Stability of Motion: From Lyapunov to the Dynamics of N–Degree of Freedom Hamiltonian Systems

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In this paper I discuss some aspects of a problem with a long history, which continues to be of current interest due to its great importance to many applications: The stability of motion in N–degree of freedom Hamiltonian systems. I will start with N small and proceed to the case of N arbitrarily large, in an attempt to understand the thermodynamic limit, where $N \to \infty$ and statistical mechanics is expected to take over from classical mechanics. Our domain is the Euclidian phase space $\mathbb{R}^{2N}$ of the $q_k, p_k, k = 1, 2, \ldots, N$, position and momentum coordinates. The dynamics is governed by Hamilton's equations of motion and the solutions (or orbits) lie on a $(2N-1)$–dimensional compact manifold (the so–called "energy surface"), defined by $H(q_1, \ldots, q_N, p_1, \ldots, p_N) = E$, where H is the Hamiltonian and E is the (constant) energy of the system. Of primary importance in our discussion is the connection between local and global dynamics, i.e. the seemingly paradoxical relevance of events occurring in small scale regions of the energy surface, to the stability of motion in large domains, affecting the properties of the system as a whole. This link is provided by a detailed study of what I call Simple Periodic Orbits (SPOs), i.e periodic solutions where all variables oscillate with equal frequencies, $\omega_k = \omega = 2\pi/T$, returning to the same values after a single maximum (and minimum) in their evolution over one period T.

We will start by recalling some fundamental concepts concerning the stability of dynamical systems, as introduced by one of the forefathers of this field, the great Russian Mathematician A. M. Lyapunov, more than 110 years ago. First, we shall review his two main methods for studying the solutions in the vicinity of equilibrium points that led to his proof of the existence of periodic solutions, as continuations of the corresponding oscillations of the linearized system of equations. We will then apply his theory of the continuation of normal modes of N–degree of freedom Hamiltonian systems to the famous Fermi–Pasta–Ulam lattice to explain how these SPOs can help resolve the paradox of the FPU recurrences. I will then discuss how the study of other SPOs, corresponding to in–phase and out–of–phase oscillations in the FPU and other Hamiltonians, help us understand the transition to large scale chaotic behavior, characterized by invariant spectra of Lyapunov exponents, as well as identify domains where the motion is still quasiperiodic, lying on invariant N–dimensional tori (on which the ω_k are rationally independent). Finally, I will report on a recent discovery of a very efficient spectrum of indices distinguishing ordered from chaotic motions in conservative dynamical systems, called the $GALI_k, k = 1, 2, \ldots, 2N$. These represent an important generalization of the SALI, used by many researchers to identify domains of chaos and order not only in N–degree–of–freedom Hamiltonian systems, but also $2N$–dimensional symplectic maps.

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1. Introduction

The subject of the stability of motion of dynamical systems is of capital importance for

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the understanding of many problems arising in the physical, astronomical, biological, economic and even social sciences. In its simplest (and perhaps most desirable) state, a dynamical system may be at equilibrium, where all variables are fixed for all time, or execute periodic oscillations, with all components returning to their starting values, after every time interval T. The first question concerning these states is their **existence**. Once this has been established, what one needs to know is their **stability**, i.e. their response to small perturbations of the initial conditions and parameter values. Two great scientists were the first to deal with these issues in a systematic and comprehensive way: The Russian mathematician Alexander Mikhailovich Lyapunov (1857–1918) and the French mathematical physicist Henri Poincaré (1854–1917). The former devoted a great deal of his efforts to local stability analysis, obtaining specific conditions for the behavior of solutions of systems of ordinary differential equations (ODEs) in the vicinity of equilibrium points [22]. The latter was primarily concerned with global properties of the dynamics, like non–integrability and the occurrence of irregular (or chaotic) solutions, wandering over large domains of the available state space [23]. Remarkably, both of them worked on periodic solutions of N–degree–of–freedom Hamiltonian systems and were fascinated by the problem of the stability of the solar system. In section 2 of this paper, I will review some of Lyapunov's famous results, regarding the analysis of the motion of systems of ODEs of the form

$$\frac{dx_k}{dt} = f_k(x_1, x_2, \ldots, x_n),\ k = 1, 2, \ldots, N \quad (1)$$

near one of their equilibrium (or fixed) points, taken to be at the origin of the phase space of the system, $(x_1, x_2, \ldots, x_n)$ in $\mathbb{R}^n$, i.e.

$$f_k(0, 0, \ldots, 0) = 0,\ k = 1, 2, \ldots, N. \quad (2)$$

The f_k functions are assumed to be analytic in all their variables, meaning that they are expressed in convergent series expansions in the x_k variables, with non–zero radius of convergence. Thus, (2) implies that the f_k contain no constant terms. Assuming that the linear terms of these series have constant coefficients, Lyapunov paid particular attention to the case where one (or more) of the eigenvalues of the matrix of these coefficients have **zero real part**. As we explain in section 2, this is essentially the beginning of what we now call bifurcation theory (see e.g. [16, 17]), as it constitutes the turning point between the case of stability of the fixed point (all eigenvalues have negative real part) and instability (at least one eigenvalue has positive real part). In particular, we will first examine the case where there is only one pair of purely imaginary eigenvalues (all others being real and negative), which implies the possibility of the existence of periodic orbits about the origin. This will allow us to extend the theory to the Hamiltonian case of interest, where $n = 2N$ and the equations of motion (1) become

$$\frac{dq_k}{dt} = \frac{\partial H}{\partial p_k},\ \frac{dp_k}{dt} = -\frac{\partial H}{\partial q_k},\ k = 1, 2, \ldots, N. \quad (3)$$

These are derived from a Hamiltonian that is expanded in power series in the variables of positions and momenta, as a sum of homogeneous polynomials H_m of degree $m \geqslant 2$

$$\begin{aligned} H &= H_2(q_1, \ldots, q_N, p_1, \ldots, p_N) \\ &+H_3(q_1, \ldots, q_N, p_1, \ldots, p_N) + \ldots = E \end{aligned} \quad (4)$$

(E is the constant energy of the system), so that the origin, $q_k = p_k = 0,\ k = 1, 2, \ldots, N$ is an equilibrium point of the system. Now, assume that the linear equations resulting from (3) and (4) with $H_m = 0$, for all $m > 2$, yield a matrix, whose eigenvalues all occur in conjugate imaginary pairs, $\pm i\lambda_k$ and provide the frequencies of the so–called normal mode oscillations of the linearized system. According to Lyapunov, if **none** of the ratios of these eigenvalues, λ_j/λ_k, is an integer, for any $j, k = 1, 2, \ldots, N$, the linear normal modes continue to exist as periodic solutions of the nonlinear system (3), when higher order terms $H_3, H_4, \ldots$ etc. are taken into account in (4). These solutions have frequencies close to those of the linear modes and are examples of what we call simple periodic orbits (SPOs), where all variables (q_k, p_k) oscillate with the same frequency $(\lambda_j =)\omega = 2\pi/T$, returning to the same values after a single maximum (and minimum) in their time evolution over one period T.

What is the importance of these nonlinear normal modes? Once we have determined that they exist, what can we say about their stability under small perturbations of their initial conditions? How do their stability properties change when we vary the total energy E in (4)? Do they only affect the motion in their immediate vicinity or can they also influence the dynamics of the system as a whole? Are there other SPOs of comparable importance that may also be useful to study from this point of view? These are the questions we shall try to answer in this paper.

In section 3, I will address these questions with reference to two physically interesting N–degree of freedom Hamiltonians: The famous Fermi–Pasta–Ulam lattice [5, 9, 13, 15, 20] and a discretized version of the Gross–Pitaevskii equation describing Bose–Einstein condensation in the tight–binding approximation [10, 19, 28, 30]. We will see that when SPOs are stable, at sufficiently small energies, they affect significantly the dynamics over relatively large regions of phase space. Sometimes, stable SPOs can be found to exist even at high energies with small but finite regions of organized motion around them! Generally, however, when they become unstable at $E > E_c(N)$, they lie at the center of wide domains of chaotic behavior, characterized by spectra of positive Lyapunov exponents, which measure the rates at which nearby orbits separate from each other. As the energy increases further, the Lyapunov spectra in these domains attain a definite functional form and can be used to calculate important statistical quantities of the system like the Kolmogorov–Sinai entropy, which is found to be extensive in the thermodynamic limit of $E \to \infty$ and $N \to \infty$, with E/N finite [1, 2, 21].

Finally, in section 4, I will discuss an important recent development in the analysis of ordered and chaotic orbits in N–degree–of–freedom Hamiltonian systems as well as $2N$–dimensional symplectic maps. In particular, in [27] we have been able to generalize the well–known SALI indicator, see [24–26], by defining a new class of indices, called $GALI_k$s, which characterize orbits by following $2 < k \leq 2N$ deviation vectors about them, unlike SALI, which uses only two. By expressing the $GALI_k$ in terms of the **norm of the "wedge" product** of these deviations, one can compute the time evolution of phase space "volumes" about a specified orbit and determine its ordered or chaotic character by the behavior of these volumes, represented by the $GALI_k$ indices.

In particular, in chaotic domains, the $GALI_k$s **decrease exponentially** to zero with exponents depending on various Lyapunov Characteristic Exponents (LCEs), while in regular domains occupied by invariant tori, they are either constant or **decay by power laws**, whose rates depend primarily on the number k of initially chosen deviation vectors. These indices constitute a major improvement over other similar indicators as they can "chart" out more rapidly and reliably whole domains of phase space, by identifying accurately their ordered and chaotic regions. Since their decay rates depend on the dimensionality of the subspace of ordered motion, they are especially well–suited for higher–dimensional systems, where they can be used to infer this dimension for orbits which "stick" for long times near invariant tori or happen to belong to systems which are partially integrable or super–integrable.

The paper ends with concluding remarks and acknowledgements. I am particularly indebted to my post–doctoral colleague Ch. Skokos and my Ph.D. student Ch. Antonopoulos, for allowing me to use their results on the distinction of chaos and order in Hamiltonian systems. Many thanks are due to my friend and organizer of the "Let's Face Chaos through Nonlinear Dynamics" conferences, Professor Marko Robnik, who has given me the opportunity to publish this paper in the present volume, dedicated to Professor Siegfried Großmann on the occasion of his 75^{th} birthday.

Siegfried was one of the first to obtain fundamental results and recognize the importance of studying chaos in simple nonlinear models of dynamical systems. He has been an inspiration to all of us for his deep and systematic approach as a researcher and exemplary didactical methods as a teacher.

2. Lyapunov's study of the stability of motion

Suppose we want to study the motion of a dynamical system described by equations (1), whose right sides are expanded in power series:

$$\frac{dx_k}{dt} = p_{k1}x_1 + p_{k2}x_2 + \ldots + p_{kn}x_n + \sum_{m_1,m_2,\ldots,m_n} P_k^{(m_1,\ldots,m_n)} x_1^{m_1} x_2^{m_2} \ldots x_n^{m_n} \quad (5)$$

where $k = 1, 2, \ldots, n$ and the summation proceeds over all $m_k > 0$ such that $m_1 + m_2 + \ldots + m_n > 1$. Since the f_k have been assumed analytic, the series in (3) are convergent for $|x_k| \leq A_k$ and by a well-known theorem of analysis (e.g. see Goursat, "Cours d' Analyse Mathematique", vol. 2 (1905), p.273) the coefficients in (5) are bounded by

$$\mid P_k^{(m_1,\ldots,m_n)} \mid \leq \frac{M_k}{{A_1}^{m_1} {A_2}^{m_2} \ldots {A_n}^{m_n}} \quad (6)$$

where M_k is an upper bound of the modulus of all terms of the form $x_1^{m_1} x_2^{m_2} \ldots x_n^{m_n}$ entering in equation (5). Lyapunov, in fact, considered the more general case, where all coefficients on the right side of (5) are continuous and bounded real functions of time for all (real) $t \geq t_0$. In our exposition, however, we shall take them all to be constant.

In his detailed analysis of the motion in the neighborhood of the equilibrium point at $x_1 = x_2 = \ldots = x_n = 0$, Lyapunov introduced two fundamental approaches, which we shall call here:

1. The series expansion method and

2. The Lyapunov function method.

The first one is local in character, since it describes solutions in a very small region around the origin and for finite intervals in time. It generalizes the treatment and the results found in Poincaré's thesis, "Sur les proprietes des functions definies par les equations aux differences partielles" (1879), of which Lyapunov learned at a later time, as he explains in the Introduction of [22]. The second one, however, is entirely his own and is based on an ingenious idea: Instead of focusing on the solutions of the direct problem, it constructs specific functions of these solutions, with well–defined geometric properties, whose development in time reveals indirectly the properties of the actual solutions for all time!

This is the famous method of Lyapunov functions, as we know it today. It is **global** in the sense that it does not refer to a finite time interval and applies to relatively large regions of phase space around the equilibrium point. However, it relies strongly on one's resourcefulness to set up the appropriate PDEs satisfied by these functions and solve them by the appropriate power series expansions.

2.1. Stability of equilibrium points

Let us be precise and speak of the notions of stability that Lyapunov himself had in mind: The first and simplest one concerns what may be called **asymptotic stability**, as it refers to the case where all solutions $x_k(t)$ of (5), starting within a domain of the origin given by $|x_k(t_0)| \leq A_k$, tend to 0 as $t \to \infty$. A less restrictive situation arises when we can prove that for every $0 < \varepsilon < \varepsilon_0$, no matter how small, all solutions starting at $t = t_0$ within a neighborhood of the origin $K(\varepsilon) \subsetneqq B(\varepsilon)$, where $B(\varepsilon)$ is a "ball" of radius ε around the origin, remain inside $B(\varepsilon)$ for all $t \geq t_0$. This weaker condition is often called **neutral or conditional** stability and is of great importance as it frequently occurs in conservative dynamical systems (among them the Hamiltonian ones), which conserve phase space volume and hence cannot come to a complete rest at any value of t, finite or infinite.

We will be primarily concerned here with the notion of conditional stability, since it characterizes precisely the systems for which Lyapunov could prove the existence of families of periodic solutions around the origin by relating them directly to a conserved quantity, known as integral of the motion. For Lyapunov, the existence of integrals was a means to an end, unlike Poincaré, who considered integrability as a primary goal in trying to show the global stability of the motion of a dynamical system.

