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M.Sc. Thesis

Application of the Compound Matrix Theory for the computation of Lyapunov Exponents of autonomous Hamiltonian systems

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Contents

Abstract

In the present thesis, the Compound Matrix Theory is applied for the computation of the Lyapunov Characteristic Exponents of autonomous Hamiltonian systems of various degrees of freedom. The method is approached by the aspect of the exterior (Grassmann) algebra and the wedge product. The advantages of this approach lie on the fact that the automation of the procedure is feasible, which is crucial for the study of high dimensional dynamical systems. The results obtained are comparable to those produced by the standard method of Benettin et al. [4], in respect of both accuracy and effectiveness. Moreover, the computation of single exponents of the spectrum is feasible without the obligation of computing the larger ones in the spectrum order, as when applying the standard method.

Introduction

The basic idea of the Compound Matrix Theory (CMT) is that for a given system of differential equations, auxiliary systems of equations, produced by the initial one, are implemented and evolved instead. More precisely, the coordinates of the initial vectors are reordered and appropriately combined with each other, following a predefined pattern, the so-called lexicographical order. This rearrangement yields new vectors, which, depending on their dimension, denote areas, volumes and hyper-volumes. The numerical integration of the time evolution of these structures instead of the initial vectors, overcomes the necessity of keeping the initial vectors linearly independent, since, as explained in the respective section, the new vectors remain independent throughout their time evolution.

In 1979 and 1985 the CMT was used by Ng and Reid [21, 22, 23], for solving eigenvalue problems of stiff ordinary differential equations, as an effort to overcome accuracy issues. The method was tested on the Orr-Sommerfeld equation, an eigenvalue equation frequently used for the study of fluid dynamics stability, yielded by the Navier-Stokes equations after considering appropriate conditions that ensure hydrodynamical stability.

In the early 80's, Froyland and Alfsen [8, 9] introduced an alternative way of computing some or all Lyapunov Characteristic Exponents (LCEs), applying a method related to the CMT, for discrete maps as well as continuous dynamical systems. They claimed that for reasonably low dimensional systems, the new method managed to compete the existing ones, with the standard method of Benettin et al. [4] being the most well known among them. The only restriction on the general application of the method concerned the dimension of the considered dynamical system, since as the dimensionality increased the auxiliary systems of equations became more complicated.

In 2002, Allen and Bridges [1] manipulated the CMT using the principles of exterior algebra (Grassmann algebra), for the study of hydrodynamic stability and atmospheric dynamics. This approach permitted the automated construction of the auxiliary systems and thus the generalization of the procedure, regardless of the dimension of the considered dynamical system.

The purpose of our study is to apply the CMT for the computation of some or all LCEs of conservative Hamiltonian systems of various degrees of freedom. Specifically, we consider the so-called variational equations that

evolve the deviation vectors through time. The deviation vectors describe small perturbations about a considered orbit, evolving on a vector space tangent to the phase space of the dynamical system. Using the principles and rules of exterior algebra, based on the work of Allen and Bridges [1] and the appendix of Skokos [29], we construct new vectors that span modified vector spaces, by reordering and combining the coordinates of the deviation vectors according to the lexicographical order. The new vectors, as has already been mentioned, are related to areas, volumes and hyper-volumes, depending on the dimensionality of the modified vector space in which they evolve. Taking advantage of the properties of the compound matrices, as proved and explained by Muldowney [19], the LCEs are computed from the time evolution of these new vectors, instead of the time evolution of the deviation vectors, according to the standard method of Benettin et al. [4]. In this way, the necessity of orthonormalizing the solutions of the considered differential systems can be overcome. Moreover, the computation of any particular LCE of the spectrum is possible, without been forced to compute all the higher order LCEs.

The 2-degree-of-freedom Hénon-Heiles Hamiltonian system [15] is used as an illustrative example, to demonstrate the basic theory. The accuracy and effectiveness of our approach is confirmed by comparison tests with results obtained by applying the well known standard method of Benettin et al. [4]. The Fermi-Pasta-Ulam β-lattice [6] is also considered for this purpose.

The present thesis is organized as follows. Chapter 1 is devoted to the general concept of dynamical systems as well as the specific case of Hamiltonian systems which is the main interest of our study. Moreover, the concept of deviation vectors is presented and explained. Specifically, in section 1.1 we present the basic definitions as well as a brief theory of the dynamical systems, the dynamical variables and the phase space. Also the notions of orbits and phase diagrams are defined. We mention the categories into which dynamical systems are divided (discrete and continuous, autonomous, conservative and dissipative) as well as the conditions of this discrimination (the appearance of the time variable in the differential equation and the preservation of the system's phase volume). Section 1.2 describes the type of dynamical systems that are the subject of our study, i.e. autonomous conservative systems, the equations that describe their time evolution and the special characteristics that are the reason of our interest. In section 1.3 we discuss the concept of deviation vectors and the variational equations that govern their time evolution, following the ideas presented in [5].

Chapter 2 is devoted to the theory and computation of the LCEs. In particular, in section 2.1 we provide a brief historical overview of the concept of the exponents. Their introduction by Lyapunov [18] and how they were gradually used for the study of dynamical systems, providing important knowledge of the characteristics and special features of the considered systems. The basic definitions and theorems are given in section 2.2, while

in section 2.3 we discuss the properties of their spectrum. The last two sections of the chapter, 2.4 and 2.5, are devoted to the presentation of numerical methods for the computation of the spectrum of LCEs like the well known standard method of Benettin et al. [4].

The CMT is described in chapter 3. More precisely, in section 3.1 a brief theory for the exterior (Grassmann) algebra and the wedge product is presented. Based on the book of Greub [11], the work of Allen and Bridges [1] and the appendix of [29], we give the definitions of exterior power and exterior algebra, we describe the wedge product and discuss its properties. Using a simple example, we explain the notion of the lexicographical order and the procedure that creates the orthonormal basis of the exterior powers. The definitions of the k-vectors and the decomposability are also included. Finally, the inner product and the norm of the k-vectors are explicitly defined. The CMT is described in section 3.2 by mainly following the work of Muldowney [19]. The relationship between the differential equations and the compound systems is clarified. The additive compound matrix is defined and the procedure of its computation is explained by illustrative examples, following two different procedures : a)by using the principles of exterior algebra and wedge product and b)by using auxiliary differential systems depending on the expected form of the solution of the initially considered differential system (see Ng and Reid [21, 22, 23]). Moreover, a basic property of additive compound matrices, which is crucial for the application of the CMT for the computation of the LCEs spectrum, is noted, [19].

In chapter 4, applications of the CMT for the computation of the LCEs spectrum and of particular individual LCEs are presented. For the computations, the FPU β -lattice is used, therefore section 4.1 is devoted to the presentation of this dynamical system, giving its equations of motion, its variational equations and its compound systems for the case of the 2-degree-of-freedom system. In section 4.2, some general information concerning the symplectic integrators, which are numerical methods used for the integration of Hamiltonian systems, are given. The particular symplectic integrator used in our study is also presented in more detail. In section 4.3 our results are presented and commented, while in 4.4 our conclusions and remarks are summarized.

We note that throughout the text, lower-case letters in bold, e.g. $\mathbf{x}$, denote vectors, while upper-case letters in bold, e.g. $\mathbf{A}$, denote matrices. The exponent T following a vector or a matrix, e.g. $\mathbf{x}^T$ or $\mathbf{A}^T$, denotes the transpose vector or matrix, respectively. The time derivative is denoted by a dot, thus the symbol $\dot{\mathbf{x}}$ stands for the derivative of the vector $\mathbf{x}$ with respect to time, t.

Chapter 1

Dynamical systems

1.1 General theory

A dynamical system is a mathematical model, described by a set of differential equations, that simulates a physical phenomenon which evolves over time, denoted by t. It consists of variables depended on time, let's denote them by $x_i(t)$ with $i = 1, 2, \ldots, n$, called the system's dynamical variables, with t being the independent variable of the system and n being the finite number of the dynamical variables, also called the dimension of the system. These variables can be considered as the coordinates of a vector $\mathbf{x}(t) = [x_1(t) \quad x_2(t) \ldots x_n(t)]^T$ that evolves on a vector space. This vector space is of dimension equal to the number of $x_i(t)$ and is called the phase space of the system, $\mathbf{S}$. Each considered time t_j, the state of the dynamical system is described by the vector $\mathbf{x}(t_j) = [x_1(t_j) \quad x_2(t_j) \ldots x_n(t_j)]^T$, depicted by a single point on $\mathbf{S}$. A set of such points, denoting the state of the system for successive times that constitute a time interval, compose a trajectory or orbit, which is the graphical representation of the time evolution of the dynamical system. Different initial vectors $\mathbf{x}_k(t_0)$, formed by different sets of initial conditions $x_{i_k}(t_0)$, where t_0 denotes the starting time of our study, delineate different orbits on the phase space. The collection of these orbits constitutes the phase diagram or phase portrait. It should be noted that every possible orbit cannot intersect with any other in the extended phase space, which is a vector space spanned by the dynamical variables and the variable of time and therefore is of dimension $n + 1$ (see for example Perko [25]).

Whether time is considered to take discrete real values, $t_j = j \cdot dt$ with $j \in \mathbf{Z}$ and dt a positive real value, or continuous real values from an interval, $t \in [t_{min}, t_{max}]$, the systems are divided into two major categories : the discrete and the continuous dynamical systems. a)The discrete dynamical systems or maps are described by the difference equations of the form :

$$\mathbf{x}_{j+1} = \mathbf{f}(\mathbf{x}_j, t_j)$$

where $\mathbf{f}$ is a set of n functions, $f_1, f_2, \ldots, f_n$, with n being the dimension of the system, and $\mathbf{x}_j = [x_{1_j} \quad x_{2_j} \ldots x_{n_j}]^T$ is the state vector at a discrete time $t_j = j \cdot dt$. b)The continuous dynamical systems or flows are described by a set of differential equations of the form :

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t)$$

where $\mathbf{f}$ is a set of n functions, $f_1, f_2, \ldots, f_n$, called the vector field, with n being the dimension of the system. If $\mathbf{f}$ does not explicitly depend on time, meaning that :

$$\frac{\partial f_i}{\partial t} = 0, \quad i = 1, \ldots, n$$

the dynamical system is called autonomous. Its vector field remains constant during t, thus, the initial time of the study does not affect the shape or the nature of the orbit, which in that case depends only on the considered initial conditions. If for an autonomous system it is :

$$div\mathbf{f} = \frac{\partial f_1}{\partial x_1} + \frac{\partial f_2}{\partial x_2} + \ldots + \frac{\partial f_n}{\partial x_n} = 0$$

the dynamical system is called conservative, meaning that it preserves its volume $\mathbf{V_D}$ on the phase space $\mathbf{S}$ during the time evolution. It is noted that $\mathbf{D}$ is a subset of the phase space ($\mathbf{D} \subset \mathbf{S}$) consisted by the system's initial conditions considered in our study. The volume of that subset, which is in fact the volume of the system for the taken initial conditions at the beginning of the study, t_0, is given by :

$$\mathbf{V_D} = \int \cdots \int_{\mathbf{D} \subset \mathbf{S}} \mathrm{d}x_1 \, \mathrm{d}x_2 \, \ldots \, \mathrm{d}x_n.$$

Hamiltonian systems, as well as symplectic maps, are considered to be representative examples of conservative dynamical systems. On the other hand, if :

$$div\mathbf{f} = \frac{\partial f_1}{\partial x_1} + \frac{\partial f_2}{\partial x_2} + \ldots + \frac{\partial f_n}{\partial x_n} < 0$$

the dynamical system is called dissipative. In that case, its volume decreases with time, forming in general a space of lower dimension than the initial vector space, which is called attractor. There exists also a third group of dynamical systems for which we get :

$$div\mathbf{f} = \frac{\partial f_1}{\partial x_1} + \frac{\partial f_2}{\partial x_2} + \ldots + \frac{\partial f_n}{\partial x_n} > 0.$$

They are called explosive systems and their solutions tend to escape to infinity. For that reason, they remain of low scientific interest.

1.2 Hamiltonian systems and equations of motion

The present study concentrates on autonomous Hamiltonian systems, which are continuous conservative dynamical systems, of N degrees of freedom described by the so-called Hamiltonian function :

$$H_N(\mathbf{q},\mathbf{p}) = T(\mathbf{p}) + V(\mathbf{q}) = \frac{1}{2}\sum_{i=1}^{N}\frac{p_i^2}{m} + V(\mathbf{q}) = h = constant$$

where $\mathbf{q} = [q_1 \quad q_2 \dots q_N]^T$ is the vector of the generalized coordinates and $\mathbf{p} = [p_1 \quad p_2 \dots p_N]^T$ is the vector of the conjugate momenta, with :

$$p_i = m_i \dot{q}_i.$$

The mass of each particle of the system is denoted by m_i. Typically, the particles of the system are considered to be of unit mass and therefore, the vector of momenta equals the system's velocities. The term $T(\mathbf{p})$ represents the kinetic energy of the system, while $V(\mathbf{q})$ is a function of the generalized coordinates representing the potential energy. The Hamiltonian equation represents the total energy of the system, therefore, due to the law of conservation of energy and if the system is considered to be isolated, the Hamiltonian remains constant over the time evolution.

A basic feature of the Hamiltonian systems, $H_N(\mathbf{q},\mathbf{p})$, is the existence of the so called integrals of motion, each one of which represents a quantity that remains constant during the time evolution of the system. A quantity $I(\mathbf{q},\mathbf{p})$ is an integral of motion if it is :

$$I = I(\mathbf{q}(t),\mathbf{p}(t)) = constant, \quad \text{or equivalently } [I, H_N] = 0$$

where $[.,.]$ is the Poisson bracket, given, for functions $f = f(\mathbf{q},\mathbf{p})$ and $g = g(\mathbf{q},\mathbf{p})$, by the following equation :

$$[f,g] = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}\right). \tag{1.1}$$

It is noted that the Hamiltonian $H_N(\mathbf{q},\mathbf{p})$ is always an integral of motion of the system, since it satisfies :

$$[H_N, H_N] = 0.$$

A Hamiltonian system $H_N(\mathbf{q},\mathbf{p})$ of N degrees of freedom is called integrable (Liouville integrability) if there exist N independent integrals of motion $I_i(\mathbf{q},\mathbf{p})$ in convolution. The above requirements are summarized at the following conditions :

$[I_i, H_N] = 0, \quad i = 1,\dots,N$: condition for the existence of N integrals

$[I_i, I_j] = 0, \quad i,j = 1,\dots,N$: condition for the convolution of the integrals.

The state of the system during its time evolution is described by the vector :

$$\mathbf{x}(t) = [\mathbf{q}(t) \quad \mathbf{p}(t)]^T = [q_1(t) \quad q_2(t) \dots q_N(t) \quad p_1(t) \quad p_2(t) \dots p_N(t)]^T.$$

The vector evolves on the $2N$-dimensional phase space $\mathbf{S}$ and is defined by the $N + N$ coordinates of the vectors $\mathbf{q}(t)$ and $\mathbf{p}(t)$, of the system. As mentioned in section 1.1, this vector taken for successive times, delineates the orbit of the system for a specific set of initial conditions and constitutes the solution of the so called Hamilton equations of motion, given in matrix form by :

$$\dot{\mathbf{x}} = \mathbf{J}_{2N} \cdot \mathbf{D}_{H_N}$$

where :

$$\mathbf{D}_{H_N} = \left[\frac{\partial H_N}{\partial \mathbf{q}} \quad \frac{\partial H_N}{\partial \mathbf{p}}\right]^T = \left[\frac{\partial H_N}{\partial q_1} \quad \frac{\partial H_N}{\partial q_2} \quad \dots \quad \frac{\partial H_N}{\partial q_N} \quad \frac{\partial H_N}{\partial p_1} \quad \frac{\partial H_N}{\partial p_2} \quad \dots \quad \frac{\partial H_N}{\partial p_N}\right]^T$$

$$\mathbf{J}_{2N} = \begin{bmatrix} \mathbf{0}_N & \mathbf{I}_N \\ -\mathbf{I}_N & \mathbf{0}_N \end{bmatrix}$$

where $\mathbf{0}_N$ is a $N \times N$ matrix with all of its elements equal to zero and $\mathbf{I}_N$ is the $N \times N$ identity matrix. Considering the above definitions, the equations of motion can take the form :

$$\dot{\mathbf{x}} = [\dot{\mathbf{q}} \quad \dot{\mathbf{p}}]^T = \left[\frac{\partial H_N}{\partial \mathbf{p}} \quad -\frac{\partial H_N}{\partial \mathbf{q}}\right]^T.$$

In order to illustrate all these, let us consider a simple example. In 1964, Hénon and Heiles [15] proposed a model to describe the nonlinear motion of stars around a galactic center, assuming for simplicity that the motion can be restricted to a 2-dimensional plane. This model, called the Hénon-Heiles Hamiltonian system, is a nonlinear 2-degree of freedom system, described by the Hamiltonian :

$$H_2 = \frac{1}{2}(p_x^2 + p_y^2) + \frac{1}{2}(x^2 + y^2) + x^2 y - \frac{1}{3}y^3.$$

According to the above-mentioned theory, its phase space $\mathbf{S}$ is of dimension 4 and the equations of motion are given by :

$$\dot{\mathbf{x}} = \begin{bmatrix} \dot{x} \\ \dot{y} \\ \dot{p_x} \\ \dot{p_y} \end{bmatrix} = \begin{bmatrix} \frac{\partial H_2}{\partial p_x} \\ \frac{\partial H_2}{\partial p_y} \\ -\frac{\partial H_2}{\partial x} \\ -\frac{\partial H_2}{\partial y} \end{bmatrix} \quad \Rightarrow$$

$$\Rightarrow \quad \begin{cases} \dot{x} = p_x \\ \dot{y} = p_y \\ \dot{p_x} = -x - 2xy \\ \dot{p_y} = y^2 - x^2 - y. \end{cases}$$

The Hénon-Heiles Hamiltonian is nonintegrable, since there doesn't exist any integral of motion other than the Hamiltonian itself.

1.3 Deviation vectors and variational equations

If $\mathbf{S}$ is the $2N$ dimensional phase space where the orbits of a dynamical system evolve on, a deviation vector $\mathbf{w}$, which describes a small perturbation of a specific orbit $\mathbf{x}$, evolves on a $2N$ dimensional space $\mathbf{T_xS}$ tangent to $\mathbf{S}$. Let us assume that the evolution of an orbit follows the rule :

$$\Phi^t : \mathbf{S} \to \mathbf{S}.$$

Then, the orbit is given in general form by the equation :

$$\mathbf{x}(t) = \Phi^t(\mathbf{x}(0))$$

while the time evolution of $\mathbf{w}$ follows the rule :

$$d_{\mathbf{x}}\Phi^t : \mathbf{T_xS} \to \mathbf{T_{\Phi^t(x)}S}$$

and the deviation vector itself is given in general form by the equation :

$$\mathbf{w}(t) = d_{\mathbf{x}}\Phi^t(\mathbf{w}(0)).$$

It is noted that $d_{\mathbf{x}}\Phi^t$ is the linear mapping that maps the tangent space $\mathbf{T_xS}$ of $\mathbf{S}$ at point $\mathbf{x}$ to the tangent space $\mathbf{T_{\Phi^t(x)}S}$ of $\mathbf{S}$ at point $\Phi^t(x)$ (see e.g. [29, 30]).

