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Conduction and Chaotic Dynamics

Relatore

Prof. Fulvio Baldovin

Laureando

Matteo Guardiani

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Abstract

In this work we analyze the Onsager theory of conduction within the context of low-dimensional nonlinear systems. After presenting the thermodynamics of conductive processes, we introduce the logistic map as a paradigmatic example for non-conservative chaotic dynamics. In the fully chaotic case, when the logistic map coincides with the Ulam map, we exactly characterize the exponential regression to equilibrium of a uniformly distributed set of initial values of particle positions. This new approach gives rise to the question of whether the Onsager theory could be generalized by introducing an adapted concept of microscopic reversibility.

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Chapter 1

Introduction

Conduction occurs when physical properties of matter within a given material are transported through time and space by the interactions of neighboring particles [1]. A valid theoretical description of conduction developed by Onsager [2, 3] uses fluctuations of non equilibrium thermodynamic quantities to link the microscopic particles' dynamics to macroscopic conduction effects under the assumption of microscopical reversibility.

It therefore becomes interesting to test whether Onsager's theory provides a good physical description of conduction even when the underlying dynamics of the particles becomes more complex. In particular, how it adapts in the context of non Hamiltonian particle trajectories and more generally when microscopic reversibility is lost. In this thesis we make an effort in this direction by exploring the thermodynamics of conduction in the case of non linear maps of the logistic class. These maps provide a simple description of chaotic behavior and for this reason they represent a natural framework for the study of conduction in a chaotic system. We will specifically focus on maps for which a closed-form solution for the dynamics is known in order to fully characterize the conductive properties of such systems.

We start by introducing the thermodynamics of conduction. In particular we explain why thermodynamic variables shall be treated as local fields. Before tackling the more complex case of conduction in chaotic systems, we apply the methods shown in Ref. [4] to the relatively simpler framework of Brownian moving particles. Finally, we focus on the analysis of conduction in the case of fully chaotic logistic-map driven particles. This has resulted in the development of a new method to derive the probability distribution function of the particles at any time given their initial distribution. This new approach to the problem of conduction of chaotic particles will be used to further develop the results in Ref. [4] by linking the microscopic non-Hamiltonian particles' dynamics to the emerging conductive properties of the system.

Chapter 2

Thermodynamics of Conduction

2.1 Entropy formulation of Thermodynamics

From a thermodynamic perspective, equilibrium states of a simple thermodynamic system are fully characterized in terms of extensive variables such as the internal energy U, the volume V and the number of particles $N_1, N_2, ..., N_r$ of the different chemical species that compose the system [5]. At equilibrium it is possible to define the entropy as a function of these extensive variables. It is then postulated that the values assumed by the extensive variables at equilibrium in the absence of internal constraints are those that maximize the entropy over the manifold of constrained equilibrium states.

The following example will make this postulate clearer. Imagine to enclose N identical particles that are in equilibrium with an energy U inside a box of volume V. It is possible to add an internal constraint on the extensive variables that define the system, for example by dividing the box into two equal compartments by means of a fixed separator. Let's further suppose such separator to be adiabatic - i.e. it does not permit any exchange of heat - but permeable to the particles. We are thus fixing the volumes $V_{(1)}$, $V_{(2)}$ and the internal energies $U_{(1)}$, $U_{(2)}$ of the two subsystems. For the sake of reasoning, we shall now accept that the energy is fixed in the two subcompartments even if the particles can flow from one side to the other. Ideally this could be obtained by controlling the temperature of the two. In addition it must still hold $N = N_{(1)} + N_{(2)}$ and the analogous relations for the energy and the volume. Let us consider all possible configurations with $N_{(1)}$ particles in (1) and $N - N_{(1)}$ in (2). If we fix each configuration - for example by making the partition instantly impermeable to particles - once equilibrium is established within each compartment it is possible to compute the constrained entropy

$$S_C\big(N_{(1)}\big) = S_C^{(1)}\big(U_{(1)}, V_{(1)}, N_{(1)}\big) + S_C^{(2)}\big(U_{(2)}, V_{(2)}, N - N_{(1)}\big).$$

The above mentioned postulate then states that once the partition has been removed and equilibrium has settled, the extensive parameters will assume the values corresponding to the maximum of the constrained manifold, i.e. $\max_{N_{(1)}} S_C\big(N_{(1)}\big)$.

The maximal information on a system at equilibrium is then given by the entropy written in terms of the extensive variables that characterize the system i.e. for a system of r different species of particles in a volume V with internal energy U, $S(U, V, N_1, N_2, ..., N_r)$. The derivative of S with respect to an extensive variable while keeping the others fixed defines the corresponding intensive variable

$$\frac{1}{T} := \frac{\partial S}{\partial U}\Big|_{V,N_1,\ldots,N_r} \qquad \frac{P}{T} := \frac{\partial S}{\partial V}\Big|_{U,N_1,\ldots,N_r} \qquad \frac{\mu_j}{T} := -\frac{\partial S}{\partial N_j}\Big|_{U,V,N_r \neq N_j} \tag{2.1}$$

where T is called temperature, P is the pressure and μ_j is the chemical potential of the j^{th} species. From now on for simplicity we will assume the system to be composed by only one chemical species and therefore drop the j subscript.

2.2 Onsager Theory

A detailed account of Onsager Theory of conductive processes can be obtained trough the continuum description. In such a context it is convenient to consider space as made up of material points. A *material point* is defined as a region of space (for sake of simplicity, let us assume it cubical) which is small enough to be considered punctiform from a macroscopic point of view. On the other hand, the same material point contains so many atoms or molecules that it is possible to consider it as a large system, where the thermodynamic limit is applicable. A classical example of a material point is a cubic portion of an ideal gas under normal conditions of side L = 1 mm. Its volume $V = 10^{-9}\,\mathrm{m}^3$ contains $N = V\ N_A \simeq 2.7 \times 10^{16}$ particles, where N_A is the Avogadro constant. This number is large enough that it is possible to apply the thermodynamic limit within the material point. Therefore in the language of continuum physics thermodynamic variables become local fields, functions of time and of the position in the space of material points.

In view of the applications that follow, we focus our discussion on a system composed of N_0 equal particles confined inside a cylinder of length L and base A (as shown in Figure 2.1). The cylinder is thermally, mechanically and chemically isolated. Moreover we reduce to a one dimensional problem by assuming the radius of the cylinder to be much smaller than the length L and particles to be uniformly distributed over any cross section. The 3D particle distribution function will therefore be referred to as $N(x, t)$. Although we will focus on diffusion, other conduction processes like the electric or thermal one can be treated similarly.

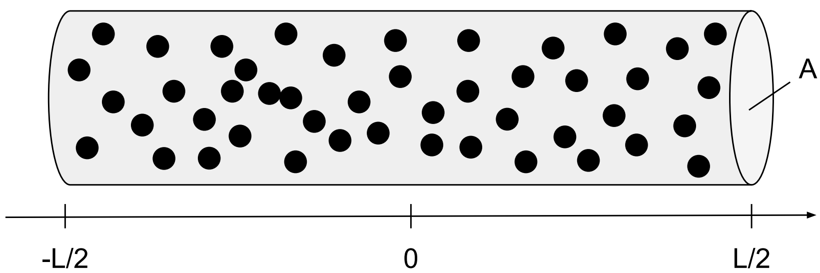

Figure 2.1: N_0 particles distributed within a cylinder of section A and length L.

2.2.1 Thermodynamics of conduction

We would now like to adapt to continuous systems the basic thermodynamic notions that were briefly recalled at the beginning of this chapter. We will assume thermodynamic equilibrium within each material point. As anticipated, the extensive variables now become local fields i.e. functions of the position in the space of material points. Since the extensive variables depend on the position, global equilibrium is lost. Therefore we will indicate the 3D distribution function as $N(x,t)$ and similarly define the analogous quantities for the energy and the volume $U(x,t), V(x,t)$. Thus, entropy becomes a functional of these extensive-variable fields $S[U(x,t), V(x,t), N(x,t)]$ under the assumption of local equilibrium. Ideally two neighboring material points will no longer be in equilibrium so they can be considered as two different constrained thermodynamic systems. For this reason entropy will not be maximum everywhere and its functional derivatives with respect to the constrained variables while keeping the other variables fixed will express the fluctuation from equilibrium. We will only take in account small (linear) fluctuations from equilibrium and for clarity we shall uniquely consider the particle-distribution dependence of the entropy, i.e. $S[N(x,t)]$. Furthermore we will apply the formalism developed so far to the cylindrical system in Fig. 2.1. We will be interested in the behavior of the 3D-distribution function's $N(x,t)$ nth-order moments

$$N_n[N] := A \int_{\mathscr{D}} x^n N(x,t)\,\mathrm{d}x$$

with $\mathscr{D} = \{x \in \mathbb{R} : -L/2 \leq x \leq L/2\}$ and A the area of the cross section of the cylinder. Under the hypothesis of local equilibrium we then define the entropy density the function $\sigma(N(x,t))$ for which the system's constrained entropy becomes

$$S[N] = A \int_{\mathscr{D}} \sigma(N(x,t))\,\mathrm{d}x\,.$$

A measure of the system's fluctuation from equilibrium can thus be computed by taking the first order variation of the entropy