2.1.1. The Method of series expansions

To illustrate Lyapunov's first method for studying the stability of a fixed point, let us consider the simple example of a one–dimensional system, $n = 1$, described by a single ODE of the Riccati type:

$$\frac{dx}{dt} = -x + x^2. \tag{7}$$

The main idea is to write its solution as a series of the form:

$$x(t) = x^{(1)} + x^{(2)} + \ldots + x^{(n)} + \ldots \tag{8}$$

where the leading term $x^{(1)}$ is the general solution of the linear part of (5), considered naturally as the most important part of the equation in a small region around the fixed point $x = 0$. This is easily written as $x^{(1)} = ae^{-t}$, and incorporates the only arbitrary constant needed for the general solution of the problem. Substituting (8) into (7) we thus obtain an infinite set of linear inhomogeneous equations for the $x^{(k)}$

$$\frac{dx^{(k)}}{dt} = -x^{(k)} + \sum_{j=1}^{k} x^{(j)} x^{(j-k)}, \quad k > 1 \tag{9}$$

for which we seek particular solutions, since the homogeneous part is already represented by $x^{(1)}(t)$. These are: $x^{(k)} = -(-a)^k e^{-kt}$, hence the general solution of (1) becomes:

$$\begin{aligned} x(t) &= x^{(1)} + x^{(2)} + \ldots \\ &= ae^{-t} - a^2 e^{-2t} + a^3 e^{-3t} - \ldots \\ &= q - q^2 + q^3 - \ldots \end{aligned} \tag{10}$$

where we have set $q = ae^{-t}$. This expression clearly converges for $|q| < 1$, which gives the region of initial conditions, at $t = 0$ with $|a| < 1$, where these solutions exist. Furthermore, in this region, all solutions tend to 0 as $t \to \infty$ and therefore 0 is an asymptotically stable equilibrium state.

Let us now see how all this works for an arbitrary n: First, we write again the general solution in the form of a series

$$x_k(t) = {x_k}^{(1)} + {x_k}^{(2)} + \ldots, \quad k = 1, 2, \ldots, n \tag{11}$$

and substituting in (5) we separate the linear system of equations for the ${x_k}^{(1)}$:

$$\frac{d{x_k}^{(1)}}{dt} = p_{k1} x_1^{(1)} + p_{k2} x_2^{(1)} + \ldots + p_{kn} x_n^{(1)} \tag{12}$$

from the rest

$$\frac{d{x_k}^{(m)}}{dt} = p_{k1} x_1^{(m)} + p_{k2} x_2^{(m)} + \ldots + p_{kn} x_n^{(m)} + R_k^{(m)}, \ m > 1 \tag{13}$$

where the $R_k^{(m)}$ contain only terms $x_s^{(j)}, s = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, m-1$, which already determined at lower orders. Thus, we first need to study the linear system (12) and obtain its general solution as a linear combination of n independent particular solutions:

$$x_k^{(1)}(t) = a_1 x_{k1}(t) + a_2 x_{k2}(t) + \ldots + a_n x_{kn}(t), \quad k = 1, 2, \ldots, n \tag{14}$$

in such a way that the initial conditions ${x_k}^{(1)}(t_0) = a_k$ are satisfied. Next, we use (14) to insert in (13) and find particular solutions of the corresponding linear inhomogeneous system at every m, so that ${x_k}^{(m)}(t_0) = 0$.

Lyapunov then obtains explicit expressions for the ${x_k}^{(m)}(t)$ and makes the additional assumption that the sets $A_1, A_2, \ldots, A_n$ and $M_1, M_2, \ldots, M_n$ (see the discussion at the beginning of section 2), considered as functions of t, have non-zero upper bound for each A_k and non–zero lower bound for each M_k, for all $t_0 \leq t \leq T$ and any T. Thus, he is able to show that the solution (11) written as power series in the quantities a_k is absolutely convergent, as long as the $|a_k|$ do not exceed some limit depending on T.

Observe now that in the general case, even though we have found the solution, it is impossible to discuss the question of stability of the origin, unless we know something about the behavior of the solutions of the linear system (12) as functions of t, as we did for the simple Riccati equation. To proceed one would have to compare first every one of the n independent solutions of (12) to an exponential function of time, with the purpose of identifying the particular exponent that would enter in such a relationship.

To achieve this, Lyapunov had the ingenious idea of introducing what he called **the characteristic number** of every function x(t), as follows: First form the auxiliary function $z(t) = x(t)e^{\lambda t}$ and define as the characteristic number λ_0 of x(t), that value of λ for which $z(t)$ vanishes for $\lambda < \lambda_0$ and becomes unbounded for $\lambda > \lambda_0$, as $t \to \infty$. Thus, this number clearly represents the "rate" of exponential decay (or growth) of $x(t)$, as time becomes arbitrarily large. With the convention that functions $x(t)$ whose $z(t)$ vanishes *for all* λ have $\lambda_0 = \infty$ and those for which $z(t)$ is unbounded for all λ have $\lambda_0 = -\infty$, one can define a unique characteristic number for every function $x(t)$.

Proceeding then to derive characteristic numbers for sums and products of functions arising in the solutions of systems of linear ODEs, Lyapunov defines what he calls a **regular system** of linear ODEs by the condition that the sum of the characteristic numbers of its solutions equals the negative of the characteristic number of the function

$$e^{-\int \sum p_{kk}(t)dt} \tag{15}$$

(see [22], p. 43). Thus, he is led to one of his most important theorems:

Theorem 1 *(see [22], p. 57): If the linear system of differential equations (12) is regular and the characteristic numbers of its independent solutions are all positive, the equilibrium point at the origin is asymptotically stable.*

It is important to note that the condition of regularity of a linear system, as defined above, can be shown to hold for all systems, whose coefficients $p_{jk}, j, k = 1, 2, \ldots, n$ are constant or periodic functions of t, and is, in fact, also verified for a much larger class of linear systems. Moreover, since we will be exclusively concerned here with the case of constant coefficients, it is necessary to identify the meaning of characteristic numbers for our problem. Indeed, as the reader can easily verify they are directly related to the eigenvalues of the nxn matrix $D = (p_{jk})/j, k = 1, 2, \ldots, n$, obtained as the n roots of the characteristic equation

$$\det(D - \lambda I_n) = 0 \tag{16}$$

$\lambda_1, \lambda_2, \ldots, \lambda_n$, I_n being the nxn identity matrix. In modern terminology, therefore, for a dynamical system (1), with an equilibrium point at $(0, 0, \ldots, 0)$ and a constant Jacobian matrix

$$D = \{p_{jk} = \frac{\partial f_j}{\partial x_k}(0, \ldots, 0)/\ j, k = 1, 2, \ldots, n\} \tag{17}$$

the above theorem translates to the following well-known result:

Theorem 2 *(see [17], p.181). If all eigenvalues of the matrix D, above, have negative real part less than $-c$, $c > 0$, there is a compact neighborhood U of the origin, such that, for all $(x_1(0), x_2(0), \ldots, x_n(0))$ in U, all solutions $x_k(t) \to 0$, as $t \to \infty$.*

Furthermore, one can show that this approach to the fixed point is exponential: Indeed, if we denote by $|.|$ the Euclidian norm in $\mathbb{R}^n$ and define $\overrightarrow{x}(t) = (x_1(t), x_2(t), \ldots, x_n(t))$, it can be proved, using simple topological arguments [17], that for all $\overrightarrow{x}(0)$ in U, $|\overrightarrow{x}(t)| \leq |\overrightarrow{x}(0)|e^{-ct}$, and $|\overrightarrow{x}(t)|$ is in U for all $t \geq 0$.

Since in his series expansions, Lyapunov expressed his solutions as sums of exponentials of the form

$$x_s{}^{(m)} = \sum C_s{}^{(m_1,m_2,\ldots,m_n)} e^{(m_1\lambda_1+m_2\lambda_2+\ldots+m_n\lambda_n)t}, \tag{18}$$

with $0 < m_1 + m_2 + \ldots + m_n < m$, when substituting these in the equations of motion (12), (13) and solving for the coefficients of these series, $C_s{}^{(m_1,m_2,\ldots,m_n)}$, one has to divide by the expression

$$m_1\lambda_1 + m_2\lambda_2 + \ldots + m_n\lambda_n. \tag{19}$$

If this ever becomes zero, this will lead to *secular terms* in the above series which will grow linearly in time. This can happen for example if one (or more) of the $\lambda_j = 0$, or if the system possesses one (or more) pairs of complex conjugate eigenvalues. Note that such *resonances* (as they are called), will never occur as long as the conditions of Theorem 2 above are satisfied and thus, in the case of $Re(\lambda_j) > 0$ all such secular terms are avoided and the convergence of the corresponding series can be proved.

2.1.2. The method of Lyapunov functions

What happens, however, to a dynamical system like (5), if one or more of the characteristic numbers of its linear part are negative, or–even worse–if they are zero? What can we say about the stability of its fixed point at the origin? It was in order to address such questions that Lyapunov came up with the following idea: Suppose that for $t \geq T$ and $|x_k| \leq H$, with T arbitrarily large and H arbitrarily small (but not zero), we can find a function $V(x_1, x_2, \ldots, x_n)$ such that:
(i) $V(x_1, x_2, \ldots, x_n)$ has a definite sign (positive or negative)
(ii) $V(x_1, x_2, \ldots, x_n) = 0$ if and only if $x_1 = x_2 = \ldots = x_n = 0$ and
(iii) $V'(x_1, x_2, \ldots, x_n) = \sum_j \frac{\partial V}{\partial x_j}\dot{x}_j$ has **opposite** sign than that of V,
where primes denotes differentiation with respect to t, the $x_k(t)$ are such that (5) are satisfied and $|x_k| \leq H$ holds for all k. We could then deduce from (i) – (iii) that as time evolves, the velocity vector $\dot{\vec{x}}(t) = (\dot{x}_1(t), \dot{x}_2(t), \ldots, \dot{x}_n(t))$ lies in a direction of decreasing V, if V is positive definite, or in a direction of increasing V, if V is negative definite. In both cases, the result of the dynamics is to move the system towards the origin, which is respectively a local minimum or a local maximum of the Lyapunov function V. Therefore, the fixed point is asymptotically stable.

Let us illustrate this by a simple example: Consider a dynamical system of the form:

$$\begin{aligned} \dot{x_1} &= -2x_1 - x_2 + R_1(x_1, x_2), \\ \dot{x_2} &= -x_1 - 2x_2 + R_2(x_1, x_2) \end{aligned} \tag{20}$$

with R_1, R_2 convergent power series starting with terms at least quadratic in x_1, x_2. This system evidently possesses a negative definite Lyapunov function of the form $V(x_1, x_2) = -({x_1}^2 - x_1x_2 + {x_2}^2)/3$, for the following reason: No matter what the R_1, R_2 are, when evaluating the total derivative of V we find that it is positive definite

$$\frac{dV}{dt} = x_1^2 + x_2^2 + R_1\frac{\partial V}{\partial x_1} + R_2\frac{\partial V}{\partial x_2} \tag{21}$$

within a sufficiently small neighborhood of the origin. Hence, according to the above argument, all solutions starting within that neighborhood will tend asymptotically to zero.

How does one find Lyapunov functions? It is often stated in the literature that it is a matter of "ingenuity and trial and error" [17]. However, this is not exactly true. Let us suppose we are given a system of ODEs of the form

$$\frac{dx_k}{dt} = p_{k1}x_1 + p_{k2}x_2 + \ldots + p_{kn}x_n + R_k, \quad k = 1, 2, \ldots, n \tag{22}$$

with R_k convergent power series, starting with terms at least quadratic in the x_k. If all the roots of the characteristic equation–see (16), (17)– have negative real parts, Lyapunov proved that one can always construct a **negative** definite quadratic form V, as a solution of PDEs of the form

$$\sum_{k=1}^{n}(p_{k1}x_1 + p_{k2}x_2 + \ldots + p_{kn}x_n)\frac{\partial V}{\partial x_k} = x_1^2 + x_2^2 + \ldots + x_n^2 = U \tag{23}$$

so that

$$\frac{dV}{dt} = x_1^2 + x_2^2 + \ldots + x_n^2 + \sum_{k=1}^{n} R_k \frac{\partial V}{\partial x_k} \tag{24}$$

just as we found in the above example. One does not have to use ingenuity and trial and error. Expanding all expressions in power series in the x_k will lead to the desired result. Since V and its total time derivative have opposite signs within a neighborhood of the origin (except at $x_1 = x_2 = \ldots = x_n = 0$), this demonstrates the asymptotic stability of the zero solution in this case.

2.2. Eigenvalues with zero real part

2.2.1. The case of one zero eigenvalue

What happens if one or more of the eigenvalues of the matrix of the associated linear system (17) have zero real part? This is where Lyapunov devotes considerable effort and obtains results of major importance: First he considers the case where only one real eigenvalue is zero and calls x the variable of the corresponding equation. Writing its ODE in the form

$$\begin{aligned}\frac{dx}{dt} &= R(x, x_1, x_2, \ldots, x_n)\\ &= gx^m + P^{(1)}x + \ldots + P^{(m-1)}x^{m-1}\\ &+ Q + S,\end{aligned} \tag{25}$$

$m \geq 2$, with the $P^{(j)}$s linear and Q quadratic in $x_1, \ldots, x_n$ and S analytic in $x, x_1, \ldots, x_n$, at least of order 3 and containing powers of x no less than m in terms of order at least $m+1$, he shows that it is always possible to make a change of variables, so that the equations for the $x_1, \ldots, x_n$

$$\begin{aligned}\frac{dx_k}{dt} &= p_{k1}x_1 + p_{k2}x_2 + \ldots + p_{kn}x_n\\ &+ R_k(x, x_1, \ldots, x_n), k = 1, 2, \ldots, n\end{aligned} \tag{26}$$

do **not depend linearly** on x. Assuming that all eigenvalues of the linear terms in (26) have negative real parts, Lyapunov proves that by solving the appropriate PDEs:

1) For m even: One can determine a function

$$V = x + U^{(1)}x + \ldots + U(m-1)x^{m-1} + W \tag{27}$$

with $U^{(j)}$ linear and W quadratic in $x_1, \ldots, x_n$, such that it is a solution of the PDE

$$\frac{dV}{dt} = g(x^m + x_1^2 + x_2^2 + \ldots + x_n^2) + T \tag{28}$$

where T is at least of order 3 in $x_1, \ldots, x_n$ and contains powers of x no less than m in terms of order at least $m+1$. Thus, we conclude that the equilibrium point at the origin will be **always unstable**, since, no matter what the sign of g, we could always find x for which V will have the same sign with its derivative.