Considering the case of an autonomous Hamiltonian system of N degrees of freedom, the time evolution of a deviation vector

$$\mathbf{w}(t) = [\delta\mathbf{q}(t) \quad \delta\mathbf{p}(t)]^T = [\delta q_1(t) \quad \delta q_2(t) \dots \delta q_N(t) \quad \delta p_1(t) \quad \delta p_2(t) \dots \delta p_N(t)]^T$$

with respect to a considered orbit $\mathbf{x}(t)$ is governed by the so-called variational equations :

$$\dot{\mathbf{w}} = \left[\mathbf{J}_{2N} \cdot \mathbf{D}^2_{H_N}(\mathbf{x}(t))\right] \cdot \mathbf{w} = \mathbf{A}(t) \cdot \mathbf{w}.$$

By $\mathbf{D}^2_{H_N}(\mathbf{x}(t))$ is denoted the $2N \times 2N$ Hessian matrix of the Hamiltonian with respect to the considered orbit, and it is given by the equation :

$$\mathbf{D}^2_{H_N}(\mathbf{x}(t)) = \begin{bmatrix} \frac{\partial^2 H_N}{\partial q_1 \partial q_1} & \cdots & \frac{\partial^2 H_N}{\partial q_1 \partial q_N} & \frac{\partial^2 H_N}{\partial q_1 \partial p_1} & \cdots & \frac{\partial^2 H_N}{\partial q_1 \partial p_N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 H_N}{\partial q_N \partial q_1} & \cdots & \frac{\partial^2 H_N}{\partial q_N \partial q_N} & \frac{\partial^2 H_N}{\partial q_N \partial p_1} & \cdots & \frac{\partial^2 H_N}{\partial q_N \partial p_N} \\ \frac{\partial^2 H_N}{\partial p_1 \partial q_1} & \cdots & \frac{\partial^2 H_N}{\partial p_1 \partial q_N} & \frac{\partial^2 H_N}{\partial p_1 \partial p_1} & \cdots & \frac{\partial^2 H_N}{\partial p_1 \partial p_N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 H_N}{\partial p_N \partial q_1} & \cdots & \frac{\partial^2 H_N}{\partial p_N \partial q_N} & \frac{\partial^2 H_N}{\partial p_N \partial p_1} & \cdots & \frac{\partial^2 H_N}{\partial p_N \partial p_N} \end{bmatrix}.$$

For the Hénon-Heiles Hamiltonian system, the tangent space $\mathbf{T_xS}$ is of dimension 4 and the variational equations are of the form :

$$\dot{\mathbf{w}} = \mathbf{A} \cdot \mathbf{w} \quad \Rightarrow$$

$$\Rightarrow \quad \dot{\mathbf{w}} = \begin{bmatrix} \mathbf{0}_2 & \mathbf{I}_2 \\ -\mathbf{I}_2 & \mathbf{0}_2 \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial^2 H_2}{\partial \mathbf{q} \partial \mathbf{q}} & \frac{\partial^2 H_2}{\partial \mathbf{q} \partial \mathbf{p}} \\ \frac{\partial^2 H_2}{\partial \mathbf{p} \partial \mathbf{q}} & \frac{\partial^2 H_2}{\partial \mathbf{p} \partial \mathbf{p}} \end{bmatrix} \cdot \mathbf{w} \quad \Rightarrow$$

$$\Rightarrow \quad \dot{\mathbf{w}} = \begin{bmatrix} \frac{\partial^2 H_2}{\partial \mathbf{p} \partial \mathbf{q}} & \frac{\partial^2 H_2}{\partial \mathbf{p} \partial \mathbf{p}} \\ -\frac{\partial^2 H_2}{\partial \mathbf{q} \partial \mathbf{q}} & -\frac{\partial^2 H_2}{\partial \mathbf{q} \partial \mathbf{p}} \end{bmatrix} \cdot \mathbf{w} \quad \Rightarrow$$

$$\Rightarrow \quad \dot{\mathbf{w}} = \begin{bmatrix} \mathbf{0}_2 & \mathbf{I}_2 \\ -\frac{\partial^2 H_2}{\partial \mathbf{q} \partial \mathbf{q}} & \mathbf{0}_2 \end{bmatrix} \cdot \mathbf{w} \quad \Rightarrow$$

$$\Rightarrow \quad \begin{bmatrix} \dot{\delta x} \\ \dot{\delta y} \\ \dot{\delta p_x} \\ \dot{\delta p_y} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -\frac{\partial^2 H_2}{\partial x^2} & -\frac{\partial^2 H_2}{\partial x \partial y} & 0 & 0 \\ -\frac{\partial^2 H_2}{\partial y \partial x} & -\frac{\partial^2 H_2}{\partial y^2} & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} \delta x \\ \delta y \\ \delta p_x \\ \delta p_y \end{bmatrix} \quad \Rightarrow$$

$$\Rightarrow \quad \begin{bmatrix} \dot{\delta x} \\ \dot{\delta y} \\ \dot{\delta p_x} \\ \dot{\delta p_y} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ (-1-2y) & -2x & 0 & 0 \\ -2x & (-1+2y) & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} \delta x \\ \delta y \\ \delta p_x \\ \delta p_y \end{bmatrix} .$$

Chapter 2

Lyapunov Characteristic Exponents

2.1 Historical review

The LCEs are asymptotic measures characterizing the average rate of growth or shrinking of small perturbations about the orbits of a dynamical system, [18, 29]. Their concept was first introduced by Lyapunov, in 1892 [18], for the study of Ordinary Differential Equations (ODEs), although, it was no sooner than 1976, [2], that the theory of the LCEs and the characterization of the nature of a dynamical system were clearly connected. A brief summary of the research during the years that intervened follows :

- In 1892, Lyapunov first used asymptotic measures to describe the rate of growth or shrinking of small perturbations about the orbits of dynamical systems, applying the theory to the study of stability of non-stationary solutions of ODEs, [18].
- In 1964, Hénon and Heiles combined the divergence rate of nearby orbits with the nature of the phase space region they belonged [15]. They chose two orbits, with initial distance of 10^6 between them, and evolved them, studying the changes of the value of that distance. They observed an exponential increase of the initial distance when the orbits were taken from a chaotic region of the phase space, while, when the orbits were chosen from a regular region, the increase of the distance was linear.
- In 1968, Oseledec proved the so-called Multiplicative Ergodic Theorem (MET), ensuring the existence and finiteness of LCEs yet without any direct reference to the relation between the LCEs and the exponential divergence of nearby orbits [24].

- This relation was established in $1976-1977$ by Benettin et al. [2], and Pesin [26], who clearly connected the LCEs with the rate of divergence.
- In 1976, Benettin et al. [2], estimated the maximum Lyapunov Exponent (mLCE) as an asymptotic measure of an appropriate quantity, related to the evolution of a chosen distance between two considered orbits.
- In 1978, Contopoulos et al. [5], came up with the idea of using deviation vectors, evolved by the variational equations, in order to compute the divergence rate. The deviation vectors refer to a single orbit and describe small perturbations about it. This approach substituted the method of choosing neighbour orbits, giving solution to the problem of the appropriate initial distance. Moreover, the use of bigger time steps was now permitted, reducing this way the CPU time needed.
- During the same year, based on the work of Oseledec [24], and Contopoulos et al. [5], Benettin et al. [3], adjusted the MET of Oseledec and developed numerical techniques for the computation of some LCEs or of the whole spectrum of them, based again on the evolution of deviation vectors.
- In 1980, Benettin et al. [4], presented the theoretical treatment as well as the numerical method for the computation of some or of all LCEs. Independently, in late 70's, Nagashima and Shimada also proposed a numerical approach for the computation of the complete set of LCEs, [20, 28].

In the rest of this chapter we will present the definition and the properties of the LCEs along with a brief mathematical theory, needed to clarify their meaning and importance.

2.2 Theory and definitions

Let us consider an $n \times n$ matrix function, $\mathbf{A}_t$, defined on the whole real axis, such that $\mathbf{A}_0 = \mathbf{I}_n$. For each time t the value of the function is a nonsingular matrix. The usual 2-norm of $\mathbf{A}_t$, $\|\mathbf{A}_t\|$, follows the 2-norm $\|\mathbf{A}\|$ of a $n \times n$ matrix $\mathbf{A}$, which is induced by the usual Euclidean 2-norm $\|\mathbf{x}\| = (\sum_{i=1}^{n} x_i^2)$ of vector $\mathbf{x}$, by :

$$\|\mathbf{A}\| = \max_{\mathbf{x}\neq 0} \frac{\|\mathbf{A}\mathbf{x}\|}{\|\mathbf{x}\|}$$

and equals the value of the largest eigenvalue of matrix $\sqrt{\mathbf{A}^T\mathbf{A}}$.

Taking a non zero vector, $\mathbf{y} \in \mathbf{R}^n$, the quantity defined by :

$$\lambda_t(\mathbf{y}) = \frac{\|\mathbf{A}_t\mathbf{y}\|}{\|\mathbf{A}_0\mathbf{y}\|} = \frac{\|\mathbf{A}_t\mathbf{y}\|}{\|\mathbf{y}\|}$$

is the coefficient of expansion in the direction of $\mathbf{y}$. It can be proved that its value is independent of the initial value of the chosen $\mathbf{y}$. If $\mathbf{A}_t$ is regular[1], the limit :

$$\chi(\mathbf{A}_t, \mathbf{y}) = \lim_{t\to\infty} \frac{1}{t} \ln \lambda_t(\mathbf{y})$$

exists, it is finite and it is called the 1-dimensional Lyapunov Characteristic Exponent or the Lyapunov Characteristic Exponent of order 1 (1-LCE) of $\mathbf{A}_t$ with respect to the vector $\mathbf{y}$. If the initial vector $\mathbf{y}$ is chosen to be unitary, the 1-LCE is simplified to the expression :

$$\chi(\mathbf{A}_t, \mathbf{y}) = \lim_{t\to\infty} \frac{1}{t} \ln\|\mathbf{A}_t\mathbf{y}\|.$$

Similarly, considering $p > 1$ linearly independent vectors, $\mathbf{y}_i \in \mathbf{R}^n$ with $i = 1, \ldots, p$, that span a p-dimensional subspace $\mathbf{E}^p \subseteq \mathbf{R}^n$, the quantity defined by :

$$\lambda_t(\mathbf{E}^p) = \frac{vol_p(\mathbf{A}_t, \mathbf{E}^p)}{vol_p(\mathbf{A}_0, \mathbf{E}^p)} = \frac{vol_p(\mathbf{A}_t, \mathbf{E}^p)}{vol_p(\mathbf{E}^p)}$$

is the coefficient of expansion in the direction of $\mathbf{E}^p$. It is noted that :

$$vol_p(\mathbf{A}_t, \mathbf{E}^p) = \|\mathbf{A}_t\mathbf{y}_1 \wedge \mathbf{A}_t\mathbf{y}_2 \wedge \ldots \wedge \mathbf{A}_t\mathbf{y}_p\|$$

represents the volume of the p-parallelogram defined by the vectors $\mathbf{A}_t\mathbf{y}_i$, with $\wedge$ denoting the wedge product of the vectors[2]. It can be proved that $\lambda_t(\mathbf{E}^p)$ is independent of the initial values of the chosen $\mathbf{y}_i$ and it only depends on the subspace $\mathbf{E}^p$. If $\mathbf{A}_t$ is regular, the limit :

$$\chi(\mathbf{A}_t, \mathbf{E}^p) = \lim_{t\to\infty} \frac{1}{t} \ln \lambda_t(\mathbf{E}^p)$$

exists, it is finite and it is called the p-dimensional Lyapunov Characteristic Exponent or the Lyapunov Characteristic Exponent of order p (p-LCE) of $\mathbf{A}_t$ with respect to the subspace $\mathbf{E}^p$. If the initial vectors $\mathbf{y}_i$ are chosen to be orthonormal, the volume $vol_p(\mathbf{E}^p)$ is unitary and the p-LCE is simplified to the expression :

$$\chi(\mathbf{A}_t, \mathbf{E}^p) = \lim_{t\to\infty} \frac{1}{t} \ln vol_p(\mathbf{A}_t, \mathbf{E}^p).$$

According to the theory presented in section 1.3, let us consider a non zero deviation vector $\mathbf{w}$ evolving on the $2N$ dimensional tangent space, $\mathbf{T_xS}$

[1] It is noted that the regularity of the matrix functions is defined in the work of Oseledec [24] and explained also in the work of Benetin et al. [4] and Skokos [29].

[2] The notion of the wedge product will be explicitly described in the section 3.1

of the $2N$ dimensional phase space $\mathbf{S}$ of an N degree of freedom dynamical system, according to the rule :

$$\mathbf{w}(t) = d_{\mathbf{x}}\Phi^t(\mathbf{w}(0)).$$

As already mentioned, the above equation describes the action of the linear mapping $d_{\mathbf{x}}\Phi^t$ over an initial deviation vector $\mathbf{w}(0)$. Applying the same rule over two successive time intervals, t and s, we get :

$$d_{\mathbf{x}}\Phi^{t+s} = d_{\Phi^s(\mathbf{x})}\Phi^t \circ d_{\mathbf{x}}\Phi^s$$

since :

$$\Phi^{t+s} = \Phi^t \circ \Phi^s.$$

The above equation can be transformed into the following one :

$$\mathbf{R}(t+s, \mathbf{x}) = \mathbf{R}(t, \Phi^s(\mathbf{x})) \cdot \mathbf{R}(s, \mathbf{x})$$

where $\mathbf{R}(t, \mathbf{x})$ is a matrix function that corresponds to the rule $d_{\mathbf{x}}\Phi^t$. Such a matrix function is called multiplicative cocycle and is a special case of the matrix functions $\mathbf{A}_t$ that were described previously. Consequently, the theory and definitions of LCEs can be valid also for this case, as long as the multiplicative cocycles are proved to be regular.

Benetin et al., [4], adjusted the MET of Oseledec [24], to Hamiltonian systems and symplectic maps, proving the regularity of the multiplicative cocycle $d_{\mathbf{x}}\Phi^t$, ensuring in this way the existence and finiteness of LCEs for such dynamical systems. Therefore, applying the already presented theory of LCEs and considering a non zero deviation vector, $\mathbf{w} \in \mathbf{T}_{\mathbf{x}}\mathbf{S}$, the coefficient of expansion in the direction of $\mathbf{w}$ is given by :

$$\lambda_t(\mathbf{w}) = \frac{\|d_{\mathbf{x}}\Phi^t\mathbf{w}\|}{\|d_{\mathbf{x}}\Phi^0\mathbf{w}\|} = \frac{\|d_{\mathbf{x}}\Phi^t\mathbf{w}\|}{\|\mathbf{w}\|}$$

and it is independent of the initial value of $\mathbf{w}$. The limit :

$$\chi(d_{\mathbf{x}}\Phi^t, \mathbf{w}) = \lim_{x\to\infty} \frac{1}{t} \ln \lambda_t(\mathbf{w})$$

exists, is finite and is the 1-LCE. If the initial deviation vector is chosen to be unitary, the 1-LCE is simplified to the following :

$$\chi(d_{\mathbf{x}}\Phi^t, \mathbf{w}) = \lim_{x\to\infty} \frac{1}{t} \ln\|d_{\mathbf{x}}\Phi^t\mathbf{w}\|.$$

If $\chi(d_{\mathbf{x}}\Phi^t, \mathbf{w}) > 0$, there occurs exponential divergence in the direction of the deviation vector, $\mathbf{w}$. It is exactly this property that Hénon and Heiles [15] used to indicate chaos.

Considering $p > 1$ and linearly independent deviation vectors, $\mathbf{w}_i \in \mathbf{T_xS}$, that span a p dimensional space $\mathbf{E}^p \subseteq \mathbf{T_xS}$, the coefficient of expansion in the direction of $\mathbf{E}^p$ is again given by :

$$\lambda_t(\mathbf{E}^p) = \frac{vol_p(d_\mathbf{x}\Phi^t, \mathbf{E}^p)}{vol_p(d_\mathbf{x}\Phi^0, \mathbf{E}^p)} = \frac{vol_p(d_\mathbf{x}\Phi^t\mathbf{E}^p)}{vol_p(\mathbf{E}^p)}$$

and it is independent of the initial values of $\mathbf{w}_i$. The quantity :

$$vol_p(d_\mathbf{x}\Phi^t, \mathbf{E}^p) = \|d_\mathbf{x}\Phi^t\mathbf{w}_1 \wedge d_\mathbf{x}\Phi^t\mathbf{w}_2 \wedge \ldots \wedge d_\mathbf{x}\Phi^t\mathbf{w}_p\|$$

is the volume of the p-parallelogram that the vectors $d_\mathbf{x}\Phi^t\mathbf{w}_i$, with $i = 1, \ldots, p$, define. The limit :

$$\chi(d_\mathbf{x}\Phi^t, \mathbf{E}^p) = \lim_{x\to\infty} \frac{1}{t} \ln \lambda_t(\mathbf{E}^p)$$

exists, is finite and is the p-LCE. If the initial deviation vectors are chosen to be orthonormal, the p-LCE is again simplified to be :

$$\chi(d_\mathbf{x}\Phi^t, \mathbf{E}^p) = \lim_{x\to\infty} \frac{1}{t} \ln vol_p(d_\mathbf{x}\Phi^t, \mathbf{E}^p).$$

All the possible different 1-LCEs of a dynamical system constitute the so-called spectrum of 1-LCEs. Furthermore, it can be induced from the MET that a p-LCE is the sum of the p largest 1-LCEs of the spectrum.

Summarizing the theory and the main conclusion of this section let us point out that an 1-LCE describes the rate of expansion of a deviation vector about a considered orbit. This vector evolves on the tangent space of the phase space of the dynamical system. A p-LCE describes the rate of expansion of a p-dimensional structure, which is formed by p linearly independent deviation vectors. A positive value of 1-LCEs or p-LCEs implies exponential divergence and, therefore, denotes the chaotic nature of the considered orbit.

In the following sections the basic properties of the spectrum of 1-LCEs, simply called LCEs, will be presented. Furthermore, the procedure of their computation will be explained.

2.3 Properties of LCEs and spectrum

The basic properties of the LCEs and p-LCEs are induced by the mathematical theory, already presented in section 2.2, and the MET [24]. They can be summarized in the following :

- The number of all the different LCEs that can be possibly computed equals the dimension n of the phase space of the system. The group

of these LCEs is called the spectrum of LCEs. The number of all the different possible p-LCEs equals the binomial coefficient :

$$\binom{n}{p} = \frac{n!}{p!(n-p)!}.$$

- The LCEs of the spectrum are ranked in descending order :

$$\chi(\mathbf{A}_t, \mathbf{y}_1) \geq \chi(\mathbf{A}_t, \mathbf{y}_2) \geq \ldots \geq \chi(\mathbf{A}_t, \mathbf{y}_n).$$

  The first one, which is the greatest exponent of the spectrum, is called the maximum LCE, mLCE.

- As already mentioned, a p-LCE equals the sum of the p largest LCEs. Therefore, given the first property above, the total number of the possible p-LCEs equals the number of the different sums of p LCEs.

- In the case of an ordered, or regular, orbit, all LCEs tent to zero exponentially, following a power law $\propto \log t/t$ [12]. On the contrary, in the case of a chaotic orbit, at least one LCE tents to a positive value. This property, combined with the one above mentioned that concerns the descending order of the LCEs, reveals the great importance of the mLCE in the study of a dynamical system, since the computation of just this exponent is sufficient for the accurate determination of the ordered or chaotic nature of an orbit.

- For a connected chaotic area the LCEs are constant, since every chaotic orbit in this area tents to densely fill it and thus different orbits may consider to be dynamically equivalent. Furthermore, chaotic orbits that belong to different chaotic areas display in general different LCEs spectrum. This property consists a simple mean for detecting weather chaotic orbits come from the same chaotic sea or not.

For simplicity, from now on the 1-LCE $\chi(\mathbf{A}_t, \mathbf{y}_i)$ will be denoted as χ_i and the p-LCE $\chi(\mathbf{A}_t, \mathbf{E}^p)$ will be denoted as χ_i^p.

Depending on the type of the considered dynamical system, the spectrum of LCEs displays a number of additional properties. For autonomous Hamiltonian systems of N degrees of freedom, as well as symplectic maps, we also have :

- Due to the preservation of their phase space (since they are conservative systems) the sum of the spectrum equals zero :

$$\sum_{i=1}^{2N} \chi_i = 0.$$

- Due to the symplecticity of the systems, the spectrum is arranged in pairs of equal absolute values and opposite signs :

$$\chi_i = -\chi_{2N-i+1}, \quad i = 1, 2, \ldots, N.$$

According to this, the spectrum takes the form :

$$\chi_1 \geq \chi_2 \geq \cdots \geq \chi_{N-1} \geq \chi_N \geq -\chi_N \geq -\chi_{N-1} \geq \cdots \geq -\chi_2 \geq -\chi_1.$$

This property can be used for testing the accuracy of the method used for the computation of the spectrum. Since the exponents are expected to form pairs, the smallness of their difference is a reliable indicator of the effectiveness of the chosen numerical method.

- For every integral of motion the dynamical system may possess, a LCEs becomes zero. Moreover, taking the previous property under consideration, it is clear that the existence of an integral of motion results in the vanishing of a pair of LCEs of the spectrum. The autonomous Hamiltonian systems have at least one integral of motion, the Hamiltonian function itself. Thus, for such systems, there is at least two LCEs equal to zero. The symplectic dynamical systems that possess as many integrals of motion as their degrees of freedom are called integrable and all their LCEs are zero.

All the above mentioned properties illustrate the importance of the LCEs spectrum in the study of a dynamical system.

2.4 Computation of LCEs and p-LCEs

Considering the general case of matrix functions $\mathbf{A}_t$ and the n-dimensional real vector space $\mathbf{R}^n$ the computation of the LCEs is achieved applying the definition, already mentioned in section 2.2 :

$$\chi(\mathbf{A}_t, \mathbf{y}) = \lim_{t\to\infty} \frac{1}{t} \ln \lambda_t(\mathbf{y})$$

for a random initial vector $\mathbf{y} \in \mathbf{R}^n$, or :

$$\chi(\mathbf{A}_t, \mathbf{y}) = \lim_{t\to\infty} \frac{1}{t} \ln\|\mathbf{A}_t\mathbf{y}\|$$

for a unitary initial vector $\mathbf{y} \in \mathbf{R}^n$. Since the same definition is used for the computation of all the possible LCEs, the different exponents of the LCEs spectrum are obtained choosing appropriate initial vectors, $\mathbf{y}$. It is reminded that the norm of the initial vectors does not affect the value of the LCEs (section 2.3). In general, there exist at most n different exponents (see section 2.3). Therefore, we need n different, appropriate vectors for the computation of the spectrum.

If the initial vector space $\mathbf{R}^n$ is analysed into appropriate subspaces of descending dimensionality, there can be induced n vector spaces, $\mathbf{V}_i$, of the form :

$$\mathbf{V}_1 \supset \mathbf{V}_2 \supset \ldots \supset \mathbf{V}_n$$

with $\mathbf{V}_1 = \mathbf{R}^n$ and dimension n, $\dim \mathbf{V}_2 = n-1$ and so on until $\dim \mathbf{V}_n = 1$. Considered n random vectors, each one taken from the respective subspace, $\mathbf{y}_i \in \mathbf{V}_i$, with $i = 1, \ldots, n$, it can be proved, [4, 24, 29], that the LCEs of the spectrum are given by :

$$\begin{aligned}
\chi_1 &= \chi(\mathbf{A}_t, \mathbf{y}_1) \quad \text{with } \mathbf{y}_1 \in \mathbf{V}_1 = \mathbf{R}^n \\
\chi_2 &= \chi(\mathbf{A}_t, \mathbf{y}_2) \quad \text{with } \mathbf{y}_2 \in \mathbf{V}_2 \\
&\vdots \\
\chi_n &= \chi(\mathbf{A}_t, \mathbf{y}_n) \quad \text{with } \mathbf{y}_n \in \mathbf{V}_n.
\end{aligned}$$

In practice, due to the computers' finite precision, all the numerically obtained deviation vectors belong to the whole $\mathbf{T_xS}$ space and thus, the computation of the different exponents of the spectrum is degenerated into the computation of the mLCE. Thus, other numerically stable procedures are needed for the actual evaluation of the spectrum.