$$\delta S[N] = A \int_{\mathscr{D}} \frac{\partial \sigma(N(x,t))}{\partial N(x,t)} \delta N(x,t)\,\mathrm{d}x = -A \int_{\mathscr{D}} \frac{\mu}{T}(N(x,t))\ \delta N(x,t)\,\mathrm{d}x$$

where we have defined $\frac{\mu}{T}(N(x,t)) := -\frac{\delta S[N]}{\delta N(x)} = -\frac{\partial \sigma(N(x,t))}{\partial N(x,t)}$ which is the translation of the last of the relations in Eq. (2.1) in the language of continuum physics. For what concerns the distribution function we must apply some conditions. In particular we require the variation of the density profile $\delta N(x,t)$ to satisfy $\delta N_0 = A \int_{\mathscr{D}} \delta N(x,t)\,\mathrm{d}x = 0$ which encodes the fact that no particles are allowed to flow in or out of the cylinder. The definition of entropy requires that for the equilibrium distribution $\delta S[N_{\mathrm{eq}}] = 0$, even though in principle N_{eq} could also be nonuniform. We highlight this concept since while for the first example we will treat (the Brownian one) we will eventually find a uniform equilibrium distribution, as we will see - e.g. in the case of the logistic-map driven dynamics - this is not always the case. However since the equilibrium distribution maximizes the entropy, it is possible to recover a conserved quantity. If we consider the reallocation of an arbitrary particle from $x_1 \in \mathscr{D}$ to $x_2 \in \mathscr{D}$ we get

$$0 = \delta S[N_{\mathrm{eq}}] = -A \int_{\mathscr{D}} \frac{\mu}{T}(N_{\mathrm{eq}}(x))\ \frac{[\delta(x-x_1) - \delta(x-x_2)]}{A}\,\mathrm{d}x = \left[\frac{\mu}{T}(N_{\mathrm{eq}}(x))\right|_{x_1}^{x_2}$$

which means that $\frac{\mu}{T}(N_{\text{eq}}(x))$ is constant on $\mathscr{D}$. To study the fluctuations of the system from equilibrium we expand S around equilibrium

$$S[N] = S[N_{\text{eq}}] + \frac{A}{2}\int_{\mathscr{D}} \frac{\partial^2 \sigma}{\partial N^2}\bigg|_{N_{\text{eq}}(x)} \delta N^2(x,t)\,\mathrm{d}x + \mathcal{O}\big(\delta N^2\big)$$

and recognize in the term

$$\frac{\delta S[N]}{\delta N(x)} = \frac{\partial^2 \sigma}{\partial N^2}\bigg|_{N_{\text{eq}}(x)} \delta N(x,t)$$

the local generalized thermodynamic force. This force is linear in the fluctuation $\delta N(x,t)$ and its intensity depends on the second derivative of the entropy density with respect to the particles' distribution function. It can physically be seen as the force that takes care of the unconstrained system's fluctuations and drives it back to equilibrium. Einstein's formula [6] shows that the probability of a fluctuation from equilibrium is proportional to the exponential of the constrained entropy, and therefore through a Gaussian integration it is possible to recover a relation for the fluctuation's expected value

$$\begin{aligned}\mathbb{E}\left[\delta N^2(x)\right] &= \int_{\Gamma} \frac{\delta N^2(x)}{\mathcal{N}} \exp\left[\frac{A}{2k_B}\int_{\mathscr{D}} \frac{\partial^2 \sigma}{\partial N^2}\bigg|_{N_{\text{eq}}(x)} \delta N^2(x)\,\mathrm{d}x\right]\mathcal{D}(\delta N(x)) = \\ &= -\frac{k_B}{AL}\left[\frac{\partial^2 \sigma}{\partial N^2}\bigg|_{N_{\text{eq}}(x)}\right]^{-1}\end{aligned}$$

where $\mathcal{N}$ is the normalization and Γ the set of all possible curves $\delta N(x)$ such that $\delta N(\pm L) = 0$. Einstein's formula is valid for any observable, once the distribution function is known. Therefore we recover an explicit relation between the thermodynamic response and the average squared fluctuation

$$\frac{\partial^2 \sigma}{\partial N^2}\bigg|_{N_{\text{eq}}(x)} = -\frac{k_B}{AL}\,\frac{1}{\mathbb{E}\left[\delta N^2(x)\right]}.$$

2.2.2 Linearly varying intensive parameter

As we have shown, for the equilibrium distribution $N_{\text{eq}}(x)$ we expect $\frac{\mu}{T}(x)$ to be a constant function of x hence for continuity - for small fluctuations from equilibrium - we assume $\frac{\mu}{T}(x,t)$ to be spatially smooth. We will now consider linear variations of $\frac{\mu}{T}(x,t)$, that will provide a clearer physical interpretation of our previous derivations. First of all since as proven in Appendix A any distribution $N(x,t)$ is fully described by its nth moments $N_n[N]$, the entropy functional $S[N]$ can be seen as an ordinary function of the particles' distribution moments [7]. Therefore it is possible to write

$$S[N] = S(N_n[N]). \tag{2.2}$$

From now on we will simply consider $S(N_0, N_1)$ which corresponds to a second order expansion of $S(N_n[N])$ (see again Appendix A), so taking the functional derivative in Eq. (2.2) we get

$$\begin{aligned}-\frac{\mu}{T}(x,t) &= \frac{\delta S[N]}{\delta N(x)} = \frac{\partial S(N_0,N_1)}{\partial N_0}\frac{\delta N_0}{\delta N(x)} + \frac{\partial S(N_0,N_1)}{\partial N_1}\frac{\delta N_1}{\delta N(x)} + \mathcal{O}\big(x^2\big) = \\ &= -\frac{\overline{\mu}}{T} + \frac{\partial S(N_0,N_1)}{\partial N_1}\,x + \mathcal{O}\big(x^2\big),\end{aligned}$$

where we have defined the global intensive parameter $\frac{\overline{\mu}}{T} := -\frac{\partial S(N_0,N_1)}{\partial N_0}$. Let us consider the Taylor expansion around $x = 0$ of $-\frac{\mu}{T}(x,t)$

$$-\frac{\mu}{T}(x,t) = -\frac{\mu}{T}(0,t) - \nabla_x \frac{\mu}{T}(0,t)\ x + \mathcal{O}\big(x^2\big),$$

by comparison with the former expression we find

$$\frac{\partial S(N_0,N_1)}{\partial N_1} = -\nabla_x \frac{\mu}{T}(0,t).$$

We have written the x derivative as a gradient to stress that this derivation can be easily generalized to the 3 dimensional case. From the last expression it is clear that the intensity of the thermodynamic force that restores equilibrium is related to the gradient of the intensive parameter $\frac{\mu}{T}$. Since we have imposed impermeable boundaries, N_0 is the number of particles which compose the system which is constant once the initial distribution in specified. With this in mind we will omit the entropy's dependence on N_0 since it is an irrelevant thermodynamic parameter and write

$$S(N_1) = S(N_{1,\mathrm{eq}}) + \frac{1}{2}\left.\frac{\partial^2 S}{\partial N_1^2}\right|_{N_{1,\mathrm{eq}}} \delta N_1^2(x,t) + \mathcal{O}\big(\delta N_1^2\big),$$

obtaining the expansion for the thermodynamic force around $x = 0$

$$\left.\frac{\partial^2 S}{\partial N_1^2}\right|_{N_{1,\mathrm{eq}}} \delta N_1(t) = -\nabla_x \frac{\mu}{T}(0,t) = -\frac{k_B}{\mathbb{E}\left[\delta N_1^2\right]}\ \delta N_1(t).$$

Let us try to interpret the $\delta N_1(t)$ term. We want to show its relation to the particle's number flux $J_N(x,t)$. Let us suppose for simplicity to be in a quasi-stationary state within the cylinder i.e. that the thermodynamic parameters are almost time independent. Such states can only occur if the number flux is uniform. In this way the number of particles entering arbitrarily small volumes in a given time interval is the same of those flowing out. Under such assumptions

$$J_N(x,t) := \overline{J}_N(t)\left[\Theta\left(x+\frac{L}{2}\right) - \Theta\left(x-\frac{L}{2}\right)\right]$$

where $\Theta(x)$ denotes the Heaviside function and taking the x gradient we find

$$\nabla_x\ J_N(x,t) = \overline{J}_N(t)\left[\delta\left(x+\frac{L}{2}\right) - \delta\left(x-\frac{L}{2}\right)\right].$$

If we write the continuity equation at a point x for $\delta N(x,t)$, and since $\delta N(x,t) = N(x,t) - N_{\mathrm{eq}}(x)$ and $N(x,t)$ have the same time dependence, we get

$$\partial_t\ \delta N(x,t) = \partial_t N(x,t) = -\nabla_x\ J_N(x,t).$$

Finally, we want to show that the variation of the first moment $\delta N_1(t)$ is the fundamental parameter in order to study regression to equilibrium. Therefore we notice that

$$\begin{aligned}\partial_t \delta N_1(t) &= A\ \partial_t \int_{\mathscr{D}} x\ \delta N(x,t)\,\mathrm{d}x = A \int_{\mathscr{D}} x\ \partial_t N(x,t)\,\mathrm{d}x = \\ &= -A \int_{\mathscr{D}} x\ \overline{J}_N(t)\left[\delta\left(x+\frac{L}{2}\right) - \delta\left(x-\frac{L}{2}\right)\right]\mathrm{d}x = AL\ \overline{J}_N(t),\end{aligned}$$

which means that the first variation of N_1, the most relevant term of the thermodynamic force that takes care of fluctuations from equilibrium, is proportional with the volume to the number flux $\overline{J}_N$.

