 1)^2}, & \text{for } -1 \leq x \leq a - 1; \\ a - 1 + \sqrt{(2 - a)^2 - (x - 1)^2}, & \text{for } a - 1 < x \leq 1. \end{cases} \quad (4.11)$$

Figure 4.4. The evolution of the average of the conjugated map (4.5) for some values of the conjugation parameter a , $a = 1.0$ (solid line, unperturbed case), $a = 0.7$ (long dashed line), and $a = 1.3$ (short dashed line).

We can see from (4.11) that $h^{-1}(x)$ is monotonously increasing therefore

$$\varrho_g^*(x) = \frac{1}{2} \frac{dh^{-1}(x)}{dx} \quad (4.12)$$

where we substituted $\varrho_f^*(t)$ from (4.7) into (4.10). Now the response $R(a)$ in (4.9) becomes

$$\begin{aligned} R(a) = \langle x \rangle &= \int_{-1}^1 x \varrho_g^*(x) dx \\ &= \frac{1}{2} \left[x h^{-1}(x) \Big|_{-1}^1 - \int_{-1}^1 h^{-1}(x) dx \right] = (a - 1) \left(1 - \frac{\pi}{2} \right). \end{aligned} \quad (4.13)$$

The response as a function of a is plotted in *Figure 4.5*.

Figure 4.5. The response $R(a)$ of the conjugated map (4.5) as a function of the conjugation or perturbation parameter a . The circles show the results of numerical calculations, the solid line is the analytical result calculated from (4.3).

From (4.13) we can see that the response $R(a)$ is proportional to the perturbation parameter a . The perturbation parameter a represents no perturbation when $a = 1$ as can be seen from (4.11) thus when we calculate the generalized susceptibility we compute the value of the derivative at $a = 1$. Finally the susceptibility is

$$\chi = \left. \frac{dR(a)}{da} \right|_{a=1} = \frac{dR(a)}{da} = 1 - \frac{\pi}{2}. \quad (4.14)$$

q.e.d.

Remark 4.2. The response $R(a)$ is not always proportional to the perturbation a , or actually the real perturbation $a - 1$. An example of this kind is shown in the following *Proposition 4.2*.

Proposition 4.2. If

i) the unperturbed map $f(t) : [-1, 1] \mapsto [-1, 1]$ is the zero centered logistic map

$$t_{n+1} = f(t_n) = 1 - 2t_n^2 \quad (4.15)$$

(see *Figure 4.6*),

ii) it is subjected to a conjugation with the conjugation function

$$x = h(t) = \begin{cases} -1 + \sqrt{a^2 - (t + 1 - a)^2}, & \text{for } -1 \leq t \leq a - 1 ; \\ 1 - \sqrt{(2 - a)^2 - (t + 1 - a)^2}, & \text{for } a - 1 < t \leq 1 \end{cases} \quad (4.2)$$

with $a \in [0, 2]$ (see *Figure 4.2*),

iii) and the initial values of t are uniformly distributed over the interval $[-1, 1]$ then

- the response $R(a)$ of the map for small perturbations, i.e., $a \ll 1$

$$R(a) \approx 0.4404(a - 1) \quad (4.16)$$

- and the generalized susceptibility is

$$\chi = \left. \frac{dR(a)}{da} \right|_{a=1} = 0.4404. \quad (4.17)$$

Proof. The proof is given in the same spirit as that adopted for the zero-centered

Figure 4.6. The zero centered logistic map (4.15).

tent map. Since the unperturbed map is the zero centered logistic map (4.15) and the perturbed map is the conjugated map $g_a(x)$

$$g_a(x) = h \circ f \circ h^{-1}, \quad (4.18)$$

(see Figure 4.7) the response $R(a)$ is given

$$R(a) = \langle x \rangle - \langle t \rangle, \quad (4.6)$$

The averaging for x takes place over the invariant distribution $\rho^*(x)$ of map $g_a(x)$ and the averaging for t takes place over the invariant distribution $\rho^*(t)$ of map (4.15) respectively. As proved in *Remark A2.9, Appendix2*, the invariant distribution of the zero centered logistic map (4.15) is

Figure 4.7. The conjugated map (4.18) with for some values of the conjugation parameter a , $a = 1.0$ (solid line, unperturbed case), $a = 0.7$ (long dashed line) and $a = 1.3$ (short dashed line).

$$\varrho^*(t) = \frac{1}{\pi\sqrt{1-t^2}}, \quad (4.19)$$

which is an even function on the interval $t \in [-1, 1]$, thereby leading to

$$\langle t \rangle = \int_{-1}^1 t \varrho^*(t) dt = \int_{-1}^1 t \frac{1}{\pi\sqrt{1-t^2}} dt = 0. \quad (4.20)$$

From (4.6) and (4.20) the response is

$$R(a) = \langle x \rangle. \quad (4.21)$$

In order to calculate $\langle x \rangle$ we need the equilibrium distribution $\varrho^*(x)$ of the perturbed map (4.18). As we proved in *Proposition A2.4, Appendix 2* the invariant

density of the conjugated map $\varrho^*(x)$ is related to the invariant density $\varrho^*(t)$ of the unperturbed map via

$$\varrho_g^*(x) = \varrho_f^*(h^{-1}(x)) \left| \frac{dh^{-1}(x)}{dx} \right|. \quad (4.22)$$

From (4.2) we get for the inverse conjugating function

$$t = h^{-1}(x) = \begin{cases} a - 1 - \sqrt{a^2 - (x + 1)^2}, & \text{for } -1 \leq x \leq a - 1; \\ a - 1 + \sqrt{(2 - a)^2 - (x - 1)^2}, & \text{for } a - 1 < x \leq 1. \end{cases} \quad (4.11)$$

(4.11) shows that $h^{-1}(x)$ is monotonously increasing thus (4.22) becomes

$$\varrho^*(x) = \frac{1}{\pi} \begin{cases} \frac{1}{\sqrt{1 - (a - 1 - \sqrt{a^2 - (x + 1)^2})^2}} \frac{x + 1}{\sqrt{a^2 - (x + 1)^2}}, & \text{for } -1 \leq x \leq a - 1; \\ \frac{1}{\sqrt{1 - (a - 1 + \sqrt{(2 - a)^2 - (x - 1)^2})^2}} \frac{1 - x}{\sqrt{(2 - a)^2 - (x - 1)^2}}, & \text{for } a - 1 < x \leq 1. \end{cases} \quad (4.23)$$

The invariant distribution $\varrho^*(x)$ (4.23) is plotted in *Figure 4.8*.

Thus the response (4.9) becomes

$$\begin{aligned} R(a) = & \frac{1}{\pi} \int_{-1}^{a-1} x \frac{1}{\sqrt{1 - (a - 1 - \sqrt{a^2 - (x + 1)^2})^2}} \frac{x + 1}{\sqrt{a^2 - (x + 1)^2}} dx \\ & + \frac{1}{\pi} \int_{a-1}^1 x \frac{1}{\sqrt{1 - (a - 1 + \sqrt{(2 - a)^2 - (x - 1)^2})^2}} \frac{1 - x}{\sqrt{(2 - a)^2 - (x - 1)^2}} dx. \end{aligned} \quad (4.24)$$

We could not evaluate this expression analytically so we used a numerical integration provided by the program package Mathematica (Wolfram 1988) and we fitted a curve to the numerical results for small values of the perturbation parameter $a - 1$ (see *Figure 4.9*). We found that the response is for small perturbation i.e., for $a - 1 \ll 1$

Figure 4.8. The invariant distribution (4.23) of the conjugated map (4.18) for some values of the conjugation parameter a , $a = 1.0$ (solid line, unperturbed case), $a = 0.7$ (long dashed line) and $a = 1.3$ (short dashed line).

$$R(a) \approx 0.4404(a - 1). \quad (4.16)$$

From (4.16) the generalized susceptibility is

$$\chi = \left. \frac{dR(a)}{da} \right|_{a=1} = 0.4404. \quad (4.17)$$

q.e.d.

Figure 4.9. The response $R(a)$ of the conjugated map (4.18) as a function of the conjugation (or perturbation) parameter a . The circles show the results of (4.24) by numerical calculations, the solid line is the fitting curve (4.16) for small perturbations.

CHAPTER 5

DETERMINISTIC BROWNIAN MOTION

In this chapter we fulfill the main goal of this work. We present two models for deterministic Brownian motion. After recalling the traditional wisdom on Brownian motion, in the first paragraph (§5.1) we present a model where the Brownian particle is coupled to a chaotic booster which is mimicked by the zero centered logistic map. The particle loses energy via a phenomenological dissipation. We use a stochastic technique for the analytical treatment and an algorithm for the numerical solution of the equations of motion.

In §5.2 we present the self consistent picture of the deterministic Brownian motion. Here the Brownian particle interacts with a chaotic booster. The result of the interaction is the fluctuation and dissipation of the energy of the particle. We test the velocity of the Brownian motion by investigating the fluctuation-dissipation and the relaxation properties. We show the deterministic Brownian motion for two kinds of chaotic boosters, the zero-centered logistic and tent maps.

§5.1 Deterministic Brownian motion with phenomenological dissipation

Remark 5.1.1. The traditional wisdom on the Brownian motion

As we mentioned in the *Introduction* Brownian motion is a result of two competing processes – the fluctuation and the dissipation. The fluctuation takes into account the action of the environment or booster on the system of interest.

In this traditional picture one assumes that the booster is robust and can have many – possibly an infinite number of – degrees of freedom and is considered to be

in thermodynamic equilibrium (statistical assumption). So the booster acts upon the system of interest in an erratic manner – this action is described by means of a random force which causes diffusion.

We assume that the system of interest is small compared to the booster therefore in its interaction with the robust booster it only slightly perturbs the dynamics of the booster. The reaction of the system to the booster takes place in a dissipative manner. The dissipation is assumed to be proportional to the velocity of the particle.

When we assume that the system of interest is small compared to the booster we use a key assumption that being the motion of the booster is fast compared to the system. In other words there is a time-scale separation between the system of interest and the booster. Due to this time-scale separation the Central Limit Theorem is applicable and one recovers the Gaussian equilibrium distribution of the velocity. In this section we shall examine two examples, when there is no time-scale separation between the booster and the variable of interest and we can not recover the Gaussian distribution.

The result of the competition between the random fluctuations and the dissipation is a dynamical equilibrium between the two processes in a way that the booster pumps as much energy into the system of interest as it receives from it by dissipation. The system of interest has a fixed average energy which is proportional to the product of the diffusion coefficient D^* and the dissipation rate γ (Einstein 1905)

$$\frac{1}{2}m \langle v^2 \rangle = \frac{1}{2}m D^* \gamma \quad (5.1.1)$$

The model above was first expressed in terms of a stochastic mathematical for-

malism by Langevin (Langevin 1908). Langevin considered a 1-dimensional system where two kinds of forces act on a particle of mass m – the dissipative force F_d which is proportional to the velocity v i.e., $F_d = -\Gamma v$ and a random force $\xi(t)$. The equation of motion reads

$$m\dot{v} = -\Gamma v + \xi(t). \quad (5.1.2)$$

After deviding by mass m (5.1.2) becomes

$$\dot{v} = -\gamma v + x(t), \quad (5.1.3)$$

where $\gamma = \Gamma/m$ and $x = \xi/m$ respectively and $x(t)$ is assumed to be delta-correlated in time

$$\langle x(t)x(0) \rangle = 2D\delta(t) \quad (5.1.4)$$

with a Gaussian distribution

$$p(x) = \frac{1}{\sqrt{4\pi D}} e^{-\frac{x^2}{4D}} \quad (5.1.5)$$

and zero average value

$$\langle x(t) \rangle = 0. \quad (5.1.6)$$

The equation (5.1.3) has the formal solution

$$v(t) = v_0 e^{-\gamma t} + e^{-\gamma t} \int_0^t e^{\gamma t'} x(t') dt', \quad (5.1.7)$$

where v_0 denotes the initial value of the velocity $v(0) = v_0$. After averaging over an ensemble of realizations of the random force (5.1.7) becomes

$$\langle v(t) \rangle = v_0 e^{-\gamma t} \quad (5.1.8)$$

where we used (5.1.6) in the averaging. For the average of the second moment we obtain from equation (5.1.7)

$$\langle v^2(t) \rangle = v_0^2 e^{-2\gamma t} + e^{-2\gamma t} \int_0^t dt' \int_0^t dt'' \langle x(t') x(t'') \rangle e^{\gamma(t'+t'')}. \quad (5.1.9)$$

Substituting equation (5.1.4) into (5.1.9) and integrating with respect to t' and t'' we get

$$\langle v^2(t) \rangle = \frac{D}{\gamma} + (v_0^2 - \frac{D}{\gamma}) e^{-2\gamma t}, \quad (5.1.10)$$

which shows that the average of the square velocity and therefore the kinetic energy reaches the equilibrium value

$$\langle v^2(\infty) \rangle = \frac{D}{\gamma} \quad (5.1.11)$$

which is the fluctuation-dissipation relation derived from the Langevin equation. We note here that the apparent difference between Einstein's fluctuation-dissipation relation (5.1.1) and (5.1.11) is the result of the fact that in (5.1.1) D^* denotes the diffusion coefficient while in (5.1.11) D denotes the correlation coefficient of the stochastic force divided by the mass. Although D and D^* are proportional to each other they are not the same. In the following we shall use equation (5.1.11) as a fluctuation- dissipation relation.