2.5 The standard method

As was explained in the previous section, any $\mathbf{y} \in \mathbf{R}^n$ randomly chosen vector will result in the computation of the mLCE. Similarly, any group of randomly chosen $\mathbf{y}_i \in \mathbf{R}^n$ with $i = 1, \ldots, p$ yet linearly independent, vectors will span a random subspace $\mathbf{E}^p \subseteq \mathbf{R}^n$, resulting in the computation of the p-mLCE. For the rest of the exponents, computational errors and finite precision arithmetic constitute obstacles to their direct evaluation. However, an indirect approach, which follows the fact that a p-LCE equals the sum of p LCEs, makes the estimation of the spectrum possible. More precisely, given that :

$$\chi_1^p = \chi_1 + \chi_2 + \ldots + \chi_p$$

with χ_1, χ_1^p being the mLCE and the p-mLCE respectively, and since these quantities can be easily computed, the other LCEs of the spectrum, apart from the mLCE, are given by the equation :

$$\chi_p = \chi_1^p - \chi_1^{p-1}, \quad p = 2, \ldots, n.$$

More specifically, it is :

$$\begin{aligned}
&\chi_2 = \chi_1^2 - \chi_1^1 = (\chi_1 + \chi_2) - \chi_1 \\
&\chi_3 = \chi_1^3 - \chi_1^2 = (\chi_1 + \chi_2 + \chi_3) - (\chi_1 + \chi_2) \\
&\vdots \quad \vdots \quad \vdots \\
&\chi_n = \chi_1^n - \chi_1^{n-1} = (\chi_1 + \chi_2 + \ldots + \chi_{n-1} + \chi_n) - (\chi_1 + \chi_2 + \ldots + \chi_{n-1}).
\end{aligned}$$

Benettin et al., [4], noticed that if an orthonormalization procedure is applied to the initially random and linearly independent p vectors, with $p = 1, \ldots, n$, the p largest LCEs of the spectrum can be computed at once, taking advantage of the above equations.

Considering p initially linearly independent vectors, $\mathbf{y}_i \in \mathbf{R}^n$, the Gram-Schmidt orthomormalization procedure, described by the following equations, force vectors to become orthogonal to all the preceded ones :

$$\begin{aligned}
\acute{\mathbf{y}}_2 &= \mathbf{y}_2 - proj_{\mathbf{y}_1}\mathbf{y}_2 \\
\acute{\mathbf{y}}_3 &= \mathbf{y}_3 - proj_{\mathbf{y}_1}\mathbf{y}_3 - proj_{\acute{\mathbf{y}}_2}\mathbf{y}_3 \\
&\vdots \\
\acute{\mathbf{y}}_p &= \mathbf{y}_p - proj_{\mathbf{y}_1}\mathbf{y}_p - proj_{\acute{\mathbf{y}}_2}\mathbf{y}_p - \ldots - proj_{\acute{\mathbf{y}}_{p-1}}\mathbf{y}_p
\end{aligned}$$

where $proj_{\mathbf{y}_i}\mathbf{y}_j$ is the projection of vector $\mathbf{y}_j$ on the line spanned by vector $\mathbf{y}_i$:

$$\begin{aligned}
proj_{\mathbf{y}_1}\mathbf{y}_2 &= \frac{< \mathbf{y}_2, \mathbf{y}_1 >}{< \mathbf{y}_1, \mathbf{y}_1 >}\mathbf{y}_1 \\
proj_{\mathbf{y}_1}\mathbf{y}_3 &= \frac{< \mathbf{y}_3, \mathbf{y}_1 >}{< \mathbf{y}_1, \mathbf{y}_1 >}\mathbf{y}_1 \\
proj_{\acute{\mathbf{y}}_2}\mathbf{y}_3 &= \frac{< \mathbf{y}_3, \acute{\mathbf{y}}_2 >}{< \acute{\mathbf{y}}_2, \acute{\mathbf{y}}_2 >}\mathbf{y}_2 \\
proj_{\mathbf{y}_1}\mathbf{y}_4 &= \frac{< \mathbf{y}_4, \mathbf{y}_1 >}{< \mathbf{y}_1, \mathbf{y}_1 >}\mathbf{y}_1 \\
proj_{\acute{\mathbf{y}}_2}\mathbf{y}_4 &= \frac{< \mathbf{y}_4, \acute{\mathbf{y}}_2 >}{< \acute{\mathbf{y}}_2, \acute{\mathbf{y}}_2 >}\mathbf{y}_2 \\
proj_{\acute{\mathbf{y}}_3}\mathbf{y}_4 &= \frac{< \mathbf{y}_4, \acute{\mathbf{y}}_3 >}{< \acute{\mathbf{y}}_3, \acute{\mathbf{y}}_3 >}\mathbf{y}_3 \\
&\vdots
\end{aligned}$$

with $< \cdot, \cdot >$ denoting the inner product. The equations above orthogonalize

the $\mathbf{y}_i$ vectors. As a last step of the procedure, each vector is normalized :

$$\begin{aligned}\hat{\mathbf{y}}_1 &= \frac{\mathbf{y}_1}{\|\mathbf{y}_1\|}\\ \hat{\mathbf{y}}_2 &= \frac{\acute{\mathbf{y}}_2}{\|\acute{\mathbf{y}}_2\|}\\ &\vdots\\ \hat{\mathbf{y}}_p &= \frac{\acute{\mathbf{y}}_p}{\|\acute{\mathbf{y}}_p\|}.\end{aligned}$$

Vectors $\hat{\mathbf{y}}_i$ are now unitary and orthogonal to each other forming an orthonormal basis of the space. Using these vectors we apply the simplified definition for the computation of p-mLCE (section 2.2).

It can be proved, [4, 29], that the volume of the p-parallelogram formed by p arbitrary orthogonal vectors $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_p$, is given by the product of their norm :

$$vol_p(\mathbf{u}_i) = \|\mathbf{u}_1 \wedge \mathbf{u}_2 \wedge \ldots \wedge \mathbf{u}_p\| = \|\mathbf{u}_1\| \cdot \|\mathbf{u}_2\| \cdot \ldots \cdot \|\mathbf{u}_p\|.$$

Combining this equation with the definition of the p-mLCE and the auxiliary equation for the computation of the LCEs of the spectrum :

$$\begin{aligned}\chi_i^p = \chi(\mathbf{A}_t, \mathbf{E}^p) &= \lim_{t\to\infty} \frac{1}{t} \ln vol_p(\mathbf{A}_t, \mathbf{E}^p)\\ &= \lim_{t\to\infty} \frac{1}{t} \ln\|\mathbf{A}_t\hat{\mathbf{y}}_1 \wedge \mathbf{A}_t\hat{\mathbf{y}}_2 \wedge \ldots \wedge \mathbf{A}_t\hat{\mathbf{y}}_p\|\\ \chi_p &= \chi_1^p - \chi_1^{p-1}, \quad p = 2, \ldots, n\end{aligned}$$

all the LCEs are now given by the equation :

$$\chi_p = \lim_{t\to\infty} \frac{1}{t} \ln \|\acute{\mathbf{y}}_p\|$$

with $\acute{\mathbf{y}}_i$ being the respective orthogonal vectors obtained by the application of the Gram-Schmidt procedure to the $\mathbf{A}_t\hat{\mathbf{y}}_i$ vectors. We note that $\mathbf{A}_t\mathbf{y}_i$ denotes the time evolution of an initial vector $\mathbf{y}_i$ according to the matrix function $\mathbf{A}_t$.

All the above mentioned procedure is also applicable to the case of our example : the autonomous conservative Hénon-Heiles Hamiltonian system. Considering 4 deviation vectors $\mathbf{w}_i \in \mathbf{T}_\mathbf{x}\mathbf{S}$, $i = 1, \ldots, 4$, which evolve in time under the rule $d_\mathbf{x}\Phi^t$ and they are orthonormalized according to the Gram-Schmidt procedure, we obtain vectors $\hat{\mathbf{w}}_i$. Then, the different exponents of the spectrum are given by :

$$\chi_p = \lim_{t\to\infty} \frac{1}{t} \ln \|\acute{\mathbf{w}}_p\|, \quad p = 1, \ldots, 4$$

where $\acute{\mathbf{w}}_i$ are the orthogonalized vectors $d_{\mathbf{x}}\Phi^t\hat{\mathbf{w}}_i$. The method described above, was introduced by Benettin et al. [4] and is widely used for the computation of the LCEs spectrum. It is known as the standard method.

Let us make some comments on the actual computation of the LCEs, using again as example the Hénon-Heiles system. This computation requires the time evolution of the deviation vectors simultaneously with the time evolution of the considered orbit. Since the equations of motion form a nonlinear system, its solution cannot be found analytically. Therefore, numerical integration methods are used, that estimate the orbit at discrete times, $k \cdot dt$, with $k = 0, 1, \ldots$ and $dt > 0$ being the integration step. As a result, the equation for the computation of the LCEs spectrum becomes :

$$\chi_p = \lim_{k\to\infty} \frac{1}{k \cdot dt} \sum_{i=1}^{k} \ln \|\acute{\mathbf{w}}_p\|, \quad p = 1, \ldots, 4.$$

In general, the norm of the deviation vectors increases rapidly. Especially in the case of a chaotic orbit, the increase is exponential. This increase leads to computational errors and eventually to the failure of the procedure due to numerical overflow. Since the initial norm of the considered deviation vectors do not affect the computation of the exponents, a normalization procedure is applied to the vectors from time to time.

In Fig. 2.1 to 2.3, we present the results of the computation of the LCEs spectrum for two ordered orbits and one chaotic of the Hénon-Heiles system. For these computations we apply the standard method of Benettin et al. [4], using an integration step $dt = 0.01$. For the numerical integration we use a symplectic integrator or the SABA family [17] and more specifically, the $SABA_2C$ integrator [3].

For the ordered orbits, the LCEs of the spectrum tent to zero exponentially, following a power law $\propto \log(t)/t$, Fig. 2.1c, 2.1d and 2.2c, 2.2d. From Fig. 2.1d and 2.2d we see that, as expected the spectrum is grouped in two pairs of opposite exponents. In the case of the chaotic orbit, Fig. 2.3, one exponent tents to retain a positive value, while two others tent exponentially to zero following the same power law as in the case of the ordered orbits.

The different nature of the orbits can clearly be obtained from the behaviour of the spectrum. These results can be also verified by inspection of the Poincaré Surface of Section (PSS) : scattered points correspond to chaotic orbits, while well defined smooth curves to ordered ones. We also not that the pair of exponents that tent to zero for both kinds of orbits gives a clear indication of the existence of only one integral of motion, i.e. the Hamiltonian itself.

[3] The symplectic integrators are presented and explained in section 4.2

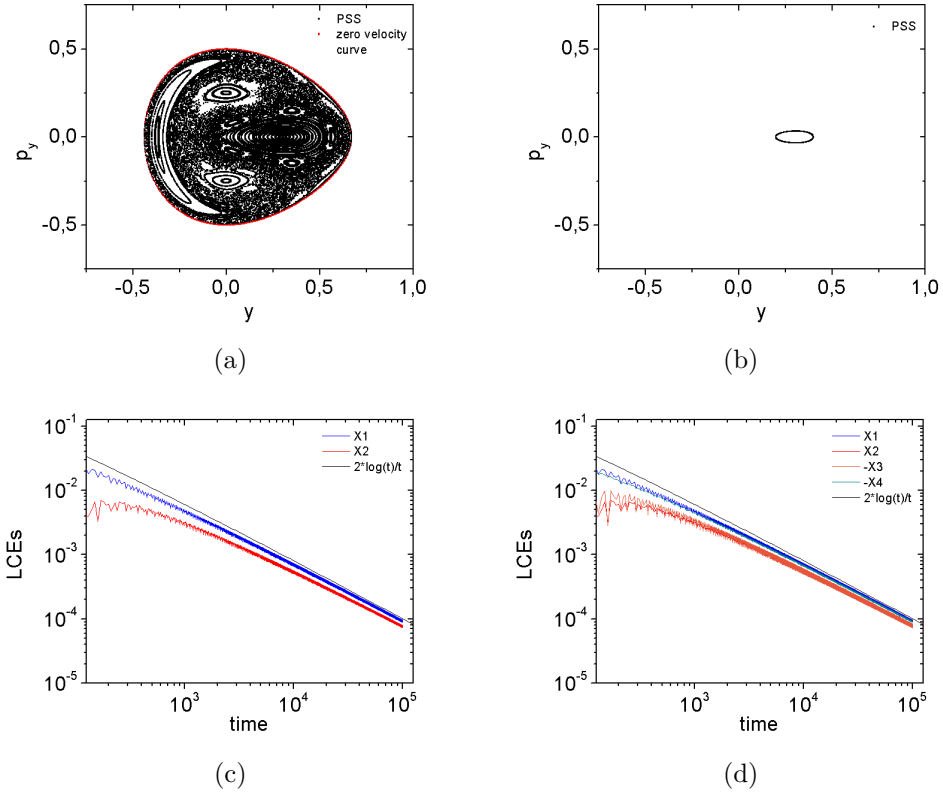


Figure 2.1: Computation of the LCEs spectrum of the Hénon-Heiles system for the ordered orbit with initial conditions $(x, y, p_y) = (0, 0.4, 0)$ for $H_0 = 0.125$. The value of the p_x variable is determined by the Hamiltonian function and is chosen to be positive. Fig. 2.1a shows the PSS of the system and Fig. 2.1b shows the PSS of the considered orbit (both plots are on the (y, p_y) plane). Fig. 2.1c shows the time evolution of the χ_1 and χ_2 exponents of the spectrum and Fig. 2.1d shows the whole spectrum of LCEs up to the $t_{max} = 10^5$ time units (both panels use log-log scales). It is noted that the exponents χ_3 and χ_4 are plotted with opposite sign. A curve proportional to $\log t/t$ is also plotted in panels 2.1c and 2.1d.

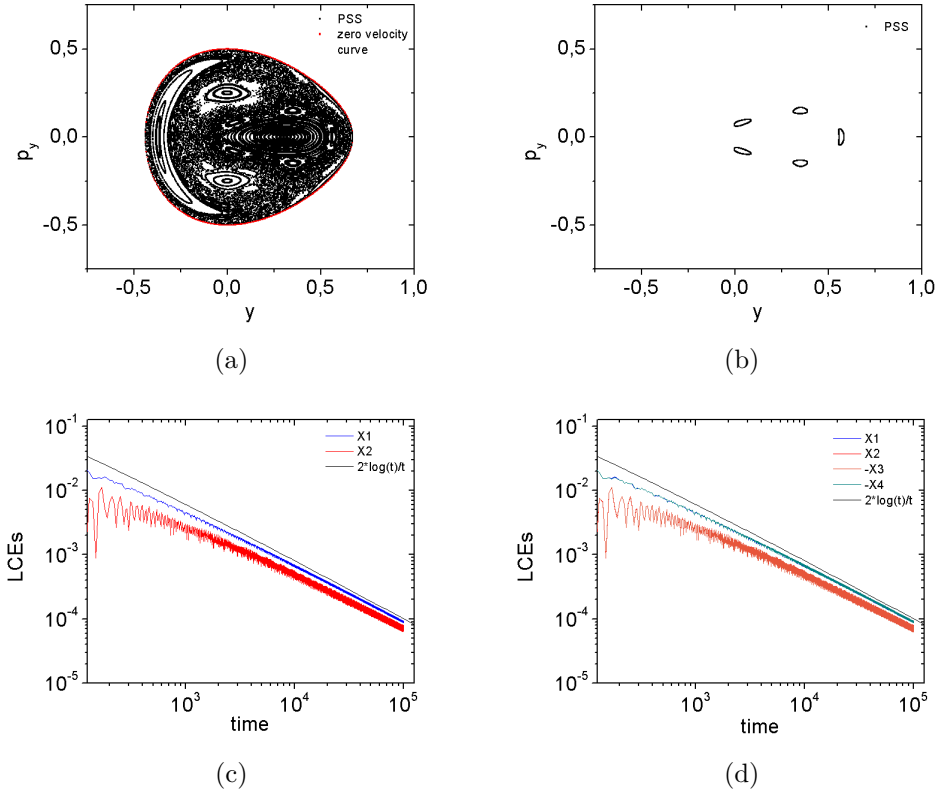


Figure 2.2: Similar plots to Fig. 2.1 for the case of the ordered orbit of the Hénon-Heiles system with initial conditions $(x, y, p_y) = (0, 0.558, 0)$ for $H_0 = 0.125$.

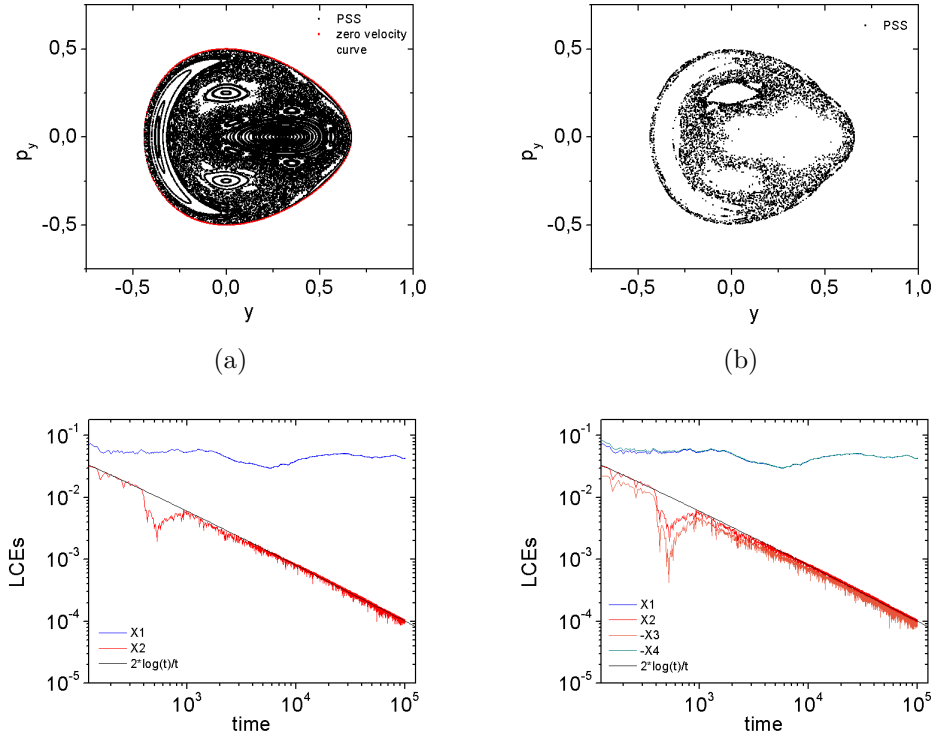


Figure 2.3: Similar plots to Fig. 2.1d and 2.2d of the Hénon-Heiles system with initial conditions $(x, y, p_y) = (0, -0.24, 0)$ for $H_0 = 0.125$.

Chapter 3

Compound Matrix Theory

3.1 Exterior Algebra and Wedge Product

In this section, based on the work of Allen and Bridges [1] and the appendix of [29], a short introduction to the exterior algebra and its principles is given.

Let us consider an n-dimensional vector space $\mathbf{V}$ over the field of real numbers $\mathbf{R}$ which is spanned by an orthonormal basis of the form $\{\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \ldots, \hat{\mathbf{e}}_n\}$. If $< \cdot, \cdot >_V$ defines an inner product in $\mathbf{V}$, then the orthonormal basis satisfies the equations :

$$< \hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j >_V = \delta_{ij}, \quad \text{where:} \quad \delta_{ij} = \begin{cases} 1 & \text{for } i = j, \\ 0 & \text{for } i \neq j. \end{cases}$$

Every vector in the $\mathbf{V}$ can be written as a linear combination of the basis vectors, thus, any two random vectors, $\mathbf{u}, \mathbf{v} \in \mathbf{V}$, can be written in the form :

$$\mathbf{u} = u_1 \cdot \hat{\mathbf{e}}_1 + u_2 \cdot \hat{\mathbf{e}}_2 + \ldots + u_n \cdot \hat{\mathbf{e}}_n$$
$$\mathbf{v} = v_1 \cdot \hat{\mathbf{e}}_1 + v_2 \cdot \hat{\mathbf{e}}_2 + \ldots + v_n \cdot \hat{\mathbf{e}}_n$$

where $u_i, v_i \in \mathbf{R}$ for $i = 1, 2, \ldots, n$.

The exterior or wedge product of these two vectors defines a new vector, which is denoted by $\mathbf{u} \wedge \mathbf{v}$ and is called a 2-vector. It is related to the area of the parallelogram that $\mathbf{u}$ and $\mathbf{v}$ form in $\mathbf{V}$, representing a 2-dimensional subspace of $\mathbf{V}$. All the possible 2-vectors generate a new vector space, called the 2nd exterior power of $\mathbf{V}$ and denoted by $\mathbf{\Lambda}^2(\mathbf{V})$. Similarly, the wedge product of k vectors, $\mathbf{u}_1 \wedge \mathbf{u}_2 \wedge \ldots \wedge \mathbf{u}_k$, with $\mathbf{u}_i \in \mathbf{V}$ for $i = 1, 2, \ldots, k$, can be related to the hyper-volume of the structure defined by these vectors, it is called a k-vector and it represents a k-dimensional subspace of $\mathbf{V}$. All the possible k-vectors generate a vector space called the k-th exterior power of $\mathbf{V}$, denoted by $\mathbf{\Lambda}^k(\mathbf{V})$.

The value of k can vary between $0 \leq k \leq n$, with $\mathbf{\Lambda}^0(\mathbf{V}) = \mathbf{R}$ and $\mathbf{\Lambda}^1(\mathbf{V}) = \mathbf{V}$. All the possible $\mathbf{\Lambda}^k(\mathbf{V})$ vector spaces are subspaces of the

$\mathbf{\Lambda}(\mathbf{V})$ vector space, which is called the exterior algebra of $\mathbf{V}$ and can be written as the direct sum of the k-th exterior powers of $\mathbf{V}$:

$$\Lambda(V) = \bigoplus_{k=0}^{n} \Lambda^k(V) = \Lambda^0(V) \oplus \Lambda^1(V) \oplus \cdots \oplus \Lambda^n(V).$$

The wedge product has the following properties :

- Associativity :

$$(\mathbf{u} \wedge \mathbf{v}) \wedge \mathbf{w} = \mathbf{u} \wedge (\mathbf{v} \wedge \mathbf{w})$$

- Bilinearity :

$$(c_1\mathbf{u} + c_2\mathbf{v}) \wedge \mathbf{w} = c_1(\mathbf{u} \wedge \mathbf{w}) + c_2(\mathbf{v} \wedge \mathbf{w})$$
$$\mathbf{w} \wedge (c_1\mathbf{u} + c_2\mathbf{v}) = c_1(\mathbf{w} \wedge \mathbf{u}) + c_2(\mathbf{w} \wedge \mathbf{v})$$

- Alternating on $\mathbf{V}$:

$$\mathbf{u} \wedge \mathbf{u} = \mathbf{0}$$

- Anticommutativity :

$$\mathbf{u} \wedge \mathbf{v} = -\mathbf{v} \wedge \mathbf{u}$$

- If at least two of the vectors $\mathbf{u}_1, \mathbf{u}_2, \ldots, \mathbf{u}_k$ are linear depended, then :

$$\mathbf{u}_1 \wedge \mathbf{u}_2 \wedge \ldots \wedge \mathbf{u}_k = \mathbf{0}$$

for $\mathbf{u}_i \in \mathbf{V}$ with $i = 1, 2, \ldots, k$ and $c_1, c_2 \in \mathbf{R}$.