2) For m odd, one can construct a function

$$V = \frac{x^2}{2} + U^{(1)}x^2 + \ldots + U(m-1)x^m + W \tag{29}$$

with $U^{(j)}$ linear and W quadratic in $x_1, \ldots, x_n$, such that its time derivative starts with a term of degree $m+1$

$$\frac{dV}{dt} = g(x^{m+1} + x_1^2 + x_2^2 + \ldots + x_n^2) + T \tag{30}$$

Now, it turns out that we can choose W to be definite and of opposite sign than g, by requiring that it satisfy the following PDE

$$\sum_{k=1}^{n}(p_{k1}x_1 + p_{k2}x_2 + \ldots + p_{kn}x_n)\frac{\partial W}{\partial x_k} + Q = g(x_1^2 + x_2^2 + \ldots + x_n^2). \tag{31}$$

This implies, therefore, that **for $g < 0$ the origin is stable** since the function V will be positive definite, while its derivative is negative definite. On the other hand, **if $g > 0$ the origin is unstable** since W is negative definite and V can take any sign, while its derivative is always positive definite in a small neighborhood about the equilibrium point.

2.2.2. The case of one pair of imaginary eigenvalues

Thus we come to the case that interests us most in this paper: It is the circumstance where a system of ODEs of the form (22) possesses one pair of imaginary eigenvalues $+i\sqrt{\lambda}, -i\sqrt{\lambda}$. Here, Lyapunov separates the two variables associated with these eigenvalues, x, y, and shows that the original system of ODEs can always be written in the form

$$\begin{aligned}\frac{dx}{dt} &= -\lambda y + X(x, x_1, x_2, \ldots, x_n) \qquad (32)\\ \frac{dy}{dt} &= \lambda x + Y(x, x_1, x_2, \ldots, x_n)\\ \frac{dx_k}{dt} &= p_{k1}x_1 + p_{k2}x_2 + \ldots + p_{kn}x_n + \alpha_k x + \beta_k y\\ &+ R_k, \quad k = 1, 2, \ldots, n. \qquad (33)\end{aligned}$$

where X, Y vanish for $x = y = 0$. It is then possible to use **polar coordinates**, $x = r\cos\theta, y = r\sin\theta$ and write the above system as follows:

$$\frac{dr}{d\theta} = rR, \quad \frac{d\theta}{dt} = \lambda + \Theta(r, x_1, \ldots, x_n) \qquad (34)$$

and

$$\begin{aligned}\frac{dx_k}{d\theta} &= q_{k1}x_1 + q_{k2}x_2 + \ldots + q_{kn}x_n\\ &+ (a_k\cos\theta + b_k\sin\theta)r + Q_k,\\ k &= 1, 2, \ldots, n. \qquad (35)\end{aligned}$$

where R, Q_k, Θ are analytic, having as coefficients in their expansions entire and rational functions of $\cos\theta, \sin\theta$ and become zero when $r = 0,\ x_1 = x_2 = \ldots = x_n = 0$. Moreover, the Q_k contain terms no less than of second degree in these variables. The new coefficients in the θ–evolution are given by

$$q_{kj} = \frac{p_{kj}}{\lambda},\ a_k = \frac{\alpha_k}{\lambda},\ b_k = \frac{\beta_k}{\lambda} \qquad (36)$$

and the q_{kj} are such that their matrix has only eigenvalues with negative real part. Lyapunov then proceeds to seek periodic solutions of the above equations as power series in an arbitrary constant $c > 0$:

$$\begin{aligned}r &= c + u^{(2)}c^2 + u^{(3)}c^3 + \ldots,\\ x_k &= u_k^{(1)}c + u_k^{(2)}c^2 + u_k^{(3)}c^3 + \ldots \qquad (37)\end{aligned}$$

$k = 1, 2, \ldots, n$, where the $u^{(j)}$, $u_k^{(j)}$ are periodic functions of θ of period 2π and independent of c. He establishes conditions for the existence of such solutions and proves the convergence of (37), for sufficiently small values of $c > 0$. It is precisely here that a crucial assumption enters concerning the eigenvalues of the matrix q_{kj}: In order for the $u^{(j)}$, $u_k^{(j)}$ to be evaluated by quadratures and be 2π–periodic in θ it is imperative that **none of these eigenvalues be an integer multiple of $i\lambda$.**

The period of the solution in the time variable t is also derived as a convergent expansion in powers of c:

$$T = \frac{2\pi}{\lambda}(1 + h_2c^2 + h_3c^3 + \ldots.). \qquad (38)$$

Finally, using similar methods as in the case of one zero eigenvalue, Lyapunov establishes conditions for the stability of the unperturbed equilibrium solution at the origin and proceeds to apply his theory to a series of remarkable examples of systems of ODEs in 3 dependent variables x, y, z. One wonders how much more he would have discovered had he the luxury of using one of our modern day computers!

2.2.3. All eigenvalues are imaginary: The case of Hamiltonian systems

Thus we come to the problem Lyapunov was eagerly interested to solve: The global stability of motion in N–degree–of–freedom Hamiltonian systems. As we pointed out in the Introduction, he was very much aware of the importance of this issue to Celestial Mechanics, much as his great contemporary fellow mathematician Henri Poincaré. Lyapunov's approach, however, was quite different. Rather than trying to prove the (non–)existence of integrals, he set out to derive rigorous conditions for the **continuation** of the fundamental periodic motions of the linearized equations to the nonlinear system obtained when higher than second degree terms are included in the Hamiltonian (4).

Let us write first the quadratic part of the Hamiltonian in canonical form,

$$\begin{aligned} H^{(2)} &= \frac{\lambda_1}{2}({x_1}^2+{y_1}^2)+\frac{\lambda_2}{2}(x_2^2+y_2^2)+\dots \\ &+ \frac{\lambda_N}{2}(x_N^2+y_N^2)=E \end{aligned} \tag{39}$$

where x_k, y_k, $k=1,2,\dots,N$ are the position and momentum coordinates and λ_k represent the frequencies of the N uncoupled oscillators of the linearized motion. Taking one of these oscillators, x_j, y_j, as an example and expressing all other variables in terms of these two, we write Hamilton's equations (3) in the form

$$\begin{aligned} -\frac{\partial H}{\partial x_j}\frac{\partial x_k}{\partial y_j}+\frac{\partial H}{\partial y_j}\frac{\partial x_k}{\partial x_j} &= \frac{\partial H}{\partial y_k}, \\ -\frac{\partial H}{\partial x_j}\frac{\partial y_k}{\partial y_j}+\frac{\partial H}{\partial y_j}\frac{\partial y_k}{\partial x_j} &= -\frac{\partial H}{\partial x_k} \end{aligned} \tag{40}$$

with $k=1,2,\dots,j-1,j+1,\dots,N$. We now designate by $H_j(x_j,y_j)$ the Hamiltonian function H with all x_k, y_k expressed as functions of x_j, y_j and seek to solve (40) for x_k, y_k as analytic functions of x_j, y_j, which vanish at $x_j=y_j=0$. As Lyapunov shows, such solutions always exist and are unique.

Evaluating now $\partial H_j/\partial x_j$ and $\partial H_j/\partial y_j$ in terms of the $\partial H/\partial x_k$ and $\partial H/\partial y_k$, using Hamilton's equations to replace them by $\dot{x}_k$ and $\dot{y}_k$ and expressing these latter ones by their partial derivatives with respect to x_j and y_j we easily reduce the PDEs (40) to the ODEs:

$$[x_j,y_j]\frac{dx_j}{dt}=\frac{\partial H_j}{\partial y_j},\quad [x_j,y_j]\frac{dy_j}{dt}=-\frac{\partial H_j}{\partial x_j}, \tag{41}$$

where $1+\sum_k\left(\frac{\partial x_k}{\partial x_j}\frac{\partial y_k}{\partial y_j}-\frac{\partial x_k}{\partial y_j}\frac{\partial y_k}{\partial x_j}\right)=[x_j,y_j]$, calling a_j and b_j the $2N$ arbitrary initial constants required to solve them. However, to ensure the successful construction of these N periodic solutions we must recall the important eigenvalue condition mentioned below (37), i.e. that

$$\frac{\lambda_j}{\lambda_k}\neq n,\quad j,k=1,2,\dots,N \tag{42}$$

where n is any integer. The N periodic solutions we shall be able to find in this way have well–defined periods, which for sufficiently small $|a_j|$ and $|b_j|$ are given by convergent expansions of the form:

$$T_j=\frac{2\pi}{\lambda_j}(1+h_j^{(1)}H_j(a_j,b_j)+h_j^{(2)}[H_j(a_j,b_j)]^2+\dots). \tag{43}$$

3. Local and global dynamics of N–degree–of–freedom Hamiltonians

The famous so–called β–FPU lattice is described by the Hamiltonian

$$\begin{aligned} H=\frac{1}{2}\sum_{j=1}^{N}\dot{x}_j^2+\sum_{j=0}^{N}\bigg(\frac{1}{2}(x_{j+1}-x_j)^2 \\ +\frac{1}{4}\beta(x_{j+1}-x_j)^4\bigg)=E \end{aligned} \tag{44}$$

where x_j are the displacements of the particles from their equilibrium position, and $\dot{x}_j$ are the corresponding canonically conjugate momenta, β is a positive real constant and E is the total energy of the system.

The BEC Hamiltonian is obtained by a discretization of a PDE of the nonlinear Schrödinger type called the Gross–Pitaevskii equation,

$$\begin{aligned} i\hbar\frac{\partial\Psi(x,t)}{\partial t} &= -\frac{\hbar^2}{2}\frac{\partial^2\Psi(x,t)}{\partial x^2}+V(x)\Psi(x,t) \\ &+g|\Psi(x,t)|^2\Psi(x,t),\ i^2=-1 \end{aligned} \tag{45}$$

where $\hbar$ is the Planck constant, g is a positive constant (repulsive interactions between atoms in the condensate) and $V(x)$ is an external potential.

This equation is related to the phenomenon of Bose–Einstein Condensation (BEC). Considering the simple case $V(x) = 0$, $\hbar = 1$ and discretizing the complex variable $\Psi(x,t) \equiv \Psi_j(t)$, we may approximate the second order derivative by

$$\Psi_{xx} \simeq \frac{\Psi_{j+1} + \Psi_{j-1} - 2\Psi_j}{\delta x^2},$$
$$\Psi_j(t) = q_j(t) + ip_j(t),\ j = 1, 2, \ldots, N \qquad (46)$$

and with

$$|\Psi(x,t)|^2 = q_j^2(t) + p_j^2(t), \qquad (47)$$

obtain a set of ODEs for the canonically conjugate variables, p_j and q_j, described by the BEC Hamiltonian

$$H = \frac{1}{2}\sum_{j=1}^{N}(p_j^2 + q_j^2) + \frac{\gamma}{8}\sum_{j=1}^{N}(p_j^2 + q_j^2)^2$$
$$-\frac{\epsilon}{2}\sum_{j=1}^{N}(p_j p_{j+1} + q_j q_{j+1}) = E \qquad (48)$$

where $\gamma > 0$ and $\epsilon = 1$ are constant parameters, $g = \frac{\gamma}{2} > 0$ with $\delta x = 1$ and E is the total energy of the system.

3.1. Simple periodic orbits

Let us focus on **Simple Periodic Orbits** (SPOs), which have well–defined symmetries and are known in closed form. By SPOs, we mean periodic solutions where all variables return to their initial state after only one maximum and one minimum in their oscillation.

Our SPOs are:

I. For FPU and BEC with **periodic boundary conditions**:

$$x_{N+k}(t) = x_k(t),\ \forall t, k \qquad (49)$$

(a) Out–of–Phase Mode (OPM), with N even

$$\hat{x}_j(t) = -\hat{x}_{j+1}(t) \equiv \hat{x}(t),\ j = 1, \ldots, N. \qquad (50)$$

(b) The In–Phase Mode (IPM) for BEC

$$\begin{aligned} q_j(t) &\equiv \hat{q}(t), \\ p_j(t) &\equiv \hat{p}(t)\ \forall j = 1, \ldots, N, \end{aligned}$$
$$N \in \mathbb{N} \ \text{ and } \ N \geq 2 \qquad (51)$$

FIG. 1. Surface of section of the BEC Hamiltonian, showing the IPM and OPM orbits on the vertical axis. The value of the norm integral is $F = 2$, while the SPOs correspond to different values of the Hamiltonian.

FIG. 2. Surface of section of the BEC Hamiltonian, showing the IPM and OPM orbits on the vertical axis. The value of the norm integral is $F = 4.1$, where the OPM on the negative p_x axis has become unstable yielding two stable SPOs one above and one below it.

II. For the FPU model and **fixed boundary conditions**:

$$x_0(t) = x_{N+1}(t) = 0,\ \forall t \qquad (52)$$

(a) The SPO1 mode, with N odd,

$$\hat{x}_{2j}(t) = 0,\ \hat{x}_{2j-1}(t) = -\hat{x}_{2j+1}(t) \equiv \hat{x}(t),\quad j = 1, \ldots, \frac{N-1}{2}. \quad (53)$$

(b) The SPO2 mode, with $N = 5 + 3m,\ m = 0, 1, 2, \ldots$ particles,

$$\begin{aligned} x_{3j}(t) &= 0,\ j = 1, 2, 3, \ldots, \frac{N-2}{3}, \\ x_j(t) &= -x_{j+1}(t) = \hat{x}(t), \\ j &= 1, 4, 7, \ldots, N-1. \end{aligned} \quad (54)$$

The FPU system with fixed boundary conditions is precisely one of those examples where we can directly apply Lyapunov's theory as described in section 2 2.2 2.2.3 above: More specifically, we can use it to **prove the existence** of SPOs as continuations of the linear normal modes of the system, whose frequencies have the well–known form [5, 9, 14, 15, 20]

$$\omega_{0q} = 2 \sin \frac{\pi q}{2(N+1)},\ \ q = 1, 2, \ldots, N. \quad (55)$$

This is so because the linear mode frequencies (55) are seen to satisfy Lyapunov's non–resonance condition (42), for all q and N.