In order to obtain the evolution of the probability density $p(v; t)$ of the velocity we have to solve the Fokker-Planck equation (Fokker 1915, Planck 1917). The Fokker-Planck equation which corresponds to the equation (5.1.3) is (Grigolini 1991)

$$\frac{\partial p(v; t)}{\partial t} = \left(\gamma \frac{\partial}{\partial v} v + D \frac{\partial^2}{\partial v^2} \right) p(v; t) \quad (5.1.12)$$

whose solution is

$$p(v; t) = \frac{1}{\sqrt{2\pi \frac{D}{\gamma} (1 - e^{-2\gamma t})}} e^{-\frac{(v - v_0 e^{-\gamma t})^2}{2(1 - e^{-2\gamma t})}}. \quad (5.1.13)$$

For long times the solution (5.1.13) of the Fokker-Planck equation approaches the Maxwell-Boltzmann-distribution i.e.,

$$p(v; \infty) = \frac{1}{\sqrt{2\pi \frac{D}{\gamma}}} e^{-\frac{v^2}{2\frac{D}{\gamma}}} \quad (5.1.14)$$

The above results represent the traditional understanding of Brownian motion.

Remark 5.1.2. From *Remark 5.1.1* we can see that the action of the booster on the velocity of the Brownian particle is represented by a random force. The chaotic and stochastic processes are similar to each other in the sense that both of them produce erratically evolving observables although the chaotic one originates from a deterministic system. Therefore it is a reasonable idea to substitute the random force, i.e., the stochastic booster in the Langevin equation (5.1.3), with a chaotic booster. In the following *Proposition 5.1.1* we show how deterministic Brownian motion emerges when a light particle interacts with a deterministic (but chaotic) booster.

Proposition 5.1.1. If

- i) the motion of a particle takes place in one dimension,
- ii) it is described by the equation of motion

$$\dot{v} = -\gamma v + x(t), \quad (5.1.14)$$

where v denotes the velocity of the particle and $x(t)$ is a chaotic variable which originates from the zero centered logistic map in its fully chaotic regime

$$x(t+1) = 1 - 2x^2(t) \quad (5.1.15)$$

then

- the velocity v reaches the equilibrium distribution $p(v; \infty) = p(v; t \rightarrow \infty)$

$$p(v; \infty) = Z^{-1} \left[1 - \frac{\gamma^2 v^2}{\langle x^2 \rangle} \right]^{\frac{1}{\gamma \tau_{chaos}} - 1}, \quad (5.1.16)$$

where τ_{chaos} is the characteristic time of the chaotic booster

$$\tau_{chaos} = \frac{1}{2} \int_0^\infty \frac{\langle x(t)x(0) \rangle}{\langle x^2 \rangle} dt \quad (5.1.17)$$

and Z^{-1} is the normalizing constant.

Proof. The proof rests on the idea that the logistic map as a booster can be mimicked by a dichotomous noise which has the same variance and characteristic time that the booster has. So we replace the chaotic $x(t)$ in (5.1.3) with a dichotomous noise and we obtain a stochastic differential equation from which we obtain the evolution of the distribution function $p(v; t)$.

The chaotic booster is the logistic map. As we showed in *Proposition A2.5, Appendix 2* the zero centered logistic map (5.1.15) has an invariant i.e., equilibrium distribution

$$\varrho^*(x) = \frac{1}{\pi \sqrt{1 - x^2}}, \quad (5.1.18)$$

the so called U-shaped distribution. It means that most of the time the booster provides values close to ± 1 and it switches back and forth between them in an erratic manner. Since the variance of the booster variable x is

$$\langle x^2 \rangle = \int_0^1 x^2 \varrho^*(x) dx = \frac{1}{2}, \quad (5.1.19)$$

we substitute the booster with the dichotomous noise

$$f(t) = \pm a, \quad (5.1.20)$$

where $a = \frac{1}{\sqrt{2}}$ and the mean value of $f(t)$

$$\langle f(t) \rangle = 0 \quad (5.1.21)$$

and the correlation function of $f(t)$ is

$$\langle f(t)f(0) \rangle = a^2 e^{-t/\tau_c}, \quad (5.1.22)$$

where τ_c is the correlation time of the dichotomous noise. Thus we replace the Langevin-equation (5.1.3) with the stochastic differential equation

$$\dot{v} = -\gamma v + f(t). \quad (5.1.23)$$

We solve equation (5.1.23) by following the procedure developed by Lindenberg and West (Lindenberg and West 1990).

From the definition of the dichotomous noise $f(t)$ we can conclude that the conditional probability $\text{Prob}\{f(t+\tau) = a | f(t) = a\}$ i.e., the probability that $f(t+\tau) = a$ at time $t+\tau$ if $f(t) = a$ at time t is

$$\begin{aligned}\text{Prob}\{f(t+\tau) = a|f(t) = a\} &= \text{Prob}\{f(t+\tau) = -a|f(t) = -a\} \\ &= \frac{1}{2} \left(1 + e^{-\tau/\tau_c}\right)\end{aligned}\quad (5.1.24)$$

and

$$\begin{aligned}\text{Prob}\{f(t+\tau) = a|f(t) = -a\} &= \text{Prob}\{f(t+\tau) = -a|f(t) = a\} \\ &= \frac{1}{2} \left(1 - e^{-\tau/\tau_c}\right).\end{aligned}\quad (5.1.25)$$

From (5.1.24) and (5.1.25) we can write the master equation for the dichotomous noise

$$\frac{\partial}{\partial t} W(a, t|f_0) = -\frac{1}{\tau_c} \frac{\partial}{\partial t} W(a, t|f_0) + \frac{1}{\tau_c} \frac{\partial}{\partial t} W(-a, t|f_0) \quad (5.1.26)$$

and

$$\frac{\partial}{\partial t} W(-a, t|f_0) = -\frac{1}{\tau_c} \frac{\partial}{\partial t} W(-a, t|f_0) + \frac{1}{\tau_c} \frac{\partial}{\partial t} W(a, t|f_0), \quad (5.1.27)$$

where $W(a, t|f_0)$ denotes the conditional probability that $f(t) = a$ at time t if $f(t) = f_0$ at time $t = 0$. Equations (5.1.26 – 27) can be rewritten in operatorial form

$$\frac{\partial}{\partial t} W(f, t|f_0) = \Pi_f W(f, t|f_0), \quad (5.1.28)$$

where

$$\Pi_f = \frac{1}{\tau_c} \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \quad (5.1.29)$$

Similarly we can write the master equation for the Langevin equation (5.1.3) as

$$\frac{\partial}{\partial t} W(v, f, t|v_0, f_0) = \left[-\frac{\partial}{\partial v} (-\gamma v + f) + \Pi_f \right] W(v, f, t|v_0, f_0), \quad (5.1.30)$$

where $W(v, f, t|v_0, f_0)$ denotes the conditional probability that $v(t) = v$ and $f(t) = f$ at time t if $v(0) = v_0$ and $f(0) = f_0$ at time $t = 0$. Substituting (5.1.20) into (5.1.30) and averaging over the initial distribution $P(f_0)$ we get

$$\begin{aligned} \frac{\partial}{\partial t} W(v, a, t|v_0) &= -\frac{\partial}{\partial v} [-\gamma v + a] W(v, a, t|v_0) - \frac{1}{\tau_c} W(v, a, t|v_0) \\ &\quad + \frac{1}{\tau_c} W(v, -a, t|v_0) \end{aligned} \quad (5.1.31)$$

$$\begin{aligned} \frac{\partial}{\partial t} W(v, -a, t|v_0) &= -\frac{\partial}{\partial v} [-\gamma v - a] W(v, -a, t|v_0) - \frac{1}{\tau_c} W(v, -a, t|v_0) \\ &\quad + \frac{1}{\tau_c} W(v, a, t|v_0). \end{aligned} \quad (5.1.32)$$

Introducing the sum and difference distributions $W_t(v, t|v_0)$ and $S_t(v, t|v_0)$ respectively (5.1.31 – 32) become

$$\frac{\partial}{\partial t} W_t(v, t|v_0) = \gamma \frac{\partial}{\partial v} v W_t(v, t|v_0) - a \frac{\partial}{\partial v} S_t(v, t|v_0) \quad (5.1.33)$$

$$\frac{\partial}{\partial t} S_t(v, t|v_0) = - \left[\frac{2}{\tau_c} - \gamma \frac{\partial}{\partial v} v \right] S_t(v, t|v_0) - a \frac{\partial}{\partial v} W_t(v, t|v_0). \quad (5.1.34)$$

We are looking for the steady state solutions $W_s(v)$ and $S_s(v)$ i.e., solutions, where the left hand sides of (5.1.33 – 34) vanish and they become

$$\gamma \frac{\partial}{\partial v} v W_s(v) = a \frac{\partial}{\partial v} S_s(v) \quad (5.1.35)$$

$$\left[\frac{2}{\tau_c} - \gamma \frac{\partial}{\partial v} v \right] S_s(v) = -a \frac{\partial}{\partial v} W_s(v) \quad (5.1.36)$$

From (5.1.35) with zero flux boundary conditions we find

$$S_s(v) = \frac{\gamma v}{a} W_s(v). \quad (5.1.37)$$

Substituting this relation into (5.1.36) and solving it again subject to zero flux boundary condition finally yields

$$W_s(v) = Z'^{-1} \frac{1}{a^2 - \gamma^2 v^2} e^{\frac{-2}{\tau_c} \int^v dv' \frac{\gamma v'}{a^2 - \gamma^2 v'^2}}, \quad (5.1.38)$$

where Z'^{-1} is the normalizing constant. After performing the integration in (5.1.38) and using (5.1.19 – 22) i.e., $\langle x^2 \rangle = a^2 = 1/2$ we obtain (5.1.16).

q.e.d

Proposition 5.1.2. If

- i) the motion of a particle takes place in one dimension,
- ii) it is described by the equation of motion

$$\dot{v} = -\gamma v + x(t), \quad (5.1.3)$$

where v denotes the velocity of the particle and $x(t)$ the chaotic variable which originates from the zero centered logistic map in its fully chaotic regime

$$x_{n+1} = 1 - 2x_n^2 \quad (5.1.15)$$

then

- the evolution of the discretized velocity is given by

$$v_{n+1} = \frac{1}{2} \left(v_{n+1}^{(1)} + v_{n+1}^{(2)} \right), \quad (5.1.39)$$

to accuracy $O(h^3)$, where

$$v_{n+1}^{(1)} = v_n - h\gamma v_n + \sqrt{h}x_n \quad (5.1.40)$$

$$v_{n+1}^{(2)} = v_n - h\gamma v_{n+1}^{(1)} + \sqrt{h}x_n, \quad (5.1.41)$$

with integration step h and

$$\tau_{chaos} \ll 1/\gamma \quad (5.1.42)$$

- the evolution of the discretized velocity is given by

$$v_{n+1} = \frac{1}{2} \left(v_{n+1}^{(1)} + v_{n+1}^{(2)} \right), \quad (5.1.39)$$

to accuracy $O(h^3)$, where

$$v_{n+1}^{(1)} = v_n - h(x_n - \gamma v_n) \quad (5.1.43)$$

$$v_{n+1}^{(2)} = v_n + h(x_n - \gamma v_{n+1}^{(1)}), \quad (5.1.44)$$

with h integration step and

$$\tau_{chaos} \gg 1/\gamma. \quad (5.1.45)$$

Proof. Proposition 5.1.1 gives the algorithm to solve equation (5.1.3) numerically. The equation (5.1.3) is a linear stochastic equation thus a modified Euler method (Gerald 1970) provides a satisfactory accuracy as a numerical solution of equation (5.1.3). The modified Euler method is a predictor-corrector method where we use the result of the Euler method as a predictor and we use this predicted value in the calculation of the corrector (Press et al. 1990). In order to show how the modified Euler-method works we consider the differential equation

$$\frac{dy}{dt} = f(y). \quad (5.1.46)$$

The Euler method gives an estimate of $y_{n+1}^{(1)}$ knowing y_n

$$y_{n+1}^{(1)} = y_n + h \left. \frac{dy}{dt} \right|_{t=t_n} = y_n + hf(y_n). \quad (5.1.47)$$

Another estimate $y_{n+1}^{(2)}$ is provided by calculating the derivative at the point $t = t_n + h$

$$y_{n+1}^{(2)} = y_n + h \left. \frac{dy}{dt} \right|_{t=t_n+h} = y_n + hf(y_{n+1}). \quad (5.1.48)$$

In order to calculate $f(y_{n+1})$ we should know y_{n+1} exactly but we do not know it. Thus we approximate it by $y_{n+1}^{(1)}$. So (5.1.46) becomes

$$y_{n+1}^{(2)} = y_n + hf(y_{n+1}^{(1)}). \quad (5.1.49)$$

We get a good estimate for y_{n+1} by taking the arithmetic mean of the predictor $y_{n+1}^{(1)}$ and corrector $y_{n+1}^{(2)}$

$$y_{n+1} = \frac{1}{2} \left(y_{n+1}^{(1)} + y_{n+1}^{(2)} \right). \quad (5.1.50)$$

In the case of $\tau_{chaos} \gg 1/\gamma$ the chaotic variable changes slowly, i.e., $x(t)$ is adiabatic variable. The addition of an adiabatic $x(t)$ to the right hand side of (5.1.46) changes (5.1.47 – 48) into the following form

$$y_{n+1}^{(1)} = y_n + hf(y_n) + hx_n \quad (5.1.51)$$

and

$$y_{n+1}^{(2)} = y_n + hf(y_{n+1}^{(1)}) + hx_n. \quad (5.1.52)$$

respectively. Identifying $y = v$ and $f(y) = -\gamma v$ (5.1.50 – 52) become (5.1.39) and (5.1.43 – 44) respectively.