Following the above mentioned properties, an orthonormal basis of each $\mathbf{\Lambda}^k(\mathbf{V})$ vector space can be constructed by the considered orthonormal basis of $\mathbf{V}$. In order to clarify this statement, we consider the example case of $\mathbf{V}$ being a 4-dimensional vector space with an orthonormal basis of the form $\{\hat{\mathbf{e}}_1, \ldots, \hat{\mathbf{e}}_4\}$. In this case the value of k can vary between $0 \leq k \leq 4$. In what follows, we will study the wedge product for the non-trivial cases of k [1].

[1] It is noted that for the trivial cases where $k = 0$ and $k = 1$ the induced spaces are the set of real numbers $\mathbf{R}$ and the initial vector space $\mathbf{V}$ respectively.

Considering the case $k = 2$ we get :

$$\begin{aligned}
\mathbf{u} \wedge \mathbf{v} &= (u_1 \cdot \hat{\mathbf{e}}_1 + u_2 \cdot \hat{\mathbf{e}}_2 + u_3 \cdot \hat{\mathbf{e}}_3 + u_4 \cdot \hat{\mathbf{e}}_4) + (v_1 \cdot \hat{\mathbf{e}}_1 + v_2 \cdot \hat{\mathbf{e}}_2 + v_3 \cdot \hat{\mathbf{e}}_3 + v_4 \cdot \hat{\mathbf{e}}_4) \\
&= u_1v_1(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_1) + u_1v_2(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2) + u_1v_3(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_3) + u_1v_4(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_4) + \\
&+ u_2v_1(\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_1) + u_2v_2(\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_2) + u_2v_3(\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_3) + u_2v_4(\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_4) + \\
&+ u_3v_1(\hat{\mathbf{e}}_3 \wedge \hat{\mathbf{e}}_1) + u_3v_2(\hat{\mathbf{e}}_3 \wedge \hat{\mathbf{e}}_2) + u_3v_3(\hat{\mathbf{e}}_3 \wedge \hat{\mathbf{e}}_3) + u_3v_4(\hat{\mathbf{e}}_3 \wedge \hat{\mathbf{e}}_4) + \\
&+ u_4v_1(\hat{\mathbf{e}}_4 \wedge \hat{\mathbf{e}}_1) + u_4v_2(\hat{\mathbf{e}}_4 \wedge \hat{\mathbf{e}}_2) + u_4v_3(\hat{\mathbf{e}}_4 \wedge \hat{\mathbf{e}}_3) + u_4v_4(\hat{\mathbf{e}}_4 \wedge \hat{\mathbf{e}}_4) \\
&= u_1v_1 \cdot 0 + u_1v_2(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2) + u_1v_3(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_3) + u_1v_4(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_4) - \\
&- u_2v_1(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2) + u_2v_2 \cdot 0 + u_2v_3(\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_3) + u_2v_4(\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_4) - \\
&- u_3v_1(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_3) - u_3v_2(\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_3) + u_3v_3 \cdot 0 + u_3v_4(\hat{\mathbf{e}}_3 \wedge \hat{\mathbf{e}}_4) - \\
&- u_4v_1(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_4) - u_4v_2(\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_4) - u_4v_3(\hat{\mathbf{e}}_3 \wedge \hat{\mathbf{e}}_4) + u_4v_4 \cdot 0 \\
&= (u_1v_2 - u_2v_1)(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2) + (u_1v_3 - u_3v_1)(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_3) + (u_1v_4 - u_4v_1)(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_4) + \\
&+ (u_2v_3 - u_3v_2)(\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_3) + (u_2v_4 - u_4v_2)(\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_4) + (u_3v_4 - u_4v_3)(\hat{\mathbf{e}}_3 \wedge \hat{\mathbf{e}}_4) \\
&= \begin{vmatrix} u_1 & v_1 \\ u_2 & v_2 \end{vmatrix} \cdot (\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2) + \begin{vmatrix} u_1 & v_1 \\ u_3 & v_3 \end{vmatrix} \cdot (\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_3) + \begin{vmatrix} u_1 & v_1 \\ u_4 & v_4 \end{vmatrix} \cdot (\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_4) + \\
&+ \begin{vmatrix} u_2 & v_2 \\ u_3 & v_3 \end{vmatrix} \cdot (\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_3) + \begin{vmatrix} u_2 & v_2 \\ u_4 & v_4 \end{vmatrix} \cdot (\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_4) + \begin{vmatrix} u_3 & v_3 \\ u_4 & v_4 \end{vmatrix} \cdot (\hat{\mathbf{e}}_3 \wedge \hat{\mathbf{e}}_4) \\
&= \bar{u}_1 \cdot \omega_1 + \ldots + \bar{u}_6 \cdot \omega_6.
\end{aligned}$$

The $\bar{u}_i \in \mathbf{R}$ elements are the coordinates of the 2-vector $\bar{\mathbf{u}} = \mathbf{u} \wedge \mathbf{v}$, while the ω_i, with $i = 1, 2, \ldots, 6$, quantities are the 2-vectors that form an orthonormal basis of the $\mathbf{\Lambda}^2(\mathbf{V})$ vector space.

The coordinates of the initially considered vectors, $\mathbf{u}, \mathbf{v}$, are reordered and combined according to a predefined pattern called the lexicographical order. More precisely, the lexicographical order is the specific order according to which all the possible permutations of the vectors of the orthonormal basis of the initial vector space should be considered, in order to form the orthonormal basis of the new vector space. It is noted that this order concerns only the permutations that yield different determinants, since any rearranging of the rows or the columns of a matrix does not change the value of its determinant. The ordering of the basis vector can be chosen arbitrarily since, as was proven in [1], it does not alter the results.

In general, the number of the ω_i k-vectors that consist the orthonormal basis and consequently the dimension of the $\mathbf{\Lambda}^k(\mathbf{V})$ vector space, is given by the binomial coefficient :

$$d_k = \binom{n}{k} = \frac{n!}{k!(n-k)!}.$$

For the case studied, the dimension of the $\mathbf{\Lambda}^2(\mathbf{V})$ space is :

$$d_2 = \binom{4}{2} = \frac{4!}{2!(4-2)!} = 6$$

and the lexicographical order was chosen to be :

$$(1,2),(1,3),(1,4),(2,3),(2,4),(3,4).$$

Similarly, considering the case where $k = 3$, the dimension of the $\mathbf{\Lambda}^3(\mathbf{V})$ vector space is :

$$d_3 = \binom{4}{3} = \frac{4!}{3!(4-3)!} = 4$$

while the lexicographical order is :

$$(1,2,3),(1,2,4),(1,3,4),(2,3,4).$$

Then, the wedge product will give the following 3-vector :

$$\begin{aligned}\mathbf{u}\wedge\mathbf{v}\wedge\mathbf{w} &= (u_1\cdot\hat{\mathbf{e}}_1+\ldots+u_4\cdot\hat{\mathbf{e}}_4)\wedge(v_1\cdot\hat{\mathbf{e}}_1+\ldots+v_4\cdot\hat{\mathbf{e}}_4)\wedge(w_1\cdot\hat{\mathbf{e}}_1+\ldots+\\ &\quad+w_4\cdot\hat{\mathbf{e}}_4)\\ &= \begin{vmatrix}u_1&v_1&w_1\\u_2&v_2&w_2\\u_3&v_3&w_3\end{vmatrix}\cdot(\hat{\mathbf{e}}_1\wedge\hat{\mathbf{e}}_2\wedge\hat{\mathbf{e}}_3)+\begin{vmatrix}u_1&v_1&w_1\\u_2&v_2&w_2\\u_4&v_4&w_4\end{vmatrix}\cdot(\hat{\mathbf{e}}_1\wedge\hat{\mathbf{e}}_2\wedge\hat{\mathbf{e}}_4)+\\ &\quad+\begin{vmatrix}u_1&v_1&w_1\\u_3&v_3&w_3\\u_4&v_4&w_4\end{vmatrix}\cdot(\hat{\mathbf{e}}_1\wedge\hat{\mathbf{e}}_3\wedge\hat{\mathbf{e}}_4)+\begin{vmatrix}u_2&v_2&w_2\\u_3&v_3&w_3\\u_4&v_4&w_4\end{vmatrix}\cdot(\hat{\mathbf{e}}_2\wedge\hat{\mathbf{e}}_3\wedge\hat{\mathbf{e}}_4)\\ &= \bar{u}_1\cdot\omega_1+\ldots+\bar{u}_4\cdot\omega_4.\end{aligned}$$

For the case where $k = n = 4$, the dimension of the $\mathbf{\Lambda}^4(\mathbf{V})$ vector space is :

$$d_4 = \binom{4}{4} = \frac{4!}{4!(4-4)!} = 1$$

and obviously the lexicographical order is :

$$(1,2,3,4).$$

The 4-vector is :

$$\begin{aligned}\mathbf{u}\wedge\mathbf{v}\wedge\mathbf{w}\wedge\mathbf{z} &= (u_1\cdot\hat{\mathbf{e}}_1+\ldots+u_4\cdot\hat{\mathbf{e}}_4)\wedge(v_1\cdot\hat{\mathbf{e}}_1+\ldots+v_4\cdot\hat{\mathbf{e}}_4)\wedge(w_1\cdot\hat{\mathbf{e}}_1+\ldots+\\ &\quad+w_4\cdot\hat{\mathbf{e}}_4)\wedge(z_1\cdot\hat{\mathbf{e}}_1+\ldots+z_4\cdot\hat{\mathbf{e}}_4)\\ &= \begin{vmatrix}u_1&v_1&w_1&z_1\\u_2&v_2&w_2&z_2\\u_3&v_3&w_3&z_3\\u_4&v_4&w_4&z_4\end{vmatrix}\cdot(\hat{\mathbf{e}}_1\wedge\hat{\mathbf{e}}_2\wedge\hat{\mathbf{e}}_3\wedge\hat{\mathbf{e}}_4)\\ &= \bar{u}_1\cdot\omega_1.\end{aligned}$$

From the previous example we understand that every k-vector $\bar{\mathbf{u}}$ in the $\mathbf{\Lambda}^k(\mathbf{V})$ space (like any vector in $\mathbf{V}$) can be written as a linear combination of the basis k-vectors ω_i, with $i = 1, \ldots, d_k$:

$$\bar{\mathbf{u}} = \sum_{i=1}^{d_k} \bar{u}_i \cdot \omega_i, \quad \bar{u}_i \in \mathbf{R}.$$

Any k-vector of $\mathbf{\Lambda}^k(\mathbf{V})$ that consists of the wedge product of k vectors of $\mathbf{V}$ is called decomposable. It must be noted that all such vectors are elements of $\mathbf{\Lambda}^k(\mathbf{V})$, but every element of $\mathbf{\Lambda}^k(\mathbf{V})$ is not necessarily a decomposable k-vector. From the theory mentioned above, as well as the previous example, it is understood that any decomposable k-vector can be generally written as follows :

$$\begin{aligned}
\bar{\mathbf{u}} &= \mathbf{u}_1 \wedge \mathbf{u}_2 \ldots \wedge \mathbf{u}_k \\
&= \sum_{i=1}^{d_k} \bar{u}_i \cdot \omega_i \\
&= \sum_{1 \le i_1 < i_2 < \ldots < i_k \le n} \begin{vmatrix} u_{i_1 1} & u_{i_1 2} & \ldots & u_{i_1 k} \\ u_{i_2 1} & u_{i_2 2} & \ldots & u_{i_2 k} \\ \vdots & \vdots & \ddots & \vdots \\ u_{i_k 1} & u_{i_k 2} & \cdots & u_{i_k k} \end{vmatrix} \cdot (\hat{\mathbf{e}}_{i_1} \wedge \hat{\mathbf{e}}_{i_2} \wedge \ldots \wedge \hat{\mathbf{e}}_{i_k}).
\end{aligned}$$

We see that each coordinate $\bar{u}_i \in \mathbf{R}$ is actually the determinant of the $n \times k$ matrix, whose columns are the coordinates of the considered k vectors of $\mathbf{V}$ and the rows are formed by taking k out of n coordinates of each vector in accordance with the lexicographical order.

An inner product on $\mathbf{V}$ induces an inner product on each vector space $\mathbf{\Lambda}^k(\mathbf{V})$. Let's see how this is done in more detail. The inner product of any two decomposable k-vectors of the form :

$$\begin{aligned}
\bar{\mathbf{u}} &= \mathbf{u}_1 \wedge \mathbf{u}_2 \wedge \ldots \wedge \mathbf{u}_k \\
\bar{\mathbf{v}} &= \mathbf{v}_1 \wedge \mathbf{v}_2 \wedge \ldots \wedge \mathbf{v}_k
\end{aligned}$$

with $\mathbf{u}_i, \mathbf{v}_i \in \mathbf{V}$ and $\bar{\mathbf{u}}, \bar{\mathbf{v}} \in \mathbf{\Lambda}^k(\mathbf{V})$, is denoted by $< \bar{\mathbf{u}}, \bar{\mathbf{v}} >_k$ and is defined by the equation :

$$< \bar{\mathbf{u}}, \bar{\mathbf{v}} >_k = \begin{vmatrix} < \mathbf{u}_1, \mathbf{v}_1 >_V & \cdots & < \mathbf{u}_1, \mathbf{v}_k >_V \\ < \mathbf{u}_2, \mathbf{v}_1 >_V & \cdots & < \mathbf{u}_2, \mathbf{v}_k >_V \\ \vdots & \ddots & \vdots \\ < \mathbf{u}_k, \mathbf{v}_1 >_V & \cdots & < \mathbf{u}_k, \mathbf{v}_k >_V \end{vmatrix}$$

where the inner product $< \mathbf{u}_i, \mathbf{v}_j >_V$ on $\mathbf{V}$ is as usual :

$$< \mathbf{u}_i, \mathbf{v}_j >_V = \sum_{r=1}^{n} u_{i_r} \cdot v_{j_r}.$$

Every element of $\mathbf{\Lambda}^k(\mathbf{V})$ can be written as a sum of decomposable elements, thus, the definition of the inner product can be extended by bilinearity to any k-vector.

Now, we can also show that the basis of $\mathbf{\Lambda}^k(\mathbf{V})$ which was formed by the wedge product of the orthonormal basis of $\mathbf{V}$, is orthonormal as was mentioned before. For the particular example of the 4-dimensional vector space $\mathbf{V}$ and the case where $k = 2$, the orthonormality of the basis can be shown as follows :

$$\begin{aligned}
< \omega_1, \omega_1 >_k &= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2 >_V \\
&= \begin{vmatrix} < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_1 >_V & < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2 >_V \\ < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_1 >_V & < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_2 >_V \end{vmatrix} \\
&= \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix} \\
&= 1
\end{aligned}$$

$$\begin{aligned}
< \omega_1, \omega_2 >_k &= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_3 >_V \\
&= \begin{vmatrix} < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_1 >_V & < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_3 >_V \\ < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_1 >_V & < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3 >_V \end{vmatrix} \\
&= \begin{vmatrix} 1 & 0 \\ 0 & 0 \end{vmatrix} \\
&= 0
\end{aligned}$$

$$\begin{aligned}
< \omega_1, \omega_3 >_k &= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_4 >_V \\
&= \begin{vmatrix} < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_1 >_V & < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_4 >_V \\ < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_1 >_V & < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_4 >_V \end{vmatrix} \\
&= \begin{vmatrix} 1 & 0 \\ 0 & 0 \end{vmatrix} \\
&= 0
\end{aligned}$$

$$\begin{aligned}
< \omega_1, \omega_4 >_k &= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_3 >_V \\
&= \begin{vmatrix} < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2 >_V & < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_3 >_V \\ < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_2 >_V & < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3 >_V \end{vmatrix} \\
&= \begin{vmatrix} 0 & 0 \\ 1 & 0 \end{vmatrix} \\
&= 0
\end{aligned}$$

$$
\begin{aligned}
< \omega_1, \omega_5 >_k &= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_4 >_V \\
&= \begin{vmatrix} < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2 >_V & < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_4 >_V \\ < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_2 >_V & < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_4 >_V \end{vmatrix} \\
&= \begin{vmatrix} 0 & 0 \\ 1 & 0 \end{vmatrix} \\
&= 0
\end{aligned}
$$

$$
\begin{aligned}
< \omega_1, \omega_6 >_k &= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3 \wedge \hat{\mathbf{e}}_4 >_V \\
&= \begin{vmatrix} < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_3 >_V & < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_4 >_V \\ < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3 >_V & < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_4 >_V \end{vmatrix} \\
&= \begin{vmatrix} 0 & 0 \\ 0 & 0 \end{vmatrix} \\
&= 0.
\end{aligned}
$$

The remaining of the possible combinations of the k-vector basis are computed in a similar way. The above computations are generalized to give :

$$< \omega_i, \omega_j >_k = \delta_{ij}, \quad i, j = 1, \ldots, d_k$$

which shows the orthonormal nature of the basis of $\mathbf{\Lambda}^k(\mathbf{V})$ vector space.

The norm of a k-vector can be computed using the already defined inner product :

$$
\begin{aligned}
\|\bar{\mathbf{u}}\| &= \|\mathbf{u}_1 \wedge \mathbf{u}_2 \ldots \wedge \mathbf{u}_k\| \\
&= \sqrt{< \bar{\mathbf{u}}, \bar{\mathbf{u}} >_k} \\
&= \left(\sum_{i=1}^{d_k} \bar{u}_i^2 \right)^{\frac{1}{2}} \\
&= \left(\sum_{1 \le i_1 < i_2 < \ldots < i_k \le n} \begin{vmatrix} u_{i_1 1} & u_{i_1 2} & \ldots & u_{i_1 k} \\ u_{i_2 1} & u_{i_2 2} & \ldots & u_{i_2 k} \\ \vdots & \vdots & \ddots & \vdots \\ u_{i_k 1} & u_{i_k 2} & \cdots & u_{i_k k} \end{vmatrix}^2 \right)^{\frac{1}{2}}.
\end{aligned}
$$

This value can be interpreted as the volume of the k-parallelogram defined by the k vectors $\mathbf{u}_i \in \mathbf{V}$.

3.2 Introduction to the Compound Matrix Theory

In 1983, Froyland [8] used an alternative procedure in order to compute some or all the LCEs. The proposed algorithm was described in a general form, concerning continuous dynamical systems as well as discrete maps, and its effectiveness was confirmed using the example of the dissipative Lorenz system, [9]. The main goal of these works was the replacement of the system of variational equations with auxiliary ones, induced from the initial system in order to avoid the constant need for orthonormalization of the deviation vectors. For at least low dimensional dynamical systems, the new approach was claimed to be faster than or comparable to the existed ones, like the standard method of Benettin et al. [4].

Around the same time, Ng and Reid [21, 22, 23] proposed the use of CMT in order to address fluid dynamics stability issues that arose from the solution of stiff nonlinear differential equations. The application of the theory suggested the handling of auxiliary systems, like the ones Froyland used in [8, 9]. Much later, Allen and Bridges [1] improved this approach by studying the CMT using the theory and principles of exterior algebra. As a result, the construction of the auxiliary systems could become automated and therefore be generalized for multidimensional dynamical systems.

Studying the application of the CMT to the computation of the LCEs from the perspective of the exterior algebra, we show that the auxiliary systems represent areas, volumes and hyper-volumes, formed by the initially considered deviation vectors which evolve with time around a given orbit. From the theory presented in section 3.1 it became clear that these structures consist vectors of modified vector spaces. The improvement of the CMT, in comparison to the standard method of [4], lies in the fact that each of the new vectors evolves on different vector space, therefore there is no need for orthonormalizing the deviation vectors. Moreover, using the properties of Compound Matrices, presented by Muldowney [19], we can see that the computation of a particular exponent of the spectrum is feasible, without the necessity of computing all the previous ones.

According to the work of Muldowney [19], for a given differential system of the form :

$$\dot{\mathbf{y}}(t) = \mathbf{A}(t) \cdot \mathbf{y}(t)$$

where $\mathbf{y}$ is a $n \times m$ solution matrix of the form :

$$\mathbf{y} = [\mathbf{y}_1 \quad \mathbf{y}_2 \dots \mathbf{y}_m], \quad \mathbf{y}_i \in \mathbf{R}^n$$

and $\mathbf{A}$ is a $n \times n$ matrix function, the k-vector $\bar{\mathbf{y}}$, constructed by the k $\mathbf{y}_i$ vectors of the solution matrix, is a solution of an auxiliary system, the so-called k-th compound system :

$$\dot{\bar{\mathbf{y}}} = \mathbf{A}^{[k]} \cdot \bar{\mathbf{y}}$$

with :

$$\bar{\mathbf{y}} = \mathbf{y}_1 \wedge \mathbf{y}_2 \wedge \ldots \wedge \mathbf{y}_k$$

and $\mathbf{A}^{[k]}$ being a new matrix called the k-th additive compound matrix of the matrix function $\mathbf{A}$.