2.2.3 Onsager's equilibrium regression

According to Onsager [2,3], the behavior of δN_1 and therefore of the thermodynamic force governing fluctuations from equilibrium shall not depend on whether the fluctuation is spontaneous or generated by an external field or reservoir. The main assumption we will make in the following derivations is that this argument holds regardless of the underlying dynamics of the system. It is a crucial one, since Onsager's theory is derived under the hypothesis of microscopic reversibility. This condition will definitely hold for our first application of conduction theory - Brownian motion - but will eventually become questionable as soon as we will move to chaotic systems due to the nonlinearity of the dynamics.

Let us now consider a small fluctuation from equilibrium at time t_0, as we know it can be monitored by $\delta N_1(t_0)$. It has been shown [8] that the most likely behavior for $\delta N_1(t_0+\tau)$, which we will denote with $\overline{\delta N_1}(t_0+\tau)$, is linear in the thermodynamic force and in time if we consider a small $|\tau|$ expansion (for $|\tau|$ larger than the molecular time scales but smaller than the macroscopic ones)

$$\overline{\delta N_1}(t_0+\tau) \overset{|\tau|\ll 1}{\simeq} \delta N_1(t_0) - |\tau| \ \frac{\Lambda}{2} \ \nabla_x \frac{\mu}{T}(0,t_0). \tag{2.3}$$

Λ is a positive coefficient which we will show to encode the transport properties of the system. Therefore,

$$\begin{aligned}\overline{J}_N(t_0+\tau) &= \frac{1}{AL} \ \partial_t \ \delta N_1(t_0+\tau) \simeq \\ &\simeq \frac{1}{AL} \frac{\overline{\delta N_1}(t_0+\tau) - \delta N_1(t_0)}{|\tau|} = -\frac{\lambda}{2AL} \ \nabla_x \frac{\mu}{T}(0,t_0).\end{aligned}$$

If we assume that the the intensive parameter can be viewed, as we did in the equilibrium case, as the chemical potential μ divided by the temperature T and that the latter is uniform along the system, then the previous relation can be written in a more convenient fashion

$$\overline{J}_N = -D \ \nabla_x N, \tag{2.4}$$

where have defined the diffusion coefficient

$$D \coloneqq \frac{\Lambda}{2AL} \ \frac{1}{T} \ \frac{\partial \mu}{\partial N}.$$

Relation (2.4) is commonly known as the *Fick's First Law* [9].

It is also possible to show [10–12] that the Λ coefficient depends on the fluctuation's autocorrelation by the Green-Kubo relation

$$\Lambda = -\frac{2}{k_B \ |\tau|} \ \left(\mathbb{E} \ [\delta N_1(t_0+\tau) \ \delta N_1(t_0)] - \mathbb{E} \ [\delta N_1^2(t_0)]\right)$$

in which $\mathbb{E} \ [\delta N_1^2(t_0)] = \mathbb{E} \ [\delta N_1^2]$ is an average over the equilibrium distribution. Instead of using Λ, we can define

$$\lambda \coloneqq \frac{k_B \ \Lambda}{\mathbb{E} \ [\delta N_1^2]}$$

and rewrite Eq.(2.3) into

$$\overline{\delta N_1}(t_0+\tau) \overset{|\tau|\ll 1}{\simeq} \delta N_1(t_0) - \frac{\lambda|\tau|}{2} \ \delta N_1(t_0).$$

Moreover, under the hypothesis of Gaussian and Markovian dynamical evolution, the Doob's theorem [13, 14] ensures that the fluctuation at larger τ follows an exponential decay

$$\overline{\delta N_1}(t_0 + \tau) = \delta N_1(t_0)\ e^{-\frac{\lambda|\tau|}{2}}. \tag{2.5}$$

In summary, we have shown that fluctuations from equilibrium of a macroscopic observable are governed by $\mathbb{E}\left[N_1^2\right]$, which determines the strength of the force that drives the system back to equilibrium. Sensible information on the conductive properties of the system encoded into λ can be gained by monitoring the time evolution of $\delta N_1(t)$.

2.3 Brownian Motion

We are now going to show how to apply the developed theory in the simple case of Brownian Motion. This will be useful to understand the actual relations between the mathematical objects we have defined in the previous chapter and their physical meaning before moving to the chaotic case.

2.3.1 Brownian Dynamics

In 1827 a botanist called Robert Brown was observing the dynamics of the pollen of Clarkia Pulchella in water. He noticed that the pollen's motion, which has then been called Brownian, appeared to be random. It was only in 1905 that Albert Einstein, in one of his first scientific contributions, arrived to a statistical-mechanics explanation of such motion as a result of collisions of the pollen with the much smaller particles of water. Even if these kind of dynamics is Hamiltonian, and therefore the analytic solution for the motion of each particle exists within Classical Mechanics, the complexity of the problem makes the classical approach impracticable.

The statistical-mechanics approach works under the assumption that the motion of the Brownian particles is compensated by the one of the smaller particles with which they interact in order to preserve energy and momentum of the system and to be in condition of null convection. The Brownian particle's motion is then affected by a stochastic term which describes the impacts of fluid particles. If we consider the position $\boldsymbol{x}(t)$ of a Brownian particle of mass m in an external bath the equation of motion will read

$$m\ddot{\boldsymbol{x}}(t) = -\frac{\dot{\boldsymbol{x}}}{\mu}(t) - \boldsymbol{\nabla} V(\boldsymbol{x}, t) + \boldsymbol{f}_{\mathrm{r}}(t). \tag{2.6}$$

The first term on the right hand side is a friction term due to viscosity, the second is the action of an external potential for example gravity and $\boldsymbol{f}_{\mathrm{r}}(t)$ is the random force. We assume the stochastic term to have mean zero. If we now consider the external potential to be zero, and we focus on the study of the overdamped limit, i.e. the viscosity term is assumed to be much bigger than the inertial one, Equation (2.6) becomes

$$\dot{\boldsymbol{x}}(x, t) = \boldsymbol{v}(\boldsymbol{x}) + \boldsymbol{\eta}(t),$$

where $\boldsymbol{v}(\boldsymbol{x}) := -\mu\boldsymbol{\nabla} V(\boldsymbol{x}, t)$ is called *deterministic velocity* and $\boldsymbol{\eta}(t) := \mu\boldsymbol{f}_{\mathrm{r}}(t)$ is called *stochastic velocity* and has zero mean. This equation is referred to as the *Langevin Equation* [15]. It is possible to use the Central Limit Theorem to support the assumption that $\boldsymbol{\eta}(t)$ is proportional to a Gaussian distribution with zero mean and standard deviation $\sqrt{2D}$, where $D \in \mathbb{R}$ is a parameter related to diffusion.

2.4 Conduction and Brownian Motion

The distribution function of the N_0 particles within the cylindrical system is

$$N(x,t) := \frac{1}{A} \sum_{i=1}^{N_0} \delta(x - x_i(t)),$$

in which $x \in \mathbb{R}$ is an Eulerian coordinate while $x_i(t) \in \mathbb{R}$ defines the Lagrangian coordinate. In this approach there are actually two sources of randomness involved. The first regards the initial particles' distribution $N(x,t_0)$, the second is due to the random term in the dynamical evolution equation. It can be shown [15] that the most likely evolution of the distribution function $\overline{N}(x,t)$ is ruled by the *Fokker-Planck Equation*

$$\partial_t \, \overline{N}(x,t) = D \, \nabla_x^2 \overline{N}(x,t). \tag{2.7}$$

The solution in the case of reflecting boundary conditions for $x = \pm\frac{L}{2}$ can be found by applying the appropriate Green function to the initial distribution $N(x_0,t_0)$

$$\overline{N}(x,t) = \frac{1}{L} \int_{\mathscr{D}} \left[1 + 2 \sum_{n=1}^{\infty} e^{-\frac{n^2\pi^2 D}{L^2}(t-t_0)} \cos\left(n\pi \frac{2x+L}{2L} \right) \cos\left(n\pi \frac{2x_0+L}{2L} \right) \right] N(x_0,t_0) \, \mathrm{d}x_0 \,.$$

The equilibrium distribution $N_{\text{eq}} = \lim_{x\to\infty} \overline{N}(x,t)$ is found to be uniform $N_{\text{eq}} = \frac{N_0}{AL}$, independently of $N(x_o,t_0)$, as the symmetry of the problem suggests. We are now interested in the first order variation $\overline{\delta N_1}(t)$ which can easily be calculated

$$\begin{aligned} \overline{\delta N_1}(t) &= A \int_{\mathscr{D}} x \, \left[\overline{N}(x,t) - N_{\text{eq}}(t) \right] \mathrm{d}x = \\ &= -4 \sum_{\substack{n=1 \\ n \text{odd}}}^{\infty} \frac{AL}{n^2\pi^2} \, e^{-\frac{n^2\pi^2 D}{L^2}(t-t_0)} \int_{\mathscr{D}} \cos\left(n\pi \frac{2x_0+L}{2L} \right) \, N(x_0,t_0) \, \mathrm{d}x_0 \,. \end{aligned}$$

If we choose $N(x_0,t_0)$ sufficiently close to N_{eq} and consider the $t \gg 1$ limit, $\overline{\delta N_1}(t)$ is dominated by the $n = 1$ term

$$\overline{\delta N_1}(t) \overset{t \gtrsim 1}{\simeq} \delta N_1(t_0) \, e^{-\frac{\pi^2 D}{L^2} t}$$

and therefore it is possible to recover the relation written in Eq. (2.5) with

$$\lambda := \frac{2\pi^2}{L^2} D.$$

We stress this exponential-decay dependence because it shows how the macroscopic properties of conduction are encoded by the local microscopic transport properties and the global geometry of the system.