In the case of $\tau_{chaos} \ll 1/\gamma$ the chaotic variable is fast therefore it is considered to be a random-like variable. The averaging over x for a time of length h takes place as it is done over the random variables. In order to do so let us consider the differential equation

$$\dot{y} = x(t), \quad (5.1.53)$$

where $x(t)$ is a delta-correlated stochastic variable with zero mean value

$$\langle x(t)x(0) \rangle = 2D\delta(t). \quad (5.1.54)$$

We know from the Central Limit Theorem (*Proposition 2.1.1*) that in this case the variable y shows diffusion

$$\langle y^2(t) \rangle = 2Dt \quad (5.1.55)$$

and at the same time y changes randomly thus it can be written as

$$y(t) = \sqrt{2Dt}\xi(t) \quad (5.1.56)$$

where $\xi(t)$ is a random variable with Gaussian distribution and variance $\langle \xi^2(t) \rangle = 1$.

Therefore the stochastic equation (5.1.53) can be discretized in the form of

$$y_{n+1} = y_n + \sqrt{2Dh}\xi(t) = y_n + \sqrt{h}x_n, \quad (5.1.57)$$

where h is the integration step.

In the case of $\tau_{chaos} \ll 1/\gamma$ the differential equation (5.1.3) is discretized by combining the discretization of the deterministic part $\dot{v} = -\gamma v$ and the random-like part $\dot{v} = x(t)$. The discretization of the deterministic part takes place by identifying $y = v$ and $f(y) = -\gamma v$ in (5.1.47), while (5.1.57) provides the discretization for the chaotic part. Thus the predictor of (5.1.3) is

$$v_{n+1}^{(1)} = v_n - h\gamma v_n + \sqrt{h}x_n \quad (5.1.40)$$

and the corrector is (5.1.41). predictor (5.1.40) and the corrector (5.1.41) yields v_{n+1} .

The only thing left to complete the proof is to show that the algorithm (5.1.39–41) and (5.1.39), (5.1.43–44) is correct to order $O(h^3)$. From (5.1.47) and (5.1.48) we get that the discretized form of (5.1.46) is

$$y_{n+1} = y_n + \frac{h}{2} [f(y_n) + f(y_n + hf(y_n))]. \quad (5.1.58)$$

Expanding the term $f(y_n + hf(y_n))$ in a Taylor-series and neglecting higher than linear terms in the expansion we realize that the algorithm we presented above

provide an accuracy of order h^2 which is satisfactory for the linear system (5.1.3) with a proper choice of integration step h .

q.e.d.

Remark 5.1.3. The algorithm we showed in *Proposition 5.1.2* was originally proposed by Rao et al. (Rao et al. 1974) and it was developed further by Sanchez (Sanchez 1982), Mannella et al. (Mannella et al. 1989) and Gard (Gard 1988) in several forms. For instance the algorithm of Mannella et al. was successfully applied for multiplicative and additive noises in nonlinear systems as well (Mannella 1989, Bonci et al. 1991).

We applied the algorithm of *Proposition 5.1.2* in 3 cases: $\gamma = 0.01$, $\gamma = 10.0$ and $\gamma = 3.0$. We calculated the equilibrium-distribution of the velocity v from 10,000 trajectories with integration step $h = 0.01$. The equilibrium distributions of the velocity v are plotted in *Figures 5.1.1a-c* for the three different dissipation parameters γ . The results of the numerical calculations are compared to the results of the theoretical investigations (5.1.16). The characteristic time of the chaotic booster (5.1.15) is calculated by (5.1.17). Since the logistic map (5.1.15) is δ -correlated (see *Proposition A2.6*), thus $\tau_{chaos} = 1$.

For the small γ case i.e., when $\gamma = 0.01$ so $\tau_{chaos} \ll 1/\gamma$ there is a large time-scale separation between the time-scale of the booster characterized by $\tau_{chaos} = 1$ and the motion of the particle characterized by time-scale $1/\gamma = 100$. Thus the particle accumulates the fluctuations of the booster and its energy or velocity-square eventually reaches the Maxwell-Boltzmann distribution which implies that the velocity follows the Gaussian distribution (see *Figure 5.1.1a*).

Figure 5.1.1a. The velocity equilibrium distribution $p(v)$ of the Brownian particle in the small γ case. The circles show the results of numerical simulations based on map (5.1.39–41) and the solid line shows the result of the theoretical investigations calculated from (5.1.16). The parameter values we used: $\tau_{chaos} = 1.0$, $\langle x^2 \rangle = 1/2$, $\gamma = 0.01$ and integration step $h = 0.1$.

In cases when the motion of the particle is faster than that of the booster (large γ) the particle is fast enough to trace the motion of the booster in a rescaled manner. Thus the equilibrium distribution of the velocity is more similar to the equilibrium distribution of the booster (see *Figure A2.3* for the equilibrium distribution of the booster). We calculated the large γ case with $\gamma = 10.0$ and plotted the result in *Figure 5.1.1b*.

Figure 5.1.1b. The velocity equilibrium distribution $p(v)$ of the Brownian particle in the large γ case. The circles show the results of numerical simulations based on map (5.1.39) and (5.1.43 – 44) and the solid line shows the result of the theoretical investigations calculated from (5.1.16). The parameter values we used: $\tau_{chaos} = 1.0$, $\langle x^2 \rangle = 1/2$, $\gamma = 10.0$ and integration step $h = 0.001$.

In the case of intermediate dissipation, i.e., when the τ_{chaos} is comparable to $1/\gamma$ the situation is a mixture of the above two cases. The equilibrium distribution of the velocity shows the properties of the booster as long as it inherits the U-shape of the equilibrium distribution of the booster but it is less steep and starts broadening. We investigated the case of $\gamma = 3.0$ and plotted the results in *Figure 5.1.1c*.

Figure 5.1.1c. The velocity equilibrium distribution $p(v)$ of the Brownian particle in the modest γ case. The circles show the results of numerical simulations based on map (5.1.39) and (5.1.43 – 44) and the solid line shows the result of the theoretical investigations calculated from (5.1.16). The parameter values we used: $\tau_{chaos} = 1.0$, $\langle x^2 \rangle = 1/2$, $\gamma = 3.0$ and integration step $h = 0.01$.

The theoretical results are in good agreement with the results of the numerical calculations for the small γ case, while the other cases show apparent deviations. This is expected since the theory so far discussed is a stochastic theory and it only works well, where the genuine stochastic properties dominate (e.g. Central Limit Theorem). In the cases, where the system is more deterministic-like we should mimick the booster with a different estimate of the statistical properties, especially as far as the second moment is concerned.

One could also wonder why the equilibrium distribution of the velocity is so different from the usual Gaussian distribution in the large and modest γ cases. The system is overdamped since it is strongly coupled to the booster and the velocity does not have time to accumulate the random actions of the booster. In other words it relaxes too fast compared to the booster.

Remark 5.1.4. There has been some efforts to derive deterministic Brownian motion (Beck 1990, Prakash et al. 1991, Trefán et al. 1991) although all of them share a common disadvantage – the presence of a phenomenological dissipation term $-\gamma v$. The appearance of a phenomenological dissipation term is an *ad hoc* assumption which forces the system from outside to obey the fluctuation- dissipation theorem. In order to have a self-consistent physical picture we need to build up a model where the dissipation is the result of the reaction of the particle on the booster and fluctuations are the result of the action of the chaotic booster on the particle. We develop this theory in the following paragraph.

§5.2 Deterministic Brownian motion – self consistent picture

Remark 5.2.1. As we pointed out in *Remark 5.1.4* the model of the Brownian motion where a phenomenological dissipative term is assumed is not satisfactory, because the dissipation is an *ad hoc* assumption. We now build up a model where both the dissipation and the fluctuation originates from the interaction of a particle with a booster. This is our goal in the present chapter, where we follow the idea developed by the author and his colleagues in (Bianucci et al. 1993b).

We consider a *1-dimensional model* where a light particle interacts with a chaotic booster. On one side the chaotic booster has a short characteristic time

τ_{chaos} and we assume that the action of the booster abruptly changes the velocity of the Brownian particle at the end of each time interval with length τ_{chaos} i.e., the particle receives an erratic kick from the booster at equidistant instants. The chaotic kicks on the particle lead to the diffusion of the velocity as we discussed earlier.

On the other side the light particle reacts on the booster. The reaction is a negative feedback which is proportional to the velocity. This feedback perturbs the booster and slightly moves it out of equilibrium. For instance, for large negative velocities the booster gives a series of chaotic kicks with positive mean values. Thus the booster produces a drift in the velocity towards its equilibrium which is a dissipation from the point of view of the velocity. This dissipation limits the otherwise unbounded growth of the velocity diffusion and as a result of the competing diffusion and dissipation the velocity of the Brownian particle reaches dynamical equilibrium with the booster. So does its average kinetic energy.

This model is expressed in mathematical form by a 2-dimensional impact mapping where the actual velocity is a sum of its previous value and a kick of a fully chaotic 1-dimensional map. The dynamics of the booster is given by a 1-parameter conjugated map of a fully chaotic map where the conjugation parameter is negatively proportional to the velocity. This conjugation, as we shall see in the following *Proposition 5.2.1*, creates the reaction or feedback which leads to a dissipation.

Proposition 5.2.1. If

- i) the 1-dimensional dynamics of a particle
- ii) is given by the following 2-dimensional impact mapping

$$v_{n+1} = v_n + x_n \tag{5.2.1}$$

$$x_{n+1} = g_a(x_n), \quad (5.2.2)$$

iii) where $g_a(x)$ is the conjugation of a zero-centered, fully chaotic map $f(t) : [-1, 1] \mapsto [-1, 1]$, $t \in [-1, 1]$ i.e.,

$$g_a(x) = h_a \circ f \circ h_a^{-1}(x), \quad (5.2.3)$$

iv) where the conjugating function $h_a(t)$ is

$$x = h_a(t) = \begin{cases} -1 + \sqrt{a^2 - (t - a + 1)^2}, & \text{for } -1 \leq t < a - 1; \\ 1 - \sqrt{(2 - a)^2 - (t - a + 1)^2}, & \text{for } a - 1 \leq t < 1; \end{cases} \quad (5.2.4)$$

where $a \in [0, 2]$,

v) and the conjugation parameter is negatively proportional to the velocity

$$a - 1 = -\Delta^2 v, \quad (5.2.5)$$

where Δ is a small reaction coefficient then

- the velocity v is indistinguishable from the velocity of a Brownian particle.

Proof. When we want to show that the velocity is that of a Brownian particle we have to show that from the map we can derive the Langevin equation

$$\dot{v} = -\gamma v + x(t) \quad (5.2.6)$$

or the Fokker-Planck equation

$$\frac{\partial}{\partial t} \varrho(v; t) = \gamma \frac{\partial}{\partial v} v + D \frac{\partial^2}{\partial v^2} \varrho(v; t). \quad (5.2.7)$$

We show this claim in the following way. First we show that (5.2.1) results in diffusion of the velocity therefore it is equivalent to an equation $\dot{v} = x(t)$, where $x(t)$ is

a random force with short correlation. Then we show that the feedback (5.2.2 – 5) is equivalent to the action of a dissipative term $-\gamma v$ in (5.2.6).

The diffusion. The fully chaotic map $f(t) : [-1, 1] \mapsto [-1, 1]$ is subjected to a conjugation. The conjugation preserves the Lyapunov spectrum (Devaney 1989) therefore it preserves the chaoticity as well. Since the feedback is small the correlation properties of the map (5.2.2) do not differ significantly from the unperturbed map $g_{a=1}(x)$ – apart from a small drift term. Since the unperturbed map $g_{a=1}(x)$ is symmetric, as we proved in *Proposition A2.6* and *Remark A2.11*, its correlation function vanishes in one step i.e., it is delta-correlated. Thus the consecutive values $x_n, x_{n+1}, \dots$ represent a sequence of short correlated kicks with same correlation time. The correlation time τ_{booster} of the booster is defined according to (2.2.8)

$$\tau_{\text{booster}} = \frac{\sum_{n=0}^{\infty} \langle x_n x_0 \rangle}{\langle x_0^2 \rangle}. \quad (2.2.8)$$

Since

$$\langle x_n x_0 \rangle = 2D \delta_{n,0}, \quad (5.2.8)$$

where

$$2D = \langle x_0^2 \rangle, \quad (5.2.9)$$

therefore

$$\tau_{\text{booster}} = 1. \quad (5.2.10)$$

Equation (5.2.1) shows that the velocity is the collector variable of the chaotic kicks with short correlation (5.2.8). Therefore the velocity v of (5.2.1) fulfills the requirements of the Central Limit theorem (*Proposition 2.1.1*) i.e., the velocity is

diffusive. Thus (5.2.1) mimicks the Langevin equation (5.2.6) without the dissipation term $-\gamma v$.

The dissipation. The feedback or the reaction of the particle on the booster is defined by equations (5.2.3 – 5). From the definition (5.2.3 – 4) of the conjugation function we can see that for $a = 1$ the conjugation function $h_a(t)$ is antisymmetric

$$h_{a=1}(-t) = -h_{a=1}(t), \quad (5.2.11)$$

so the conjugated map $g_a(x)$ is symmetric for $a = 1$.

$$g_{a=1}(-x) = g_{a=1}(x). \quad (5.2.12)$$

Thus the map $g_a(x)$ with $a = 1$ produces a sequence of x -s with zero mean value

$$\langle x_n \rangle_{a=1} = 0, \quad (5.2.13)$$

where $\langle \dots \rangle_{a=1}$ denotes the averaging over an ensemble of the dynamics of $g_{a=1}(x_n)$ when $a = 1$. We refer to the case with $a = 1$ as the unperturbed booster or the booster with unperturbed dynamics. From (5.2.5) we can see that the dynamics is unperturbed when the velocity $v = 0$.