The characteristics of the additive compound matrix are illustrated in the following example. We consider again the variational equations of the Hénon-Heiles system :

$$\dot{\mathbf{w}} = \mathbf{A}(t) \cdot \mathbf{w}$$

where :

$$\mathbf{A}(t) = \begin{bmatrix} \mathbf{0}_2 & \mathbf{I}_2 \\ -\mathbf{V}_{q_i q_{j\,2}} & \mathbf{0}_2 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ (-1-2y) & -2x & 0 & 0 \\ -2x & (-1+2y) & 0 & 0 \end{bmatrix}.$$

Its tangent space is of dimension 4, therefore, the possible $\mathbf{\Lambda}^k(\mathbf{T_x S})$ vector spaces exist for $0 \leq k \leq 4$. For each vector space, except the trivial cases of $\mathbf{\Lambda}^0(\mathbf{T_x S}) = \mathbf{R}$ and $\mathbf{\Lambda}^1(\mathbf{T_x S}) = \mathbf{T_x S} \Rightarrow \mathbf{A}^{[1]} = \mathbf{A}$, the respective auxiliary system is given by :

$$\dot{\mathbf{w}}^{(k)} = \mathbf{A}^{[k]}(t) \cdot \mathbf{w}^{(k)}$$

where $\mathbf{w}^{(k)}$ is a k-vector and $\mathbf{A}^{[k]}(t)$ is the k-th additive compound matrix.

The k-vector $\mathbf{w}^{(k)}$ is the wedge product of the k initial, arbitrarily chosen deviation vectors and is of dimension $d_k \times 1$. The k-th additive compound matrix, $\mathbf{A}^{[k]}(t)$, is constructed by the $\mathbf{A}(t)$ matrix of the variational equations and is of dimension $d_k \times d_k$, with $d_k = \binom{n}{k}$. According to [19], each element of $\mathbf{A}^{[k]}(t)$ is given as the inner product $A_{ij}^{[k]} =< \omega_i, \mathbf{A}(t)\omega_j >_k$, with $i, j = 1, \ldots, d_k$, on the $\mathbf{\Lambda}^k(\mathbf{T_x S})$ vector space. We note that for :

$$\bar{\mathbf{u}} = \mathbf{u}_1 \wedge \mathbf{u}_2 \wedge \ldots \wedge \mathbf{u}_k, \quad \mathbf{u}_i \in \mathbf{T_x S}, \quad i = 1, \ldots, k$$

we get :

$$\begin{aligned} \mathbf{A}\bar{\mathbf{u}} &= \mathbf{A}\mathbf{u}_1 \wedge \mathbf{u}_2 \wedge \ldots \wedge \mathbf{u}_k + \mathbf{u}_1 \wedge \mathbf{A}\mathbf{u}_2 \wedge \ldots \wedge \mathbf{u}_k + \ldots + \mathbf{u}_1 \wedge \mathbf{u}_2 \wedge \ldots \wedge \mathbf{A}\mathbf{u}_k \\ &= \sum_{i=1}^{k} \mathbf{u}_1 \wedge \mathbf{u}_2 \wedge \ldots \wedge \mathbf{A}\mathbf{u}_i \wedge \ldots \wedge \mathbf{u}_k. \end{aligned}$$

Therefore, for the $k = 2$ case and for the already used lexicographical order, the elements of the 2nd additive compound matrix $\mathbf{A}^{[2]}$, which is a 6×6

matrix, are :

$$
\begin{aligned}
A_{11}^{[2]} &= < \omega_1, \mathbf{A}\omega_1 >_k \\
&= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \mathbf{A}(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2) >_k \\
&= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2 >_k + < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_1 \wedge \mathbf{A}\hat{\mathbf{e}}_2 >_k \\
&= \begin{vmatrix} < \hat{\mathbf{e}}_1, \mathbf{A}\hat{\mathbf{e}}_1 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2 >_{\mathbf{T_x S}} \\ < \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_1 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_2 >_{\mathbf{T_x S}} \end{vmatrix} + \begin{vmatrix} < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_1 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_1, \mathbf{A}\hat{\mathbf{e}}_2 >_{\mathbf{T_x S}} \\ < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_1 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_2 >_{\mathbf{T_x S}} \end{vmatrix} \\
&= \begin{vmatrix} A_{11} & 0 \\ A_{21} & 1 \end{vmatrix} + \begin{vmatrix} 1 & A_{12} \\ 0 & A_{22} \end{vmatrix} \\
&= A_{11} + A_{22} \\
&= 0
\end{aligned}
$$

$$
\begin{aligned}
A_{12}^{[2]} &= < \omega_1, \mathbf{A}\omega_2 >_k \\
&= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \mathbf{A}(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_3) >_k \\
&= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_3 >_k + < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_1 \wedge \mathbf{A}\hat{\mathbf{e}}_3 >_k \\
&= \begin{vmatrix} < \hat{\mathbf{e}}_1, \mathbf{A}\hat{\mathbf{e}}_1 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_3 >_{\mathbf{T_x S}} \\ < \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_1 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3 >_{\mathbf{T_x S}} \end{vmatrix} + \begin{vmatrix} < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_1 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_1, \mathbf{A}\hat{\mathbf{e}}_3 >_{\mathbf{T_x S}} \\ < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_1 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_3 >_{\mathbf{T_x S}} \end{vmatrix} \\
&= \begin{vmatrix} A_{11} & 0 \\ A_{12} & 0 \end{vmatrix} + \begin{vmatrix} 1 & A_{13} \\ 0 & A_{23} \end{vmatrix} \\
&= 0 + A_{23} \\
&= 0
\end{aligned}
$$

$$
\begin{aligned}
A_{13}^{[2]} &= < \omega_1, \mathbf{A}\omega_3 >_k \\
&= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \mathbf{A}(\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_4) >_k \\
&= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_4 >_k + < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_1 \wedge \mathbf{A}\hat{\mathbf{e}}_4 >_k \\
&= \begin{vmatrix} < \hat{\mathbf{e}}_1, \mathbf{A}\hat{\mathbf{e}}_1 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_4 >_{\mathbf{T_x S}} \\ < \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_1 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_4 >_{\mathbf{T_x S}} \end{vmatrix} + \begin{vmatrix} < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_1 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_1, \mathbf{A}\hat{\mathbf{e}}_4 >_{\mathbf{T_x S}} \\ < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_1 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_4 >_{\mathbf{T_x S}} \end{vmatrix} \\
&= \begin{vmatrix} A_{11} & 0 \\ A_{21} & 0 \end{vmatrix} + \begin{vmatrix} 1 & A_{14} \\ 0 & A_{24} \end{vmatrix} \\
&= 0 + A_{24} \\
&= 1
\end{aligned}
$$

$$
\begin{aligned}
A_{14}^{[2]} &= < \omega_1, \mathbf{A}\omega_4 >_k \\
&= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \mathbf{A}(\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_3) >_k \\
&= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_3 >_k + < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_2 \wedge \mathbf{A}\hat{\mathbf{e}}_3 >_k \\
&= \begin{vmatrix} < \hat{\mathbf{e}}_1, \mathbf{A}\hat{\mathbf{e}}_2 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_3 >_{\mathbf{T_x S}} \\ < \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_2 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3 >_{\mathbf{T_x S}} \end{vmatrix} + \begin{vmatrix} < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_1, \mathbf{A}\hat{\mathbf{e}}_3 >_{\mathbf{T_x S}} \\ < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_2 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_3 >_{\mathbf{T_x S}} \end{vmatrix} \\
&= \begin{vmatrix} A_{12} & 0 \\ A_{22} & 0 \end{vmatrix} + \begin{vmatrix} 0 & A_{13} \\ 1 & A_{23} \end{vmatrix} \\
&= 0 - A_{13} \\
&= -1
\end{aligned}
$$

$$
\begin{aligned}
A_{15}^{[2]} &= < \omega_1, \mathbf{A}\omega_5 >_k \\
&= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \mathbf{A}(\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_4) >_k \\
&= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_2 \wedge \hat{\mathbf{e}}_4 >_k + < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_2 \wedge \mathbf{A}\hat{\mathbf{e}}_4 >_k \\
&= \begin{vmatrix} < \hat{\mathbf{e}}_1, \mathbf{A}\hat{\mathbf{e}}_2 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_4 >_{\mathbf{T_x S}} \\ < \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_2 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_4 >_{\mathbf{T_x S}} \end{vmatrix} + \begin{vmatrix} < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_1, \mathbf{A}\hat{\mathbf{e}}_4 >_{\mathbf{T_x S}} \\ < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_2 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_4 >_{\mathbf{T_x S}} \end{vmatrix} \\
&= \begin{vmatrix} A_{12} & 0 \\ A_{22} & 0 \end{vmatrix} + \begin{vmatrix} 0 & A_{14} \\ 1 & A_{24} \end{vmatrix} \\
&= 0 - A_{14} \\
&= 0
\end{aligned}
$$

$$
\begin{aligned}
A_{16}^{[2]} &= < \omega_1, \mathbf{A}\omega_6 >_k \\
&= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \mathbf{A}(\hat{\mathbf{e}}_3 \wedge \hat{\mathbf{e}}_4) >_k \\
&= < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_3 \wedge \hat{\mathbf{e}}_4 >_k + < \hat{\mathbf{e}}_1 \wedge \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3 \wedge \mathbf{A}\hat{\mathbf{e}}_4 >_k \\
&= \begin{vmatrix} < \hat{\mathbf{e}}_1, \mathbf{A}\hat{\mathbf{e}}_3 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_4 >_{\mathbf{T_x S}} \\ < \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_3 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_4 >_{\mathbf{T_x S}} \end{vmatrix} + \begin{vmatrix} < \hat{\mathbf{e}}_1, \hat{\mathbf{e}}_3 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_1, \mathbf{A}\hat{\mathbf{e}}_4 >_{\mathbf{T_x S}} \\ < \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3 >_{\mathbf{T_x S}} & < \hat{\mathbf{e}}_2, \mathbf{A}\hat{\mathbf{e}}_4 >_{\mathbf{T_x S}} \end{vmatrix} \\
&= \begin{vmatrix} A_{13} & 0 \\ A_{23} & 0 \end{vmatrix} + \begin{vmatrix} 0 & A_{14} \\ 0 & A_{24} \end{vmatrix} \\
&= 0.
\end{aligned}
$$

The remaining elements are computed similarly. Therefore, the final matrix

is :

$$\mathbf{A}^{[2]} = \begin{bmatrix} A_{11}+A_{22} & A_{23} & A_{24} & -A_{13} & -A_{14} & 0 \\ A_{32} & A_{11}+A_{33} & A_{34} & A_{12} & 0 & -A_{14} \\ A_{42} & A_{43} & A_{11}+A_{44} & 0 & A_{12} & A_{13} \\ -A_{31} & A_{21} & 0 & A_{22}+A_{33} & A_{34} & -A_{24} \\ -A_{41} & 0 & A_{21} & A_{43} & A_{22}+A_{44} & A_{23} \\ 0 & -A_{41} & A_{31} & -A_{42} & A_{32} & A_{33}+A_{44} \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 1 & -1 & 0 & 0 \\ -2x & 0 & 0 & 0 & 0 & 0 \\ -(1-2y) & 0 & 0 & 0 & 0 & 1 \\ 1+2y & 0 & 0 & 0 & 0 & -1 \\ 2x & 0 & 0 & 0 & 0 & 0 \\ 0 & 2x & -(1+2y) & 1-2y & -2x & 0 \end{bmatrix}.$$

Following the same procedure, the 3×3 matrix $\mathbf{A}^{[3]}$ is :

$$\mathbf{A}^{[3]} = \begin{bmatrix} A_{11}+A_{22}+A_{33} & A_{34} & -A_{24} & A_{14} \\ A_{43} & A_{11}+A_{22}+A_{44} & A_{23} & -A_{13} \\ -A_{42} & A_{32} & A_{11}+A_{33}+A_{44} & A_{12} \\ A_{41} & -A_{31} & A_{21} & A_{22}+A_{33}+A_{44} \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1-2y & -2x & 0 & 0 \\ -2x & 1+2y & 0 & 0 \end{bmatrix}$$

and the 1×1 matrix $\mathbf{A}^{[4]}$ is :

$$\mathbf{A}^{[4]} = A_{11}+A_{22}+A_{33}+A_{44} = Tr(\mathbf{A}) = 0.$$

At this point, a comment about the computation of the auxiliary systems without applying the tools of exterior algebra and wedge product should be made. Ng and Reid [21, 22, 23], while studying the Orr-Sommerfeld equation using the approach of CMT, produced matrices of coefficients, identical to the k-th additive compound matrices for the various values of k, following an indirect way. They considered the inhomogeneous linear system :

$$\phi'(x) = \mathbf{A}(x) \cdot \phi(x) + \mathbf{f}(x) = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix} \cdot \phi(x) + \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{bmatrix} \quad (3.1)$$

where $\phi(x), \mathbf{f}(x) \in \mathbf{R}^4$ and $\mathbf{A}(x)$ is a 4×4 matrix. Note that the symbol $\phi'(x)$ stands for the derivative of ϕ with respect to the independent variable x, $\phi'(x) = \frac{d\phi}{dx}$. They sought solutions of the form :

$$\phi = \mathbf{g} + \alpha\mathbf{u} + \beta\mathbf{v}$$

where $\alpha, \beta \in \mathbf{R}$, the vectors $\mathbf{u}, \mathbf{v} \in \mathbf{R}^4$ are linear independent solutions of the homogeneous system obtained from the initial inhomogeneous one and the vector $\mathbf{g} \in \mathbf{R}^4$ is a partial solution of the initial inhomogeneous system, with respect to the given boundary conditions of the problem. They combined these vectors together forming two solution matrices, $\mathbf{M}_1 = [\mathbf{uv}]$ and $\mathbf{M}_2 = [\mathbf{guv}]$, where $\mathbf{M}_1 \in \mathbf{R}^{4\times 2}$ and $\mathbf{M}_2 \in \mathbf{R}^{4\times 3}$, whose columns are the solution vectors, and then they considered all the possible different determinants of these matrices, according to a specific lexicographical order, as coordinates of new vectors, $\mathbf{y}$ and $\mathbf{z}$, named the second and third compound matrices respectively. It is easily understood that these vectors are the 2-vector and 3-vector that can be produced applying the exterior algebra theory. The time evolution of these vectors was given by the following equations :

$$\mathbf{y}' = \mathbf{B}(x) \cdot \mathbf{y} \tag{3.2}$$

$$\mathbf{z}' = \mathbf{C}(x) \cdot \mathbf{z} + \mathbf{D} \cdot \mathbf{f}. \tag{3.3}$$

Considering the above equations and keeping in mind that the vectors $\mathbf{u}, \mathbf{v}$ are the solutions of the homogeneous equation and $\mathbf{g}$ is a solution of the inhomogeneous equation (3.1) the matrices $\mathbf{B}$ and $\mathbf{C}$ are easily constructed. These matrices are identical to the 2-nd and 3-rd additive compound matrices that the application of exterior algebra produces.

More precisely, the vector $\mathbf{y}$ has 6 coordinates, each one of which is a minor of the matrix $\mathbf{M}_1$. In particular, we have :

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \end{bmatrix} = \begin{bmatrix} \begin{vmatrix} u_1 & v_1 \\ u_2 & v_2 \end{vmatrix} \\ \begin{vmatrix} u_1 & v_1 \\ u_3 & v_3 \end{vmatrix} \\ \begin{vmatrix} u_1 & v_1 \\ u_4 & v_4 \end{vmatrix} \\ \begin{vmatrix} u_2 & v_2 \\ u_3 & v_3 \end{vmatrix} \\ \begin{vmatrix} u_2 & v_2 \\ u_4 & v_4 \end{vmatrix} \\ \begin{vmatrix} u_3 & v_3 \\ u_4 & v_4 \end{vmatrix} \end{bmatrix}.$$

Now, following equation (3.2) and considering the y_1 coordinate we get :

$$y_1' = \begin{vmatrix} u_1 & v_1 \\ u_2 & v_2 \end{vmatrix}' = (u_1v_2 - u_2v_1)' = u_1'v_2 + u_1v_2' - u_2'v_1 - u_2v_1'$$

$$= (A_{11}u_1 + A_{12}u_2 + A_{13}u_3 + A_{14}u_4)v_2 + u_1(A_{21}v_1 + A_{22}v_2 + A_{23}v_3 + A_{24}v_4) -$$
$$- (A_{21}u_1 + A_{22}u_2 + A_{23}u_3 + A_{24}u_4)v_1 - u_2(A_{11}v_1 + A_{12}v_2 + A_{13}v_3 + A_{14}v_4)$$

$$= (A_{11} + A_{22})(u_1v_2 - u_2v_1) + A_{23}(u_1v_3 - u_3v_1) + A_{24}(u_1v_4 - u_4v_1) -$$
$$- A_{13}(u_2v_3 - u_3v_2) - A_{14}(u_2v_4 - u_4v_2)$$

$$= (A_{11} + A_{22}) \cdot y_1 + A_{23} \cdot y_2 + A_{24} \cdot y_3 - A_{13} \cdot y_4 - A_{14} \cdot y_5$$

As it can be understood, the coefficients A_{ij} with $i, j = 1, 2, 3, 4$ are the elements of the first row of the $A^{[2]}$ additive compound matrix. All the other elements are similarly produced. A similar construction holds for the elements of the $A^{[3]}$ additive compound matrix, related to the $\mathbf{z}$ vector.

According to [19], a k-th additive compound matrix, $\mathbf{A}^{[k]}$, of an initial matrix $\mathbf{A}$ has the following property : If $x_1, x_2, \ldots, x_k$ are the eigenvectors of $\mathbf{A}$ and $\lambda_1, \lambda_2, \ldots, \lambda_k$ are the respective eigenvalues, then the k-vector $x_1 \wedge x_2 \wedge \ldots \wedge x_k$ is an eigenvector of $\mathbf{A}^{[k]}$ and its eigenvalue is $\lambda_1 + \lambda_2 + \ldots + \lambda_k$.

For the various cases of k for an n-dimensional system, all the LCEs of the spectrum can be computed using the appropriate compound system. More precisely, considering the case of the 4-dimensional Hénon-Heiles system and the possible cases of $k = 1, 2, 3, 4$, the computation of the respective exponents is done as follows (Oseledec [24]) :

- $k = 1$:
  This is the trivial case where the compound system is identical to the initial system of variational equations. Therefore, any random deviation vector leads to the computation of the mLCE of the spectrum.

- $k = 2$:
  For this case the 2-nd compound system is used :

  $$\dot{\mathbf{w}}^{(2)} = \mathbf{A}^{[2]} \cdot \mathbf{w}^{(2)}.$$

  Similar to the previous case and considering the additive matrix property mentioned previously, any random 2-vector $\mathbf{w} \in \mathbf{\Lambda}^2(\mathbf{T_x S})$ leads to the computation of the sum of the 2 largest LCEs, $X_2 = \chi_1 + \chi_2$. If the mLCE is known, the computation of the χ_2 is obvious.

- $k = 3$:
  For this case the 3-nd compound system is used :

  $$\dot{\mathbf{w}}^{(3)} = \mathbf{A}^{[3]} \cdot \mathbf{w}^{(3)}.$$

Following a similar approach, any random 3-vector $\mathbf{w} \in \mathbf{\Lambda}^3(\mathbf{T_x S})$ leads to the computation of the sum of the 3 largest LCEs, $X_3 = \chi_1 + \chi_2 + \chi_3$. This allows the computation of χ_3 if χ_1 and χ_2 are known.

- $k = 4$:
  For this case the 4-nd compound system takes the form :

$$\begin{aligned} \dot{\mathbf{w}}^{(4)} &= \mathbf{A}^{[4]} \cdot \mathbf{w}^{(4)} \\ &= Tr(\mathbf{A}) \cdot \mathbf{w}^{(4)} \\ &= \mathbf{0}. \end{aligned}$$

  This equation is in accordance with the fact that the sum of LCEs should be zero, since the dynamical system considered is conservative. Following the same procedure as before, the computation of the last exponent of the spectrum is done.

From the previous example it became clear the importance of automating the construction of the additive compound matrices and the important role of the exterior algebra and wedge product towards this direction. Moreover, we should mention another advantage of the CMT, besides the already mentioned fact that no orthonormalization is needed. This approach permits the computation of single LCEs, without the obligation of computing all the previous ones, as is done with the standard method [4]. If, for example, the value of the χ_5 exponent of a 5-degree-of-freedom dynamical system, having 10-dimensional phase space, is needed, then we can only use the following two sets of equations :

$$\begin{aligned} \dot{\mathbf{w}}^{(4)} = \mathbf{A}^{[4]} \cdot \mathbf{w}^{(4)} \quad &\Rightarrow \quad X_4 = \chi_1 + \chi_2 + \chi_3 + \chi_4 \\ \dot{\mathbf{w}}^{(5)} = \mathbf{A}^{[5]} \cdot \mathbf{w}^{(5)} \quad &\Rightarrow \quad X_5 = \chi_1 + \chi_2 + \chi_3 + \chi_4 + \chi_5. \end{aligned}$$

The value of χ_5 is then obtained from a simple subtraction, $\chi_5 = X_5 - X_4$. This characteristic could be of importance for the detection of the existence of additional integrals of motion, which lead to the vanishing of more pairs of Lyapunov exponents. In addition, for high-dimensional systems, the computation of single exponents is possible, for less computational time.

In the following chapter, the CMT is applied for the computation of the LCEs spectrum, as well as for the computation of single exponents for the FPU β-lattice, which facilitates the use of models with different degrees of freedom.

Chapter 4

Application of the Compound Matrix Theory

In this chapter, we apply the CMT for the computation of the spectrum of LCEs, as well as of individual exponents. For our study, we consider the system of the FPU β-lattice, as we can easily change the dimensionality of the model by adding new lattice points. In addition, this model favours the automation of the proposed procedure. Due to the nonlinearity of the system, its solution can be obtained only numerically. Among the available symplectic integrators, we choose to apply methods belonging to the SABA family of integrators [17] because they exhibit a quite satisfactory behaviour. In the following sections information about the FPU β-lattice and the symplectic integration techniques are given, before the final presentation of the obtained results.

4.1 The FPU lattice

The FPU lattice describes a vibrating string of nearest-neighbour coupled oscillators. The system was initially studied in 1953 by Fermi, Pasta, Ulam and Tsingou [6], who observed a peculiar behaviour different from a priori expectations : the system showed a complicated quasi-periodic behaviour instead of initially anticipated chaotic one.