Chapter 3

Chaotic Dynamics

At the end of the nineteenth century, French mathematician Henri Poincaré was probably the first scientist to address the problem of chaotic dynamics. He was studying the three-body problem in celestial dynamics. What he had discovered is that given a set of initial points in the phase space of certain planets or stars, the resulting orbits - which are now called *chaotic* - are nonperiodic even though they are limited and they do not approach any fixed point. We are briefly going to explain what Chaos Theory is, in particular by focusing on nonlinear maps of the logistic class.

3.1 Dynamical Systems

First of all we introduce the definition of a dynamical system. From a mathematical point of view it is possible to define a dynamical system as follows.

Definition 3.1.1. (*Dynamical System*) A *dynamical system* is the set $\langle \mathcal{M}, f, \mathcal{T} \rangle$, with $\mathcal{M}$ a manifold, $\mathcal{T}$ the domain for time - e.g. non-negative reals, the integers, ... - and f an evolution rule $t \mapsto f(t)$ (with $t \in \mathcal{T}$ such that $f(t)$ is a diffeomorphism of the manifold to itself. So, $f(t)$ is a diffeomorphism, for every time t in the domain $\mathcal{T}$.

Therefore, a dynamical system is a deterministic prescription for the time evolution of the state of a system [16]. The most common example of a dynamical system widely treated in Physics is given by

$$\dot{\boldsymbol{x}}(t) = -\boldsymbol{\mathcal{F}}[\boldsymbol{x}(t)],$$

in which $\boldsymbol{x}(t)$ and $\boldsymbol{\mathcal{F}}[\boldsymbol{x}(t)]$ are N-dimensional vectors. Known the initial state of the system $\boldsymbol{x}(t)$ it is possible to solve the equation for its evolution at any t. The space in which the N coordinates are defined is called *phase space*. Paths in the phase space followed by a system that evolves in time are called *orbits* or *trajectories*. The last key mathematical definition we would like to introduce is the one of attractor. An *attractor* is a bounded subset of the phase space to which regions of initial condition of nonzero phase-space measure asymptote as time increases. As a consequence of Poincaré recurrence theorem, conservative dynamical systems do not have attractors.

3.1.1 Nonlinear Mappings

The simplest setting in which it is possible to develop a theory of chaos is the one-dimensional. Of course in higher dimensions, complex patterns emerge almost naturally, but in principle the one dimensional case provides an easier and simple enough framework to approach chaos. We will consider only discrete, integer-valued time maps which can be written in the form

$$x_{n+1} = f(x_n),$$

in which x_{n+1} is usually called the (time) *iterate* of x_n. A map f is said to be invertible if given x_{n+1}, there exists one and only one x_n such that $x_n = f^{-1}(x_{n+1})$. f^{-1} is then called the inverse of the map f. If the map is invertible then there can be no chaos unless the dimension of the *phase space* $d \geq 2$ [16]. For such reason to find chaotic patterns in $d = 1$ we have to look for non invertible maps. One of the simplest one-dimensional non-invertible maps is the *tent map* discussed in Appendix B. This map is important since it is linear, but nonetheless extremely sensitive to initial conditions [16]. A main point we want to clarify is that chaotic behavior can arise even in completely deterministic systems - i.e. systems in which a univocal evolution law has been specified. The chaotic behavior of the system is then related to the non predictability of the dynamics, which corresponds to the fact that two arbitrarily close initial points, even at small t, can be mapped into very distant iterates.

In the language of dynamical systems a measure of the exponential separation of two adjacent points is called *Lyapunov exponent* and is usually indicated with λ. Thus, if two initial points x_0 and $x_0 + \delta$ are separated by a distance δ and after iterating N times the map they reach a distance $l \coloneqq ||f^N(x_0 + \delta) - f^N(x_0)||$, the *Lyapunov exponent* can be defined as

$$l = \delta e^{N\lambda}.$$

Nonlinear mappings, like the logistic one which we are about to discuss, are indeed maps in which f is nonlinear. Nonlinear maps can definitely produce positive Lyapunov exponents.

3.2 Chaotic Dynamics

3.2.1 Physical Applications

The physical applications of chaos theories are potentially countless. On the one side this is because chaotic patterns can arise from the most simple dynamical system - e.g. the harmonic oscillator in Classical Mechanics. This is due to the separation in phase space of two arbitrary close initial values [17, 18]. On the other side it is possible to provide examples of intrinsically chaotic dynamics that are not even *deterministic* [16] in the Classical-Mechanic sense. In general examples of chaotic behavior can be largely found all over in Nature. The rise of computers has made it possible to find numerical solutions for many dynamical systems, and has shown the importance of a deep understanding of the behavior of chaos in the *complex-system* framework.

3.2.2 Logistic Map

The *logistic map* was introduced in 1976 by the biologist Robert May as a discretization of Verhulst's *logistic equation.* It was used to represent a rough ecological model for the yearly variations in the population of an insect species [16]. Let us suppose that these insects hatch out of eggs every spring. They eat, grow, mate, lay eggs and then die. If we assume the same condition every year, i.e. the same weather, predator population, etc., the population at year $n+1$ is only determined by the one at year n. Moreover, imagining that each insect every year lays on average $r > 1$ eggs, the following year the population will grow from z_n to $z_{n+1} = rz_n$, i.e. it will experience an exponential growth. However, if the population grows too much the food supplies might become scarce. If we suppose that the number of eggs laid for each insect decreases linearly with the population, for example of a factor $r(1 - \frac{z_n}{\overline{z}})$ where $\overline{z}$ represents the theoretical *carrying capacity* of the environment minus the current population and letting $y_n := \frac{z_n}{\overline{z}}$ we get

$$y_{n+1} = ry_n(1 - y_n). \tag{3.1}$$

If we require $y \in [0, 1]$ we obtain $r \in [0, 4]$. Eq. (3.1) is the *logistic map* evolution equation. Its relative simplicity makes it a widely used point of entry into chaos theory. In view of the applications that follow we will consider a different representation of the map

$$x_{t+1} = 1 - \mu x_t^2, \tag{3.2}$$

where $x_t \in [-1, 1]$ and $\mu \in [0, 2]$ is the control parameter of the map. The two representations in Eq. (3.1) and Eq. (3.2 can be topologically conjugated for $r \in (2, 4]$. We show how it is possible to pass from one representation to the other in Appendix F.

The logistic map iterates behavior is extremely sensitive to variations in the control parameter r or μ. Exponential divergence of sequences of iterates for certain values of the control parameters show the connection between chaos and unpredictability and are encoded by positive Lyapunov exponents. Hence, predictions about future states become progressively - indeed, exponentially - worse when there are even very small errors in the knowledge of the initial state.

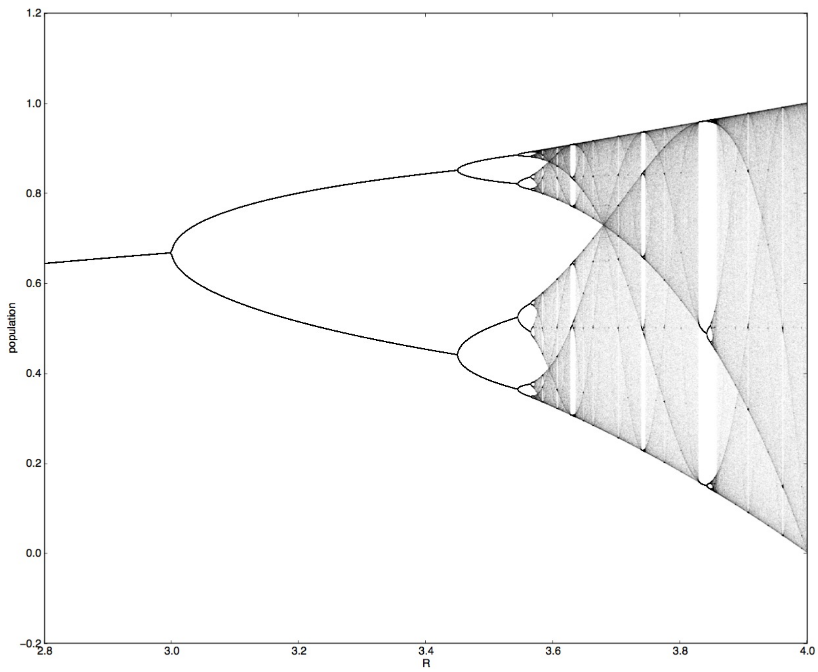

Figure 3.1: Logistic Map bifurcation diagram as a function of the control parameter r.

In Fig. (3.1) we show the logistic map bifurcation diagram in the r representation of the map. The bifurcation diagram displays the set of values of x visited asymptotically from almost all initial conditions by the iterates of the logistic equation at a fixed r value. We see that while for example for certain values of r, i.e. between 0 and 3, the iterates converge to a certain attractor (1-cycle), for other values the dynamics is completely different. Beyond $r \simeq 3.56995$ - that is called the *onset of chaos* - at the end of the period-doubling cascade, we fall into the chaotic end of the map. From almost every initial condition, we no longer see oscillations of finite period.