Now let us see what happens when the velocity reaches a large positive value. When v is large and positive then from (5.2.5) the perturbation parameter $a - 1$ is small

$$|a - 1| \ll 1. \quad (5.2.14)$$

It means that the dynamics of the booster $g_a(x)$ is subjected to a small, negative perturbation. In this case the booster provides a series of x -s with a modest negative mean

$$\langle x_n \rangle_{a < 1} < 0. \quad (5.2.15)$$

From (5.2.5) the perturbation is negatively proportional to the velocity v . To small perturbations the booster responds proportionally to the strength of the perturbation $a - 1$

$$\langle x_n \rangle = \langle g_a(x_n) \rangle = (a - 1)\chi, \quad (5.2.16)$$

where χ denotes the generalized susceptibility

$$\chi = \left. \frac{\partial \langle x_n \rangle}{\partial a} \right|_{a=1}. \quad (5.2.17)$$

From (5.2.16 – 17) and (5.2.5) we obtain

$$\langle x_n \rangle = \langle g_a(x_n) \rangle = -\Delta^2 \chi \langle v_n \rangle. \quad (5.2.18)$$

From (5.2.1) we can see that this negative mean (5.2.18) is accumulated in the velocity v thus forcing the velocity from its large positive value to tend to zero. This mechanism is the dissipation. Since the booster variable x couples directly to the velocity v we can identify the coefficient $-\Delta^2 \chi$ as the dissipation parameter γ i.e.,

$$\gamma = \Delta^2 \chi \quad (5.2.19)$$

From the aboves we can conclude that the impact map (5.2.1 – 5) represents a Langevin equation with the dissipation coefficient (5.2.19) and fluctuation coefficient

$$D = \frac{1}{2} \langle x_n^2 \rangle \tau_{\text{booster}} \quad (2.2.2)$$

Thus the fluctuation – dissipation relation for map (5.2.1 – 5) reads

$$\langle v^2 \rangle = \frac{D}{\gamma} = \frac{1}{2} \frac{\langle x_0^2 \rangle \tau_{booster}}{\Delta^2 \chi}. \quad (5.2.20)$$

q.e.d

Remark 5.2.2. In the followings we show two examples for the realization of *Proposition 5.2.1*.

In the first example we consider the case where the map (5.2.2) is the conjugate of the zero-centered tent map

$$t_{n+1} = 1 - 2|t_n| \quad (4.1)$$

with the conjugation function (5.2.3 – 4). If the velocity is that of a Brownian particle then, as we showed in *Remark 5.1.1*, its average relaxes according to (5.1.8)

$$\langle v_n \rangle = v_0 e^{-\gamma n} \quad (5.1.8)$$

and the average kinetic energy or average velocity square evolves according to (5.1.10)

$$\langle v_n^2 \rangle = \frac{D}{\gamma} + (v_0^2 - \frac{D}{\gamma}) e^{-\gamma n}, \quad (5.1.10)$$

where n denotes the discrete time.

We can determine the fluctuation coefficient D from (2.2.2), where $\langle x_0^2 \rangle$ denotes the variance of the unperturbed dynamics of the conjugated map. Using the results of (4.12) $\langle x_0^2 \rangle$ becomes

$$\langle x_0^2 \rangle = \int_{-1}^1 x_0^2 \ell_g^*(x_0) dx_0 = \frac{1}{2} \int_{-1}^1 x_0^2 \frac{dh^{-1}(x_0)}{dx_0} dx_0, \quad (5.2.21)$$

where $h^{-1}(x)$ is the inverse of the conjugation function (5.2.4) given by (4.11)

$$h^{-1}(x) = \begin{cases} a - 1 - \sqrt{a^2 - (x + 1)^2}, & \text{for } -1 \leq x < a - 1; \\ a - 1 + \sqrt{(2 - a)^2 - (x - 1)^2}, & \text{for } a - 1 \leq x \leq 1. \end{cases} \quad (4.11)$$

Substituting (4.11) into (5.2.21) and evaluating the integral for the unperturbed case ($a = 1$) we get

$$\langle x_0^2 \rangle = 1 + \int_{-1}^0 x \sqrt{1 - (x + 1)^2} dx - \int_0^1 x \sqrt{1 - (x - 1)^2} dx = \frac{5}{3} - \frac{\pi}{2} = 0.0959. \quad (5.2.22)$$

From (2.2.22), (5.2.22) and (5.2.10) the fluctuation coefficient D is

$$D = \frac{1}{2} \left(\frac{5}{3} - \frac{\pi}{2} \right) = 0.0480. \quad (5.2.23)$$

The dissipation coefficient γ we determine from (5.2.19). We showed in *Proposition 4.1* that if the zero centered tent map is subjected to perturbation by conjugation with the conjugating function (5.2.4) then the generalized susceptibility χ is

$$\chi = \frac{\pi}{2} - 1. \quad (4.4)$$

Thus from (5.2.19) and from (4.4) the dissipation coefficient is

$$\gamma = -\Delta^2 \left(\frac{\pi}{2} - 1 \right). \quad (5.2.24)$$

We executed computer calculations to monitor the relaxation of the average velocity.

The initial velocity v_0 was chosen to be $v_0 = 100$, the reaction parameter Δ was

chosen to be small in order to keep the perturbation small and the booster was initially placed into the equilibrium of the unperturbed map. The way to place the booster in unperturbed equilibrium is to place the tent map in equilibrium initially i.e., to start the evolution of the tent map from uniformly distributed random initial values on the interval $[-1, 1]$. The average was taken over 10,000 different initial conditions. The resulting velocity relaxation is plotted in *Figure 5.2.1*. The results of the computer calculations are compared to the theoretical results obtained from (5.1.8) with (5.2.23) and (5.2.24).

Figure 5.2.1. Relaxation of the velocity of map (5.2.1 – 5) with reaction parameter $\Delta = 0.01$. (5.2.3) is the conjugate of the tent map . The velocity is set initially to $v_0 = 100$ and the average is taken over 10,000 samples. The circles show the results of numerical calculations and the solid line represents the theoretical prediction of (5.1.8) with (5.2.23) and (5.2.24).

We also calculated the evolution of the average kinetic energy for some values of the reaction parameter. Δ was chosen to be 0.005, 0.006, ..., 0.01. The velocity was initially set to $v_0 = 0$ and the booster started its evolution from its unperturbed equilibrium. The results on the evolution of the average velocity square are plotted in *Figure 5.2.2*. We compared the results of computer calculations to the theoretical results calculated from (5.1.10) with (5.2.23) and (5.2.24).

Figure 5.2.2. Evolution of the average velocity square from map (5.2.1 – 5) for some values of the reaction parameter Δ . (5.2.3) is the conjugate of the tent map. The velocity was initially set to $v_0 = 0$ and the average was taken over 10,000 trajectories. The circles represent the results of computer calculations and the solid line shows the theoretical results using (5.1.10) with (5.2.23) and (5.2.24).

The second example is where map (5.2.2) is the conjugate of the zero-centered logistic map

$$t_{n+1} = 1 - 2t_n^2 \quad (4.15)$$

with the conjugating function (5.2.3 – 5). Here again we monitor the the evolution of the average velocity square and the relaxation of the average velocity. In order to do so we need the fluctuation coefficient D and dissipation coefficient γ .

The fluctuation coefficient D is determined from (2.2.22), where in the calculation of the variance $\langle x_0^2 \rangle$ the average must be taken over the invariant distribution (4.21). The inverse conjugation function is (4.11) so for D we obtain

$$D = 0.1134. \quad (5.2.25)$$

The dissipation coefficient γ was determined from (5.2.19) using the result of *Proposition 4.2*, where we showed that the generalized susceptibility χ of the perturbed logistic map, if the perturbation was represented by the conjugating function (5.2.4), is

$$\chi = 0.4404. \quad (5.2.26)$$

We realized (5.2.1 – 5) on the computer and monitored the relaxation of the average velocity starting from a non-equilibrium position $v_0 = 100$. The reaction parameter was chosen to be small, $\Delta = 0.01$ and the booster started to evolve from its unperturbed equilibrium. The average was taken over 10,000 samples. The results are plotted in *Figure 5.2.3*.

We also monitored the evolution of the velocity square when the velocity was set initially to $v_0 = 0$. We used several values of the reaction parameter Δ and plotted the results in *Figure 5.2.4*.

Figure 5.2.3. Relaxation of the velocity of map (5.2.1 – 5) with reaction parameter $\Delta = 0.01$. (5.2.3) is the conjugate of the logistic map. The velocity is set initially to $v_0 = 100$ and the average is taken over 10,000 samples. The circles show the results of numerical calculations and the solid line represents the theoretical prediction of (5.1.8) with (5.2.25) and (5.2.26).

From *Figures 5.2.1-4* we can see that the results of numerical calculations and the theory are in good agreement.

Figure 5.2.4. Evolution of the average velocity square from map (5.2.1 – 5) for some values of the reaction parameter Δ . (5.2.3) is the conjugate of the logistic map. The velocity was initially set to $v_0 = 0$ and the average was taken over 10,000 trajectories. The circles represent the results of computer calculations and the solid line shows the the theoretical results using (5.1.10) with (5.2.23) and (5.2.24).

CHAPTER 6

CONCLUSION

We have shown that a rigorously microscopic derivation of the Fokker-Planck equation rests on the rigorously microscopic derivation of both diffusion and friction from the interaction of the system of interest with the same "thermal bath".

The problem of deriving diffusion from a deterministic process has been addressed and successfully solved by many groups (Chirikov 1979, Rechester and White 1980, Cary et al. 1981, Schell et al. 1982, Doran and Fishman 1988). We have shown that the standard diffusion behind the Fokker-Planck equation essentially rests on the Central Limit Theorem, and, consequently, on the possibility of deriving from a deterministic process of a given variable x a decaying correlation function. The so called sensitive dependence of chaos on initial conditions insures this possibility.

The problem of deriving friction from the interaction with a fully deterministic bath, that we term booster, was much more difficult to solve. We have carefully addressed this problem and we have shown that the solution of this problem essentially rests on the linear response of a booster to an external perturbation.

This raises a long-standing problem, that of the Kubo linear response theory and of the strong criticism by van Kampen against this theory. The Kubo linear response theory is based on a perturbation treatment of the Liouville equation, which, in turn, is expected to be totally equivalent to a first-order perturbation treatment of single trajectories. Since the boosters are chaotic, and chaos is essential to generate diffusion, the single trajectories are highly unstable and do not respond linearly to weak external perturbation.

To deal with this intriguing problem we have replaced the continuous-time representation with a discrete-time picture. In other words, we have adopted maps as boosters of our Brownian particle, and we have therefore addressed the problem of the response of a chaotic booster to an external perturbation.

We have noticed that a chaotic mapping is characterized by an invariant measure which is a continuous function of the control parameters of the map. Consequently if the external perturbation is made to act on a control parameter of the map, we have that the booster distribution undergoes slight modifications as an effect of weak external perturbation, thereby leading to a linear response of the mean value of the perturbed variable of the booster. This approach to the linear response bypasses completely the criticism of van Kampen.

The joint use of these two ingredients, diffusion and friction stemming from the interaction of the Brownian particle with the same booster, making possible for us to derive (Bianucci et al. 1993b) what, to the best of our knowledge, must be considered as being the microscopic derivation of a Fokker-Planck equation.

The comparison of the analytic to the simulation results are extremely good. We can construct a fully chaotic deterministic process as close as we want to the dynamical behavior of a Fokker-Planck equation. However, there are many problems left for future investigation. First of all, we have shown how to derive a linear response to a chaotic system, in spite of the warnings of van Kampen. The warnings of van Kampen focus on the adoption of a perturbation approach to the linear response, and do not concern the possibility itself of deriving a linear response out of a chaotic system.

Thus, we have now to face the problem of whether or not our approach to the linear response conflicts with the approach of Kubo. There are preliminary results showing that the Kubo approach to the derivation of the time asymptotic value of

the susceptibility leads to an exact result. We believe that the theoretical analysis carried out in this dissertation proves to be of fundamental importance in explaining why it is so. We have indeed shown that the invariant distributions are stable against external perturbation and this stability makes it possible to successfully adopt a perturbation treatment.

Encouraged by these results, we do hope that we shall be able to successfully address a more difficult problem, that of deriving the Fokker-Planck equation from a fully Hamiltonian picture, within a continuous time representation.

The problem of deriving statistical mechanics from chaos, as we have tried to do it in this dissertation, cannot be really carried out if we ignore that microscopic dynamics is in fact driven by quantum mechanics. For the foundation of statistical physics one needs to use chaotic systems, thus the classically chaotic quantum systems are of paramount interest from the point of view of statistical physics. In fact, the manifestation of chaos in classically chaotic quantum systems is a subject of active research (Casati et al. 1979, Izrailev 1990). On the other hand the origin of irreversibility in quantum mechanics is a very difficult problem.