The system's Hamiltonian function contains a quadratic (α-lattice) or a cubic (β-lattice) nonlinear term. In our study we consider the β-lattice, having the Hamiltonian :

$$H_N = H_N(\mathbf{p}, \mathbf{q}) = \sum_{i=1}^{N} \frac{p_i^2}{2} + \sum_{i=0}^{N} \left[\frac{(q_{i+1} - q_i)^2}{2} + \frac{\beta (q_{i+1} - q_i)^4}{4} \right] \tag{4.1}$$

where N is the number of the movable particles. Note that the particles at the boundaries (particles with numbers 0 and $N + 1$) are fixed during the

time evolution, therefore we have $q_0 = p_0 = 0$ and $q_{N+1} = p_{N+1} = 0$, $\forall t$. The system's equations of motion are given by :

$$\begin{cases} \dot{q_i} = \frac{\partial H_N}{\partial p_i} \\ \dot{p_i} = -\frac{\partial H_N}{\partial q_i} \end{cases} \Rightarrow$$

$$\Rightarrow \quad \begin{cases} \dot{q_i} = p_i \\ \dot{p_i} = (q_{j+1} - q_j)(\delta^i_j - \delta^i_{j+1}) + \beta(q_{j+1} - q_j)^3(\delta^i_j - \delta^i_{j+1}) \end{cases}$$

with $1 \leq i \leq N$ and δ^i_j denoting the Kronecker delta, which is equal to 1 if $i = j$ and 0 otherwise. The equation of motion for the momentum p_i of particle i is :

$$\begin{aligned} \dot{p_i} = &\ldots + (q_{i-1} - q_{i-2})(\delta^i_{i-2} - \delta^i_{i-1}) + \beta(q_{i-1} - q_{i-2})^3(\delta^i_{i-2} - \delta^i_{i-1}) + \\ &+ (q_i - q_{i-1})(\delta^i_{i-1} - \delta^i_i) + \beta(q_i - q_{i-1})^3(\delta^i_{i-1} - \delta^i_i) + \\ &+ (q_{i+1} - q_i)(\delta^i_i - \delta^i_{i+1}) + \beta(q_{i+1} - q_i)^3(\delta^i_i - \delta^i_{i+1}) + \\ &+ (q_{i+2} - q_{i+1})(\delta^i_{i+1} - \delta^i_{i+2}) + \beta(q_{i+2} - q_{i+1})^3(\delta^i_{i+1} - \delta^i_{i+2}) + \ldots \\ = &\ldots + 0 + 0 + (q_i - q_{i-1})(-1) + \beta(q_i - q_{i-1})^3(-1) + \\ &+ (q_{i+1} - q_i) + \beta(q_{i+1} - q_i)^3 + 0 + 0 + \ldots \\ = &\, q_{i+1} - 2q_i + q_{i-1} + \beta\left[(q_{i+1} - q_i)^3 - (q_i - q_{i-1})^3\right]. \end{aligned}$$

Thus, the total set of equations of motion is given by :

$$\dot{\mathbf{x}} = \begin{bmatrix} \dot{q_i} \\ \dot{p_i} \end{bmatrix} = \begin{bmatrix} p_i \\ q_{i+1} - 2q_i + q_{i-1} + \beta\left[(q_{i+1} - q_i)^3 - (q_i - q_{i-1})^3\right] \end{bmatrix} \tag{4.2}$$

for $1 \leq i \leq N$. The equations of motion of the first ($i = 1$) and last ($i = N$) particle, taking into account the specific boundary conditions, are :

$$\begin{bmatrix} \dot{q_1} \\ \dot{p_1} \end{bmatrix} = \begin{bmatrix} p_1 \\ q_2 - 2q_1 + \beta\left[(q_2 - q_1)^3 - q_1^3\right] \end{bmatrix}, \quad \text{particle } i = 1$$

$$\begin{bmatrix} \dot{q_N} \\ \dot{p_N} \end{bmatrix} = \begin{bmatrix} p_N \\ -2q_N + q_{N-1} + \beta\left[(-q_N)^3 - (q_N - q_{N-1})^3\right] \end{bmatrix}, \quad \text{particle } i = N.$$

The variational equations governing the time evolution of deviation vectors are :

$$\dot{\mathbf{w}} = \begin{bmatrix} \dot{\delta\mathbf{q}} \\ \dot{\delta\mathbf{p}} \end{bmatrix} = \begin{bmatrix} \mathbf{0}_N & \mathbf{I}_N \\ -\mathbf{D}^2_{H_N}(\mathbf{q}) & \mathbf{0}_N \end{bmatrix} \cdot \begin{bmatrix} \delta\mathbf{q} \\ \delta\mathbf{p} \end{bmatrix} \quad \Rightarrow \quad \begin{cases} \dot{\delta q_i} = \delta p_i \\ \dot{\delta p_i} = -\sum_{j=1}^N \frac{\partial^2 H_N}{\partial q_i \partial q_j} \delta q_j \end{cases} \tag{4.3}$$

where $1 \leq i \leq N$ and the square matrix of the coefficients is of dimension $2N \times 2N$. According to equation (4.2), it is :

$$-\frac{\partial^2 H_N}{\partial q_i \partial q_j} = \begin{cases} -2 - 3\beta\left[(q_{j+1} - q_j)^2 + (q_j - q_{j-1})^2\right] & \text{if } i = j \\ 1 + 3\beta(q_i - q_j)^2 & \text{if } |i-j| = 1 \\ 0 & \text{if } |i-j| > 1 \end{cases}$$

and therefore, the variational equations of particle i is :

$$\begin{bmatrix} \dot{\delta q_i} \\ \dot{\delta p_i} \end{bmatrix} = \begin{bmatrix} \delta p_i \\ -\sum_{j=1}^{N} \frac{\partial^2 H_N}{\partial q_i \partial q_j} \delta q_j \end{bmatrix} = \begin{bmatrix} \delta p_i \\ \frac{\partial^2 H_N}{\partial q_i \partial q_{i-1}} \delta q_{i-1} + \frac{\partial^2 H_N}{\partial q_i^2} \delta q_i + \frac{\partial^2 H_N}{\partial q_i \partial q_{i+1}} \delta q_{i+1} \end{bmatrix}.$$

Consequently, the variational equations are given by :

$$\dot{\mathbf{w}} = \begin{bmatrix} \dot{\delta q_1} \\ \vdots \\ \dot{\delta q_N} \\ \dot{\delta p_1} \\ \vdots \\ \dot{\delta p_N} \end{bmatrix} = \begin{bmatrix} 0 & 0 & \dots & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 & 0 & \dots & 1 \\ -\frac{\partial^2 H_N}{\partial q_1^2} & -\frac{\partial^2 H_N}{\partial q_1 \partial q_2} & \dots & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & -\frac{\partial^2 H_N}{\partial q_N \partial q_{N-1}} & -\frac{\partial^2 H_N}{\partial q_N^2} & 0 & \dots & 0 \end{bmatrix} \cdot \begin{bmatrix} \delta q_1 \\ \vdots \\ \delta q_N \\ \delta p_1 \\ \vdots \\ \delta p_N \end{bmatrix}.$$

In the general case of the N-degree-of-freedom Hamiltonian (4.1), the application of the CMT results to the construction of k-vectors with $0 \leq k \leq 2N$. Obviously, the case of $k = 0$ corresponds to the space $\Lambda^0(\mathbf{T_x S}) = \mathbf{R}$. Let us illustrate the construction of the differential equations governing the evolution of hyper-volumes in the system's tangent space by considering the particular case of the 2-degree-of-freedom system ($N = 2$). Then, the different compound matrices take the form :

- For $k = 1$:
  In this case the system is identical to the system of variational equations (4.3).

- For $k = 2$:

The additive matrix is a 6×6 matrix, given by :

$$\mathbf{A}^{[2]} = \begin{bmatrix} A_{11}+A_{22} & A_{23} & A_{24} & -A_{13} & -A_{14} & 0 \\ A_{32} & A_{11}+A_{33} & A_{34} & A_{12} & 0 & -A_{14} \\ A_{42} & A_{43} & A_{11}+A_{44} & 0 & A_{12} & A_{13} \\ -A_{31} & A_{21} & 0 & A_{22}+A_{33} & A_{34} & -A_{24} \\ -A_{41} & 0 & A_{21} & A_{43} & A_{22}+A_{44} & A_{23} \\ 0 & -A_{41} & A_{31} & -A_{42} & A_{32} & A_{33}+A_{44} \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 1 & -1 & 0 & 0 \\ -\frac{\partial^2 H_2}{\partial q_1 \partial q_2} & 0 & 0 & 0 & 0 & 0 \\ -\frac{\partial^2 H_2}{\partial q_2^2} & 0 & 0 & 0 & 0 & 1 \\ \frac{\partial^2 H_2}{\partial q_1^2} & 0 & 0 & 0 & 0 & -1 \\ \frac{\partial^2 H_2}{\partial q_2 \partial q_1} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{\partial^2 H_2}{\partial q_2 \partial q_1} & -\frac{\partial^2 H_2}{\partial q_1^2} & \frac{\partial^2 H_2}{\partial q_2^2} & -\frac{\partial^2 H_N}{\partial q_1 \partial q_2} & 0 \end{bmatrix}.$$

Therefore, the compound system is the following :

$$\dot{\mathbf{w}}^{(2)} = \mathbf{A}^{[2]} \cdot \mathbf{w}^{(2)}$$

where, $\mathbf{w}^{(2)} \in \Lambda^2(\mathbf{T_x S})$ is a 2-vector.

- For $k = 3$:
  The additive matrix $\mathbf{A}^{[3]}$ is a 4×4 matrix and it is given by :

$$\mathbf{A}^{[3]} = \begin{bmatrix} A_{11}+A_{22}+A_{33} & A_{34} & -A_{24} & A_{14} \\ A_{43} & A_{11}+A_{22}+A_{44} & A_{23} & -A_{13} \\ -A_{42} & A_{32} & A_{11}+A_{33}+A_{44} & A_{12} \\ A_{41} & -A_{31} & A_{21} & A_{22}+A_{33}+A_{44} \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ \frac{\partial^2 H_2}{\partial q_2^2} & -\frac{\partial^2 H_2}{\partial q_1 \partial q_2} & 0 & 0 \\ -\frac{\partial^2 H_2}{\partial q_2 \partial q_1} & \frac{\partial^2 H_2}{\partial q_1^2} & 0 & 0 \end{bmatrix}.$$

Therefore, the compound system is the following :

$$\dot{\mathbf{w}}^{(3)} = \mathbf{A}^{[3]} \cdot \mathbf{w}^{(3)}$$

where, $\mathbf{w}^{(3)} \in \Lambda^3(\mathbf{T_x S})$ is a 3-vector.

- For $k = 4$:

This is the trivial case where the additive compound matrix is an element matrix defined by the trace of the matrix of coefficients of the variational equations :

$$\mathbf{A}^{[4]} = [A_{11} + A_{22} + A_{33} + A_{44}] = [Tr(\mathbf{A})] = \mathbf{0}$$

Therefore, the compound system takes the form :

$$\dot{\mathbf{w}}^{(4)} = \mathbf{0}$$

The solution of this system, $\mathbf{w}^{(4)} = ct$, is in accordance with the property that conservative systems preserve their phase space volume during their evolution. This corresponds to the fact that the sum of all the LCEs of the spectrum is zero and, consequently, no volume change is observed.

The computation of the LCEs spectrum is achieved by integrating the above systems, as already explained in section 3.2. The system of the case $k = 1$, which is merely the initial system of variational equations, leads to the computation of the mLCE χ_1, while the integration of the systems for $k = 2$ and $k = 3$ allows the computation of the χ_2 and χ_3 exponents respectively. The χ_4 exponent is computed considering the fact that the sum of all LCEs is equal to zero. A similar procedure is followed for all the studied FPU systems of higher degrees of freedom.

We note that the k-vectors of the compound systems can be constructed by the initial deviation vectors applying the definition given in section 3.1. These k-vectors are taken initially to be random, as is also done with the usual deviation vectors. We have tested and verified that the initial values of the k-vectors do not affect the computation of the LCEs.

4.2 Symplectic integrators

In sections 1.1 and 1.2, we mentioned that Hamiltonian systems preserve their phase space volume during their evolution. More precisely, if $(\mathbf{q}(t), \mathbf{p}(t))$ are the dynamical variables of the system, then (see for example [31, 32, 33]) the mapping from $(\mathbf{q}(0), \mathbf{p}(0))$ to $(\mathbf{q}' = \mathbf{q}(dt), \mathbf{p}' = \mathbf{p}(dt))$ along the solution is symplectic, meaning that the symplectic structure :

$$d\mathbf{q} \wedge d\mathbf{p} = d\mathbf{q}' \wedge d\mathbf{p}'$$

is conserved. In addition to this property, all autonomous Hamiltonian systems also preserve their energy during their evolution in time. The common numerical integrators, such as the Euler method or the Runge-Kutta methods [13, 14], cannot retain the symplectic character of these systems and preserve the value of the energy. Moreover, Ge and Marsden [10] claimed

that it is impossible for a numerical integrator to preserve simultaneously both the symplecticity of the system and its energy for nonlinear and non-integrable systems, since in that case, the solution would be identical to the analytic one. Instead, it is possible the construction of integrators that can preserve one of these properties. The ones that succeed to preserve the symplectic nature of a Hamiltonian system are called symplectic integrators.

Symplectic integrators are divided into two major categories, the explicit and the implicit ones. The explicit schemes are commonly applied for the numerical integration of Hamiltonians that can be written in the form :

$$H_N(\mathbf{q},\mathbf{p}) = T(\mathbf{p}) + V(\mathbf{p}),$$

where T denotes the system's kinetic energy and V its potential. Some of the integrators of this category can be found in [7, 17, 31, 32, 33].

The implicit schemes are applied to Hamiltonian systems that cannot be divided into parts of the kinetic and the potential energy. For example, in [13, 14] all the symplectic integrators of the Runge-Kutta Gauss-Legendre family along with the conditions that must fulfil in order to be symplectic are explained in detail. These conditions are also explained in detail by Lasagni [16] and Sanz-Serna [27], where it is clarified that symplectic integrators of the Runge-Kutta family are only implicit schemes. In [27] is also noted that in the case of linear problems the condition that renders these methods symplectic also guarantees the exact conservation of the system's.

In our study, the 4th order symplectic integrator $SABA_2C$ of the SABA family with a corrector term is used. According to this method, the symplectict operator $e^{\tau L_H} = e^{\tau(L_T+L_V)}$ is approached by an integrator of multiple steps, which is composed of the operators ([17, 30]) :

$$e^{c_i\tau L_T} : \begin{cases} \mathbf{q}' = \mathbf{q} + \mathbf{p}c_i\tau \\ \mathbf{p}' = \mathbf{p} \end{cases},$$

$$e^{d_i\tau L_V} : \begin{cases} \mathbf{q}' = \mathbf{q} \\ \mathbf{p}' = \mathbf{p} - \frac{\partial V(\mathbf{q})}{\partial \mathbf{q}_i} d_i\tau \end{cases}.$$

The integrator is given by :

$$SABA_{2n} : e^{c_1\tau L_T} e^{d_1\tau L_V} \dots e^{d_n\tau L_V} e^{c_{n+1}\tau L_T} e^{d_n\tau L_V} \dots e^{d_1\tau L_V} e^{c_1\tau L_T}.$$

The corrector term is given by :

$$e^{g_i\tau L_C} : \begin{cases} \mathbf{q}' = \mathbf{q} \\ \mathbf{p}' = \mathbf{p} - \frac{\partial C(\mathbf{q})}{\partial \mathbf{q}_i} g_i\tau \end{cases}$$

where :

$$C = [V,[V,T]] = \sum_{i=1}^{N} \left(\frac{\partial V(\mathbf{q})}{\partial \mathbf{q}_i} \right)^2$$

with [., .] being the Poisson bracket, (1.1). Therefore the general form of the equations is :

$$SABA_{2n}C : e^{-\frac{g_i}{2}\tau^3 L_C} SABA_{2n} e^{-\frac{g_i}{2}\tau^3 L_C}.$$

The values of $c_i, d_i, g_i \in \mathbf{R}$ and can be found in [17].

This integrator will be used for the simultaneous integration of the equations of motion and the compound systems, as indicated by the so-called Tangent Map method, [30].

The application of the $SABA_2C$ integrator to the studied Hamiltonian systems is based on the fact that the Hamiltonian can be divided into two parts, the kinetic and potential energy. The FPU β-lattice as well as the induced set of variational equations satisfy this condition. Unfortunately, it doesn't happen the same with the corresponding compound systems, as it can be understood by the form of the additive compound matrix $\mathbf{A}^{[2]}$. Among the compound systems constructed from the initial set of variational equations, only the cases where $k = 1$ (trivial) and $k = 2N - 1$ produce separable systems.

For low dimensional systems, up to $N = 4$ particles, this problem can be addressed as follows. For a time interval equal to the time step dt, the coefficients of the additive matrices, which are related to the dynamical variables of the Hamiltonian, are assumed to be constant. As a result, the compound system is treated as a set of ODEs. Its analytic parametric integration is feasible and the system is set to the appropriate form for the application of the $SABA_2C$ integrator. From that point on, the followed procedure is the same as for the equations of motion and the variational equations. We note that the parametric solution is obtained with the aid of the Mathematica software due to its capability of performing symbolic computations. In our study we followed this procedure.

Another approach to deal with this problem is to seek an appropriate numerical integrator for non separable systems. The Runge-Kutta Gauss-Legendre implicit integrators is considered to be a reliable choice ([13, 14, 16, 27, 31, 32, 33]). Another available option is the explicit Runge-Kutta methods of high order accuracy, such as the 5th order Dopr5 and the 8th order Dopr853 integrator [13, 14], which both are integrators of adaptive stepsize. Nevertheless, we did not include in our study these alternatives.

4.3 Results

In this section, we present the computation of the LCEs spectrum of the FPU β-lattice (4.1) using the well known standard method of Benettin et al. [4] and the CMT, developed in chapter 3. The spectrum has been computed for the N-degree-of-freedom β-lattice, with $N = 2, 3, 4, 10$, and for three cases of the system energy, $E = H_N = 1, 10, 30$, while the coefficient

β was fixed at $\beta = 1.5$. For the computations, the symplectic integrator $SABA_2C$ of the $SABA_n$ family of symplectic integrators [17] has been used. The numerical integrations were performed up to final time $t_{max} = 10^5$ time units with a time step fixed at $dt = 0.01$. We note that all graphs are depicted in log-log scale.

Fig. 4.1 shows the spectrum of LCEs for a regular orbit of the 2-degree-of-freedom FPU β-lattice, with the energy of the system fixed at $E = 1.0$. As was explained in section 2.3, the LCEs are grouped into two pairs of equal exponents with opposite signs (χ_1, χ_4) and (χ_2, χ_3), as we see from Figs. 4.1a, 4.1c, 4.1b and 4.1d. The ordering of the spectrum is also satisfied, since the absolute value of exponents χ_1 and χ_4 is greater than the absolute value of exponents χ_2 and χ_3. Moreover, both pairs tend to zero, due to the presence of an integral of motion, i.e. the Hamiltonian, the regular nature of the considered orbit is evident as the LCEs tent to zero following a power law, which is well approximated by the function :

$$2\frac{\log(t)}{t}.$$

Comparing the results obtained by the standard method (Figs. 4.1a and 4.1c) with the ones obtained by the CMT (Figs. 4.1b and 4.1d) one can realize that the CMT gives results of the same accuracy with the ones of the standard method, since the form of the spectrum for both methods is practically identical. Furthermore, the ordering of the exponents is correct for both methods. The difference between the two methods is detected in Figs. 4.1e and 4.1f, where the absolute value of the sum of the exponents of each pair is plotted. In these figures it is shown that the properties :

$$\chi_1 = -\chi_4 \quad \text{and} \quad \chi_2 = -\chi_3$$

are verified more accurately by the standard method, since the difference of the exponents' value is varying from 10^{-3} down to values of the order of 10^{-6}, while the corresponding ones obtained by the CMT reach accuracy levels between 10^{-2} to 10^{-5}.

As the energy of the system increases, in Figs. 4.2 and 4.3, the spectrum retains the same form as shown in Fig. 4.1 for both computation methods. Considering the sum of the exponents' values of each pair, we see a change in the form of the results as large fluctuations appear that increase as the energy increases (compare Figs. 4.2e and 4.2f with 4.3e and 4.3f). The accuracy levels of the CMT remain similar to the ones presented in Fig. 4.1f, while these of the standard method become slightly worse (see Fig. 4.3e).

We note that in the six plots of the sum of the exponents for energy $E = 1.0, 10.0, 30.0$ (Figs. 4.1, 4.2, 4.3) the curve of $\chi_1 + \chi_4$ is overlapped by the curve of $\chi_2 + \chi_3$.