3.2. Linear stability analysis and local chaos

The stability analysis of SPOs can be easily performed by studying the eigenvalues of the monodromy matrix. For example, consider the SPO1 mode of FPU: The equations of motion

$$\begin{aligned} \ddot{x}_j(t) &= x_{j+1} - 2x_j + x_{j-1} \\ &+\beta\Big((x_{j+1} - x_j)^3 - (x_j - x_{j-1})^3\Big), \\ &j = 1, \ldots, N \end{aligned} \quad (56)$$

for fixed boundary conditions collapse to a single second order ODE:

$$\ddot{\hat{x}}(t) = -2\hat{x}(t) - 2\beta\hat{x}^3(t). \quad (57)$$

Its solution is well–known in terms of Jacobi elliptic functions

$$\hat{x}(t) = \mathcal{C}\,\mathrm{cn}(\lambda t, \kappa^2) \quad (58)$$

where

$$\mathcal{C}^2 = \frac{2\kappa^2}{\beta(1-2\kappa^2)},\ \ \lambda^2 = \frac{2}{1-2\kappa^2} \quad (59)$$

and κ^2 is the modulus of the cn elliptic function. Its stability is analyzed setting $x_j = \hat{x}_j + y_j$ and keeping up to linear terms in y_j to get the variational equations

$$\ddot{y}_j = (1 + 3\beta\hat{x}^2)(y_{j-1} - 2y_j + y_{j+1}),\ j = 1, \ldots, N \quad (60)$$

where $y_0 = y_{N+1} = 0$.

We now separate these variational equations into N uncoupled Lamé equations

$$\ddot{z}_j(t) + 4(1 + 3\beta\hat{x}^2)\sin^2\left(\frac{\pi j}{2(N+1)}\right) z_j(t) = 0,\quad j = 1, \ldots, N \quad (61)$$

where the z_j variations are simple linear combinations of the y_j's. Changing variables to $u = \lambda t$, this equation takes the form

$$\begin{aligned} &z_j''(u) + 2\big(1 + 4\kappa^2 - 6\kappa^2 \mathrm{sn}^2(u, \kappa^2)\big) \\ &\sin^2\left(\frac{\pi j}{2(N+1)}\right) z_j(u) = 0,\ j = 1, \ldots, N \end{aligned} \quad (62)$$

where primes denote differentiation with respect to u.

Equation (62) is an example of Hill's equation

$$z''(u) + Q(u)z(u) = 0 \quad (63)$$

where $Q(u)$ is a T–periodic function ($Q(u) = Q(u+T)$). According to Floquet theory, its solutions are bounded (or unbounded) depending on whether the eigenvalues of the matrix of its fundamental solutions evaluated at the period T (monodromy matrix) lie on the unit circle or not. The first variation $z_j(u)$ to become unbounded as κ^2 increases is $j = \frac{N-1}{2}$ and the energy values

$E_c/N \propto 1/N$ at which this happens are plotted below.

In fact, all these periodic solutions are found to experience a first destabilization at energy densities:

$$\frac{E_c}{N} \propto N^{-\alpha}, \ \alpha = 1, \ or, \ 2, \ N \to \infty. \tag{64}$$

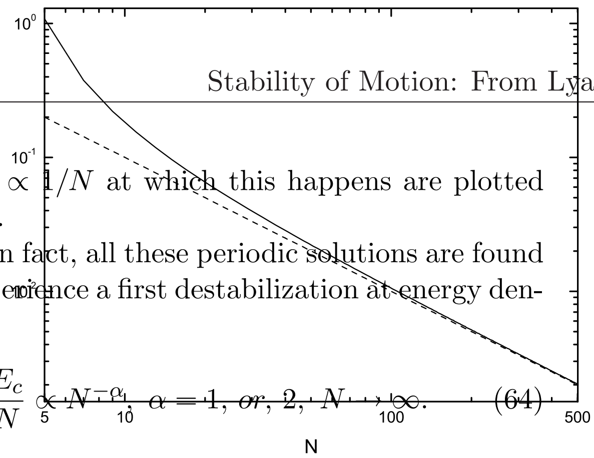

FIG. 3. The solid curve corresponds to the energy per particle $\frac{E_c}{N}$, for $\beta = 1.04$, of the first destabilization of the SPO1 nonlinear mode of the FPU system obtained by the numerical evaluation of the monodromy matrix, while the dashed line corresponds to the function $\propto \frac{1}{N}$. Note that both axes are logarithmic.

The OPMs of the FPU and BEC Hamiltonians become unstable, as the eigenvalues of their monodromy matrix exit the unit circle on the real axis: For FPU at -1 (period–doubling bifurcation) and for BEC at $+1$ (pitchfork bifurcation). Interestingly enough, the IPM of the BEC Hamiltonian remains stable for all the energies and number of degrees of freedom we studied!

3.3. An analytical criterion for "weak" chaos

As was mentioned above, using Lyapunov's theorem, we can prove that the linear modes of the FPU β–model, with frequencies (55) can be continued as SPOs of the corresponding nonlinear lattice. In fact, it was recently shown in [14] that the energy threshold for the destabilization of the low $q \ll N$ modes coincides with the "weak" chaos threshold shown by de Luca and Lichtenberg (1995)[11] to be associated with the breakup of the famous FPU recurrences.

Thus, using different approaches, these authors report an approximate formula for the destabilization energy of the mode with $q = 3$ given by

$$E_c \approx \frac{\pi^2}{6\beta(N+1)}. \tag{65}$$

We have discovered that this energy threshold also coincides with the instability threshold of our SPO2 mode! In Fig. 4 we compare the approximate formula (dashed line) with our destabilization threshold for SPO2 obtained by the monodromy matrix analysis(solid line), for $\beta = 0.0315$, and find excellent agreement.

FIG. 4. The solid curve corresponds to the energy $E_{2u}(N)$ of the first destabilization of the SPO2 for $\beta = 0.0315$ obtained by the numerical evaluation of the eigenvalues of the monodromy matrix, while the dashed line corresponds to the approximate formula for the $q = 3$ nonlinear normal mode.

3.4. Lyapunov exponents and global chaos

3.4.1. Lyapunov spectra and their convergence

We now evaluate, in the neighborhood of our SPOs the **Lyapunov spectra**:

$$L_i,\ i=1,\ldots,2N,\ L_1 \equiv L_{\max} > L_2 > \ldots > L_{2N}. \tag{66}$$

If at least one of them, the largest one, $L_1 \equiv L_{\max} > 0$, the orbit is chaotic. Benettin *et al.* [3, 4] have proposed an efficient algorithm which allows us to compute them all: In particular, $L_i \equiv L_i(\vec{x}(t))$ for a given orbit $\vec{x}(t)$ is the limit for $t \to \infty$ of the quantities

$$K_t^i = \frac{1}{t}\ln\frac{\parallel \vec{w}_i(t) \parallel}{\parallel \vec{w}_i(0) \parallel}, \tag{67}$$

$$L_i = \lim_{t\to\infty} K_t^i \tag{68}$$

where $\vec{w}_i(0)$ and $\vec{w}_i(t)$, $i=1,\ldots,2N$ are deviation vectors from the given orbit $\vec{x}(t)$, at times $t=0$ and $t>0$. In practice, of course, one stops their evaluation after some time T_i, ortho–normalizes the vectors $\vec{w}_i(t)$ and repeats the calculation for the next time interval T_{i+1}, etc. thus obtaining finally L_i as an average over many T_j, $j=1,2,\ldots,n$

$$L_i = \frac{1}{n}\sum_{j=1}^{n} K_{T_j}^i,\ n\to\infty. \tag{69}$$

For fixed N we have found that as E is increased, the Lyapunov spectrum for all our unstable SPOs falls on a smooth curve [1, 2, 21]. Observe that in Fig. 5 below we have plotted the Lyapunov spectrum of both the OPM and of the SPO1 mode of the FPU Hamiltonian for $N=16$ and periodic boundary conditions at the energy $E=6.82$ where both of them are unstable. We clearly see that the two Lyapunov spectra are almost identical at this energy suggesting that their chaotic regions have become "connected".

Let us see this in more detail by plotting in Fig. 6(a) the Lyapunov spectra of two neighboring orbits of the SPO1 and SPO2 modes, of the FPU system with fixed boundary conditions, for $N=11$ degrees of freedom and energy values $E_1=1.94$ and $E_2=0.155$ respectively, where the SPOs have just destabilized. Here, the maximum Lyapunov exponents L_1, are very small ($\approx 10^{-4}$) and the corresponding Lyapunov spectra are quite distinct.

FIG. 5. The Lyapunov spectrum of the OPM of the FPU Hamiltonian, for $N=16$ and the SPO1 mode of the same Hamiltonian and N, for periodic boundary conditions practically coincide at $E=6.82$ where both of them are destabilized.

Raising the energy, now, we observe in Fig. 6(b) that at the value $E=2.1$, the Lyapunov spectra for both SPOs are closer to each other, even though their maximal Lyapunov exponents L_1 are still different. At $E=2.62$, we see that the two spectra have nearly converged to the same exponentially decreasing function,

$$L_i(N) \propto e^{-\alpha\frac{i}{N}}, i=1,2,\ldots,K(N) \tag{70}$$

at least up to $K(N)\approx\frac{3N}{4}$, while their maximal Lyapunov exponents are virtually the same. The α exponents for the SPO1 and SPO2 are found to be approximately 2.3 and 2.32 respectively. Fig. 6(d) finally shows that this coincidence of Lyapunov spectra persists at higher energies.

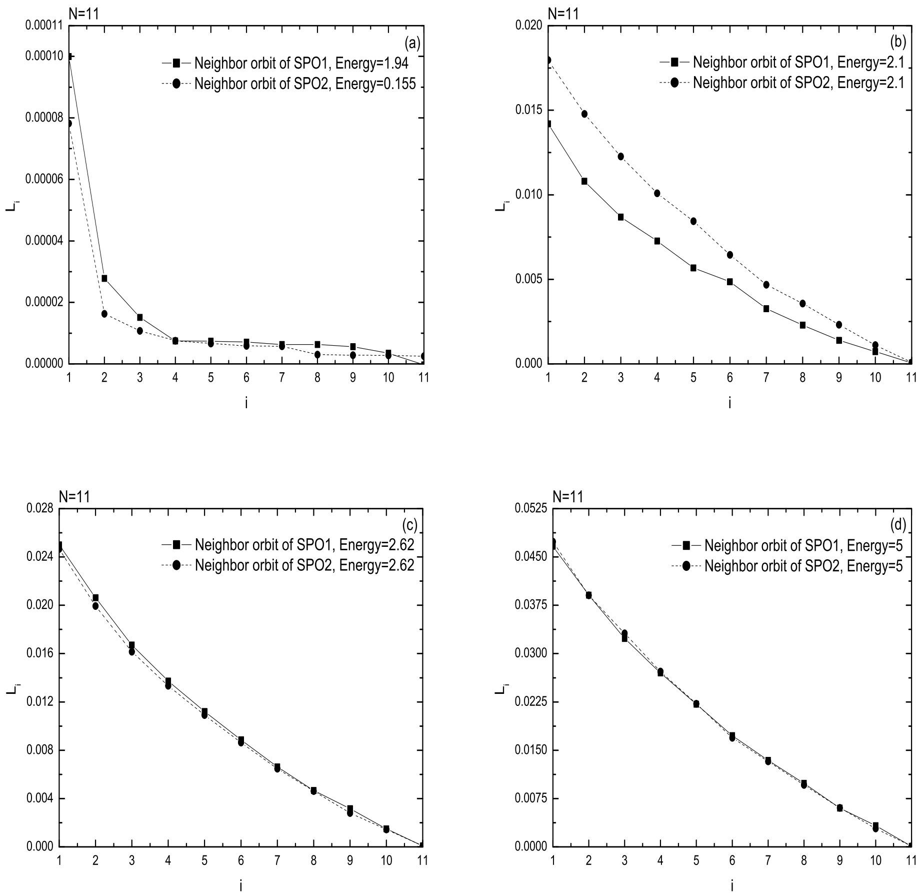

FIG. 6. (a) Lyapunov spectra of neighboring orbits of SPO1 and SPO2 respectively for $N = 11$ at energies $E = 1.94$ and $E = 0.155$, where they respectively have just destabilized. (b) Same as in panel (a) at energy $E = 2.1$ for both SPOs, where the spectra are still distinct. (c) Convergence of the Lyapunov spectra of neighboring orbits of the two SPOs at energy $E = 2.62$ where both of them are unstable. (d) Coincidence of Lyapunov spectra continues at higher energy $E = 5$. All initial distances between nearby trajectories are $\simeq 10^{-2}$.

3.5. Lyapunov spectra and the thermodynamic limit

Choosing now again as initial conditions the unstable OPMs of both Hamiltonians, let us determine some important statistical properties of the dynamics in the so–called **thermodynamic limit** where E and N grow indefinitely, while E/N is kept constant. In particular, we compute the spectrum of the Lyapunov exponents of the FPU and BEC systems starting at the OPM solutions for energies where these orbits are unstable. We thus find that the Lyapunov exponents are well approximated for both systems by smooth curves of the form $L_i \propto e^{-\alpha i/N}$.