The Ulam map At the very end of the chaotic region of the map for $r = 4$ we are in what is called the fully chaotic case. In the μ representation the iteration equation becomes

$$x_{n+1} = 1 - 2x_n^2$$

and is also referred to as the *Ulam Map*. This map has several simplifying properties which are not generally valid for the complete logistic map. One of them is that it can be topologically conjugated to the linear *tent map* as we have shown in Appendix B. A fundamental property is the existence of one of the two closed-form solutions of the logistic map [19, 20], i.e. a function for the iterate x_t at any time t, given the initial value x_0

$$x_t = 2\sin^2\left[2^t \arcsin\sqrt{\frac{1}{2}(x_0+1)} - 1\right]. \tag{3.3}$$

The other known exact solution [19] is for $r = 2$ and therefore is a 1-cycle solution.

3.3 Conduction in chaotic systems

Now that the explicit solution for the Ulam map has been presented, we are going to focus on the main subject of the thesis, i.e. the study conduction in chaotic systems. Our derivations will still adapt to the cylindrical system in Fig. (2.1) but without loss of generality we choose to fix $|L| = 2$. We will use the μ representation of the map, which is defined for $x \in [-1, 1]$ and therefore can be more easily adapted to the system. Mimicking what we did for Brownian motion, we would like to find an equivalent to the *Fokker-Planck* equation for N chaotically moving particles, for which the dynamics is governed by the logistic map iteration equation

$$x_i(t) = 1 - \mu x_i^2(t-1),$$

where $x_i(t) \in [-1, 1]$ are the Lagrangian coordinates and $t \in \mathbb{N}_0$ represents the (discrete) time and $\mu \in [0, 2]$ the control parameter of the map. For simplicity we will drop the i subscript and assume the following relations to hold for each particle that composes the system. To shorten the notation we additionally define the Lagrangian coordinate as $x_t := x_i(t)$. If we introduce Eulerian coordinates it is possible to write the probability of finding a particle at a certain point x and time t

$$p(x,t) = \int_{\mathscr{D}} p(x_t|y_{t-1})\; p(y_{t-1})\, \mathrm{d}y\,,$$

and since we know that the evolution of the Lagrangian coordinate is given by the logistic map we get that the transition probability is a Dirac δ-function

$$p(x_t|y_{t-1}) = \delta(x_t - (1 - \mu y_{t-1}^2)).$$

With all this in mind it is possible to write

$$\begin{aligned} p(x,t) &= \int_{\mathscr{D}} \delta[x_t - 1 + \mu y_{t-1}^2]\; p(y_{t-1})\, \mathrm{d}y = \\ &= \int_{-1}^{0} \delta[x_t - 1 + \mu y_{t-1}^2]\; p(y_{t-1})\, \mathrm{d}y + \int_{0}^{1} \delta[x_t - 1 + \mu y_{t-1}^2]\; p(y_{t-1})\, \mathrm{d}y\,. \end{aligned}$$

If we consider the change of variables

$$u := 1 - \mu y^2 \implies y = \pm\sqrt{\frac{1-u}{\mu}} \quad \text{and} \quad \mathrm{d}y = \pm\frac{\mathrm{d}u}{2\sqrt{\mu(1-u)}},$$

where the plus sign applies for $y \in [-1, 1-\mu]$ and the minus for $y \in [1-\mu, 1]$ we get

$$\begin{aligned} p(x,t) &= \int_{1-\mu}^{1} \delta(x-u) \left.\left[\frac{p\left(-\sqrt{\frac{1-u}{\mu}}\right)}{2\sqrt{\mu(1-u)}}\right]\right|_{t-1} \mathrm{d}u - \int_{1}^{1-\mu} \delta(x-u) \left.\left[\frac{p\left(+\sqrt{\frac{1-u}{\mu}}\right)}{2\sqrt{\mu(1-u)}}\right]\right|_{t-1} \mathrm{d}u = \\ &= \begin{cases} 0 & \text{if } x \in [-1, 1-\mu]; \\ \left.\left[\frac{p\left(-\sqrt{\frac{1-x}{\mu}}\right) + p\left(+\sqrt{\frac{1-x}{\mu}}\right)}{2\sqrt{\mu(1-x)}}\right]\right|_{t-1} & \text{if } x \in [1-\mu, 1]. \end{cases} \end{aligned} \tag{3.4}$$

Let us check that it behaves as a probability distribution function, i.e. that it is correctly normalized to 1.

$$\begin{aligned}\int_{-1}^{1} p(x,t)\,\mathrm{d}x &= \int_{1-\mu}^{1} \left[\frac{p\left(-\sqrt{\frac{1-x}{\mu}}\right) \; + \; p\left(+\sqrt{\frac{1-x}{\mu}}\right)}{2\sqrt{\mu(1-x)}}\right]\Bigg|_{t-1} \mathrm{d}x = \\ &= \int_{0}^{1} \left[\frac{2\mu u}{2\sqrt{\mu(\mu u^2)}} p(u)\right]\Bigg|_{t-1} \mathrm{d}u + \int_{-1}^{0} \left[\frac{2\mu u}{2\sqrt{\mu(\mu u^2)}} p(u)\right]\Bigg|_{t-1} \mathrm{d}u = \\ &= \int_{0}^{1} \Big[p(u)\Big]\Big|_{t-1} \mathrm{d}u + \int_{-1}^{0} \Big[p(u)\Big]\Big|_{t-1} \mathrm{d}u = \\ &= 1\end{aligned}$$

which shows the correct normalization, provided of course that $p(x, 0)$ is normalized to 1. So Eq. (3.4) represents the probability distribution function of finding a certain particle in x at time t. An interesting property of the map is the equilibrium probability distribution function p_{eq}, that should satisfy

$$p_{\mathrm{eq}}(x) = \frac{p_{\mathrm{eq}}\left(\sqrt{\frac{1-x}{\mu}}\right) + p_{\mathrm{eq}}\left(-\sqrt{\frac{1-x}{\mu}}\right)}{2\sqrt{\mu(1-x)}}. \tag{3.5}$$

In order to find the equilibrium distribution we shall introduce the transfer operator method [21]. Given a probability density function $p(x, t)$, it is possible to define the *Perron-Frobenius operator* $\mathcal{L}$ as

$$p(x,t) = \mathcal{L}\;[p(x,t-1)].$$

In the logistic map case such operator acts as we have shown in Eq 3.4. This operator therefore encodes the time evolution of the dynamical system. Actually, it can be seen as the analogous of the the Liouville operator $\hat{L}[f] \coloneqq -i\{f, \mathcal{H}\}$ in Classical Mechanics where $\{\,\cdot\,,\,\cdot\,\}$ denotes the *Poisson bracket* and $\mathcal{H}$ the Hamiltonian of the system. In this analogy the role of $\mathcal{L}$ is assumed by $\mathcal{L}_{\mathcal{H}} \coloneqq \exp\left[-i\hat{L}t\right]$, where t is the time interval in which the evolution has taken place. Looking for an invariant distribution means searching for a fixed point of the *Perron-Frobenius operator* of the specific map. The fixed point is indeed an entire function, the equilibrium probability density function $p_{\mathrm{eq}}(x)$. No analytic expression has been found [21] for the invariant distribution of the logistic map for values of μ different from 0 and 2.

3.3.1 The Fully Chaotic Case

Let us focus on the fully chaotic case. As we have stated previously, this case is obtained for $\mu = 2$. It can be shown (see Appendix B) that the equilibrium distribution in this case is

$$p_{\mathrm{eq}}(x) = \frac{1}{\pi\,\sqrt{1-x^2}}. \tag{3.6}$$

We now address the problem of finding the probability distribution $p(x, t)$ at a point x and time t for the fully chaotic case $\mu = 2$. We will use the general approach viewed above and adapt it to the case in which the analytic solution of the dynamics is known.

First of all let's recover the explicit solution Eq. (3.3). Accordingly to what we have done previously, the probability distribution $p(x,t)$ can be found passing to Eulerian coordinates $x \in [-1,1]$. Having a closed-form solution though means that it is possible to compute $p(x,t)$ directly from the initial distribution that we call $p(y_0)$

$$p(x,t) = \int_{\mathscr{D}} p(x,t|y,0)\; p(y,0)\,\mathrm{d}y\,.$$

The transition probability $p(x,t|y,0)$ is still given by a Dirac δ-function

$$p(x,t|y,0) = \delta\left[x - \left(2\sin^2\left[2^t \arcsin\sqrt{\frac{1}{2}(y+1)}\right] - 1\right)\right].$$

Let's now call $u(y) \coloneqq 2\sin^2\left[2^t \arcsin\sqrt{\frac{1}{2}(y+1)}\right] - 1$. Inverting this change of variable is a crucial but tricky calculation that has been explicitly worked out in Appendix C. After performing this variable change we are left with

$$p(x,t) = \sum_{k=0}^{2^t-1} \int_{I_k} \delta(x-u)\; \tilde{p}(u,0)\,\mathrm{d}u\,, \tag{3.7}$$

where $\tilde{p}(u,0) \coloneqq p(y(u),0)$. We also recall our definition of

$$I_k(t) \coloneqq [-\cos(2^{-t}k\pi), -\cos(2^{-t}(k+1)\pi)]$$

that are the intervals of monotonicity of the function $u(y)$ i.e. those on which it is possible to invert the function in order to compute $p(x,t)$ from Eq. (3.7). A straightforward calculation, reported in Appendix C yields to

$$p(x,t) = \sum_{k=0}^{2^t-1} \frac{\sin\left[2^{-t}\left(\arccos\left[(-1)^{k+1}x\right] + k\pi\right)\right]}{2^t\sqrt{1-x^2}}\; p\Big(-\cos\left[2^{-t}\Big(\arccos[(-1)^{k+1}x] + k\pi\Big)\right], 0\Big).$$

Now that the probability distribution function is known, it is possible to test Onsager's approach. All the calculations that follow are explained in detail in Appendix D. We analyze relaxation to equilibrium for different initial particles' distributions. For the sake of clarity we have chosen to report only the crucial passages in order to deliver the main picture.