This difficulty lies in the fact that in classical systems chaoticity means that two, initially close orbits depart from each other in an exponential manner. This very rapid divergence of orbits results in the motions of two, initially close orbits becoming independent of each other in a short time. Thus a chaotic environment behaves like a random environment which results in irreversibility. The corresponding quantum mechanical average orbits follow the classical path, but the overlap of the orbits grows exponentially like the divergence of averages. The overlap keeps the wave functions of the corresponding classical orbits in phase and it provides a robust cohesion of the wavefunction. Thus the exponential separation of classical orbits does not result in dephasing, i.e., uncorrelated motion, thus a classically chaotic

quantum system does not produce relaxation. In other words quantum mechanics means that the instability of trajectories is lost, and that the long-range correlations, in time and space, are established. Consequently the problem of quantum irreversibility is very difficult, nevertheless there have been successful attempts at describing irreversibility in classically chaotic quantum systems (Bonci et al. 1992, Roncaglia 1992). Thus this disertation is the first step on a long road whose end is the extremely difficult enterprise of establishing a dynamical basis of quantum statistical mechanics.

A promising way of approaching the problem of irreversibility of quantum mechanical origin is to study classical systems of weak chaos. Quantum uncertainty tends to spread all over the region of the classical phase space occupied by chaotic clouds. For this reason, an approach to the canonical equilibrium distribution through the Fokker-Planck equation, which do not rest on the total ergodicity of the system, can be very useful. The traditional approach to the canonical equilibrium distribution, is, more or less, as follows. One assumes ergodicity first. This means a microcanonical equilibrium distribution. Then, one makes a contraction over the irrelevant degrees of freedom of this microcanonical equilibrium distribution, and one gets a canonical equilibrium distribution. From the point of view of quantum mechanics the microcanonical distribution might become an enormous quantum cloud. If we derive the canonical equilibrium distribution by means of our Fokker-Planck approach, we can rederive the classical statistical mechanics as well.

Another possible direction of research could be exploring quantum maps (Berry et al. 1979, Tabor 1983), where one could attempt to understand what the conjugation means and if it is possible to build up a feedback by conjugation in quantum maps.

APPENDIX 1

THE ZWANZIG PROJECTION TECHNIQUE

In *Chapter 2*, §2.3 we studied the deterministic diffusion in the standard map and we derived the diffusion coefficient using the Zwanzig projection technique. The Zwanzig projection technique, which is a quantum mechanics-like formalism, was developed originally for continuous classical systems (Nakajima 1958, Zwanzig 1960) and it was applied to various physical systems (Grabert 1982). In this appendix we show the basic ideas and definitions. We introduce the projection operator and we derive a master equation using it. Then we show how a memory kernel arises in simple cases and how one can calculate the averages of observables of interest.

Let us consider a classical physical system with a set of "relevant" variables or variables of interest $\vec{a}$ and a set of "irrelevant" variables or variables of the environment $\vec{b}$. Since the system is classical the equations of motion for the probability distribution ρ is given in terms of the Liouville-operator $\hat{L}$

$$\frac{\partial}{\partial t} \rho(\vec{a}, \vec{b}; t) = \hat{L} \rho(\vec{a}, \vec{b}; t). \quad (\text{A1.1})$$

Let us assume that $\hat{L}$ may be written as

$$\hat{L} = \hat{L}_a + \hat{L}_b + \hat{L}_I, \quad (\text{A1.2})$$

where $\hat{L}_a$ and $\hat{L}_b$ describe the evolution of the distribution due to variables $\vec{a}$ and $\vec{b}$, and $\hat{L}_I$ expresses the evolution of ρ due to the interaction between the variables $\vec{a}$ and $\vec{b}$. Let us assume furthermore that $\hat{L}_b$ admits an equilibrium distribution

$$\hat{L}_b \rho_{eq}(\vec{b}) = 0. \quad (\text{A1.3})$$

Thus the projection operator P is defined

$$P \rho(\vec{a}, \vec{b}; t) \equiv \rho_{eq}(\vec{b}) \sigma(\vec{a}; t) \equiv \rho_{eq}(\vec{b}) \int d\vec{b} \rho(\vec{a}, \vec{b}; t). \quad (\text{A1.4})$$

If $\rho_{eq}(\vec{b})$ is normalized the operator P is idempotent

$$P^2 = P. \quad (A1.5)$$

We introduce the densities ρ_1 and ρ_2 which correspond to the projection operator P and its conjugate Q in the following way

$$\rho = \rho_1 + \rho_2, \quad (A1.6)$$

where

$$\rho_1 = P\rho \quad (A1.7)$$

and

$$\rho_2 = Q\rho = (1 - P)\rho. \quad (A1.8)$$

Thus the evolution equation (A1.1) becomes

$$\frac{\partial}{\partial t}\rho = \hat{L}(\rho_1 + \rho_2). \quad (A1.9)$$

Applying operators P and Q on both sides of (A1.9) becomes

$$\frac{\partial}{\partial t}\rho_1 = P\hat{L}(\rho_1 + \rho_2) \quad (A1.10)$$

and

$$\frac{\partial}{\partial t}\rho_2 = Q\hat{L}(\rho_1 + \rho_2). \quad (A1.11)$$

Equation (A1.11) is a first order inhomogenous equation with the formal solution

$$\rho_2(t) = e^{Q\hat{L}t}Q\rho(0) + \int_0^t ds e^{Q\hat{L}s}Q\hat{L}P\rho(t-s)\rho(0). \quad (A1.12)$$

Substituting (A1.12) into (A1.10) we obtain the master equation

$$\frac{\partial}{\partial t}\rho_1(t) = P\hat{L}P\rho(t) + \int_0^t ds P\hat{L}e^{Q\hat{L}s}Q\hat{L}P\rho(t-s) + P\hat{L}e^{Q\hat{L}t}Q\rho(0). \quad (A1.13)$$

Equation (A1.13) can be rewritten in terms of the memory kernel

$$K(t) = P\hat{L}e^{Q\hat{L}t}Q\hat{L}P \quad (A1.14)$$

in the form

$$\frac{\partial}{\partial t}\rho_1(t) = P\hat{L}P\rho(t) + \int_0^t ds K(s)\rho(t-s) + P\hat{L}e^{Q\hat{L}t}Q\rho(0). \quad (A1.15)$$

In the Markovian approximation the kernel (A1.14) is a δ -function and in some cases the inhomogeneous term can be neglected (Grigolini 1976).

The Markovian assumption can not be applied always but we can express the memory kernel in terms of the correlation functions of the variables of interest. In order to do so we shall use the interaction picture instead of the Schrödinger picture (A1.1). In the interaction picture the equation of motion of the density $\tilde{\rho}$ reads

$$\frac{\partial}{\partial t}\tilde{\rho}(t) = \hat{L}_I(t)\tilde{\rho}(t), \quad (A1.16)$$

where

$$\tilde{\rho} = e^{\hat{L}_0 t} \rho \quad (A1.17)$$

and

$$\hat{L}_I(t) = e^{\hat{L}_0 t} \hat{L}_I e^{\hat{L}_0 t} \quad (A1.18)$$

where $\hat{L}_0$ denotes

$$\hat{L}_0 = \hat{L}_a + \hat{L}_b. \quad (A1.19)$$

Repeating the calculations (A1.1 – 13) we obtain obtain the master equation

$$\begin{aligned} \frac{\partial}{\partial t} P \tilde{\rho}(t) = & P \hat{L}_I(t) P \tilde{\rho}(t) + \int_0^t ds P \hat{L}_I(t) \overleftarrow{\text{exp}} \left[\int_s^t ds_1 Q \hat{L}_I(s_1) \right] Q \hat{L}_I(s) P \tilde{\rho}(s) \\ & + P \hat{L}_I(t) \overleftarrow{\text{exp}} \left[\int_0^t ds Q \hat{L}_I(s) \right] Q \tilde{\rho}(0). \end{aligned} \quad (A1.20)$$

The roughest approximation is to replace the time ordered exponential with unity and if the inhomogeneous term can be neglected too the master equation (A1.20) becomes

$$\frac{\partial}{\partial t} \tilde{\rho}_1(t) = \int_0^t ds P \hat{L}_I(t) \hat{L}_I(s) \tilde{\rho}(s). \quad (A1.21)$$

In deriving (A1.21) we assumed that $P \hat{L}_I(t) P = 0$. Using the general properties of the projection operator P and $\hat{L}_b$ that $e^{\hat{L}_b t} P = P$ and $P e^{\hat{L}_b t} = P$ the memory kernel becomes

$$K(t-s) = e^{\hat{L}_I(t-s)} K_b(t-s), \quad (A1.22)$$

where

$$K_b(t-s) \equiv P \hat{L}_I e^{(\hat{L}_a + \hat{L}_b)(t-s)} \hat{L}_I P. \quad (A1.23)$$

$K_b(t)$ is a correlation operator providing information on the relaxation properties of the bath.

The average value of an observable A , where A depends on the variables of interest $\vec{a}$, by definition is

$$\langle A(t) \rangle = \int A(\vec{a}) \rho(\vec{a}, \vec{b}; t) d\vec{a} d\vec{b} = \int A \left[e^{\hat{L}t} \rho(\vec{a}, \vec{b}; 0) \right] d\vec{a} d\vec{b}. \quad (A1.24)$$

Since observable A depends only on the variables of interest $\vec{a}$ in calculating $\langle A(t) \rangle$ one may use the reduced density $\sigma(\vec{a}; t)$ so (A1.24) becomes

$$\langle A(t) \rangle = \int A \sigma(\vec{a}; t) d\vec{a}, \quad (A1.25)$$

where $\sigma(\vec{a}; t)$ is defined by the projection operator P in (A1.4) which we rewrite in the following form

$$\sigma(\vec{a}; t) \equiv \frac{\rho_1(\vec{a}, \vec{b}; t)}{\rho_{eq}(\vec{b})}, \quad (A1.26)$$

where $\rho_1(\vec{a}, \vec{b}; t)$ is the part of interest of $\rho(\vec{a}, \vec{b}; t)$ defined by (A1.7). Since $\rho_1(\vec{a}, \vec{b}; t)$ is given as the solution of the master equation (A1.13) we can calculate $\langle A(t) \rangle$ from (A1.25) and (A1.26) by solving (A1.13).

APPENDIX 2

PROBABILISTIC DESCRIPTION OF CHAOTIC MAPS –

THE FROBENIUS OPERATOR

Chaotic motion of physical observables means an erratically evolving variable. In this sense the chaotic motion is reminiscent of the stochastic motion. Therefore it is a good idea to use the probabilistic formalism in the discription of chaotic phenomena.

In this Appendix we present a probabilistic description of chaotic maps. Since in the study of stochastic processes the quantities of primary importance are the probability density and correlation functions we define density functions for maps and investigate its evolution in an operatorial formalism. Several, practically useful definitions of the evolution operator are given for 1- and 2-dimensional maps.

Because the conjugation plays an important role in studies of maps we study the conjugation and its action on the density and the correlation properties of maps.

Finally we prove that all the symmetric maps have quickly vanishing correlation functions.

Definition A2.1. Let us consider a map $f(x) : [0, 1] \mapsto [0, 1]$ i.e.,

$$x_{n+1} = f(x_n), \quad (A2.1)$$

where $x_n \in [0, 1]$. The asymptotic density function $\varrho^*(x)$ is defined as

$$\varrho^*(x) = \lim_{\substack{m(I) \rightarrow 0 \\ I \rightarrow x}} \lim_{n \rightarrow \infty} \sum_{j=0}^{n-1} \chi_I[f_j(x_0)], \quad (A2.2)$$

where x_0 is the initial condition, $m(I)$ denotes the Lebesgue measure of interval $I \subset [0, 1]$ and χ_I its characteristic function (1 if x inside of I , 0 elsewhere). The asymptotic density function $\varrho^*(x)$ is a useful tool of calculations for instance the average of x denoted by $\langle x \rangle$ is calculated as

$$\langle x \rangle = \int_{\text{all possible } x} x \varrho^*(x) dx. \quad (A2.3)$$

Remark A2.1. Consecutive applications of a map on a set of initial condiditons which is described by an initial distribution have the density function evolved. Our goal is to derive the evolution of an initial density function in terms of an operatorial formalism. Therefore let us consider a large number N of initial states $x_1^0, x_2^0, \dots, x_N^0$. The evolution takes place by the application of map (A2.1)

$$x_1^1 = f(x_1^0), x_2^1 = f(x_2^0), \dots, x_N^1 = f(x_N^0). \quad (A2.4)$$

We approximate the density function $\varrho_0(x)$ of the initial state with the characteristic function $\chi_{I_0}(x_j^0)$, for every (not too small) interval $I \subset [0, 1]$

$$\int_{I_0} \varrho_0(u) du \simeq \frac{1}{N} \sum_{j=1}^N \chi_{I_0}(x_j^0). \quad (A2.5)$$

Similarly the density function $\varrho_1(x)$ of the states $x_1^0, x_2^0, \dots, x_N^0$ satisfies, for $I \subset [0, 1]$

$$\int_I \varrho_1(u) du = \frac{1}{N} \sum_{j=1}^N \chi_I(x_j^1). \quad (A2.6)$$

For any $I \subset [0, 1]$

$$x_j^1 \in I \text{ if and only if } x_j \in f^{-1}(I), \quad (A2.7)$$

where $f^{-1}(I)$ denotes the preimage of I i.e., the set of points which are mapped into I by applying 1 iteration

$$f^{-1}(I) = \{x : f(x) \in I\}. \quad (A2.8)$$

So we have the relation

$$\chi_I(f(x)) = \chi_{f^{-1}(I)}(x). \quad (A2.9)$$

with which we can rewrite equation (A2.6) in the form

$$\int_I \varrho_1(u) du \simeq \frac{1}{N} \sum_{j=1}^N \chi_{f^{-1}(I)}(x_j^0). \quad (A2.10)$$

We note that our choice of I_0 and I are arbitrary so we can use the choice

$$I_0 = f^{-1}(I). \quad (A2.11)$$

With this choice the right-hand sides of (A2.5) and (A2.10) are equal therefore

$$\int_I \varrho_1(u) du = \int_{f^{-1}(I)} \varrho_0(u) du. \quad (A2.12)$$

The relationship (A2.12) expresses the conservation of states under the evolution dynamics (A2.1).