Specifically, as we see in Fig. 7 in the case of the OPM of the FPU Hamiltonian for $\frac{E}{N} = \frac{3}{4}$ we find

$$L_i(N) \propto \; e^{-2.76\frac{i}{N}}, \tag{71}$$

while, in the case of the OPM of the BEC Hamiltonian for fixed $\frac{E}{N} = \frac{3}{2}$, a similar behavior is ob-

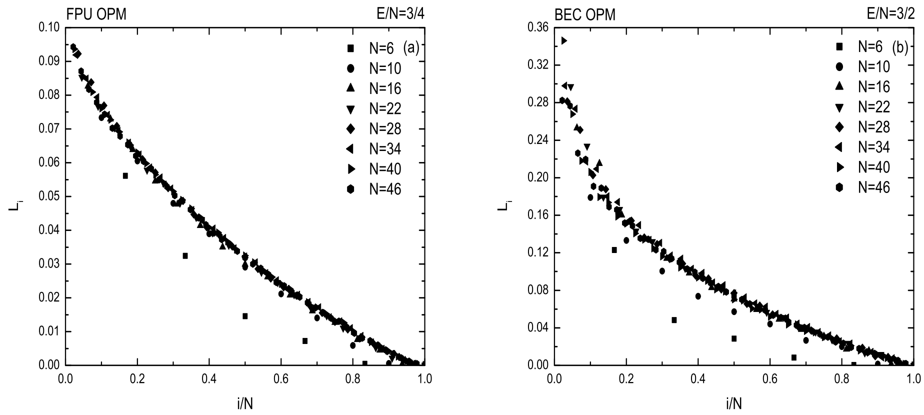

FIG. 7. (a) Positive Lyapunov exponents spectrum of the OPM (50) of the FPU Hamiltonian (44) for fixed $\frac{E}{N} = \frac{3}{4}$. (b) Positive Lyapunov exponents spectrum of the OPM (50) of the BEC Hamiltonian (48) for fixed $\frac{E}{N} = \frac{3}{2}$. In both panels i runs from 1 to N.

served,

$$L_i(N) \propto e^{-3.33\frac{i}{N}}. \tag{72}$$

Next, we compute the well–known Kolmogorov–Sinai entropy $h_{KS}(N)$ (solid curves), which is defined as the sum of the positive Lyapunov exponents,

$$h_{KS}(N) = \sum_{i=1}^{N-1} L_i(N),\ L_i(N) > 0. \tag{73}$$

In this way, we verify, for both Hamiltonians, that $h_{KS}(N)$ is an **extensive thermodynamic quantity** as it is clearly seen in Fig. 8 to grow linearly with N, i.e.,

$$h_{KS}(N) \propto N \tag{74}$$

demonstrating that in their chaotic regions the FPU and BEC Hamiltonians behave as ergodic systems of statistical mechanics.

3.6. Distinguishing order from chaos by the SALI method

3.6.1. Definition of the SALI method

To estimate the "size" of islands of regular motion around stable SPOs we have used the Smaller Alignment Index (SALI) method to distinguish between regular and chaotic orbits in the FPU and BEC Hamiltonians [24–26]. In order to compute the SALI, one follows simultaneously the time evolution of a reference orbit along with two deviation vectors with initial conditions $\vec{w}_1(0)$, $\vec{w}_2(0)$, normalizing them, at every time step to 1,

$$\hat{w}_i(t) = \frac{\vec{w}_i(t)}{\|\vec{w}_i(t)\|},\ \ i = 1, 2. \tag{75}$$

The SALI is then defined as:

$$\mathrm{SALI}(t) = \min\left\{\|\hat{w}_1(t) + \hat{w}_2(t)\|, \|\hat{w}_1(t) - \hat{w}_2(t)\|\right\}, \tag{76}$$

whence it is evident that $\mathrm{SALI}(t) \in [0, \sqrt{2}]$.

It has been shown in the past [24–26] that:

(A) In the case of **chaotic orbits**, the deviation vectors $\hat{w}_1$, $\hat{w}_2$ eventually become aligned in the direction of the maximal Lyapunov exponent and $\mathrm{SALI}(t)$ falls exponentially to zero as

$$\mathrm{SALI}(t) \propto e^{-(L_1 - L_2)t} \tag{77}$$

L_1, L_2 being the two largest LCEs.

(B) In the case of **ordered motion**, on the other hand, the orbit lies on a torus and eventually the vectors $\hat{w}_1$, $\hat{w}_2$ fall on the tangent space

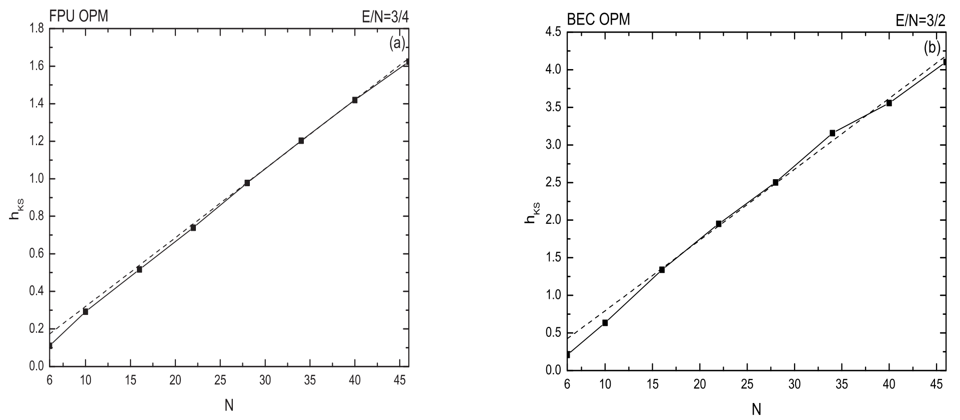

FIG. 8. (a) The $h_{KS}(N)$ entropy near the OPM of the FPU Hamiltonian for fixed $\frac{E}{N} = \frac{3}{4}$ (solid curve) and the approximate formula (dashed curve). (b) The $h_{KS}(N)$ entropy near the OPM of the BEC Hamiltonian for fixed $\frac{E}{N} = \frac{3}{2}$ (solid curve) and the approximate formula (dashed curve).

of the torus, following a t^{-1} time dependence. In this case, the SALI oscillates about values that are different from zero, i.e

$$\text{SALI} \approx \text{const.} > 0, \;\; t \to \infty. \tag{78}$$

Exploiting these different behaviors of SALI for regular and chaotic orbits, we can estimate approximately the "size" of regions of regular motion (or, "islands" of stability) in phase space, by computing SALI at points further and further away from a stable periodic orbit checking whether the orbits are still on a torus (SALI$\geq 10^{-8}$) or have entered a chaotic "sea" (SALI$< 10^{-8}$) up to the final integration time $t_f = 4000$. The initial conditions are chosen perturbing all the positions of the stable SPO by the same quantity dq and all the canonically conjugate momenta by the same dp while keeping always constant the integral F, of the BEC Hamiltonian and the energy E in the case of the FPU Hamiltonian. In this way, we are able to estimate the approximate "magnitude" of the islands of stability in every case varying the energy E and the number of degrees of freedom N (see [1] for more details).

4. The $GALI_k(t)$ indicators of order and chaos in Hamiltonian dynamics

4.1. Geometric interpretation of the SALI

Let us observe, first, that seeking to minimize the two positive quantities in (76) (which are bounded above by $\sqrt{2}$) is essentially equivalent to the evaluation of the product

$$P(t) = \|\hat{w}_1(t) - \hat{w}_2(t)\| \cdot \|\hat{w}_1(t) + \hat{w}_2(t)\|, \tag{79}$$

at every value of t. Indeed, if the minimum of these two quantities is zero (as in the case of a chaotic reference orbit, see below), then so will be the value of $P(t)$. On the other hand, if it is not zero, $P(t)$ will be proportional to the constant about which this minimum oscillates (as in the case of ordered motion, see below). This suggests that, instead of computing the SALI(t) from (76), one might as well evaluate the "exterior" or "wedge" product of the two deviation vectors $\hat{w}_1 \wedge \hat{w}_1$ for which it holds [27]

$$\|\hat{w}_1 \wedge \hat{w}_2\| = \frac{\|\hat{w}_1 - \hat{w}_2\| \cdot \|\hat{w}_1 + \hat{w}_2\|}{2}. \tag{80}$$

Thus, in terms of the wedge product, the SALI is related to the **"area"** between the 2 deviation vectors, $\hat{w}_1$, $\hat{w}_2$. Generalizing to more than two deviations $\hat{w}_1, \hat{w}_2, \ldots, \hat{w}_k$, $2 \leq k \leq 2N$, we introduce an index that is proportional to the **"volume" of the parallelepiped** that has these vectors as vertices [27].

4.2. Definition of the wedge product

Following an introduction to the theory of wedge products as presented in textbooks such as [29], let us consider an M–dimensional vector space V over the field of real numbers $\mathbb{R}$. The exterior algebra of V is denoted by $\Lambda(V)$ and its multiplication, known as the wedge product or the exterior product, is written as $\wedge$. The wedge product is associative, bilinear and alternating on V,

$$\vec{u} \wedge \vec{v} = -\vec{v} \wedge \vec{u} \tag{81}$$

from which it follows that

$$\vec{u} \wedge \vec{u} = \vec{0} \tag{82}$$

for all vectors $\vec{u} \in V$. Thus, we have that

$$\vec{u}_1 \wedge \vec{u}_2 \wedge \cdots \wedge \vec{u}_k = \vec{0} \tag{83}$$

whenever $\vec{u}_1, \vec{u}_2, \ldots, \vec{u}_k \in V$ are linearly dependent.

Let $\{\hat{e}_1, \hat{e}_2, \ldots, \hat{e}_M\}$ be an orthonormal basis of V, i. e. $\hat{e}_i$, $i = 1, 2, \ldots, M$ are linearly independent vectors of unit magnitude

$$\hat{e}_i \cdot \hat{e}_j = \delta_{ij} \tag{84}$$

where $(\cdot)$ denotes the inner product in V.

It can be easily seen that the set

$$\{\hat{e}_{i_1} \wedge \hat{e}_{i_2} \wedge \cdots \wedge \hat{e}_{i_k} \mid 1 \leq i_1 < i_2 < \cdots < i_k \leq M\} \tag{85}$$

is a basis of $\Lambda^k(V)$ since any wedge product of the k–vector $\vec{u}_1 \wedge \vec{u}_2 \wedge \cdots \wedge \vec{u}_k$ can be written as a linear combination of the basis vectors $\hat{e}_i$, $i = 1, 2, \ldots, M$.

The wedge product $\vec{u}_1 \wedge \vec{u}_2 \wedge \cdots \wedge \vec{u}_k$ is defined by

$$\begin{aligned} &\vec{u}_1 \wedge \vec{u}_2 \wedge \cdots \wedge \vec{u}_k \\ &= \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq M} \begin{vmatrix} u_{1i_1} & u_{1i_2} & \cdots & u_{1i_k} \\ u_{2i_1} & u_{2i_2} & \cdots & u_{2i_k} \\ \vdots & \vdots & & \vdots \\ u_{ki_1} & u_{ki_2} & \cdots & u_{ki_k} \end{vmatrix} \\ &\hat{e}_{i_1} \wedge \hat{e}_{i_2} \wedge \cdots \wedge \hat{e}_{i_k} \end{aligned} \tag{86}$$

where the sum is performed over all possible combinations of k indices out of the M total indices. Thus, the coefficient of a particular k–vector $\hat{e}_{i_1} \wedge \hat{e}_{i_2} \wedge \cdots \wedge \hat{e}_{i_k}$ is the determinant of the $k \times k$ submatrix of the $k \times M$ matrix of coefficients appearing in equation (87) formed by its i_1, i_2, …, i_k columns.

Let us write these relations in matrix form

$$\begin{bmatrix} \vec{u}_1 \\ \vec{u}_2 \\ \vdots \\ \vec{u}_k \end{bmatrix} = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1M} \\ u_{21} & u_{22} & \cdots & u_{2M} \\ \vdots & \vdots & & \vdots \\ u_{k1} & u_{k2} & \cdots & u_{kM} \end{bmatrix} \cdot \begin{bmatrix} \hat{e}_1 \\ \hat{e}_2 \\ \vdots \\ \hat{e}_M \end{bmatrix} = \mathbf{C} \cdot \begin{bmatrix} \hat{e}_1 \\ \hat{e}_2 \\ \vdots \\ \hat{e}_M \end{bmatrix} \tag{87}$$

$\mathbf{C}$ being the matrix of the coefficients of vectors $\vec{u}_i$, $i = 1, 2, \ldots, k$ with respect to the orthonormal basis $\hat{e}_i$, $i = 1, 2, \ldots, M$ and v_{ij}, $i = 1, 2, \ldots, k$, $j = 1, 2, \ldots, M$ are real numbers.

Let us consider an autonomous Hamiltonian system of N degrees of freedom having a Hamiltonian function

$$H(q_1, q_2, \ldots, q_N, p_1, p_2, \ldots, p_N) = h = \text{const.} \tag{88}$$

where q_i and p_i, $i = 1, 2, \ldots, N$ are the generalized coordinates and conjugate momenta respectively. An orbit of this system is defined by a vector $\vec{x}(t) = (q_1(t), q_2(t), \ldots, q_N(t), p_1(t), p_2(t), \ldots, p_N(t))$, with $x_i = q_i$, $x_{i+N} = p_i$, $i = 1, 2, \ldots, N$. The time evolution of this orbit is governed by

Hamilton's equations of motion

$$\frac{d\vec{x}}{dt} = \vec{\mathcal{V}}(\vec{x}) = \left(\frac{\partial H}{\partial \vec{p}}, -\frac{\partial H}{\partial \vec{q}}\right), \quad (89)$$

while the time evolution of an initial deviation vector $\vec{w}(0) = (dx_1(0), dx_2(0), \ldots, dx_{2N}(0))$ from the $\vec{x}(t)$ solution of (89) obeys the variational equations

$$\frac{d\vec{w}}{dt} = \mathbf{M}(\vec{x}(t))\,\vec{w}\,, \quad (90)$$

where $\mathbf{M} = \partial\vec{\mathcal{V}}/\partial\vec{x}$ is the Jacobian matrix of $\vec{\mathcal{V}}$.