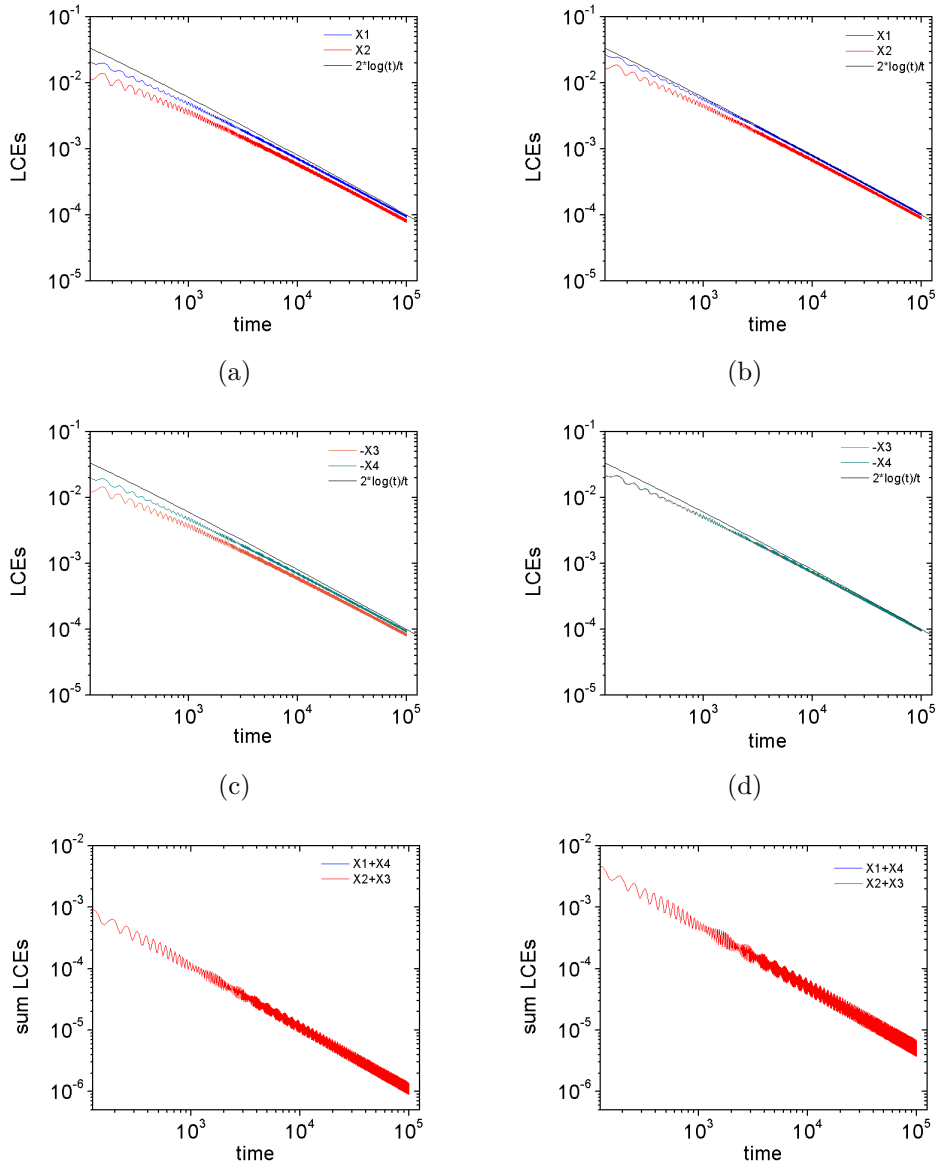


Figure 4.1: Computation of the spectrum of LCEs of the FPU β-lattice (4.1) with $N = 2$ and $E = 1.0$, for the regular orbit with $q_i = 0$ and $p_i = (-1.32913, -0.48313)$, for $i = 1, 2$. Plots in the left column are computed by the standard method and those in the right by the Compound Matrix method. Figs. 4.1a and 4.1b show the computation of the χ_1 and χ_2 exponents, while Figs. 4.1c and 4.1d show the computation of $-\chi_3$ and $-\chi_4$. Figs. 4.1e and 4.1f depict the sum of the pairs of exponents, (χ_1, χ_4) and (χ_2, χ_3).

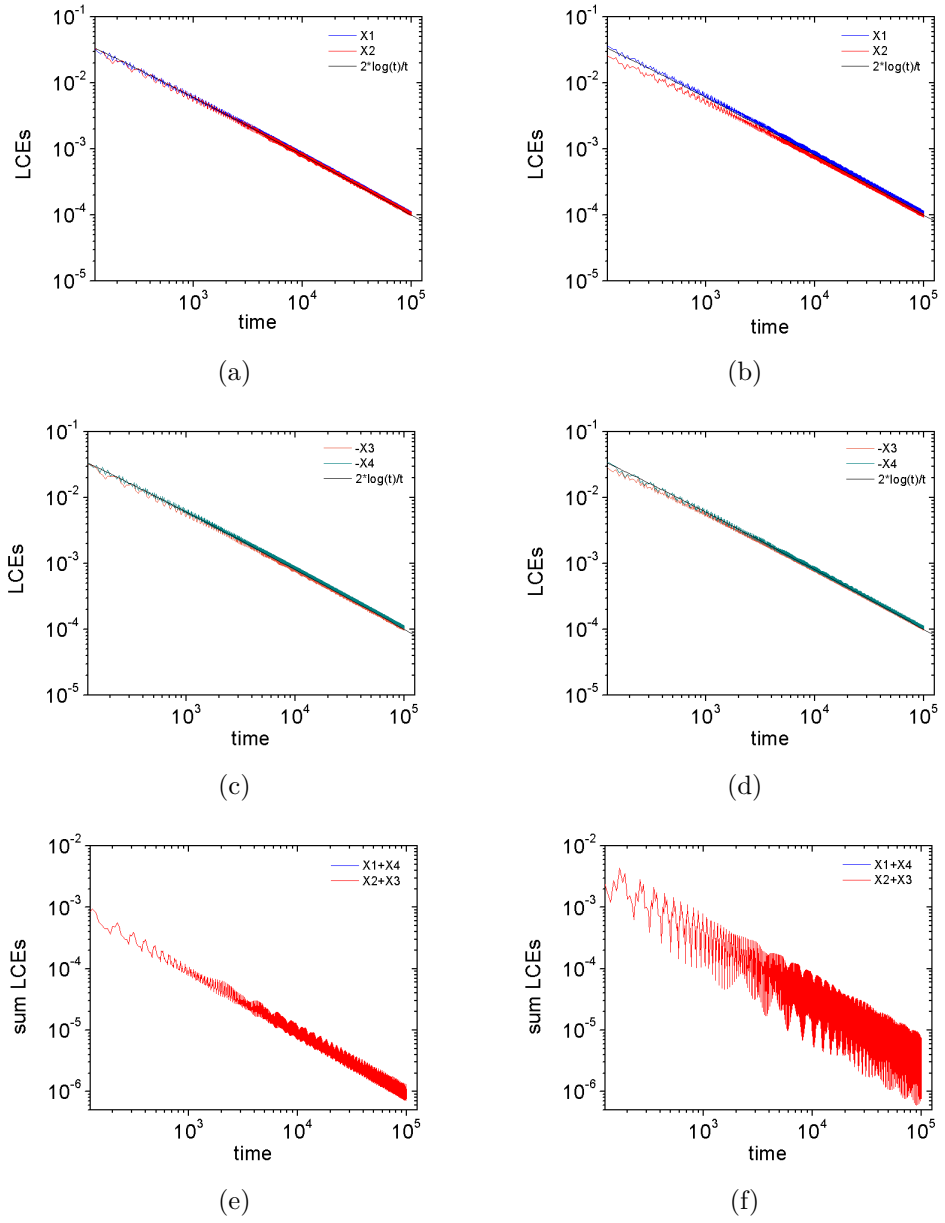


Figure 4.2: Computation of the spectrum of LCEs of the FPU β-lattice (4.1) with $N = 2$ and $E = 10.0$, for the regular orbit with $q_i = 0$ and $p_i = (-2.17060, -3.91005)$, for $i = 1, 2$. The panels follow the same arrangement as in Fig. 4.1.

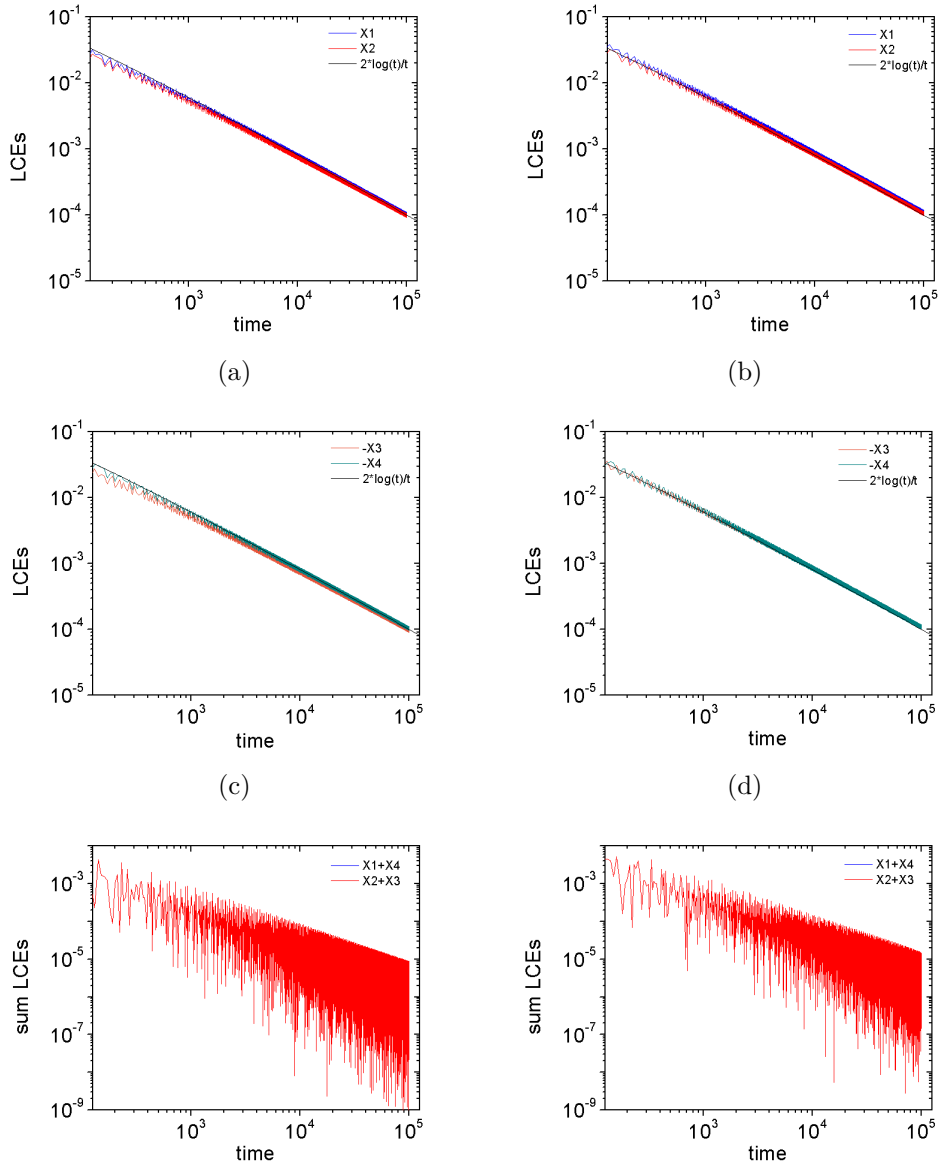


Figure 4.3: Computation of the spectrum of LCEs of the FPU β-lattice (4.1) with $N = 2$ and $E = 30.0$, for the regular orbit with $q_i = 0$ and $p_i = (7.26151, 2.69637)$, for $i = 1, 2$. The panels follow the same arrangement as in Fig. 4.1.

Fig. 4.4 shows the spectrum of a regular orbit of a 3-degree-of-freedom FPU β-lattice, as well as the sums of the tree pairs of the opposite exponents, (Figs. 4.4e and 4.4f). We see that the form of the spectrum computed by the standard method (Figs. 4.4a and 4.4c) and the one computed by the CMT (Figs. 4.4b and 4.4d) are comparable. Similar to Fig. 4.1-4.3 the exponents tend to zero following the function $2\frac{\log(t)}{t}$. From the values of the sums, we conclude that the accuracy of the obtained results is of the same order for both methods. We notice some fluctuations in the sum of the 3rd pair of exponents, $(\chi_3+\chi_4)$. The fluctuations of the results of the standard method are more intense.

Figs. 4.5 and 4.6 show the LCEs spectrum for chaotic orbits of the 3-degree-of-freedom system of Fig. 4.4. Again, the standard method and the CMT give similar results, as in all the previous cases. The sums of the pairs of exponents, however, present a different form in comparison with the form of the previous regular orbits in Figs. 4.1, 4.2, 4.3. Now we do not observe any fluctuations and the accuracy levels are the same for both methods. It is worth noting that the order of the sums is different : in Figs. 4.5e, 4.5f, 4.6e and 4.6f, the pair that gives the larger sum is not always the same. Moreover, the accuracy of the sums for $E = 10.0$ is better than the one for $E = 30.0$, being 10^{-6} and 10^{-5} respectively.

Similar observations are also seen in the case of a 4-degree-of-freedom FPU β-lattice (Figs. 4.7, 4.8 and 4.9). The spectrum is of the same form and the accuracy levels of the sums deteriorate as the energy of the system increases, while no particular ordering of the sum is seen.

Figs. 4.10 to 4.12 show the computation of only one pair of exponents, χ_1 and χ_{20} of a 10-degree of freedom FPU β-lattice, applying the standard method and the CMT. Also in this case, the accuracy and effectiveness of the CMT becomes evident as it produces results similar to the ones obtained by the standard method.

Finally, in Fig. 4.13 we plot the CPU time needed for the computation of all the previous results of Figs. 4.1 to 4.12, by the two methods. We see that the CMT demands more CPU time than the standard method even for low-dimensional systems, with $N = 3, 4$. However, this figure also clarifies a big advantage of the CMT in comparison with the standard method. For the case where the computation of only one exponent is of interest (Figs. 4.10 to 4.12), the CMT requires considerably less CPU time than the standard method, which also requires from the user to compute all the exponents of the spectrum of order higher than the one we are interested in.

4.4 Comments

From the results of, Figs. 4.1 to 4.12 it becomes evident that the computation of the LCEs spectrum is feasible by applying the CMT. Using this

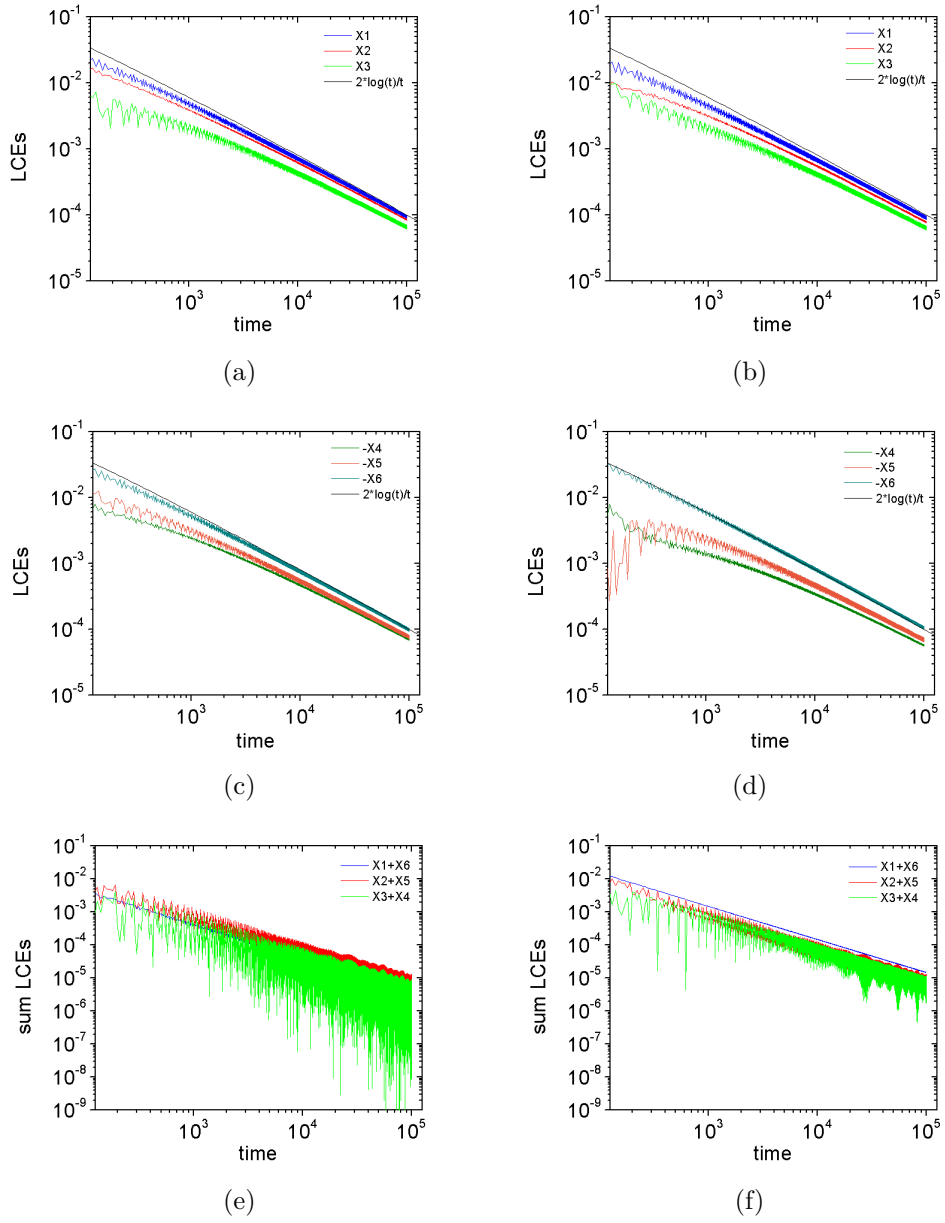


Figure 4.4: Computation of the spectrum of LCEs of the FPU β-lattice (4.1) with $N = 3$ and $E = 1.0$, for the regular orbit with $q_i = 0$ and $p_i = (0.69545, -1.17790, 0.35903)$ for $i = 1, 2, 3$. Plots in the left column are computed by the standard method and those in the right by the Compound Matrix method. Figs. 4.4a and 4.4b show the computation of χ_1, χ_2 and χ_3 exponents, while Figs. 4.4c and 4.4d show the computation of $-\chi_4$, $-\chi_5$ and $-\chi_6$. Figs. 4.4e and 4.4f depict the sum of the pairs of exponents, (χ_1, χ_6), (χ_2, χ_5) and (χ_3, χ_4).

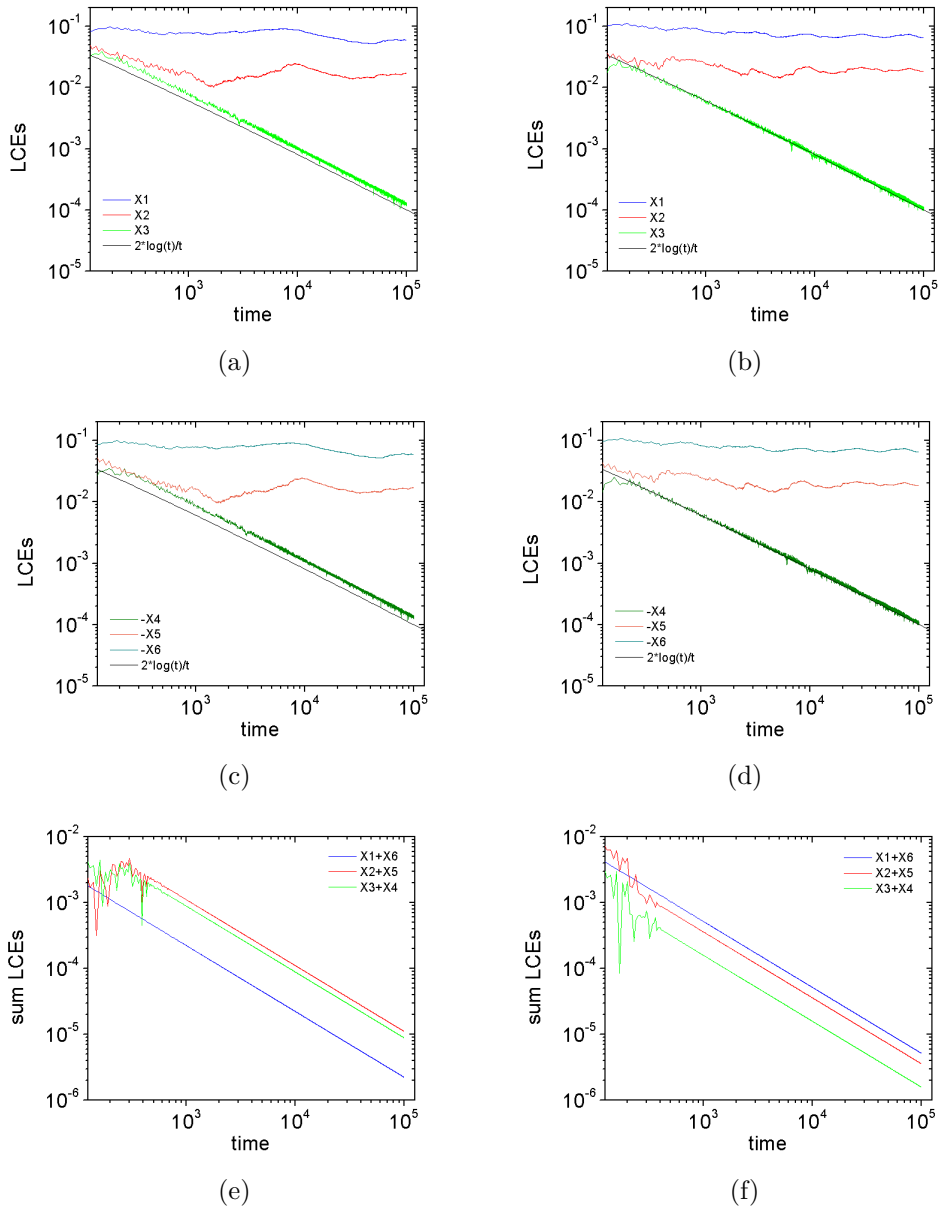


Figure 4.5: Computation of the spectrum of LCEs of the FPU β-lattice (4.1) with $N = 3$ and $E = 10.0$, for the chaotic orbit with $q_i = 0$ and $p_i = (3.91870, -1.27957, 1.73392)$, for $i = 1, \ldots, 3$. The panels follow the same arrangement as in Fig. 4.4.