If I is an interval, say $I = [a, x]$ we can obtain an explicit representation for ϱ_1 since equation (A2.12) becomes

$$\int_a^x \varrho_1(u) du = \int_{f^{-1}([a, x])} \varrho_0(u) du. \quad (A2.13)$$

and differentiating with respect to x gives

$$\varrho_1(x) = \frac{d}{dx} \int_{f^{-1}([a, x])} \varrho_0(u) du. \quad (A2.14)$$

This observation leads us to the following definition.

Definition A.2.2. The *Frobenius operator* which describes the evolution of a density function under the dynamics f is defined

$$\varrho_{n+1}(x) = \hat{P}\varrho_n(x) = \frac{d}{dx} \int_{f^{-1}([0,x])} \varrho_n(u) du. \quad (A2.15)$$

Definition A.2.3. The density function $\varrho^*(x)$ which is unchanged under the action of the Frobenius operator, i.e.,

$$\hat{P}\varrho^*(x) = \varrho^*(x) \quad (A2.16)$$

is called the *invariant distribution function*. The invariant distribution in stationary deterministic systems plays the role of a probability density.

Proposition A2.1. If

- i) we consider dynamics $f : [0, 1] \mapsto [0, 1]$ given by
- ii)

$$f(x) = rx \quad \text{mod } 1, \quad (A2.17)$$

- iii) where r is integer then

- the invariant distribution of f is the uniform distribution i.e.,

$$\varrho^*(x) = 1. \quad (A2.18)$$

The map (A2.17) for $r = 3$ is shown in *Figure A2.1*.

Proof. We pick up an arbitrary interval $[0, x] \subset [0, 1]$. So the preimage of the interval $[0, x]$ is given by

$$f^{-1}([0, x]) = \cup_{i=0}^{r-1} \left[\frac{i}{r}, \frac{i}{r} + \frac{x}{r} \right]. \quad (A2.19)$$

Figure A2.1. The map (A2.17) for $r = 3$.

Applying the Frobenius operator on the uniform density we get

$$\hat{P}1 = \frac{d}{dx} \sum_{i=0}^{r-1} \int_{\frac{i}{r}}^{\frac{i+1}{r}} 1 du = \frac{d}{dx} \sum_{i=0}^{r-1} \frac{x}{r} = 1, \quad (\text{A2.20})$$

which means that the uniform distribution is invariant under the evolution of map (A2.17).

q.e.d.

Remark A2.2. In a very similar way we can prove that

- i) linear piecewise maps $f(x) : [0, 1] \mapsto [0, 1]$ composed of n branches
- ii) where the i -th branch maps the interval $I_i = [a_i, b_i]$ onto the interval $[0, 1]$
i.e., $I_i = [a_i, b_i] \mapsto [0, 1]$
- iii) in a way that $f(a_i) = 0$ or $f(a_i) = 1$ and $f(b_i) = 0$ or $f(b_i) = 1$

iv) and $a_{i+1} = b_i$

v) and within a branch the map has the same nonzero slope i.e., it is not broken within the unit circle (A2.21)
then

- map (A2.21) has a uniform invariant distribution.

A map like this is shown in *Figure A2.2*.

Figure A2.2. The map (A2.21).

Remark A2.3. If we restrict ourselves to maps which are invertible we can give different definitions for the Frobenius operator. In the following propositions we show that those definitions are equivalent.

Definition A2.4. The *Frobenius operator* $\hat{P}$ for an invertible and differentiable map $f : [0, 1] \mapsto [0, 1]$ is defined

$$\hat{P}\varrho(x) = \varrho(f^{-1}(x)) \left| \frac{d}{dx} [f^{-1}(x)] \right|. \quad (A2.22)$$

Proposition A2.2. If

- i) the map $f : [0, 1] \mapsto [0, 1]$ is invertible
- ii) and f is differentiable

then

- *Definitions A.2.2 and A2.4* of the Frobenius operator are equivalent.

Proof. Suppose that f is an increasing function. Then

$$f^{-1}([a, x]) = [f^{-1}(a), f^{-1}(x)] \quad (A2.23)$$

and from the *Definition A2.2.* i.e., from equation (A2.15)

$$\begin{aligned} \hat{P}\varrho(x) &= \frac{d}{dx} \int_{f^{-1}(a)}^{f^{-1}(x)} \varrho(s) ds = \frac{d}{dx} [R(f^{-1}(x)) - R(f^{-1}(a))] \\ &= \varrho(f^{-1}(x)) \frac{d}{dx} [f^{-1}(a)], \end{aligned} \quad (A2.24)$$

where $R(s)$ denotes the indefinite integral function of $\varrho(s)$. If f is decreasing the sign of the right hand side is reversed. Thus in the general 1-dimensional case

$$\hat{P}\varrho(x) = \varrho(f^{-1}(x)) \left| \left[\frac{d}{dx} f^{-1}(x) \right] \right|. \quad (A2.25)$$

q.e.d.

Definition A2.5. The *Frobenius operator* $\hat{P}$ for an invertible and differentiable 1-dimensional map $f : [0, 1] \mapsto [0, 1]$ is defined by

$$\hat{P}\varrho(x) = \varrho(f^{-1}(x)) J^{-1}(x) \quad (A2.26)$$

where $J^{-1}(x)$ denotes the Jacobian of the of the inverse map.

Proposition A2.3 If

- i) the map $f : [0, 1] \mapsto [0, 1]$ is invertible
- ii) and differentiable

then

- *Definition A2.4* and *Definition A2.5* of the Frobenius operator are equivalent.

Proof. For 1-dimensional dynamical systems the Jacobian is defined as

$$J(x) = \left| \frac{d}{dx} f(x) \right|. \quad (A2.27)$$

Introducing the notation $J^{-1}(x)$ for the Jacobian of the inverse map

$$J^{-1}(x) = \left| \frac{d}{dx} f^{-1}(x) \right|. \quad (A2.28)$$

and comparing (A2.28) to equation (A2.25) we end up with equation (A2.26).

q.e.d.

Remark A2.4. The *Definition A2.5* is important from the point of view of generalization since the Frobenius operator is defined for more than 1-dimensional systems too, where we have to use the Jacobian and the preimage of a given n-dimensional volume element.

Definition A2.6. The *Frobenius operator* $\hat{P}$ of a 2-dimensional map $f(x, y)$ is acting on a density function $\varrho(x, y)$

$$\hat{P}\varrho(x, y) = \frac{\partial^2}{\partial x \partial y} \int \int_{f^{-1}([a, x] \times [b, y])} \varrho(s, t) ds dt, \quad (A2.29)$$

where $f^{-1}([a, x] \times [b, y])$ denotes the preimage of the rectangle $[a, x] \times [b, y]$.

Remark A2.4. Besides the *Definition A2.2* and *Definition A2.4* we can give another definition for the Frobenius operator. It is based on the idea that maps are completely deterministic and their evolution can be expressed in terms of a δ -function. Thus the evolution of the density function can be given in terms of δ -function too.

$$\varrho_{n+1}(x) = \int \delta(x - f(y)) \varrho(y) dy \quad (A2.30)$$

Using the properties of the δ -functions (for example in Messiah 1961) (A2.30) can be written in the form of

$$\varrho_{n+1}(x) = \sum_i \frac{\varrho_n(y_i(x))}{|f'(y_i(x))|}, \quad (A2.31)$$

where $y_i(x)$ are the solutions of the equation

$$x = f(y). \quad (A2.32)$$

Thus we can define the Frobenius operator as follows:

Definition A2.7. Let us consider a map $f : [0, 1] \mapsto [0, 1]$. The Frobenius operator $\hat{P}$ is given by its action

$$\varrho_{n+1}(x) = \hat{P}\varrho_n(x) = \sum_i \frac{\varrho_n(y_i(x))}{|f'(y_i(x))|}, \quad (A2.33)$$

where $y_i(x)$ are the solutions of the equation (A2.32).

Remark A2.5. *Definition A2.7* allows us to generalize the Frobenius operator for 2-dimensional maps.

Definition A2.8. Let us consider the 2-dimensional invertible map $f = f(x, y) : [0, 1] \times [0, 1] \mapsto [0, 1] \times [0, 1]$. The Frobenius operator is given by its action on a density function $\varrho_n(x, y)$

$$\varrho_{n+1}(x, y) = \hat{P}\varrho_n(x, y) = \frac{1}{|\text{Det}Df|_{f^{-1}(x, y)}} \varrho_n(f^{-1}(x, y)), \quad (\text{A2.34})$$

where $f^{-1}(x, y)$ denotes the inverse of map $f(x, y)$ and $|\text{Det}Df|$ denotes the Jacobian of map f .

Remark A2.6. The knowledge of the Frobenius operator and the evolution of a density function is important. It is also important to know how the map evolves in a transformed space. This is what we investigate in the next few statements following the idea of Halmos (Halmos 1956), Ulam (Ulam 1960), Smale and Williams (Smale and Williams 1976) and Grossmann (Grossmann 1979).

Definition A2.9. Let us consider a map $f : I \mapsto I$ which is defined on variable $t \in I$

$$t_{n+1} = f(t_n) \quad (\text{A2.35})$$

and let us consider a map $g : J \mapsto J$ which is defined on variable $x \in J$. Maps f and g are *conjugate* if there exist a one-to-one map $h : I \mapsto J$ such that

$$g(x) = h(f[h^{-1}(x)]) = h \circ f \circ h^{-1}(x). \quad (A2.36)$$

Remark A2.7. In the following *Proposition A2.3* we show an example of conjugated maps.

Proposition A2.2. If

i) the tent map $f : [0, 1] \mapsto [0, 1]$

$$t_{n+1} = f(t_n) = 1 - 2 \left| \frac{1}{2} - t_n \right| \quad (A2.37)$$

ii) is subjected to a conjugation via the conjugating function

$$x = h(t) = \sin^2\left(\frac{\pi}{2}t\right) \quad (A2.38)$$

then

• the conjugated map $g(x)$ is the logistic map

$$x_{n+1} = g(x_n) = 4x_n(1 - x_n). \quad (A2.39)$$

Proof. We can obtain the conjugated map $g(x)$ from its definition (A2.36). First we need to calculate $h^{-1}(x)$ then $f[h^{-1}(x)]$ finally $h(f[h^{-1}(x)])$. We get from (A2.38)

$$t = h^{-1}(x) = \frac{2}{\pi} \arcsin \sqrt{x}. \quad (A2.40)$$

Thus

$$f[h^{-1}(x)] = 1 - 2 \left| \frac{1}{2} - \frac{2}{\pi} \arcsin \sqrt{x} \right|. \quad (A2.41)$$

Finally for $h(f[h^{-1}(x)])$ we get

$$\begin{aligned} g(x) &= h(f[h^{-1}(x)]) = \sin^2 \left[\frac{\pi}{2} \left(1 - 2 \left| \frac{1}{2} - \frac{2}{\pi} \arcsin \sqrt{x} \right| \right) \right] \\ &= \cos^2 \left(\left| \frac{1}{2} - \frac{2}{\pi} \arcsin \sqrt{x} \right| \pi \right) = \cos^2 \left(\frac{\pi}{2} - 2 \arcsin \sqrt{x} \right) \\ &= \sin^2 (2 \arcsin \sqrt{x}) = 4 \sin^2(\arcsin \sqrt{x}) \cos^2(\arcsin \sqrt{x}) \\ &= 4x(1-x). \end{aligned} \quad (A2.42)$$

q.e.d.

Remark A2.8. The conjugation is a useful tool from practical point of view since say we have a complicated map but we can find a conjugation which results in a simpler map. Then we do our investigations on the simple map and by an inverse conjugation we transform the results back to the space of the complicated map. For instance in the case of chaotic maps the quantity of paramount importance is the density function. In the next *Proposition A2.4* we show how the density behaves under conjugation.

Proposition A2.4. If

i) the map $f(t) = f: I \mapsto I, t \in I$

$$t_{n+1} = f(t_n) \quad (A2.43)$$

ii) has the invariant density $\varrho_f(t)$,

- iii) a conjugation $t = h(x)$ $h : I \mapsto J$
- iv) results in map $g(x) = g : J \mapsto J$, $x \in J$
- v) and the map g has an invariant density $\varrho_g(x)$

then

- the invariant densities $\varrho_g(x)$ and $\varrho_f(t)$ are related via

$$\varrho_g(x) = \varrho_f[h^{-1}(x)] \left| \frac{dh^{-1}(x)}{dx} \right| \quad (A2.44)$$

Proof. The probability $P(x)$ that x is between x and $x + dx$

$$P(x) = \varrho_g(x)dx. \quad (A2.45)$$

Similarly the probability $P(t)$ that t is between t and $t + dt$

$$P(t) = \varrho_f(t)dt. \quad (A2.46)$$

From the conservation of probabilities

$$P(x) = P(t), \quad (A2.47)$$

which after substituting the conjugation function $t = h^{-1}(x)$ immediately leads us to the result (A2.44).

Remark A2.9. Now we show an example how one can find the invariant density of the logistic map, which is difficult to obtain by a straightforward calculation, with the help of a proper conjugation.