All normalized deviation vectors $\hat{w}_i$, $i = 1, 2, \ldots, 2N$, belong to the $2N$–dimensional tangent space of the Hamiltonian flow. Using as a basis of this space the usual set of orthonormal vectors, any such unit deviation vector $\hat{w}_i$ can be written as

$$\hat{w}_i = \sum_{j=1}^{2N} w_{ij}\hat{e}_j, \;\; i = 1, 2, \ldots, k \quad (91)$$

where w_{ij} are real numbers satisfying

$$\sum_{j=1}^{2N} w_{ij}^2 = 1, \;\; i = 1, 2, \ldots, k. \quad (92)$$

Thus, equation (87) gives

$$\begin{bmatrix} \hat{w}_1 \\ \hat{w}_2 \\ \vdots \\ \hat{w}_k \end{bmatrix} = \begin{bmatrix} w_{11} & w_{12} & \cdots & w_{1\,2N} \\ w_{21} & w_{22} & \cdots & w_{2\,2N} \\ \vdots & \vdots & & \vdots \\ w_{k1} & w_{k2} & \cdots & w_{k\,2N} \end{bmatrix} \cdot \begin{bmatrix} \hat{e}_1 \\ \hat{e}_2 \\ \vdots \\ \hat{e}_{2N} \end{bmatrix}. \quad (93)$$

Using then equation (86) the wedge product of these k deviation vectors takes the form

$$\hat{w}_1 \wedge \hat{w}_2 \wedge \cdots \wedge \hat{w}_k = \sum_{1 \le i_1 < i_2 < \cdots < i_k \le 2N} \begin{vmatrix} w_{1i_1} & w_{1i_2} & \cdots & w_{1i_k} \\ w_{2i_1} & w_{2i_2} & \cdots & w_{2i_k} \\ \vdots & \vdots & & \vdots \\ w_{ki_1} & w_{ki_2} & \cdots & w_{ki_k} \end{vmatrix} \hat{e}_{i_1} \wedge \hat{e}_{i_2} \wedge \cdots \wedge \hat{e}_{i_k}. \quad (94)$$

If at least two of the normalized deviation vectors $\hat{w}_i$, $i = 1, 2, \ldots, k$ are linearly dependent, all the $k \times k$ determinants appearing in equation (94) will become zero making the "volume" vanish. Equivalently the quantity

$$\|\hat{w}_1 \wedge \hat{w}_2 \wedge \cdots \wedge \hat{w}_k\| = \left\{ \sum_{1 \le i_1 < i_2 < \cdots < i_k \le 2N} \begin{vmatrix} w_{1i_1} & w_{1i_2} & \cdots & w_{1i_k} \\ w_{2i_1} & w_{2i_2} & \cdots & w_{2i_k} \\ \vdots & \vdots & & \vdots \\ w_{ki_1} & w_{ki_2} & \cdots & w_{ki_k} \end{vmatrix}^2 \right\}^{1/2} \quad (95)$$

which we call the "norm" of the wedge product, will also become zero. Thus, we define this quantity as the Generalized Alignment Index (GALI) of order k

$$\mathrm{GALI}_k(t) = \|\hat{w}_1(t) \wedge \hat{w}_2(t) \wedge \cdots \wedge \hat{w}_k(t)\|\,. \quad (96)$$

Consequently, if at least one of the deviation vectors **becomes linearly dependent** on the remaining ones, $\mathrm{GALI}_k(t)$ will tend to zero as the volume of the parallelepiped having the vectors $\hat{w}_i$ as edges shrinks to zero. On the other hand, if $\mathrm{GALI}_k(t)$ remains far from zero, as t grows arbitrarily, this would indicate the **linear independence** of the deviation vectors and the existence of a corresponding parallelepiped, whose volume is different from zero for all time.

4.3. Theoretical results for the Time Evolution of GALI

4.3.1. Exponential decay of GALI for chaotic orbits

Let us first investigate the dynamics in the vicinity of a chaotic orbit of the Hamiltonian system, with N degrees of freedom. Let

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{2N} \tag{97}$$

be the "local Lyapunov exponents" oscillating about their time averaged values

$$\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{N-1} \geq \sigma_N = \sigma_{N+1} = 0 \geq \sigma_{N+2} \geq \cdots \geq \sigma_{2N} \tag{98}$$

which are the "global" LCEs. Assuming that the λ_i, $i = 1, 2, \ldots, 2N$ do not fluctuate significantly, the evolution of any initial deviation vector $\vec{w}_i$ may be written as

$$\vec{w}_i(t) = \sum_{j=1}^{2N} c_j^i \, e^{\sigma_j t} \, \hat{u}_j. \tag{99}$$

A leading order estimate of the deviation vector's Euclidean norm, for long enough times, is

$$\|\vec{w}_i(t)\| \approx |c_1^i| e^{\sigma_1 t}. \tag{100}$$

Consequently, the matrix $\mathbf{C}$ in (87) of coefficients of k normalized deviation vectors $\hat{w}_i(t) = \vec{w}_i(t)/\|\vec{w}_i(t)\|$, $i = 1, 2, \ldots, k$ with $2 \leq k \leq 2N$, using as basis of the vector space the set $\{\hat{u}_1, \hat{u}_2, \ldots, \hat{u}_{2N}\}$ becomes

$$\mathbf{C}(t) = [c_{ij}] = \begin{bmatrix} s_1 & \frac{c_2^1}{|c_1^1|} e^{-(\sigma_1 - \sigma_2)t} & \frac{c_3^1}{|c_1^1|} e^{-(\sigma_1 - \sigma_3)t} & \cdots & \frac{c_{2N}^1}{|c_1^1|} e^{-(\sigma_1 - \sigma_{2N})t} \\ s_2 & \frac{c_2^2}{|c_1^2|} e^{-(\sigma_1 - \sigma_2)t} & \frac{c_3^2}{|c_1^2|} e^{-(\sigma_1 - \sigma_3)t} & \cdots & \frac{c_{2N}^2}{|c_1^2|} e^{-(\sigma_1 - \sigma_{2N})t} \\ \vdots & \vdots & & \cdots & \vdots \\ s_k & \frac{c_2^k}{|c_1^k|} e^{-(\sigma_1 - \sigma_2)t} & \frac{c_3^k}{|c_1^k|} e^{-(\sigma_1 - \sigma_3)t} & \cdots & \frac{c_{2N}^k}{|c_1^k|} e^{-(\sigma_1 - \sigma_{2N})t} \end{bmatrix}, \tag{101}$$

with $s_i = \text{sign}(c_1^i)$ and $i = 1, 2, \ldots, k$, $j = 1, 2, \ldots, 2N$ and so we have

$$\left[\, \hat{w}_1 \;\; \hat{w}_2 \;\; \ldots \;\; \hat{w}_k \,\right]^{\mathrm{T}} = \mathbf{C} \cdot \left[\, \hat{u}_1 \;\; \hat{u}_2 \;\; \ldots \;\; \hat{u}_{2N} \,\right]^{\mathrm{T}} \tag{102}$$

with $(^{\mathrm{T}})$ denoting the transpose of a matrix. The wedge product of the k normalized deviation vectors is then computed as in equation (94) by:

$$\hat{w}_1(t) \wedge \hat{w}_2(t) \wedge \cdots \wedge \hat{w}_k(t) = \sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq 2N} \begin{vmatrix} c_{1i_1} & c_{1i_2} & \cdots & c_{1i_k} \\ c_{2i_1} & c_{2i_2} & \cdots & c_{2i_k} \\ \vdots & \vdots & & \vdots \\ c_{ki_1} & c_{ki_2} & \cdots & c_{ki_k} \end{vmatrix} \hat{u}_{i_1} \wedge \hat{u}_{i_2} \wedge \cdots \wedge \hat{u}_{i_k}. \tag{103}$$

Note that the quantity

$$S_k = \left(\sum_{1 \leq i_1 < i_2 < \cdots < i_k \leq 2N} \begin{vmatrix} c_{1i_1} & c_{1i_2} & \cdots & c_{1i_k} \\ c_{2i_1} & c_{2i_2} & \cdots & c_{2i_k} \\ \vdots & \vdots & & \vdots \\ c_{ki_1} & c_{ki_2} & \cdots & c_{ki_k} \end{vmatrix}^2 \right)^{\frac{1}{2}} \tag{104}$$

is *not identical* with the norm (95) of the k-vector $\hat{w}_1(t) \wedge \hat{w}_2(t) \wedge \cdots \wedge \hat{w}_k(t)$ as the wedge product in equation (103) is not expressed with respect to the usual basis. Thus one should consider the transformation

$$\left[\ \hat{u}_1\ \ \hat{u}_2\ \ \ldots\ \ \hat{u}_{2N}\ \right]^{\mathrm{T}} = \mathbf{T}_c \cdot \left[\ \hat{e}_1\ \ \hat{e}_2\ \ \ldots\ \ \hat{e}_{2N}\ \right]^{\mathrm{T}}, \tag{105}$$

between the two bases, with $\mathbf{T}_c$ denoting the transformation matrix. Thus, if we consider the wedge product of *fewer* than $2N$ deviation vectors, the norm (95) and the quantity S_k (104) are not related through a simple expression. We shall proceed, however, to obtain results using (104) instead of (95), because: First, we note that both quantities are zero, when at least two of the k deviation vectors are linearly dependent. In addition, the transformation matrix $\mathbf{T}_c$ is not singular as the sets $\{\hat{u}_i\}$ and $\{\hat{e}_i\}$, $i = 1, 2, \ldots, 2N$ continue to be valid bases of the vector space.

The determinants appearing in the definition of S_k (see equation (104)) can be divided in two categories depending on whether or not they contain the first column of matrix $\mathbf{C}$. Using standard properties of determinants, we see that those that do contain the first column yield

$$D_{1,j_1,j_2,\ldots,j_{k-1}} = \begin{vmatrix} s_1 & \frac{c^1_{j_1}}{|c^1_1|}e^{-(\sigma_1-\sigma_{j_1})t} & \ldots & \frac{c^1_{j_{k-1}}}{|c^1_1|}e^{-(\sigma_1-\sigma_{j_{k-1}})t} \\ s_2 & \frac{c^2_{j_1}}{|c^2_1|}e^{-(\sigma_1-\sigma_{j_1})t} & \ldots & \frac{c^2_{j_{k-1}}}{|c^2_1|}e^{-(\sigma_1-\sigma_{j_{k-1}})t} \\ \vdots & \vdots & & \vdots \\ s_k & \frac{c^k_{j_1}}{|c^k_1|}e^{-(\sigma_1-\sigma_{j_1})t} & \ldots & \frac{c^k_{j_{k-1}}}{|c^k_1|}e^{-(\sigma_1-\sigma_{j_{k-1}})t} \end{vmatrix} = \begin{vmatrix} s_1 & \frac{c^1_{j_1}}{|c^1_1|} & \cdots & \frac{c^1_{j_{k-1}}}{|c^1_1|} \\ s_2 & \frac{c^2_{j_1}}{|c^2_1|} & \cdots & \frac{c^2_{j_{k-1}}}{|c^2_1|} \\ \vdots & \vdots & & \vdots \\ s_k & \frac{c^k_{j_1}}{|c^k_1|} & \cdots & \frac{c^k_{j_{k-1}}}{|c^k_1|} \end{vmatrix} \times e^{-t\left[(\sigma_1-\sigma_{j_1})+(\sigma_1-\sigma_{j_2})+\cdots+(\sigma_1-\sigma_{j_{k-1}})\right]} \tag{106}$$

with $1 < j_1 < j_2 < \ldots < j_{k-1} \le 2N$. Thus, the time evolution of $D_{1,j_1,j_2,\ldots,j_{k-1}}$ is mainly determined by the exponential law

$$D_{1,j_1,j_2,\ldots,j_{k-1}} \propto e^{-\left[(\sigma_1-\sigma_{j_1})+(\sigma_1-\sigma_{j_2})+\cdots+(\sigma_1-\sigma_{j_{k-1}})\right]t}. \tag{107}$$

Similarly, we deduce that the determinants that do *not* contain the first column of matrix $\mathbf{C}$ (101) have a form $D_{j_1,j_2,\ldots,j_k}$, with $1 < j_1 < j_2 < \ldots < j_{k-1} < j_k \le 2N$, that also tends to zero following an exponential law

$$D_{j_1,j_2,\ldots,j_k} \propto e^{-\left[(\sigma_1-\sigma_{j_1})+(\sigma_1-\sigma_{j_2})+\cdots+(\sigma_1-\sigma_{j_{k-1}})+(\sigma_1-\sigma_{j_k})\right]t}. \tag{108}$$

Clearly, from all determinants appearing in the definition of S_k, (104), the one that decreases the *slowest* is the one containing the first k columns of matrix $\mathbf{C}$ in (101):

$$D_{1,2,3,\ldots,k} \propto e^{-[(\sigma_1-\sigma_2)+(\sigma_1-\sigma_3)+\cdots+(\sigma_1-\sigma_k)]t} \tag{109}$$

yielding the approximation that GALI_k tends to zero as above, i.e.

$$\mathrm{GALI}_k(t) \propto e^{-[(\sigma_1-\sigma_2)+(\sigma_1-\sigma_3)+\cdots+(\sigma_1-\sigma_k)]t}. \tag{110}$$

Note that in the previous analysis we assumed that $\sigma_1 > \sigma_2$ so that the norm of each deviation vector can be well approximated by equation (100). If the first m Lyapunov exponents, with $1 < m < k$, are equal, or very close to each other, i.e. $\sigma_1 \simeq \sigma_2 \simeq \cdots \simeq \sigma_m$ equation (110) becomes

$$\mathrm{GALI}_k(t) \propto e^{-[(\sigma_1-\sigma_{m+1})+(\sigma_1-\sigma_{m+2})+\cdots+(\sigma_1-\sigma_k)]t}, \tag{111}$$

which still describes an exponential decay.

4.3.2. The evaluation of GALI for ordered orbits

As is well–known, ordered orbits of an N degree of freedom Hamiltonian system (88) typically lie on N–dimensional tori, which can be described by a local transformation to action–angle variables, so that the equations of motion, locally become

$$\begin{array}{rcl} \dot{J}_i & = & 0 \\ \dot{\theta}_i & = & \omega_i(J_1, J_2, \ldots, J_N) \end{array}, \; i = 1, 2, \ldots, N. \tag{112}$$

These can be easily integrated to give

$$\begin{array}{rcl} J_i(t) & = & J_{i0} \\ \theta_i(t) & = & \theta_{i0} + \omega_i(J_{10}, J_{20}, \ldots, J_{N0})\, t, \\ & & i = 1, 2, \ldots, N, \end{array} \tag{113}$$

where J_{i0}, θ_{i0}, $i = 1, 2, \ldots, N$ are the initial conditions.

By denoting as ξ_i, η_i, $i = 1, 2, \ldots, N$ small deviations of J_i and θ_i respectively, the variational equations of system (112), can be solved to yield:

$$\begin{array}{rcl} \xi_i(t) & = & \xi_i(0) \\ \eta_i(t) & = & \eta_i(0) + \left[\sum_{j=1}^{N} \omega_{ij}\xi_j(0)\right] t, \\ & & i = 1, 2, \ldots, N. \end{array} \tag{114}$$

Thus, we see that an initial deviation vector $\vec{w}(0)$ evolves in time in such a way that its action coordinates remain constant, while its angle coordinates increase linearly in time. This implies an almost linear increase of the norm of the deviation vector, whose time evolution is given by

$$\|\vec{w}(t)\|^2 = 1 + \left[\sum_{i=1}^{N}\left(\sum_{j=1}^{N}\omega_{ij}\xi_j(0)\right)\right] t^2 + 2\left[\sum_{i=1}^{N}\left(\eta_i(0)\sum_{j=1}^{N}\omega_{ij}\xi_j(0)\right)\right] t. \tag{115}$$

Therefore, this normalized deviation vector tends to **fall on the tangent space of the torus**, since its coordinates perpendicular to the torus (i. e. the coordinates along the action directions) vanish following a t^{-1} rate.