Uniform distribution Considering a uniform initial distribution $p(x,0) = \frac{1}{2}, \forall x \in \mathscr{D}$, from Eq. (3.7) we see that

$$p(x,t) = \frac{1}{2}\sum_{k=0}^{2^t-1} \frac{\sin\left[2^{-t}\left(\arccos\left[(-1)^{k+1}x\right] + k\pi\right)\right]}{2^t\sqrt{1-x^2}}.$$

Therefore

$$\begin{aligned}\delta N_1(t) &\coloneqq N_1(t) - N_{1,\mathrm{eq}} = N_1(t) = \\ &= \frac{A}{\pi}\sum_{k=0}^{2^t-1}\int_{\mathscr{D}} x\, \frac{\sin\left[2^{-t}\left(\arccos\left[(-1)^{k+1}x\right] + k\pi\right)\right]}{2^{t+1}\sqrt{1-x^2}}\,\mathrm{d}x = \\ &= \frac{A}{\pi}\sum_{k=0}^{2^t-1} d_k(t),\end{aligned}$$

having defined

$$d_k(t) := \int_{\mathscr{D}} x \; \frac{\sin\left[2^{-t}\big(\arccos\left[(-1)^{k+1}x\right] + k\pi\big)\right]}{2^{t+1}\sqrt{1-x^2}} \,\mathrm{d}x\,.$$

Analogously to what we have shown in Appendix D for the small linear perturbation, the sum has then been evaluated with *Mathematica* giving the following output

$$\begin{aligned}\delta N_1(t) &= \frac{A}{\pi}\left[\frac{\cos^2\left[2^{-t-1}\,\pi\right]}{4^t-1} + \frac{1}{2}\sum_{k=1}^{2^t-1}(-1)^k\;\frac{\cos\left[2^{-t}\pi\;a_1(k)\right] + \cos\left[2^{1-t}\pi\;a_2(k)\right]}{4^t-1}\right] = \\ &= \frac{A}{\pi}\;\frac{1}{4^t-1}.\end{aligned}$$

Step distribution function The last interesting initial distribution we are going to analyze is the one in which the particles are all uniformly distributed within the positive x half of the cylinder, i.e.

$$p(x,0) = \begin{cases} 0, & \text{if } x \in [-1,0) \\ 1, & \text{if } x \in [0,1] \end{cases}$$

Remembering that

$$p(x,t) = \sum_{k=0}^{2^t-1} \frac{\sin\left[z_k(x,t)\right]}{2^t\sqrt{1-x^2}}\; p(z_k(x,t),0)$$

and

$$z_k(x,t) = -\cos\left[2^{-t}\Big(\arccos[(-1)^{k+1}x] + k\pi\Big)\right] \implies \begin{cases} z_k(x,t) < 0, & \text{if } 0 \le k \le 2^{t-1}-1 \\ z_k(x,t) \ge 0, & \text{if } 2^{t-1} \le k \le 2^t-1, \end{cases}$$

in this case $p(x,t)$ assumes the following form

$$p(x,t) = \sum_{k=2^{t-1}}^{2^t-1} \frac{\sin\left[2^{-t}\big(\arccos\left[(-1)^{k+1}x\right] + k\pi\big)\right]}{2^t\sqrt{1-x^2}}.$$

Finally calculating the fluctuation

$$\begin{aligned}\delta N_1(t) &:= N_1(t) - N_{1,\mathrm{eq}} = N_1(t) = \\ &= \frac{A}{\pi}\sum_{k=2^{t-1}}^{2^t-1}\int_{\mathscr{D}} x\;\frac{\sin\left[2^{-t}\big(\arccos\left[(-1)^{k+1}x\right] + k\pi\big)\right]}{2^t\sqrt{1-x^2}}\,\mathrm{d}x = \\ &= \frac{A}{\pi}\sum_{k=2^{t-1}}^{2^t-1}(-1)^k\;\frac{\cos\left[2^{-t}\pi\;a_1(k)\right] + \cos\left[2^{1-t}\pi\;a_2(k)\right]}{4^t-1} = \\ &= \frac{A}{\pi}\;\frac{1}{4^t-1}\end{aligned}$$

where as in the previous cases (see Appendix C and D) we have used *Mathematica* to find the proper coefficients of the sum.

Just as in the Brownian case, we see that the dominant time dependence of the fluctuation $\delta N_1(t)$ tipically follows an exponential law.

Chapter 4

Conclusions

In this work we have shown how a fully chaotic system relaxes to equilibrium. As seen at the end of the previous chapter, the fluctuation of the first moment of the particle-distribution function tipically follows an exponential decay. In the Brownian case, when the microscopic dynamics was ruled by the *Fokker-Planck equation* Eq. (2.7), we were able to find a relation between the exponent $-\lambda t$ of the fluctuation from equilibrium $\delta N_1(t)$ and both the dynamical and geometric properties of the system

$$\lambda = \frac{2\pi^2}{L^2} D.$$

In the chaotic case this translates to

$$\delta N_1(t) \sim \frac{1}{4^t} = e^{-\gamma t},$$

with $\gamma \coloneqq \log(4) = \log[\mu L]$.
The last explicit formulation for $\gamma = \log[\mu L]$, although being an heuristic one, exhibits a possible link between the emerging thermodynamic properties of a conductive system and the underlying microscopic dynamics. If this relation will be proven to hold for all values of the control parameter $\mu \in [0, 2]$, Onsager theory could be generalized to non-Hamiltonian systems characterized by a chaotic dynamics. Future work then might involve testing if the same exponential relaxation to equilibrium pattern can be found when the control parameter of the logistic map r is set to 2. Indeed, $r = 2$ is the only other value of the control parameter for which a closed-form solution for the dynamics is known. As for the $\mu = 2$ case this would mean that it is possible to find an analytic expression for $\delta N_1(t)$. The study of such quantity could bring additional evidence of the correct parametrization of the exponential decay of the fluctuation suggested above as encoding the microscopic dynamical information together with the geometric properties of the system. This would definitely link the underlying microscopic properties of particles' dynamics to the emerging (macroscopic) conductive ones. Furthermore, of particular interest would be to analyze relaxation processes at the onset of chaos, where the Lyapunov exponent vanishes.

Chapter 5

Appendices

5.1 Appendix A

Moments' characterization of a distribution function N(x,t) Let us consider a distribution function $N(x, t)$. This function can equivalently be written in its Fourier representation in the $k \in \mathbb{R}$ Fourier space

$$\hat{N}(k,t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} N(x,t)\ e^{-ikx}\,\mathrm{d}x\,.$$

It is now possible to perform a Taylor expansion around $k = k_0$ (without losing generality we can take $k_0 = 0$)

$$\begin{aligned}
\hat{N}(k,t) &= \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} \int_{\mathbb{R}} x^n\ N(x,t)\ e^{-ikx}\,\mathrm{d}x \Big|_{k=0} = \\
&= \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{\infty} \frac{(-ik)^n}{n!} N_n[N]
\end{aligned}$$

that shows that the distribution $N(x, t)$ is fully characterized in terms of its moments multiplied by appropriate coefficients. Anti-transforming

$$\begin{aligned}
N(x,t) =& \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \hat{N}(k,t)\ e^{ikx}\,\mathrm{d}k = \frac{1}{2\pi} \sum_{n=0}^{\infty} \frac{N_n[N]}{n!} \int_{\mathbb{R}} (-ik)^n\ e^{ikx}\,\mathrm{d}k = \\
=& \frac{1}{2\pi} \sum_{n=0}^{\infty} \frac{N_n[N]}{n!} \int_{\mathbb{R}} (-1)^n\ \frac{\mathrm{d}^n}{\mathrm{d}x^n} e^{ikx}\,\mathrm{d}k = \\
=& \sum_{n=0}^{\infty} \frac{(-1)^n}{n!}\ N_n[N]\ \frac{\mathrm{d}^n}{\mathrm{d}x^n} \left(\frac{1}{2\pi} \int_{\mathbb{R}} e^{ikx}\,\mathrm{d}k \right) = \\
=& \sum_{n=0}^{\infty} \frac{(-1)^n}{n!}\ N_n[N]\ \delta^{(n)}(x)
\end{aligned}$$

we find the final expression for $N(x, t)$ as a function of its moments, in which we have of course denoted $\delta^{(n)}(x) := \frac{\mathrm{d}^n}{\mathrm{d}x^n}\delta(x)$.