Proposition A2.5. If

i) we consider the logistic map $g : [0, 1] \mapsto [0, 1]$

$$x_{n+1} = g(x_n) = 4x_n(1 - x_n) \quad (\text{A2.48})$$

then

- its invariant density is

$$\varrho^*(x) = \frac{1}{\pi\sqrt{x(1-x)}}. \quad (\text{A2.49})$$

Proof. As we proved in *Proposition A2.3* the logistic map (A2.48) is the conjugate of the tent map (A2.37) with the conjugation function (A2.38). In *Proposition A2.1* we proved that the tent map (A2.37) has a uniform distribution

$$\varrho_f(t) = 1. \quad (\text{A2.50})$$

Thus from *Proposition A2.4* we get

$$\varrho_g(x) = 1 \left| \frac{dh^{-1}(x)}{dx} \right|. \quad (\text{A2.51})$$

From (A2.38) we get

$$\frac{dh^{-1}(x)}{dx} = \frac{2}{\pi} \frac{d}{dx} \arcsin \sqrt{x} = -\frac{1}{\pi\sqrt{x(1-x)}}. \quad (\text{A2.52})$$

Substituting (A2.52) into (A2.51) we obtain (A2.49). The invariant distribution (A2.49) of the logistic map (A2.48) is presented in *Figure A2.3*.

q.e.d.

Figure A2.3. The invariant distribution (A2.49) of the logistic map (A2.48).

Remark A2.10. As we mentioned in *Remark A2.8* the quantity of primary importance of chaotic maps is their invariant density functions. From the point of view of dynamics it is also important to know their correlation properties. In the next *Proposition A2.6* we show how one can obtain the correlation function of the logistic map.

Proposition A2.6. If

i) we consider the zero centered logistic map $f(x) : [-1, 1] \mapsto [-1, 1]$

$$x_{n+1} = f(x_n) = 1 - 2x_n^2 \quad (A2.53)$$

then

- its correlation function

$$c_n = \langle x_n x_0 \rangle = \langle x_0^2 \rangle \delta_{n,0}, \quad (A2.54)$$

where $\delta_{n,0}$ denotes the Kronecker symbol.

Proof. The proof is based purely on symmetry arguments. The correlation function is an equilibrium property therefore we have to assume that the initial values x_0 are distributed according to the invariant density

$$\varrho^*(x) = \frac{1}{\pi \sqrt{1-x^2}}. \quad (A2.55)$$

The invariant density (A2.55) of the zero centered logistic map is obtained by a simple rescaling from the invariant density (A2.49) of the non-zero centered logistic map. We observe that (A2.55) is an even function.

$$\varrho^*(x) = \varrho^*(-x) \quad x \in [-1, 1]. \quad (A2.56)$$

Thus the correlation function from its definition is given as

$$c_0 = \langle x_0 x_0 \rangle = \langle x_0^2 \rangle = \int_{-1}^1 x_0^2 \varrho^*(x_0) dx_0 \quad (A2.56)$$

and

$$c_1 = \langle x_1 x_0 \rangle = \langle f(x_0) x_0 \rangle = \int_{-1}^1 f(x_0) x_0 \varrho^*(x_0) dx_0 = 0, \quad (\text{A2.57})$$

because $f(x_0)$ and $\varrho^*(x_0)$ are even and x_0 is odd function. Thus the integrand is an odd function whose integral on the interval $[-1, 1]$ vanishes. Since all the further iterates $f^n(x_0)$ ($n \geq 1$) are even (see for instance *Figure A2.4*), the argument above is valid and

$$c_n = \langle x_n x_0 \rangle = 0 \quad \text{for } n \geq 1 \quad (\text{A2.58})$$

q.e.d.

Figure A2.4. The iterates $f^1(x)$ and $f^2(x)$ of the zero centered logistic map (A2.53).

Remark A2.11. The results of *Proposition A2.6* are obviously generalized to symmetric maps

$$f(x) = f(-x) \quad x \in [-1, 1]. \quad (A2.59)$$

All the fully chaotic symmetric maps have 1-step vanishing correlation functions.

APPENDIX 3

THE LINEAR RESPONSE THEORY OF KUBO AND THE
GEOMETRICAL LINEAR RESPONSE THEORY
FOR CLASSICAL CONTINUOUS SYSTEMS

In this Appendix first we review the conventional Linear Response Theory of Kubo. Then we show the difficulties emerge in the justification of this theory. In the second part of the Appendix we show how one can bypass the difficulties of the conventional theory of Kubo by presenting the Geometrical Linear Response Theory.

Proposition A3.1. The Linear Response Theory of Kubo.

If

i) the considered physical system is a classical N particle system i.e., its phase space Γ

$$\Gamma = \{\vec{q}_j, \vec{p}_j\} \quad j = 1, 2, \dots, N, \quad (\text{A3.1})$$

ii) its unperturbed dynamics is described by the Hamiltonian H_0

$$H_0 = H_0(\vec{q}_j, \vec{p}_j), \quad (\text{A3.2})$$

iii) it is subjected to a perturbation KH_1

$$KH_1 = H_1(\{\vec{q}_j, \vec{p}_j\}, t), \quad (\text{A3.3})$$

where the perturbation parameter is K ,

iv) the perturbation is small i.e., a first order perturbation calculation can be applied,

v) the integration with respect to time and the phase space variables independent,

vi) and initially (before the perturbation) the system is in equilibrium of the unperturbed system

then

- the generalized susceptibility $\chi(t)$ with respect to observable $A = A(\Gamma)$ is

$$\chi(t) = \int_0^t d\vartheta \left\langle A(\vartheta) \hat{L}_1 \right\rangle_{\varrho_{\text{eq}}(\Gamma)} \quad (\text{A3.4})$$

where $\hat{L}_1$ is the Liouville operator associated with the perturbation Hamiltonian H_1 and $\varrho_{\text{eq}}(\Gamma)$ is the equilibrium phase space density of the unperturbed system and $\langle \rangle_{\varrho_{\text{eq}}(\Gamma)}$ denotes the averaging over the density $\varrho_{\text{eq}}(\Gamma)$.

Proof. We follow the method of Kubo (Kubo 1957) in the proof. The above considered physical system evolves under the action of the total Hamiltonian H

$$H = H_0 + KH_1. \quad (\text{A3.5})$$

The evolution of the phase space density $\varrho(\Gamma, t)$ is given by the Liouville-operator $\hat{L}(t)$

$$\frac{\partial \varrho(\Gamma, t)}{\partial t} = \hat{L}(t) \varrho(\Gamma, t) = \left[\hat{L}_0 + K \hat{L}_1(t) \right] \varrho(\Gamma, t), \quad (\text{A3.6})$$

where

$$\hat{L}_0 \varrho(\Gamma, t) = \{H_0, \varrho(\Gamma, t)\}_{\text{Poisson}} = \sum_{j=1}^{3N} \left(\frac{\partial H_0}{\partial p_j} \frac{\partial}{\partial q_j} - \frac{\partial H_0}{\partial q_j} \frac{\partial}{\partial p_j} \right) \varrho(\Gamma, t), \quad (\text{A3.7})$$

and

$$\hat{L}_1(t) \varrho(\Gamma, t) = K \{H_1(t), \varrho(\Gamma, t)\}_{\text{Poisson}} = K \sum_{j=1}^{3N} \left(\frac{\partial H_1}{\partial p_j} \frac{\partial}{\partial q_j} - \frac{\partial H_1}{\partial q_j} \frac{\partial}{\partial p_j} \right) \varrho(\Gamma, t). \quad (\text{A3.8})$$

The total Liouville operator $\hat{L}$ is separated into two parts, $\hat{L}_0$ which describes the evolution of the density $\varrho(\Gamma, t)$ of the unperturbed system and $\hat{L}_1$ which describes

the evolution of the density $\varrho_1(\Gamma, t)$ purely due to the perturbation respectively. In terms of the densities the total density $\varrho(\Gamma, t)$ consist of two parts, the equilibrium density of the unperturbed system $\varrho_{\text{eq}}(\Gamma)$ and the density $\varrho_1(\Gamma, t)$ which is the result of the perturbation itself

$$\varrho(\Gamma, t) = \varrho_{\text{eq}}(\Gamma) + \varrho_1(\Gamma, t) \quad (\text{A3.9})$$

Substituting (A3.9) into the evolution equation (A3.6) we obtain

$$\frac{\partial \varrho_{\text{eq}}(\Gamma)}{\partial t} + \frac{\partial \varrho_1(\Gamma, t)}{\partial t} = \hat{L}_0 \varrho_{\text{eq}}(\Gamma) + K \hat{L}_1(t) \varrho_{\text{eq}}(\Gamma) + \hat{L}_0 \varrho_1(\Gamma, t) + K \hat{L}_1(t) \varrho_1(\Gamma, t). \quad (\text{A3.10})$$

The equilibrium condition reads

$$\frac{\partial \varrho_{\text{eq}}(\Gamma)}{\partial t} = \hat{L}_0 \varrho_{\text{eq}}(\Gamma) = 0. \quad (\text{A3.11})$$

Thus the Liouville equation for the perturbed density $\varrho_1(\Gamma, t)$ becomes

$$\frac{\partial \varrho_1(\Gamma, t)}{\partial t} = K \hat{L}_1(t) \varrho_{\text{eq}}(\Gamma) + \hat{L}_0 \varrho_1(\Gamma, t) + K \hat{L}_1(t) \varrho_1(\Gamma, t). \quad (\text{A3.12})$$

The last term is considered to be of second order therefore it is neglected so the Liouville equation for $\varrho_1(\Gamma, t)$ becomes

$$\frac{\partial \varrho_1(\Gamma, t)}{\partial t} = K \hat{L}_1(t) \varrho_{\text{eq}}(\Gamma) + \hat{L}_0 \varrho_1(\Gamma, t). \quad (\text{A3.13})$$

We use the assumption *vi)* that the perturbation is applied at time $t = 0$ and before this instant the density ϱ is the equilibrium density of the unperturbed dynamics

$$\varrho_1(\Gamma, 0) = \varrho_{\text{eq}}(\Gamma) = \frac{e^{-\beta H_0}}{Z}, \quad (\text{A3.14})$$

where

$$\beta = \frac{1}{k_B T} \quad (A3.15)$$

with k_B the Boltzmann-constant and T absolute temperature and Z is the partition function

$$Z = \int_{\text{all } \Gamma} d\vec{q}_j d\vec{p}_j e^{-\beta H_0(\vec{q}_j, \vec{p}_j)}. \quad (A3.16)$$

The assumption above allows us to rewrite the perturbation operator $K\hat{L}_1(t)$ in the form of

$$K\hat{L}_1(t) = K\hat{L}_1(t)\theta(t), \quad (A3.17)$$

where we separated the phase space and time dependent parts by introducing the step-function $\theta(t)$. With this notation the Liouville equation (A3.13) becomes

$$\frac{\partial \varrho_1(\Gamma, t)}{\partial t} = K\theta(t)\hat{L}_1\varrho_{\text{eq}}(\Gamma) + \hat{L}_0\varrho_1(\Gamma, t) \quad (A3.18)$$

whose formal solution is

$$\varrho_1(\Gamma, t) = K \int_0^t dt' e^{\hat{L}_0(t-t')} \hat{L}_1 \varrho_{\text{eq}}(\Gamma). \quad (A3.19)$$

Now we can calculate the response with respect to an observable A . The observable A of the perturbed system at time t has the mean value $\langle A \rangle_e$ where $\langle \rangle_e$ denotes the averaging over a distribution ϱ

$$\langle A \rangle_e = \int_{\text{all } \Gamma} d\Gamma A(\Gamma) \varrho(\Gamma, t). \quad (A3.20)$$

Since

$$\langle A \rangle_{\varrho} = \langle A \rangle_{\varrho_{\text{eq}} + \varrho_1} = \langle A \rangle_{\varrho_{\text{eq}}} + \langle A \rangle_{\varrho_1} \quad (\text{A3.21})$$

the response R_A in observable A is the difference between its perturbed and unperturbed values

$$R_A = \langle A \rangle_{\varrho} - \langle A \rangle_{\varrho_{\text{eq}}} = \langle A \rangle_{\varrho_1}, \quad (\text{A3.22})$$

thus from (A3.19) and (A3.22)

$$R_A = K \int_{\text{all } \Gamma} d\Gamma \int_0^t dt' A(\Gamma) e^{\hat{L}_0(t-t')} \hat{L}_1 \varrho_{\text{eq}}(\Gamma). \quad (\text{A3.23})$$

Using the assumption $v)$ of the exchangeability of integrations with respect to time and to phase space variables and applying the operator $e^{\hat{L}_0(t-t')}$ to the left of $A(\Gamma)$ in (A3.23) we obtain for the response R_A

$$R_A = K \int_0^t dt' \int_{\text{all } \Gamma} d\Gamma A(t-t') \hat{L}_1 \varrho_{\text{eq}}(\Gamma). \quad (\text{A3.24})$$

Introducing $\vartheta = t - t'$ the response R_A is given in terms of a cross-correlation function

$$R_A = K \int_0^t d\vartheta \left\langle A(\vartheta) \hat{L}_1 \right\rangle_{\varrho_{\text{eq}}}. \quad (\text{A3.25})$$

Equation (A3.25) is the *Kubo formula* for classical systems. Since the *Kubo formula* is linear in the perturbation parameter K the generalized susceptibility $\chi(t)$ is

$$\chi(t) = \frac{\partial R_A}{\partial K} \quad (\text{A3.26})$$

which leads us to equation (A3.4).

q.e.d.