Using as a basis of the $2N$–dimensional phase space the $2N$ unit vectors $\{\hat{v}_1, \hat{v}_2, \ldots, \hat{v}_{2N}\}$, such that the first N of them, $\hat{v}_1, \hat{v}_2, \ldots, \hat{v}_N$ correspond to the N action variables and the remaining ones, $\hat{v}_{N+1}, \hat{v}_{N+2}, \ldots, \hat{v}_{2N}$ to the N conjugate angle variables, any unit deviation vector $\hat{w}_i$, $i = 1, 2, \ldots$ can be written as

$$\hat{w}_i(t) = \frac{1}{\|\vec{w}(t)\|} \cdot \left[\sum_{j=1}^{N}\xi_j^i(0)\,\hat{v}_j + \sum_{j=1}^{N}\left(\eta_j^i(0) + \sum_{k=1}^{N}\omega_{kj}\xi_j^i(0)t\right)\hat{v}_{N+j}\right]. \tag{116}$$

Note that if the initial deviation vector *lies in the tangent space of the torus* it will remain constant for all time having norm 1! In particular, such a vector has the form

$$\hat{w}(t) = (0, 0, \ldots, 0, \eta_1(0), \eta_2(0), \ldots, \eta_N(0)). \tag{117}$$

Let us now study the case of k, general, linearly independent unit deviation vectors $\{\hat{w}_1, \hat{w}_2, \ldots, \hat{w}_k\}$ with $2 \leq k \leq 2N$. Using as vector basis the set $\{\hat{v}_1, \hat{v}_2, \ldots, \hat{v}_{2N}\}$ we get:

$$\left[\, \hat{w}_1 \;\; \hat{w}_2 \;\; \ldots \;\; \hat{w}_k \,\right]^{\mathrm{T}} = \mathbf{D} \cdot \left[\, \hat{v}_1 \;\; \hat{v}_2 \;\; \ldots \;\; \hat{v}_{2N} \,\right]^{\mathrm{T}}. \tag{118}$$

If *no* deviation vector is initially located in the tangent space of the torus, matrix $\mathbf{D}$ has the form

$$\mathbf{D} = [d_{ij}] = \frac{1}{\prod_{m=1}^{k} \|\vec{w}_m(t)\|} \cdot \mathbf{D}^{0,k}(t) \tag{119}$$

where $i = 1, 2, \ldots, k$ and $j = 1, 2, \ldots, 2N$. Recalling our earlier discussion, the norm of vector $\vec{w}_i(t)$ for long times, grows linearly with t as

$$M_i(t) = \|\vec{w}_i(t)\| \propto t. \tag{120}$$

The matrix $\mathbf{D}$ then assumes the much simpler form

$$\mathbf{D}(t) = \frac{1}{t^k} \cdot \mathbf{D}^{0,k}(t). \tag{121}$$

Since, in general, we choose the initial deviation vectors randomly (insisting only that they be linearly independent), the most common situation is that none of the initial deviation vectors is tangent to the torus. However, as this may not always hold, we need to consider also the possibility that $0 < m \leq N$ of our deviation vectors are initially in the tangent space of the torus. For $2 \leq k < N$, this will make no difference, as the GALI_k will still tend to a non–zero constant. However, for $N < k \leq 2N$, GALI_k goes to zero by a power law and the fact that m vectors are already in the tangent space, at $t = 0$, can significantly affect the decay rate of the index. Thus, in such cases, the behavior of GALI needs to be treated separately.

4.3.3. The case of $m > 0$ tangent initial deviation vectors

Let us start with the case where k is lower than the dimension of the tangent space of the torus, i. e. $2 \leq k \leq N$. The fastest increasing determinants in this case are the determinants, whose k columns are chosen among the last N columns of matrix $\mathbf{D}^{0,k}$. Thus, using standard properties of determinants, we easily see that their time evolution is mainly dictated by the time evolution of determinants of the form

$$\left|\, \omega_{j_1 m_1} \boldsymbol{\xi}^{0,k}_{m_1} t \;\; \omega_{j_2 m_2} \boldsymbol{\xi}^{0,k}_{m_2} t \;\; \cdots \;\; \omega_{j_k m_k} \boldsymbol{\xi}^{0,k}_{m_k} t \,\right| = \propto t^k, \tag{122}$$

where $m_i \in \{1, 2, \ldots, N\}$, $i = 1, 2, \ldots, k$, with $m_i \neq m_j$, for all $i \neq j$. Thus, we conclude that the contribution to the behavior in S'_k (S'_k is a quantity analogous to S_k in (104)) of the determinants related to $\Delta^{0,k}_{j_1, j_2, \ldots, j_k}$ is to provide constant terms. All other determinants appearing in the definition of S'_k, not being of the form of $\Delta^{0,k}_{j_1, j_2, \ldots, j_k}$, contain at least one column from the first N columns of matrix $\mathbf{D}^{0,k}$ and introduce terms that grow at a rate *slower* than t^k, proportional to $t^{k-m}/t^k = 1/t^m$ ($1 < m \leq k$) and tending to zero as t grows. Thus, the overall behavior of S'_k will be of the form t^k, which yields the important result

$$\mathrm{GALI}_k(t) \approx \text{constant} \;\; \text{for} \;\; 2 \leq k \leq N. \tag{123}$$

Next, let us turn to the more subtle case of k deviation vectors with $N < k \leq 2N$. The fastest growing determinants are again those containing the last N columns of the matrix $\mathbf{D}^{0,k}$: Thus, the time evolution of these determinants is mainly determined by $\propto t^{2N-k}$ which contribute to the time evolution of S'_k by introducing terms proportional to

$$t^{2N-k}/t^k = 1/t^{2(k-N)}. \tag{124}$$

All other determinants appearing in the definition of S'_k introduce terms that tend to zero faster than $1/t^{2(k-N)}$ since they contain more than $k - N$ time independent columns of the form $\boldsymbol{\xi}^{0,k}_i$, $i = 1, 2, \ldots, N$. Thus the GALI_ks tend to zero following a power law of the form:

$$\mathrm{GALI}_k(t) \propto \frac{1}{t^{2(k-N)}} \;\; \text{for} \;\; N \leq k \leq 2N. \tag{125}$$

Finally, let us consider the behavior of GALI_k in the case where m deviation vectors, with $m \leq k$ and $m \leq N$, are initially located in the tangent space of the torus. Here, all determinants appearing in the definition of S'_k have as a common factor the quantity $1/\prod_{i=1}^{k-m} M_{m+i}(t)$, which decreases to zero following a power law

$$\frac{1}{\prod_{i=1}^{k-m} M_{m+i}(t)} \propto \frac{1}{t^{k-m}}. \tag{126}$$

Proceeding in exactly the same manner as in the $m = 0$ case, we deduce that, in the case of $2 \leq k < N$ the fastest growing $k \times k$ determinants are of the form:

$$\left| \boldsymbol{\eta}_{i_1}^k \;\; \boldsymbol{\eta}_{i_2}^k \;\; \cdots \;\; \boldsymbol{\eta}_{i_m}^k \;\; \omega_{i_{m+1}n_1}\boldsymbol{\xi}_{n_1}^{0,k}t \;\; \omega_{i_{m+2}n_2}\boldsymbol{\xi}_{n_2}^{0,k}t \;\; \cdots \;\; \omega_{i_k n_{k-m}}\boldsymbol{\xi}_{n_{k-m}}^{0,k}t \right| \propto t^{k-m}, \tag{127}$$

with $i_l \in \{1, 2, \ldots, N\}$, $l = 1, 2, \ldots, k$ with $i_l \neq i_j$ and $n_l \in \{1, 2, \ldots, N\}$, $l = 1, 2, \ldots, k-m$ with $n_l \neq n_j$, for $l \neq j$. Hence, we conclude that the behavior of S'_k, and consequently of GALI_k is defined by the behavior of determinants having the form of (127) which, when combined with (126) implies that

$$\mathrm{GALI}_k(t) \approx \text{const. for } 2 \leq k \leq N. \tag{128}$$

The case of $N < k \leq 2N$ deviation vectors, however, with $m > 0$ initially tangent vectors, yields a considerably different result. Following entirely analogous arguments as in the $m = 0$ case, we find that, if $m < k-N$, S'_k and GALI_k evolve proportionally to $t^{2N-k}/t^{k-m} = 1/t^{2(k-N)-m}$. On the other hand, if $m \geq k-N$, one can show that the fastest growing determinant is proportional to t^{N-m}. In this case, S'_k and GALI_k evolve in time following a quite *different* power law:

$$t^{N-m}/t^{k-m} = 1/t^{k-N}. \tag{129}$$

Summarizing the results of this section, we see that GALI_k remains essentially constant when $k \leq N$, while it tends to zero for $k > N$ following a power law which depends on the number m ($m \leq N$ and $m \leq k$) of deviation vectors initially tangent to the torus. In conclusion, we have shown that:

$$\mathrm{GALI}_k(t) \propto \begin{cases} \text{const.} & \text{if } 2 \leq k \leq N \\ \frac{1}{t^{2(k-N)-m}} & \text{if } N < k \leq 2N \text{ and } 0 \leq m < k-N \\ \frac{1}{t^{k-N}} & \text{if } N < k \leq 2N \text{ and } m \geq k-N \end{cases} \tag{130}$$

4.4. Numerical verification and applications

We will apply these theoretical results first to the example of 2 (2D) degrees of freedom: the Hénon–Heiles Hamiltonian [20]

$$H_2 = \frac{1}{2}(p_x^2+p_y^2)+\frac{1}{2}(x^2+y^2)+x^2y-\frac{1}{3}y^3, \tag{131}$$

and then study the higher–dimensional 15D Fermi–Pasta–Ulam (FPU) model

$$H_{15} = \frac{1}{2}\sum_{i=1}^{15} p_i^2 + \sum_{i=1}^{15}\left[\frac{1}{2}(q_{i+1}-q_i)^2 + \frac{1}{4}\beta(q_{i+1}-q_i)^4\right]. \quad (132)$$

4.4.1. A 2D Hamiltonian system

Let us consider a chaotic orbit of the 2D Hamiltonian (131), with initial conditions $x = 0$, $y = -0.25$, $p_x = 0.42$, $p_y = 0$. In Fig. 9(a) we see the time evolution of $L_1(t)$ of this orbit, which is a good approximation of the maximal LCE, σ_1. Actually, for $t \approx 10^5$, we find $\sigma_1 \approx 0.047$. We recall that 2D Hamiltonian systems have only one positive LCE σ_1, since the second largest is $\sigma_2 = 0$. It also holds that $\sigma_3 = -\sigma_2$ and $\sigma_4 = -\sigma_1$ and thus formula (110), which describes GALI_k for chaotic orbits, gives

$$\text{GALI}_2(t) \propto e^{-\sigma_1 t},\ \ \text{GALI}_3(t) \propto e^{-2\sigma_1 t},\ \ \text{GALI}_4(t) \propto e^{-4\sigma_1 t}. \quad (133)$$

Note in the above figure one of the main advantages of GALI_k over the computation of Lyapunov exponents. Due to the large fluctuations of LCEs, one often has to wait very long (about 10^4 time units) before concluding that $L_1(t)$ actually converges to a non zero value in Fig. 9(a). By contrast, the GALIs of Fig. 9(b) have revealed the chaotic nature of the orbit already after about $t = 600$ units!

Now, for an ordered orbit of the 2D Hamiltonian (131) and a random choice of initial deviation vectors, we expect the GALI indices to behave as

$$\text{GALI}_2(t) \propto \text{constant},\ \ \text{GALI}_3(t) \propto \frac{1}{t^2},\ \ \text{GALI}_4(t) \propto \frac{1}{t^4}. \quad (134)$$

We now use the smooth curve of a quasiperiodic orbit on the PSS of the system (131) to choose initial deviation vectors **tangent to a torus**. From the morphology of two closed curves plotted on x, p_x and y, p_y surfaces of section, it is easy to verify that deviation vectors $\hat{e}_1 = (1, 0, 0, 0)$ and $\hat{e}_4 = (0, 0, 0, 1)$ are tangent to the torus.

In Fig. 10, we plot the time evolution of SALI, GALI_2, GALI_3 and GALI_4 for an ordered orbit, for various choices of initial deviation vectors. In Fig. 10(a) the initial deviation vectors are randomly chosen so that none of them is tangent to the torus. In Fig. 10(b) we present results when $m = 1$ initial deviation vector is tangent to the torus (in particular vector $\hat{e}_1$). Finally, in Fig. 10(c) we have plotted our results using $m = 2$ initial deviation vectors tangent to the torus (vectors $\hat{e}_1$ and $\hat{e}_4$).

Figs. 9(b) and 10 clearly illustrate that GALI_3 and GALI_4 tend to zero both for ordered and chaotic orbits, but with different time rates. In particular, both indices tend to zero exponentially for chaotic orbits, while they follow a power law for ordered ones. We may use this difference of rates to distinguish between chaotic and ordered motion following a different approach than SALI or GALI_2.

Let us illustrate this by considering the computation of GALI_4: From (133) and (134), we expect $\text{GALI}_4 \propto e^{-4\sigma_1 t}$ for chaotic orbits and $\text{GALI}_4 \propto 1/t^4$ for ordered ones. These time rates imply that, in general, the time needed for the index to become zero is much larger for ordered orbits. Thus, instead of simply registering the value of the index at the end of a given time interval (as we do with SALI or GALI_2), let us record the time, t_{th}, needed for GALI_4 to reach a very small threshold, e. g. 10^{-12}, and color each grid point according to the value of t_{th}.