5.2 Appendix B

Invariant distribution for $\mu = 2$ We find the invariant distribution for the mapping

$$f(x) = 1 - 2x^2$$

where $x \in [-1, 1]$. This is also known as the *Ulam map*.
First off, we notice that the change of variable $u := \frac{1}{\pi}\arccos(-x) =: \phi^{-1}(x),\ u \in [0,1]$ transforms the map into a topologically conjugated map g(u) for which

$$-\cos(\pi g(u)) = 1 - 2\cos^2(\pi u) = -\cos(2\pi u).$$

Let us now introduce another map, the *tent map*. Since the topological conjugation of an invariant density is still invariant, we want to show that the tent map has a simple invariant density distribution and that it is possible to make a topological conjugation of its invariant density to the one of the Ulam map. The tent map is defined as follows

$$f(x) = \begin{cases} 2x, & \text{if } x \in [0, \frac{1}{2}] \\ 2(1-x), & \text{if } x \in (\frac{1}{2}, 1] \end{cases}$$

where $x \in [0, 1]$. As Fig. (5.1) suggests, this map preserves the length of arbitrary intervals. In other words, the preimages l'_1, l'_2 of an interval of length l satisfy

$$l = l'_1 + l'_2.$$

It is then clear that the uniform distribution function $p_{\text{eq}}(x) = 1$ is an invariant probability density.

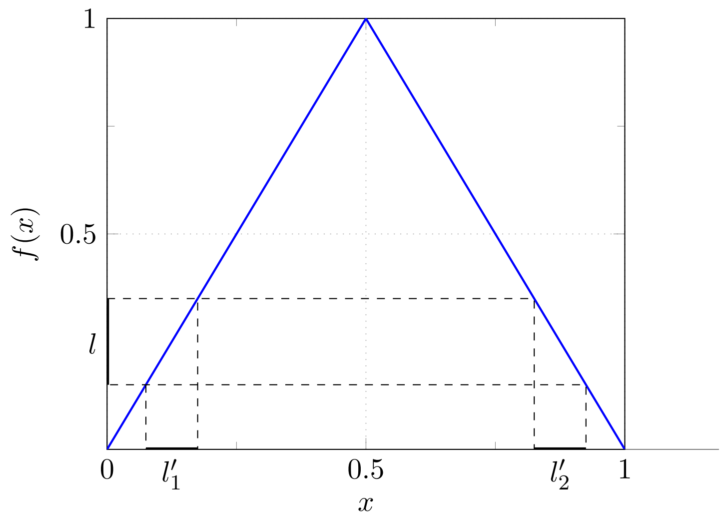

Figure 5.1: The *tent map* and the length conservation $l = l'_1 + l'_2$.

Finally it is possible to find the invariant density for the Ulam map. The invariant density should satisfy the conservation of probability relation

$$p_{x,eq}(x) = p_{u,eq}(u)\ |\det J_{\phi^{-1}}|$$

where $J_{\phi^{-1}}$ is the Jacobian of $u = \phi^{-1}(x)$ that clearly becomes the x derivative in one dimension. Since for the tent map $p_{u,eq}(u) = 1$, differentiating we get

$$p_{x,eq}(x) = \left|\frac{\mathrm{d}\phi^{-1}}{\mathrm{d}x}\right| = \frac{1}{\pi\,\sqrt{1-x^2}}.$$

Let's focus on the properties of $p_{\mathrm{eq}}(x)$. First of all we notice that it is an even function, secondly we check that it satisfies Eq. (3.5). Since $p_{\mathrm{eq}}(x)$ is even it suffices that it verifies

$$p_{\mathrm{eq}}(x) = \frac{p_{\mathrm{eq}}\left(\sqrt{\frac{1-x}{\mu}}\right)}{\sqrt{\mu(1-x)}}$$

for $\mu = 2$. Plugging in our definition of $p_{\mathrm{eq}}(x)$ we obtain

$$\begin{aligned}\frac{p_{\mathrm{eq}}\left(\sqrt{\frac{1-x}{2}}\right)}{\sqrt{2(1-x)}} &= \frac{1}{\pi}\frac{1}{\sqrt{1-\frac{1-x}{2}}}\frac{1}{\sqrt{2\,(1-x)}} = \frac{1}{\pi}\frac{1}{\sqrt{1+x}}\frac{1}{\sqrt{1-x}} = \\ &= \frac{1}{\pi\,\sqrt{1-x^2}} = p_{\mathrm{eq}}(x).\end{aligned} \tag{5.1}$$

5.3 Appendix C

Change of variable We will now discuss in detail the change of variable performed in Eq. (3.7). Specifically we would like to compute the integral

$$p(x,t) = \int_{-1}^{1} \delta\left[x - \left(2\sin^2\left[2^t \arcsin\sqrt{\frac{1}{2}(y+1)}\right] - 1\right)\right] p(y,0)\,\mathrm{d}y$$

introducing

$$u(y) \coloneqq 2\sin^2\left[2^t \arcsin\sqrt{\frac{1}{2}(y+1)}\right] - 1 = -\cos\left[2^t \arccos(-y)\right],$$

with $u, y \in [-1,1]$. In order to perform the substitution we need to compute $\left|\frac{\mathrm{d}y}{\mathrm{d}u}\right|$ and therefore we must find $y(u) \coloneqq u^{-1}(y)$. First of all Let us consider the following inequalities

$$-1 \leq y \leq 1 \implies 0 \leq \arccos(-y) \leq \pi \implies 0 \leq 2^t \arccos(-y) \leq 2^t\pi.$$

In order to invert the cosine we need to divide the interval $[0, 2^t\pi]$ into 2^t contiguous intervals of span π

$$k\pi \leq 2^t \arccos(-y) \leq (k+1)\pi$$

with $k = 0, 1, ..., 2^t - 1$, so that multiplying by -2^{-t} within each interval

$$2^{-t}(k+1)\pi \leq -\arccos(-y) \leq 2^{-t}k\pi.$$

Notice that $z \coloneqq -\arccos(-y) \in [0,\pi]$ and therefore $\cos(z)$ is monotonically increasing in its domain of definition. Solving for y we get

$$\cos\big(2^{-t}(k+1)\pi\big) \leq -y \leq \cos\big(2^{-t}k\pi\big) \implies -\cos\big(2^{-t}k\pi\big) \leq y \leq -\cos\big(2^{-t}(k+1)\pi\big).$$

Hence we define $I_k(t) \coloneqq \big\{y \in \mathbb{R} : y \in [-\cos\big(2^{-t}k\pi\big), -\cos\big(2^{-t}(k+1)\pi\big)]\big\}$. Finally, within each interval $I_k(t)$ it is possible to invert

$$u(y) = -\cos\left[2^t \arccos(-y)\right].$$

Let $v(y) \coloneqq 2^t \arccos(-y)$. Omitting for clarity the y dependencies, the previous relation becomes $\cos(v) = -u$ and $v \in [k\pi, (k+1)\pi]$. Inversion gives

$$\begin{cases} v = \arccos(-u) + k\pi, & \text{if } k \text{ is even} \\ v = \arccos(u) + k\pi, & \text{if } k \text{ is odd} \end{cases}$$

or more compactly

$$v = \arccos\Big((-1)^{k+1}u\Big) + k\pi$$

and since $v(y) \coloneqq 2^t \arccos(-y)$ eventually we get

$$y = -\cos\left[2^{-t}\Big(\arccos\Big((-1)^{k+1}u\Big) + k\pi\Big)\right].$$

It is now possible to compute $\left|\frac{\mathrm{d}y}{\mathrm{d}u}\right|$, needed to perform the change of variable

$$\left|\frac{\mathrm{d}y}{\mathrm{d}u}\right| = \left|(-1)^k \, \frac{2^{-t}\sin\left[2^{-t}\big(\arccos\left[(-1)^{k+1}u\right] + k\pi\big)\right]}{\sqrt{1-u^2}}\right|$$

and therefore

$$
\begin{aligned}
p(x,t) &= \int_{-1}^{1} \delta\left[x - \left(2\sin^2\left[2^t \arcsin\sqrt{\frac{1}{2}(y+1)}\right] - 1\right)\right] p(y,0)\,\mathrm{d}y = \\
&= \int_{u(-1)}^{u(1)} \delta(x-u)\ \tilde{p}(u,0)\ \left|\frac{\mathrm{d}y}{\mathrm{d}u}\right| \mathrm{d}u = \\
&= \sum_{k=0}^{2^t-1} \int_{I_k(t)} \delta(x-u)\ \tilde{p}(u,0)\ \left|\frac{2^{-t}\sin\left[2^{-t}\big(\arccos\left[(-1)^{k+1}u\right] + k\pi\big)\right]}{\sqrt{1-u^2}}\right| \mathrm{d}u = \\
&= \sum_{k=0}^{2^t-1} \left|\frac{\sin\left[2^{-t}\big(\arccos\left[(-1)^{k+1}x\right] + k\pi\big)\right]}{2^t\sqrt{1-x^2}}\right| \tilde{p}(x,0) = \\
&= \sum_{k=0}^{2^t-1} \left|\frac{\sin\left[2^{-t}\big(\arccos\left[(-1)^{k+1}x\right] + k\pi\big)\right]}{2^t\sqrt{1-x^2}}\right| p\Big(-\cos\Big[2^{-t}\Big(\arccos[(-1)^{k+1}x] + k\pi\Big)\Big], 0\Big),
\end{aligned}
$$

where we have indicated with $\tilde{p}(u,0) \coloneqq p(y(u),0)$. Moreover, the absolute value can be removed noticing that the only possibly negative quantity is given by

$$
\sin\left[2^{-t}\left(\arccos\left[(-1)^{k+1}x\right] + k\pi\right)\right].
$$

But since $k = 0, ..., 2^{t-1}$, if we call $z \coloneqq \left[2^{-t}\big(\arccos\left[(-1)^{k+1}x\right] + k\pi\big)\right]$ the argument of the sine

$$
0 \le \arccos\left[(-1)^{k+1}x\right] \le \pi \implies 0 \le 2^t\ z \le (k+1)\ \pi.
$$

Therefore it becomes clear that

$$
0 = \left[2^{-t}k\right]\Bigg|_{k=0} \le z \le \left[2^{-t}\ (k+1)\ \pi\right]\Bigg|_{k=2^t-1} = \pi
$$

and $\sin(z)$ is non negative.