Remark A3.1. Kubo's linear response formula (A3.4) is an approximate result based on a first order perturbation theory. There are two important assumption in the derivation of it. One of them is the exchangeability of the integration with respect to time and phase space variables. The other assumption is that one can neglect the term $\hat{L}_1(t)\varrho_1(\Gamma, t)$ in the evolution of the distribution. Neither of these two assumptions are well established. Especially the latter one was criticized by van Kampen (van Kampen 1971) who pointed out that the neglect of the term $\hat{L}_1(t)\varrho_1(\Gamma, t)$ is essentially a linearization of the trajectories. Although linearization of the trajectories can yield correct results only in linear systems at the same time these systems do not produce relaxation to equilibrium.

In the following *Proposition A3.2* we show a linear response theory which recovers Kubo's Linear Response Theory without linearizing the individual trajectories. In *Proposition A3.2* we follow the way was developed by Bianucci et al. (Bianucci et al 1993b).

Proposition A3.2. The Geometrical Linear Response Theory.

If

- i) the considered unperturbed physical system is described by the Hamiltonian

$$H_0 = \frac{m_1 \pi^2}{2} + \frac{m_2 \nu^2}{2} + U_0(\xi, \zeta), \quad (\text{A3.27})$$

- ii) where the potential $U(\xi, \zeta)$ is a modified Henon-Heiles potential (see *Figure A3.1*)

$$U_0(\xi, \zeta) = \frac{\xi^2}{2} + \frac{\zeta^2}{2} + \xi\zeta^2 - \frac{\xi^3\zeta}{3} + \xi^4\zeta^4, \quad (\text{A3.28})$$

Figure A3.1. The modified Henon-Heiles potential (A3.28).

iii) the perturbed physical system is described by the Hamiltonian

$$H = H_0 + U_0(\xi, \zeta) - K\xi\theta(t), \quad (\text{A3.29})$$

where $\theta(t)$ is the step-function,

iv) and the unperturbed system is chaotic i.e., the parameters

$$m_1 = 1; \quad m_2 = 0.54; \quad E = H_0 = 0.8 \quad (\text{A3.30})$$

then

- the generalized susceptibility $\chi = \chi(\infty)$ with respect to the perturbation parameter K

$$\chi = -\frac{1}{2} \frac{\xi_R - \xi_L}{U'_0(\xi_R, \zeta^*)} \quad (A3.31)$$

where ξ_R and ξ_L are the largest and smallest values of variable ξ in the Poincarè surface of sections of plane (π, ξ) .

Proof. The proof is based on the following idea. The perturbation is applied to the variable ξ . The action of the perturbation is monitored in its action upon the Poincarè surface of section of the plane (π, ξ) with ζ and ν fixed. The Poincarè surface of sections in the unperturbed case gives a uniformly filled circle in the (π, ξ) plane which is stretched along the ξ axis due to the perturbation (see *Figure A3.2*). This distortion is manifested in

$$\langle \xi(K) \rangle_{\text{perturbed}} \neq \langle \xi(K) \rangle_{\text{unperturbed}} = 0, \quad (A3.32)$$

from which the generalized susceptibility χ is determined in the usual way

$$\chi = \frac{\partial}{\partial K} \left(\langle \xi(K) \rangle_{\text{perturbed}} - \langle \xi(K) \rangle_{\text{unperturbed}} \right) \Big|_{K=0}. \quad (A3.32)$$

The Poincarè surface of sections and the average values of the physical quantities are calculated within the framework of the microcanonical formalism.

Thus the proof consist of two parts. First we calculate the dominion of the Poincarè surface of sections using the energy conservation then we calculate the

Figure A3.2. The deformation of the Poincaré surface of sections due to perturbation. The solid line shows the boundary of the Poincaré surface of sections of the plane (π, ξ) when the motion takes place in the modified Henon-Heiles potential (A3.28) i.e., the motion is unperturbed. The dashed line shows the boundary of the Poincaré surface of sections of the perturbed motion.

response with the help of this dominion.

Determination of the dominion of the Poincaré surface of sections.

Let us consider the system with the Hamiltonian (A3.27)

$$H_0 = \frac{m_1 \pi^2}{2} + \frac{m_2 \nu^2}{2} + U_0(\xi, \zeta). \quad (\text{A3.27})$$

The parameters m_1, m_2 and the total energy E are chosen in a way that the system is chaotic (see assumption *iii*). This chaotic system is microcanonical (Rasetti 1986, Katok et al. 1986). We assume also that the system is ergodic which is an

obvious assumption. Thus the time average of a variable can be replaced by an average over the microcanonical density distribution which is defined by

$$d\mu \equiv \frac{\delta(E - H(\xi, \pi, \zeta, \nu))d\xi d\pi d\zeta d\nu}{\int \delta(E - H(\xi, \pi, \zeta, \nu))d\xi d\pi d\zeta d\nu}. \quad (A3.33)$$

Therefore the probability that the system explores a certain region of the phase space is proportional to the volume of this region. So the mean value $\langle f(\xi) \rangle$ is

$$\langle f(\xi) \rangle = \int d\mu f(\xi), \quad (A3.34)$$

where $d\mu$ is given by (A3.33).

The energy E is a constant of motion so we can eliminate one of the phase space variables say ν . The δ -function in (A3.33) is rewritten in terms of ν

$$\delta(E - H_0) = \frac{\delta(\nu - \bar{\nu})}{\bar{\nu}}, \quad (A3.35)$$

where

$$\bar{\nu} = \sqrt{\frac{2}{m_2} \left(E - \frac{m_1 \pi^2}{2} - U(\xi, \zeta) \right)}. \quad (A3.36)$$

Thus the microcanonical density distribution (A3.33) becomes

$$\begin{aligned} d\mu &= \frac{1}{\bar{\nu}} \frac{d\xi d\pi d\zeta}{\int_{\Omega(E)} \frac{d\xi d\pi d\zeta}{\bar{\nu}}} \\ &= \frac{1}{\sqrt{\frac{2}{m_2} \left(E - \frac{m_1 \pi^2}{2} - U(\xi, \zeta) \right)}} \frac{d\xi d\pi d\zeta}{\int_{\Omega(E)} \frac{d\xi d\pi d\zeta}{\sqrt{\frac{2}{m_2} \left(E - \frac{m_1 \pi^2}{2} - U(\xi, \zeta) \right)}}}, \end{aligned} \quad (A3.37)$$

where $\Omega(E)$ is the integration domain i.e., the domain of space ξ, ζ, π , where

$$\bar{\nu}^2 \geq 0. \quad (A3.38)$$

The domain $\Omega(E)$ is bounded by a surface $S = S(E)$. The surface $S(E)$ is defined by the region of the space where

$$\bar{\nu} = 0 \quad (A3.39)$$

i.e., the region, where

$$E - \frac{m_1 \pi^2}{2} - U(\xi, \zeta) = 0. \quad (A3.40)$$

From the surface $S(E)$ and (A3.40) we can determine the range of integration of variable π . It is

$$\pi \in [-\pi_E, \pi_E], \quad (A3.41)$$

where

$$\pi_E = \pi_E(\xi, \zeta) = \sqrt{\frac{2}{m_1} (E - U(\xi, \zeta))}. \quad (A3.42)$$

Thus the mean value $\langle f(\xi) \rangle$ i.e., (A3.34) can be written

$$\begin{aligned} \langle f(\xi) \rangle &= \frac{\int_{\Omega(E)} \frac{f(\xi)}{\bar{\nu}} d\xi d\zeta d\pi}{\int_{\Omega(E)} \frac{d\xi d\zeta d\pi}{\bar{\nu}}} \\ &= \frac{\int_{\zeta_L}^{\zeta_R} d\zeta \int_{\xi_L}^{\xi_R} d\xi f(\xi) \int_{-\pi_E}^{\pi_E} \frac{d\pi}{\sqrt{\frac{2}{m_2} \left(E - \frac{m_1 \pi^2}{2} - U(\xi, \zeta) \right)}}}{\int_{\zeta_L}^{\zeta_R} d\zeta \int_{\xi_L}^{\xi_R} d\xi \int_{-\pi_E}^{\pi_E} \frac{d\pi}{\sqrt{\frac{2}{m_2} \left(E - \frac{m_1 \pi^2}{2} - U(\xi, \zeta) \right)}}} \\ &= \frac{\int_{\zeta_L}^{\zeta_R} d\zeta \int_{\xi_L(\zeta)}^{\xi_R(\zeta)} d\xi f(\xi)}{\int_{\zeta_L}^{\zeta_R} d\zeta \int_{\xi_L(\zeta)}^{\xi_R(\zeta)} d\xi} = \frac{\int_{\zeta_L}^{\zeta_R} d\zeta [F(\xi_R(\zeta)) - F(\xi_L(\zeta))]}{\int_{\zeta_L}^{\zeta_R} d\zeta [\xi_R(\zeta) - \xi_L(\zeta)]}, \end{aligned} \quad (A3.43)$$

where $F(\xi)$ is the indefinite integral function of $f(\xi)$, $\xi_R(\zeta)$ and $\xi_L(\zeta)$ are the solutions of the equation

$$E - U(\xi, \zeta) = 0 \quad (A3.44)$$

so it is considered being the extrema of the range of integration of ξ with E and ζ fixed, ζ_L and ζ_R are the extrema of the range of integration of the variable ζ at fixed energy E .

Now we can calculate the average value $\langle f(\xi) \rangle$ only using the Poincaré surface of sections of the system. $\Omega(E)$ is a 3-dimensional range of the phase space (ξ, ζ, π) . Fixing $\zeta = \zeta^*$ and plotting the phase space coordinates (ξ, π) whenever the trajectory hits the plane $\zeta = \zeta^*$ from the same direction, we get a closed domain of the (ξ, π) plane which is uniformly filled. This domain of the phase space is the Poincaré surface of section.

From (A3.43) we can see that the invariant measure derived by the Poincaré map $d\mu(\xi, \zeta^*)$ with respect to variable ξ corresponds to a uniformly distributed ξ i.e.,

$$d\mu(\xi, \zeta^*) = \frac{d\xi}{\xi_R(\zeta^*) - \xi_L(\zeta^*)}. \quad (A3.45)$$

Thus from (A3.45) and (A3.43) we get average $\langle f(\xi) \rangle$

$$\langle f(\xi) \rangle = \frac{F(\xi_R(\zeta^*)) - F(\xi_L(\zeta^*))}{\xi_R(\zeta^*) - \xi_L(\zeta^*)} \quad (A3.46)$$

which in the case of $f(\xi) = \xi$ is simplified to

$$\langle \xi \rangle = \frac{1}{2} (\xi_R(\zeta^*) + \xi_L(\zeta^*)). \quad (A3.47)$$

Determination of the linear response

In order to determine the generalized susceptibility we need to calculate the average of ξ with the perturbation acting which value is denoted by $\langle \xi \rangle_K$. The average of ξ for the unperturbed case is given by (A3.47). We can determine $\langle \xi \rangle_K$ using the energy conservation and the calculations above.

At time $t = 0$ the perturbation starts acting although the system remains conservative as the Hamiltonian (A3.29) shows. The Hamiltonian also shows that the energy E_p of the perturbed system is

$$E_p = E + K(\xi - \xi(0)), \quad (\text{A3.48})$$

where $\xi(0)$ denotes the value of the variable ξ at time $t = 0$.

Now we can repeat the calculations we did previously using the energy E_p . Thus the corresponding equations to equation (A3.44) becomes

$$E - U(\xi, \zeta) - K(\xi - \xi(0)) = 0, \quad (\text{A3.49})$$

from which $\xi_R(\zeta^*)$ and $\xi_L(\zeta^*)$ can be determined.

From the definition (A3.32) and from (A3.46) we can see that the generalized susceptibility χ becomes

$$\chi = \frac{1}{2} \left[\left. \frac{\partial \xi_R(\zeta^*)}{\partial K} \right|_{K=0} + \left. \frac{\partial \xi_L(\zeta^*)}{\partial K} \right|_{K=0} \right]. \quad (\text{A3.50})$$

In order to obtain the susceptibility χ we also need

$$\frac{\partial \xi_L(\zeta^*)}{\partial K} = - \frac{\partial f}{\partial K} \left(\frac{\partial f}{\partial \xi} \right)^{-1} \Big|_{\xi=\xi_L} = - \frac{\xi - \xi(0)}{U'(\xi, \zeta^*) + K} \Big|_{\xi=\xi_L} \quad (\text{A3.51})$$

and

$$\frac{\partial \xi_R(\zeta^*)}{\partial K} = -\frac{\partial f}{\partial K} \left(\frac{\partial f}{\partial \xi} \right)^{-1} \Big|_{\xi=\xi_R} = -\frac{\xi - \xi(0)}{U'(\xi, \zeta^*) + K} \Big|_{\xi=\xi_R} \quad (A3.52)$$

where

$$U'(\xi, \zeta^*) = \frac{d}{d\xi} U(\xi, \zeta^*). \quad (A3.53)$$

Substituting (A3.51) and (A3.52) into (A3.50) the generalized susceptibility χ takes the simple form of

$$\chi = -\frac{1}{2} \left[\frac{\xi_R - \xi(0)}{U'(\xi_R, \zeta^*)} + \frac{\xi_L - \xi(0)}{U'(\xi_L, \zeta^*)} \right], \quad (A3.54)$$

where $\xi_R(\zeta^*)$ and $\xi_L(\zeta^*)$ denote the extrema of the domain accessible of the unperturbed map.

Since our potential fulfills the symmetry

$$U'(\xi_R, \zeta^*) = -U'(\xi_L, \zeta^*), \quad (A3.55)$$

the generalized susceptibility is simplified to (A3.31).

q.e.d.

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