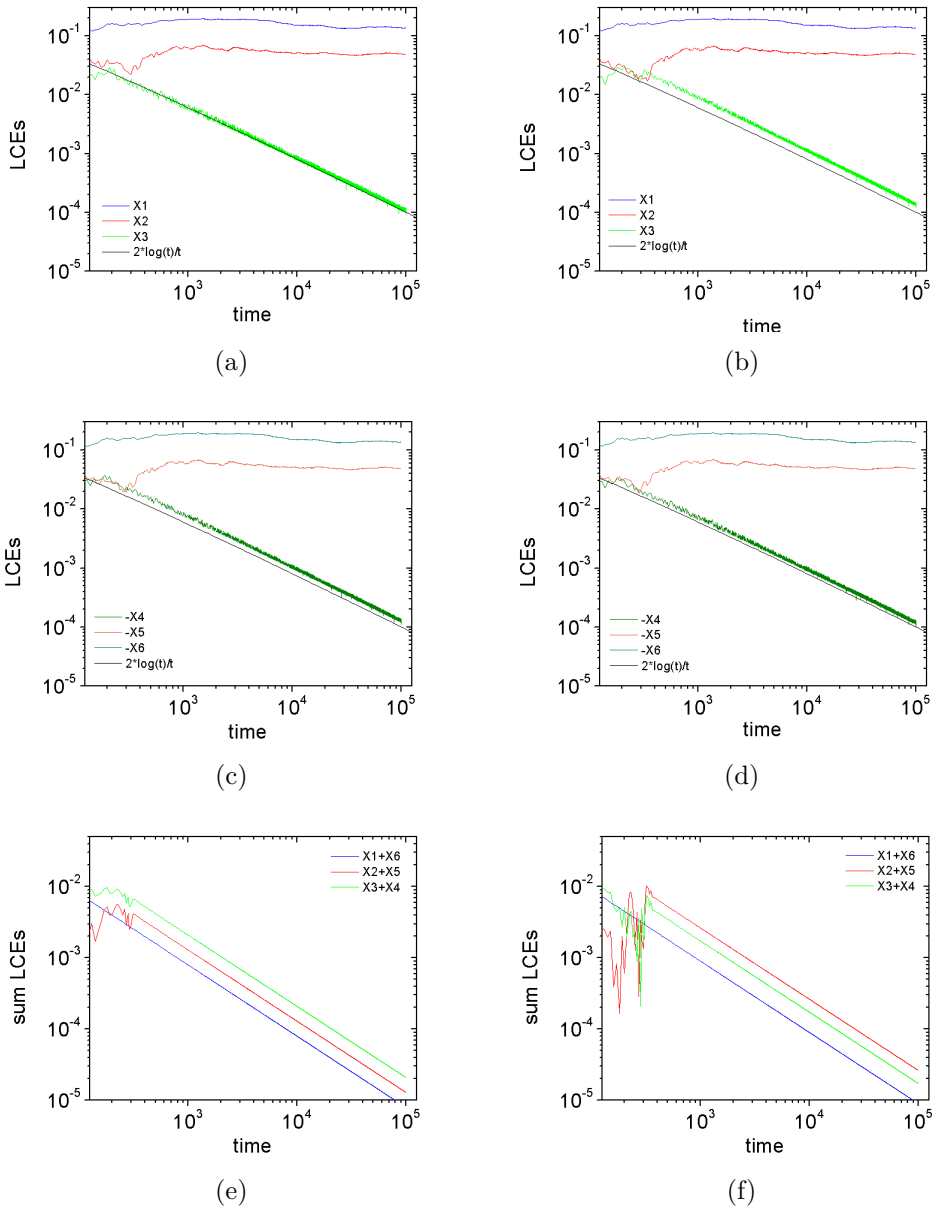


Figure 4.6: Computation of the spectrum of LCEs of the FPU β-lattice (4.1) with $N = 3$ and $E = 30.0$, for the chaotic orbit with $q_i = 0$ and $p_i = (-4.37489, -4.09722, 4.90644)$, for $i = 1, \ldots, 3$. The panels follow the same arrangement as in Fig. 4.4.

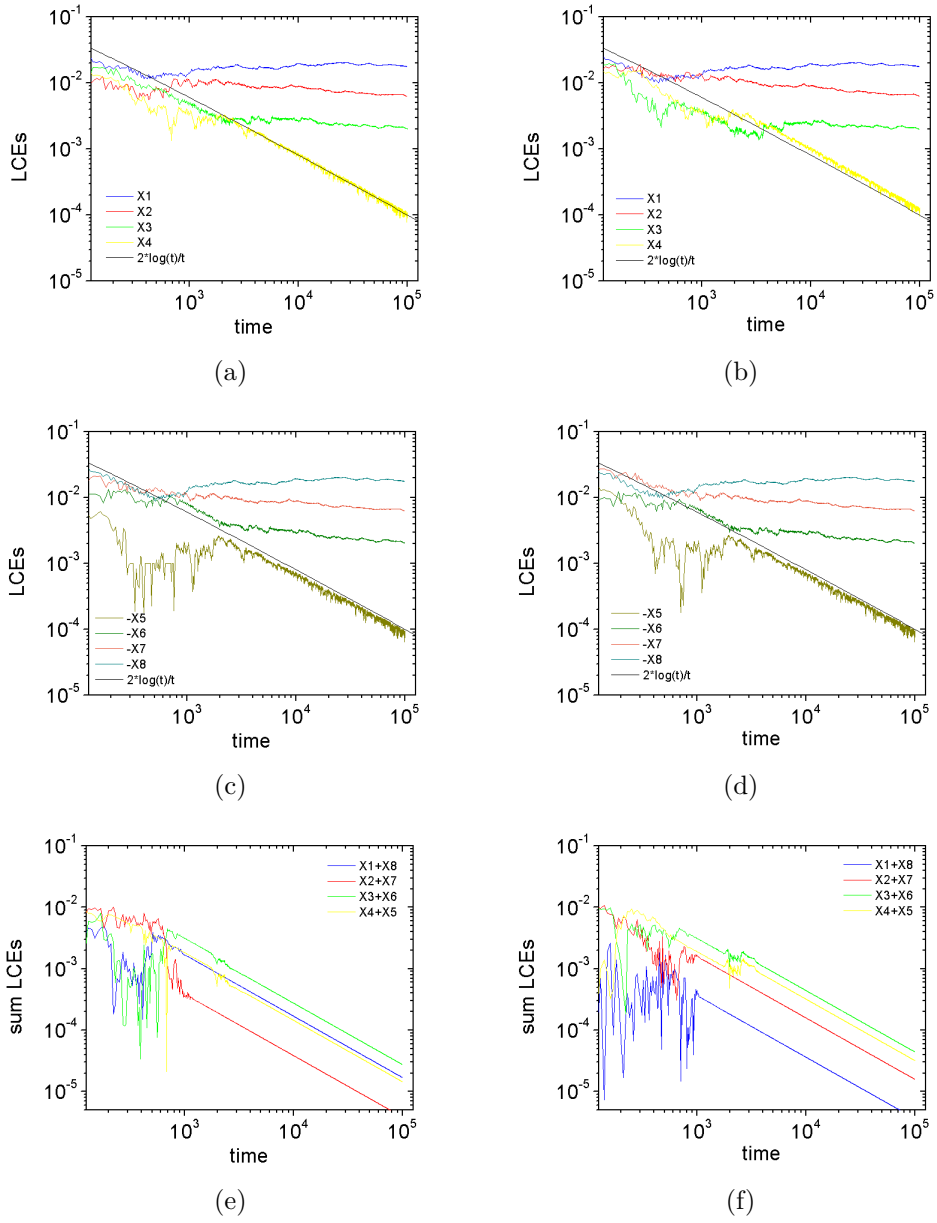


Figure 4.7: Computation of the spectrum of LCEs of the FPU β-lattice (4.1) with $N = 4$ and $E = 1.0$, for the chaotic orbit with $q_i = 0$ and $p_i = (0.97028, -0.45587, 0.11756, 0.91483)$ for $i = 1, 2, 3, 4$. Plots in the left column are computed by the standard method and those in the right by the Compound Matrix method. Figs. 4.7a and 4.7b show the computation of χ_1, χ_2, χ_3 and χ_4 exponents, while Figs. 4.7c and 4.7d show the computation of $-\chi_5$, $-\chi_6$, $-\chi_7$ and $-\chi_8$. Figs. 4.7e and 4.7f depict the sum of the pairs of exponents, (χ_1, χ_8), (χ_2, χ_7), (χ_3, χ_6) and (χ_4, χ_5).

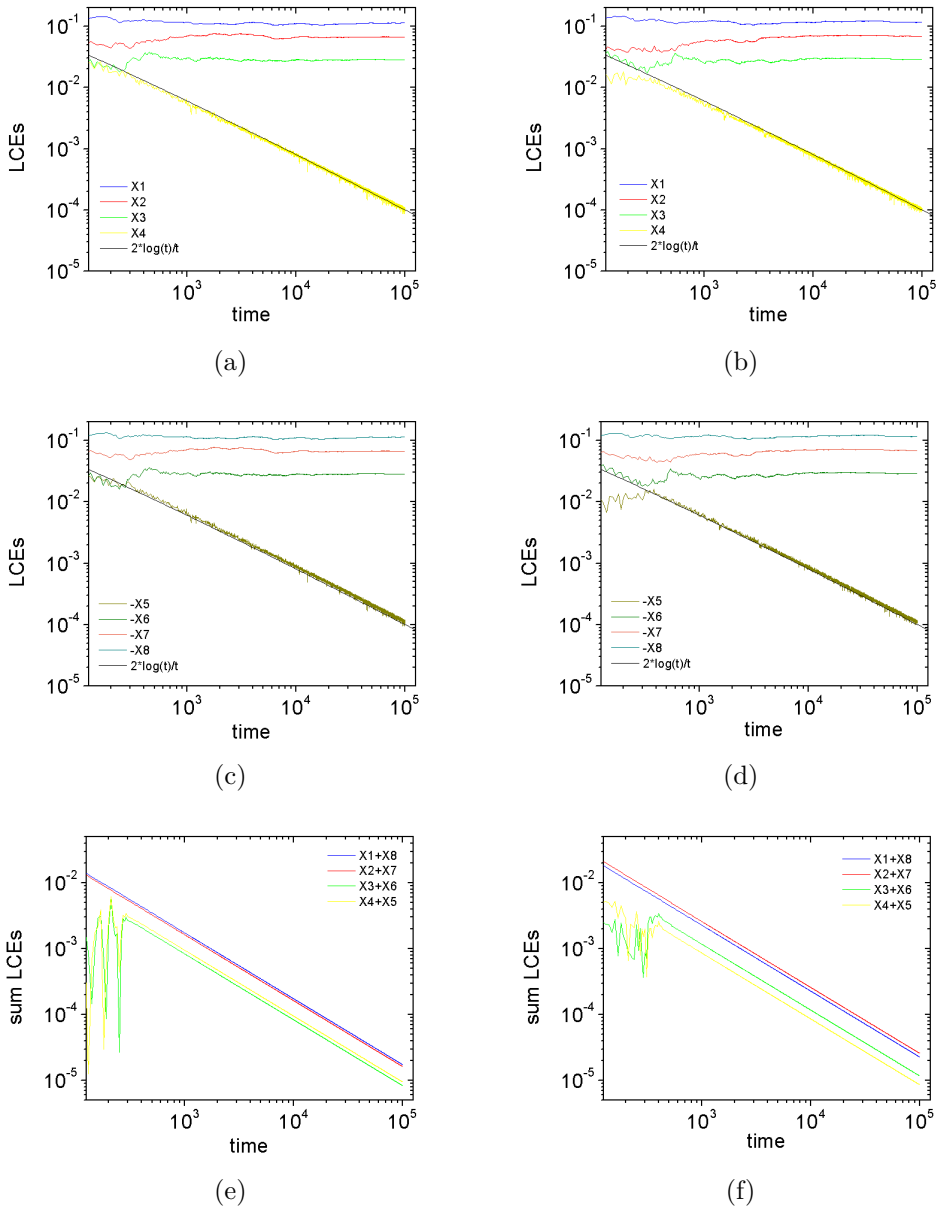


Figure 4.8: Computation of the spectrum of LCEs of the FPU β-lattice (4.1) with $N = 4$ and $E = 10.0$, for the chaotic orbit with $q_i = 0$ and $p_i = (-3.24235, 2.41708, -0.68840, 1.78073)$, for $i = 1, \ldots, 4$. The panels follow the same arrangement as in Fig. 4.7.

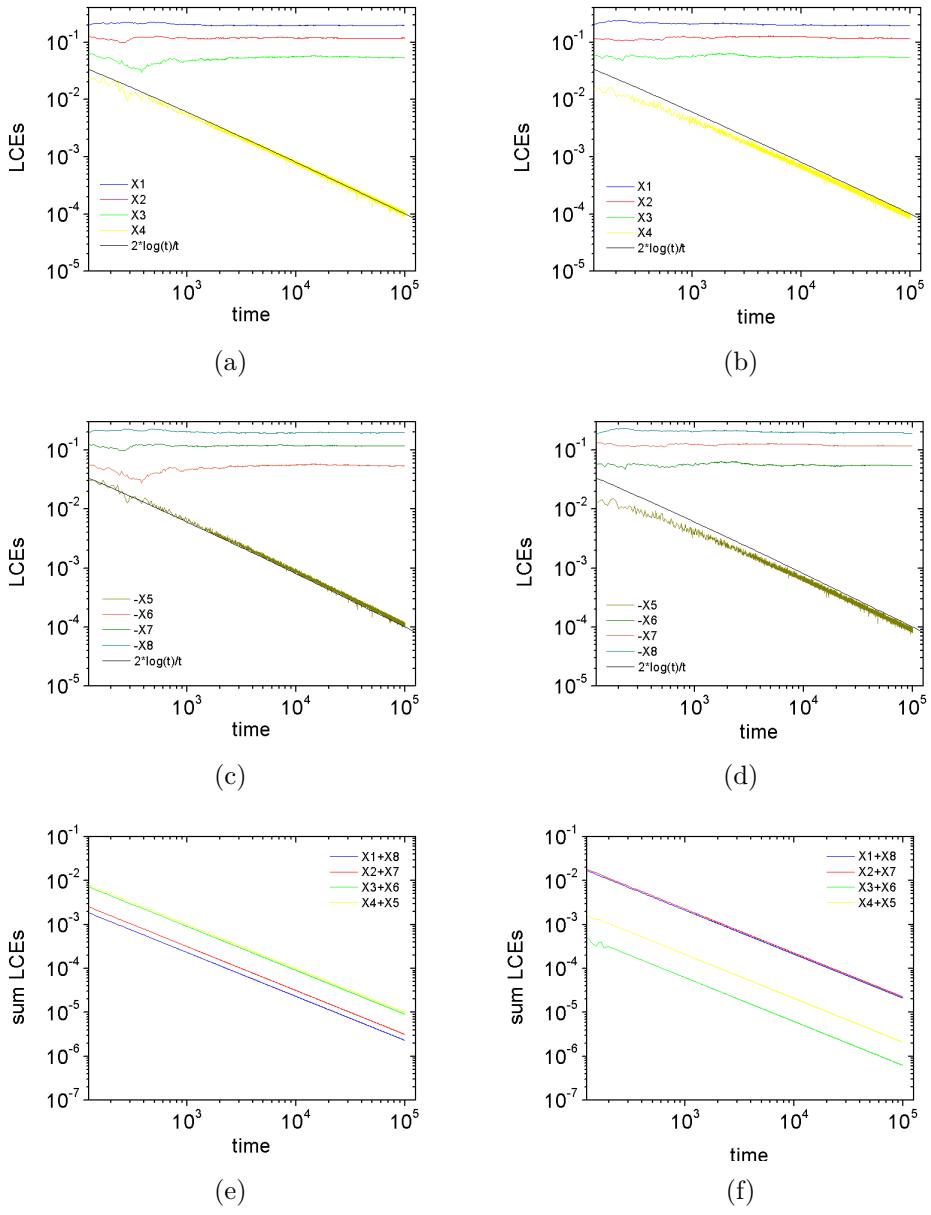
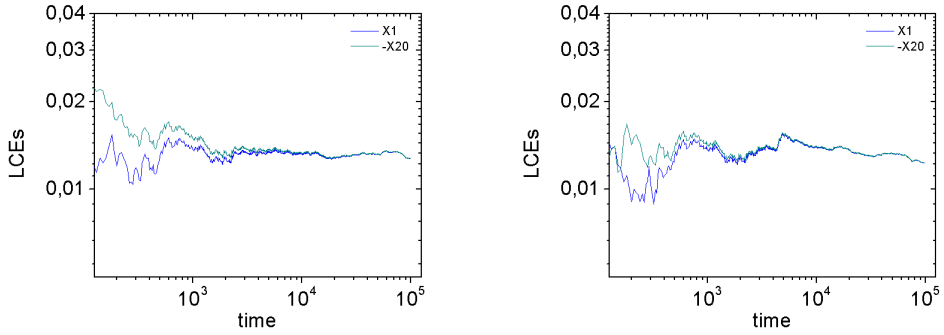
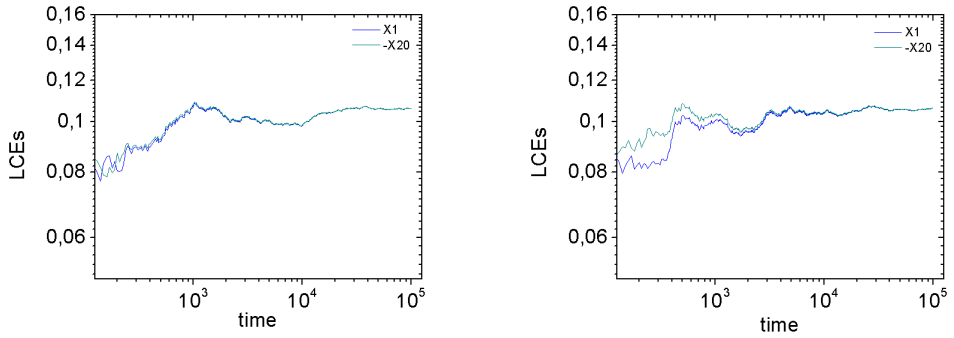


Figure 4.9: Computation of the spectrum of LCEs of the FPU β-lattice (4.1) with $N = 4$ and $E = 30.0$, for the chaotic orbit with $q_i = 0$ and $p_i = (-5.43191, 5.15383, 1.362307, -1.44099)$, for $i = 1, \ldots, 4$. The panels follow the same arrangement as in Fig. 4.7.



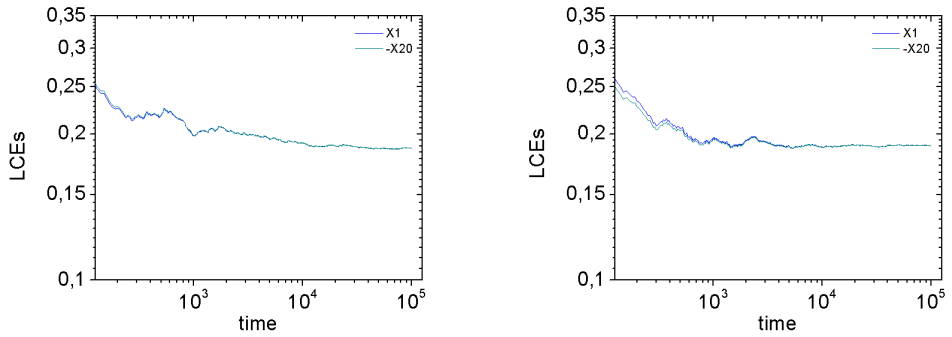
(a) (b)

Figure 4.10: Computation of the χ_1 and $-\chi_{20}$ exponents of the FPU β-lattice (4.1) with $N = 10$ and $E = 1.0$, for the chaotic orbit with $q_i = 0$ and $p_i = (0.30123, -0.39090,$
$-0.49109, 0.42709, 0.59279, -0.46748, -0.40343, 0.65692, -0.41051, -0.01043)$, for $i = 1, \ldots 10$. Fig. 4.10a is computed by the standard method, while Fig. 4.10b by the Compound Matrix method.



(a) (b)

Figure 4.11: Computation of the χ_1 and $-\chi_{20}$ exponents of the FPU β-lattice (4.1) with $N = 10$ and $E = 10.0$, for the chaotic orbit with $q_i = 0$ and $p_i = (-2.09583, 1.21986,$
$0.00537, 2.12219, 1.75060, 1.29881, 1.66538, 0.03062, 1.04788, 0.99585)$, for $i = 1, \ldots, 10$. Fig. 4.11a is computed by the standard method, while Fig. 4.11b by the Compound Matrix method.



(a) (b)

Figure 4.12: Computation of the χ_1 and $-\chi_{20}$ exponents of the FPU β-lattice (4.1) with $N = 10$ and $E = 30.0$, for the chaotic orbit with $q_i = 0$ and $p_i = (-0.77404, 1.84736, 4.48308, -0.78350, 3.25791, -4.33036, -1.54221, -1.28921, -0.71101, 1.16801)$, for $i = 1, \ldots, 10$. Fig. 4.12a is computed by the standard method, while Fig. 4.12b by the Compound Matrix method.

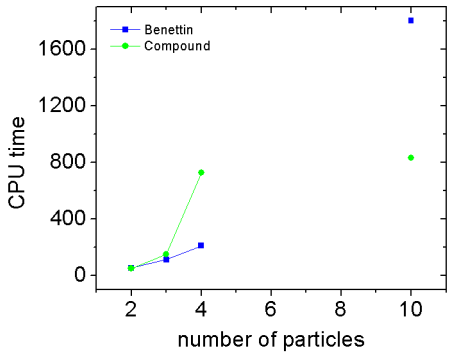


Figure 4.13: The CPU time needed for the computation of the spectrum of LCEs for $N = (2, 3, 4)$ of the FPU β-lattice (4.1) and for the computation of the mLCE χ_1 and of the last exponent, χ_{20}, for the case of $N = 10$.

method we obtaining comparable results, with the ones produced by the standard method of Benettin et al. [4], with respect to the achieved accuracy. Moreover, the computation of a single LCE without the necessity of computing all the previous ones in the spectrum, as it is done by the standard method, is possible as we saw from the results of Figs. 4.10 to 4.12.

As it is shown in Fig. 4.13, the CMT method requires more CPU time than the standard method for the computation of the whole spectrum, even for low dimensional systems. On the contrary, the difference of the computational time needed when a single exponent is of interest, especially for the case of high dimensional systems is significant.

An important disadvantage of the CMT method is that the compound systems that are constructed from the variational equations, become more complicated as the dimensionality of the studied systems increases. Moreover, the auxiliary compound systems cannot be explicitly divided into parts of variables that evolve independently, as for the case of $H_N = T(\mathbf{p}) + V(\mathbf{p})$ Hamiltonians. As a result, the SABA family integrators are not the suitable choice for their integration. New integrators should be sought in order to obtain a desired accuracy.

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