The outcome of this procedure for the 2D Hénon–Heiles system (131) is presented in Fig. 11. Each orbit is integrated up to $t = 500$ units and if the value of GALI_4, at the end of the integration is larger than 10^{-12} the corresponding grid point is colored by the light gray color used for $t_{th} \geq 400$. At the border between them we find points having intermediate values of t_{th}

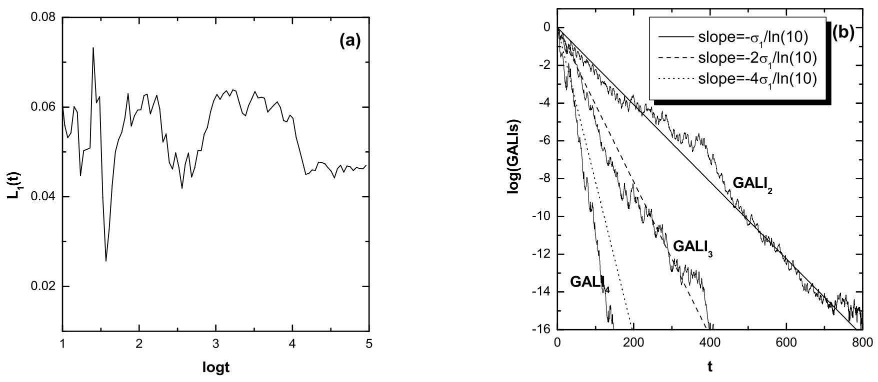

FIG. 9. (a) The evolution of $L_1(t)$ for a chaotic orbit with initial conditions $x = 0$, $y = -0.25$, $p_x = 0.42$, $p_y = 0$ of the 2D system (131). (b) The evolution of GALI_2, GALI_3 and GALI_4 of the same orbit. The plotted lines correspond to functions proportional to $e^{-\sigma_1 t}$ (solid line), $e^{-2\sigma_1 t}$ (dashed line) and $e^{-4\sigma_1 t}$ (dotted line) for $\sigma_1 = 0.047$. Note that the t-axis is linear.

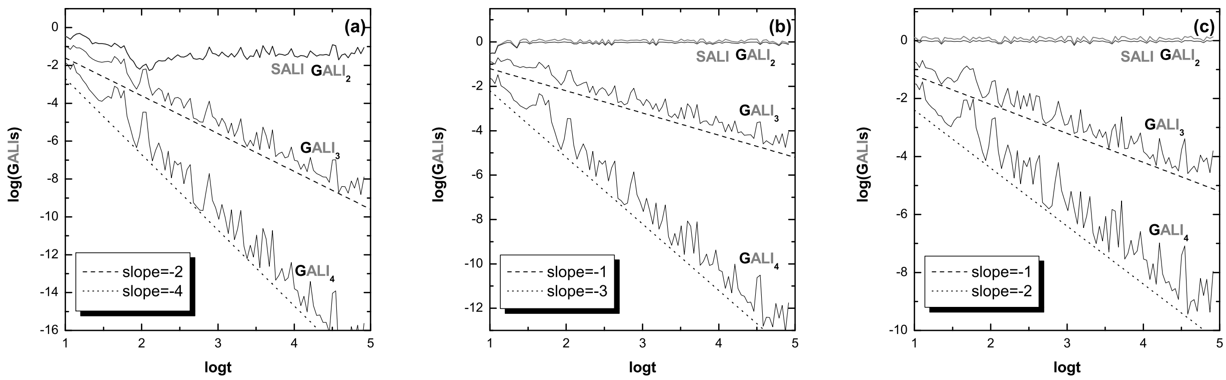

FIG. 10. Time evolution of SALI (gray curves), GALI_2, GALI_3 and GALI_4 for an ordered orbit in log-log scale for different values of the number m of deviation vectors initially tangent to the torus: (a) $m = 0$, (b) $m = 1$ and (c) $m = 2$. We note that in panel (a) the curves of SALI and GALI_2 are very close to each other and thus cannot be distinguished. In every panel, dashed lines corresponding to particular power laws are also plotted.

which belong to the so–called "sticky" chaotic regions.

4.4.2. A multi–dimensional Hamiltonian system

Let us finally turn to a much higher–dimensional Hamiltonian system having 15 degrees of freedom, i. e. the one described b the FPU Hamiltonian (132). Using fixed boundary conditions

$$q_0(t) = q_{16}(t) = 0, \ \forall t \qquad (135)$$

it is known that there exists, for all energies, $H_{15} = E$, a simple periodic orbit, which we called SPO1 above

$$q_{2i}(t) = 0, q_{2i-1}(t) = -q_{2i+1}(t) = q(t), \quad i = 1, 2, \ldots, 7. \qquad (136)$$

For the parameter values $H_{15} = 26.68777$ and $\beta = 1.04$ used in an earlier study [1], we know

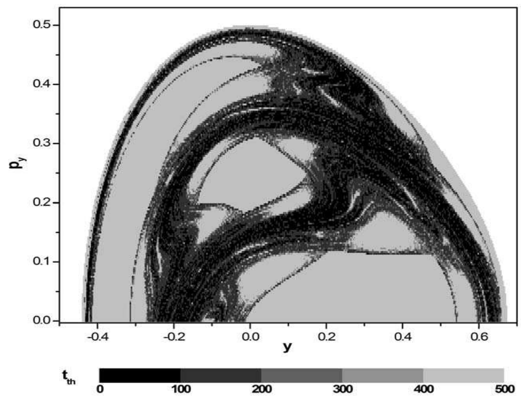

FIG. 11. Regions of different values of the time t_{th} needed for GALI_4 to become less than 10^{-12} on the PSS defined by $x = 0$ of the 2D Hénon–Heiles Hamiltonian (131).

that this orbit is unstable and has a sizable chaotic region around it. As initial conditions for (136) we take

$$q(0) = 1.322 \text{ and } p_i(0) = 0,\ i = 1, 2, \ldots, 15. \tag{137}$$

First, we consider a chaotic orbit which is located in the **immediate neighborhood** of this periodic solution, by taking as initial conditions $q_1(0) = q(0)$, $q_3(0) = q_7(0) = q_{11}(0) = -q(0) + 10^{-7}$, $q_5(0) = q_9(0) = q_{15}(0) = q(0) - 10^{-7}$, $q_{2i} = 0$ for $i = 1, 2, \ldots, 7$ and $p_i(0) = 0$ for $i = 1, 2, \ldots, 14$, $p_{15}(0) = 0.00323$. The chaotic nature of this orbit is revealed by the fact that it has positive LCEs (see Fig. 12(a)). In fact, from the results of Fig. 12(a) we deduce reliable estimates of the system's four largest Lyapunov exponents: $\sigma_1 \approx 0.132$, $\sigma_2 \approx 0.117$, $\sigma_3 \approx 0.104$ and $\sigma_4 \approx 0.093$. Here, we have a case where the largest two LCEs are very close to each other. The behavior of the GALIs is again quite accurately approximated by the theoretically predicted exponential laws (110). This becomes evident by the results presented in Fig. 12(b), where we plot the time evolution of GALI_2, GALI_3 and GALI_4 as well as the exponential laws that theoretically describe the evolution of these indices. In this case, SALI decays to zero relatively slowly since σ_1 and σ_2 have similar values and hence, using GALI_3, GALI_4 or a GALI of higher order, one can determine the chaotic nature of the orbit much faster.

5. Conclusions

After reviewing the classical results of A. M. Lyapunov on the global stability of motion of nonlinear dynamical systems, I described in this paper how he was led to his famous proof of the continuation of normal modes of coupled, non–degenerate harmonic oscillators to the nonlinear case, where polynomial terms (of degree higher than 2) are allowed in the Hamiltonian. These so–called nonlinear normal modes are examples of what we call **simple periodic orbits** (SPOs), i.e. solutions where all variables oscillate in or out of phase with each other, with the same frequencies. We then went on to study such SPOs in a number of Hamiltonian systems, from the point of view of their **local** stability analysis and described a number of interesting results, which appear to hold for arbitrarily large values of N and total energy E, demonstrating that such solutions are indeed very important for the global properties of motion in these systems. In particular:

1) We studied the connection between local and global dynamics of different N degrees of freedom Hamiltonian systems, known as the FPU and BEC systems. We focused on simple periodic orbits (SPOs) and showed that the energy per particle of their first destabilization decays with a simple power–law

$$E_c/N \propto N^{-\alpha},\ \alpha = 1,\ or,\ 2. \tag{138}$$

One notable exception is the IPM orbit of the BEC Hamiltonian, which is found to be stable for any energy and number of degrees of freedom we considered!

2) We showed in the FPU β–model that the local properties of a relatively high $q = 2(N+1)/3$ mode of the linear lattice, called SPO2, are very important for the global dynamics of the system. It destabilizes as $E_2/N \propto N^{-2}$, much faster than

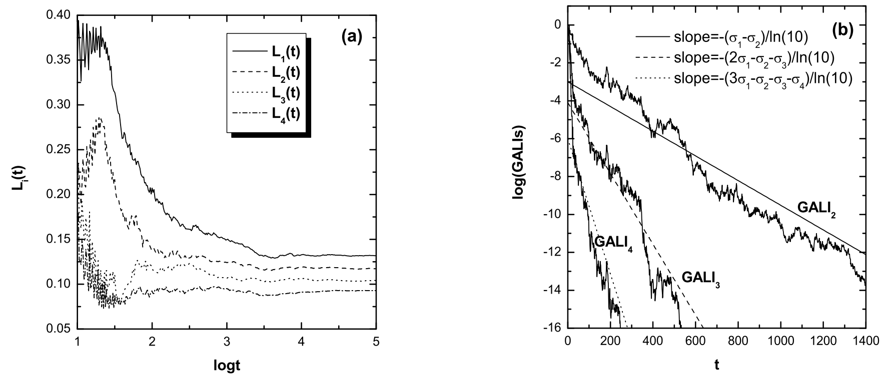

FIG. 12. (a) The evolution of $L_1(t)$, $L_2(t)$, $L_3(t)$ and $L_4(t)$ for a chaotic orbit of the 15D system (132). (b) The evolution of GALI_2, GALI_3 and GALI_4 for the same orbit. The plotted lines correspond to functions proportional to $e^{-(\sigma_1-\sigma_2)t}$, $e^{-(2\sigma_1-\sigma_2-\sigma_3)t}$ and $e^{-(3\sigma_1-\sigma_2-\sigma_3-\sigma_4)t}$, for $\sigma_1 = 0.132$, $\sigma_2 = 0.117$, $\sigma_3 = 0.104$, $\sigma_2 = 0.093$. Note that the t-axis is linear.

another mode called SPO1, which corresponds to the $q = (N+1)/2$ mode of the linear system, which destabilizes at $E_1/N \propto N^{-1}$. We discovered that the SPO2 destabilization threshold,

$$E_c \approx \frac{\pi^2}{6\beta(N+1)}. \tag{139}$$

coincides with the one found by other researchers for the breakdown of FPU recurrences ("weak" chaos) and the destabilization of the $q = 3$ mode.

3) We calculated the Lyapunov spectra characterizing chaotic dynamics in the vicinity of all our SPOs solutions. We thus found that, as E increases, the Lyapunov spectra in these regions attain the **same functional form**,

$$L_i(N) \propto e^{-\alpha\frac{i}{N}}, i = 1, 2, \ldots, K(N) \tag{140}$$

implying that their chaotic regions have "merged" and large scale chaos has spread in the FPU lattice. Using this exponential law, we were able to show that the associated Kolmogorov–Sinai entropies per particle increase linearly with N

$$h_{KS}(N) = \sum_{i=1}^{N-1} L_i(N) \propto N,\ L_i(N) > 0 \tag{141}$$

in the thermodynamic limit of $E \to \infty$ and $N \to \infty$ and fixed E/N and, therefore, behave as **extensive** quantities of statistical mechanics.

4) Generalizing the SALI method, we introduced and applied the **Generalized Alignment Indices, GALI$_k$**, to study local and global dynamics in conservative dynamical systems. The Smaller Alignment Index (SALI) follows the evolution of *two* initially different deviation vectors and already represents an improvement over the calculation of Lyapunov Characteristic Exponents (LCEs). Motivated by the observation that the SALI is proportional to the "area" of a parallelogram, having as edges the two normalized deviation vectors, we generalized it by defining a quantity called GALI_k, representing the "volume" of a parallelepiped having as edges $k > 2$ initially independent deviation vectors. GALI_k is computed as the "norm" of the "exterior" or wedge product of the k normalized deviation vectors. We have shown analytically that for chaotic orbits these indices decay exponentially fast:

$$\mathrm{GALI}_k(t) \propto e^{-[(\sigma_1-\sigma_2)+(\sigma_1-\sigma_3)+\cdots+(\sigma_1-\sigma_k)]t}. \tag{142}$$

For ordered trajectories the situation is more subtle:

$$\mathrm{GALI}_k(t) \approx \text{const. for } 2 \leq k \leq N \tag{143}$$

while for $N < k \leq 2N$, the GALI$_k$s tend to zero following a power law of the form:

$$\mathrm{GALI}_k(t) \propto \frac{1}{t^{2(k-N)}} \text{ for } N \leq k \leq 2N. \quad (144)$$

In the case where $m > 0$ of the initial deviation vectors that lie in the tangent space of the ordered motion, the following behaviors of the GALI$_k$s were derived:

$$\mathrm{GALI}_k(t) \propto \begin{cases} \text{const.} & \text{if } 2 \leq k \leq N \\ \frac{1}{t^{2(k-N)-m}} & \text{if } N < k \leq 2N \;\&\; 0 \leq m < k-N. \\ \frac{1}{t^{k-N}} & \text{if } N < k \leq 2N \;\&\; m \geq k-N \end{cases} \quad (145)$$

5) We presented numerical results, on two examples of Hamiltonian systems, which verify the theoretical estimates and show that the GALI$_k$s can be successfully applied to:

a) Distinguish very rapidly chaotic orbits, for $2 \leq k \leq N$, where the GALI$_k$s decay exponentially to zero (with a rate which depends on several LCEs), from ordered orbits, for which GALI$_k$ fluctuates around non–zero values.

b) Determine the dimensionality N of the subspace of ordered motion, for $N < k \leq 2N$, since GALI$_k$ tends to zero following a power law, whose exponent depends on N. This may also help identify, for example, partially integrable systems, as well as cases where the motion occurs on cantori of dimension $d < N$ and the orbits become "sticky" on island chains.

c) Efficiently chart large domains of phase space, characterizing the dynamics in the various regions, ranging from ordered to chaotic, by different behaviors (constant, exponential decrease or power law decays) of the indices.

d) Obtain analogous results also for $2N$–dimensional symplectic maps.

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