Hence we are left with

$$
p(x,t) = \sum_{k=0}^{2^t-1} \frac{\sin\left[2^{-t}\big(\arccos\left[(-1)^{k+1}x\right] + k\pi\big)\right]}{2^t\sqrt{1-x^2}}\ p\Big(-\cos\Big[2^{-t}\Big(\arccos[(-1)^{k+1}x] + k\pi\Big)\Big], 0\Big).
$$

5.4 Appendix D

Explicit calculation of $\delta N_1(t)$ First of all we show how a linear perturbation at $t = 0$ of the equilibrium distribution

$$p(x,0) = \frac{1}{\pi\,\sqrt{1-x^2}} + \epsilon\, x$$

with $0 < \epsilon \ll 1$, evolves in time.

For $t > 0$ we get

$$\begin{aligned}
p(x,t) &= \sum_{k=0}^{2^t-1} \frac{\sin\left[2^{-t}\big(\arccos\left[(-1)^{k+1}x\right] + k\pi\big)\right]}{2^t\sqrt{1-x^2}}\; p\Big(-\cos\Big[2^{-t}\Big(\arccos[(-1)^{k+1}x] + k\pi\Big)\Big], 0\Big) = \\
&= \sum_{k=0}^{2^t-1} \frac{\sin\left[2^{-t}\big(\arccos\left[(-1)^{k+1}x\right] + k\pi\big)\right]}{2^t\sqrt{1-x^2}} \left(\frac{1}{\pi\,\sqrt{1-\cos^2(z_k(x,t))}} - \epsilon\cos(z_k(x,t))\right) = \\
&= \sum_{k=0}^{2^t-1} \frac{1-\epsilon\sin(z_k(x,t))\cos(z_k(x,t))}{2^t\;\pi\sqrt{1-x^2}} = \frac{1}{\pi\sqrt{1-x^2}} - \epsilon\sum_{k=0}^{2^t-1}\frac{\sin(z_k(x,t))\cos(z_k(x,t))}{2^t\;\pi\sqrt{1-x^2}}
\end{aligned}$$

where we have called $z_k(x,t) \coloneqq 2^{-t}\big(\arccos[(-1)^{k+1}x] + k\pi\big)$.

From this relation it is possible to find the variation of the number of the particles

$$\begin{aligned}
\delta N_1(t) \coloneqq N_1(t) - N_{1,\mathrm{eq}} &= \\
&= A\epsilon \sum_{k=0}^{2^t-1} \int_{\mathscr{D}} x\; \frac{\sin\left[z_k(x,t)\right]\cos\left[z_k(x,t)\right]}{2^t\;\pi\sqrt{1-x^2}}\,\mathrm{d}x = \\
&= \frac{A\epsilon}{\pi}\sum_{k=0}^{2^t-1} c_k(t),
\end{aligned}$$

having defined

$$\begin{aligned}
c_k(t) &\coloneqq \int_{\mathscr{D}} x\;\frac{\sin\left[z_k(x,t)\right]\cos\left[z_k(x,t)\right]}{2^t\sqrt{1-x^2}}\,\mathrm{d}x = \\
&= \int_{-1}^{1} x\;\frac{\sin\left[2^{-t}\big(\arccos[(-1)^{k+1}x] + k\pi\big)\right]\cos\left[2^{-t}\big(\arccos[(-1)^{k+1}x] + k\pi\big)\right]}{2^t\sqrt{1-x^2}}\,\mathrm{d}x\,.
\end{aligned}$$

The computation of $c_k(t)$ performed on *Mathematica* leads us to the following result

$$c_k(t) = \begin{cases} 2\;\dfrac{\cos^2\left[2^{-t}\;\pi\right]}{4^t-4}, & \text{if } k = 0 \\[2ex] (-1)^k\;\dfrac{\cos\left[2^{1-t}\pi\;a_1(k)\right] + \cos\left[2^{2-t}\pi\;a_2(k)\right]}{4^t-4}, & \text{if } k > 0 \end{cases}$$

with

$$a_1(k) \coloneqq 2\left\lfloor\frac{k}{2}\right\rfloor + 1 \quad \text{and} \quad a_2(k) \coloneqq \left\lfloor\frac{k+1}{2}\right\rfloor + 1,$$

where $\lfloor\,\cdot\,\rfloor$ denotes the *floor* function. Hence, we finally find

$$\delta N_1(t) = \frac{A\epsilon}{\pi}\,\frac{1}{4^t-4}\left[2\cos^2\left[2^{-t}\;\pi\right] + \sum_{k=1}^{2^t-1}(-1)^k\;\Big(\cos\left[2^{1-t}\pi\;a_1(k)\right] + \cos\left[2^{2-t}\pi\;a_2(k)\right]\Big)\right].$$

5.5 Appendix E

Odd perturbations of the equilibrium distribution function We show that any odd perturbation of the equilibrium distribution function reduces to the invariant distribution after one time step. Consider at time $t = 0$ any odd perturbation of the invariant density

$$p(x,0) = \frac{1}{\pi\ \sqrt{1-x^2}} + x^{2n+1} = p_{\rm eq}(x) + x^{2n+1}$$

with $n \in \mathbb{N}$.

Adapting the iteration rule Eq. (3.4),

$$p(x,t=1) = \begin{cases} 0 & \text{if } x \in [-1, 1-\mu]; \\ \left[\dfrac{p\Big(-\sqrt{\frac{1-x}{\mu}}\Big) \ + \ p\Big(+\sqrt{\frac{1-x}{\mu}}\Big)}{2\sqrt{\mu(1-x)}} \right]\Bigg|_{t=0} & \text{if } x \in [1-\mu, 1] \end{cases}$$

and using Eq. (5.1)

$$= \begin{cases} 0 & \text{if } x \in [-1, 1-\mu]; \\ p_{\rm eq}(x) + \left[\dfrac{\Big(-\sqrt{\frac{1-x}{\mu}}\Big)^{2n+1} \ + \ \Big(+\sqrt{\frac{1-x}{\mu}}\Big)^{2n+1}}{2\sqrt{\mu(1-x)}} \right]\Bigg|_{t=0} & \text{if } x \in [1-\mu, 1] \end{cases}$$

$$= \begin{cases} 0 & \text{if } x \in [-1, 1-\mu]; \\ p_{\rm eq}(x) & \text{if } x \in [-1, 1-\mu]. \end{cases}$$

5.6 Appendix F

Different representations of the logistic map We show how to topologically conjugate the two different representations of the logistic map in Eq. (3.1) and Eq. (3.2), explicitly

$$y_{n+1} = ry_n(1-y_n) = g(y_n) \quad \longmapsto \quad x_{n+1} = 1 - \mu x_n^2 = f(x_n), \tag{5.2}$$

where $y \in [0,1]$, $r \in [0,4]$ and $x \in [-1,1]$, $\mu \in [0,2]$. We are looking for a change of variable $x \coloneqq \psi(y)$ such that

$$x_{n+1} = f(x_n) = \psi(y_{n+1}) = \psi(g(y_n)) \quad \Longrightarrow \quad f(x_n) = \psi(g(y_n)).Le$$

If we put in Eq. (5.2) the ansatz of a linear transformation, thus

$$\psi(y) = Ay + B$$

we get

$$x_{n+1} = \psi(y_{n+1}) = \psi[ry_n(1-y_n)] \overset{!}{=} 1 - \mu x_n^2 = 1 - \mu[\psi(y_n)]^2$$

and therefore

$$\psi[ry_n(1-y_n)] = 1 - \mu[\psi(y_n)]^2 \implies A[ry_n(1-y_n)] + B = 1 - \mu[Ay_n + B)]^2.$$

Rearranging the terms, supposing $A \neq 0$ and comparing equal powers of y_n we get

$$\begin{cases} \mu A - r = 0 \\ Ar + 2AB\mu = 0 \\ B^2\mu + B - 1 = 0 \end{cases} \implies \begin{cases} A = \dfrac{1}{\mu}\left[\sqrt{1+4\mu}+1\right] \\ B = -\dfrac{1}{2\mu}\left[\sqrt{1+4\mu}+1\right] \\ r = \sqrt{1+4\mu}+1 \end{cases}$$

and therefore

$$\psi(y) = \left(y - \frac{1}{2}\right)\frac{1}{\mu}\left[\sqrt{1+4\mu}+1\right].$$

We stress that such conjugation is valid only in the case $r \in (2,4]$.

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