Lyapunov exponents from unstable periodic orbits in the FPU-$\beta$ model

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In the framework of a recently developed theory for Hamiltonian chaos, which makes use of the formulation of Newtonian dynamics in terms of Riemannian differential geometry, we obtained analytic values of the largest Lyapunov exponent for the Fermi-Pasta-Ulam-$\beta$ model (FPU-$\beta$) by computing the time averages of the metric tensor curvature and of its fluctuations along analytically known unstable periodic orbits (UPOs). The agreement between our results and the Lyapunov exponents obtained by means of standard numerical simulations supports the fact that UPOs are reliable probes of a general dynamical property as chaotic instability.

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1. INTRODUCTION

Unstable periodic orbits (UPOs) are widely studied in the framework of classical nonlinear dynamical systems, since they form the "skeleton" of the phase space of these systems and are very sensitive to local characteristic features of the dynamics. Among the applications of the studies of UPOs we can mention: a characterization of dynamical systems, control of classical chaos, semiclassical quantization. Furthermore, they are useful for a characterization of quantum chaos and for the description of some thermodynamical properties of dynamical systems with many degrees of freedom.

The present paper aims at lending further credit to the common wisdom of relevance of UPOs for chaotic dynamics. Our contribution to this subject stems from a Riemannian geometric approach to the study of Hamiltonian systems. However, since the mentioned time averages are in general not analytically knowable, one has to replace them with microcanonical averages which coincide with time averages when the number of degrees of freedom is large and the dynamics is chaotic. In fact, integrating the tangent dynamics equation

$$\frac{d^2\xi_i}{dt^2} + \left(\frac{\partial^2 V}{\partial q^i \partial q^j}\right)_{q(t)} \xi^j = 0,$$  \hspace{1cm} (1)

along a reference trajectory $q(t) = [q_1(t), ..., q_N(t)]$, and then $\lambda_1 = \lim_{t \to \infty} 1/2t \log(\Sigma_{i=1}^N [\xi_i^2(t)] + \xi_i^2(0)) / \Sigma_{i=1}^N [\xi_i^2(0) + \xi_i^2(t)])$. In the conventional theory of chaos, dynamical instability is caused by homoclinic intersections of perturbed separatrices, but this theory seems not adequate to treat chaos in Hamiltonian systems with many degrees of freedom. In this case, the direct numerical simulation is the only way to compute $\lambda_1$.

Recently, it has been proposed by Pettini to tackle Hamiltonian chaos in a different theoretical framework with respect to that of homoclinic intersections. This new method resorts to a well known formulation of Hamiltonian dynamics in the language of Riemannian differential geometry: the mechanical trajectories of a dynamical system can be viewed as geodesics of a Riemannian manifold endowed with a suitable metric. In this framework, it is possible to relate the instability of a geodesics flow with the curvature properties of the underlying “mechanical” manifold through two geometric quantities: the Ricci curvature and its fluctuations. These two geometric quantities, in principle averaged along a generic geodesic, enter a formula, derived by Pettini et al. in Ref, which allows the analytic computation of the largest Lyapunov exponent for a generic Hamiltonian system. However, since the mentioned time averages are in general not analytically knowable, one has to replace them with microcanonical averages which coincide with time averages when the number of degrees of freedom is large and the dynamics is chaotic. In fact,
under these circumstances, the measure of regular orbits in phase space - at physically meaningful energies - is vanishingly small, thus the dynamics is \textit{bona fide} ergodic and mixing.

Therefore, the analytic computation of the largest Lyapunov exponent can be done whenever the simplifying hypotheses of Ref. [6] are justified and the microcanonical averages of the mentioned geometric quantities are analytically computable. This is just the case of the FPU-\(\beta\) model which has been considered in Ref. [7].

It is the purpose of the present work to show that, in some special case, the above mentioned replacement of some unstable periodic orbits, a reasonable analytic estimate of the values of \(\lambda_1\) can be obtained without resorting to microcanonical averages. It is somewhat surprising, and undoubtedly very interesting, that unstable periodic orbits make something like an “importance sampling” of the relevant geometric features of configuration space which are needed to estimate the average degree of chaoticity of the dynamics, measured by \(\lambda_1\). A similar problem was already addressed in Ref. [5], where the authors gave an analytical estimate of the largest Lyapunov exponent at high energy density for the Fermi-Pasta-Ulam-\(\beta\) model by computing the average of the modulational instability growth rates associated to unstable modes.

2. GEOMETRY AND DYNAMICS

Let us summarize the geometrization of Newtonian dynamics tackled in Ref. [2]. It applies to standard autonomous systems described by the Lagrangian function (all the indices run from 1 to \(N\) degrees of freedom)

\[
L(q, \dot{q}) = \frac{1}{2} \sum_{ik} a_{ik}(q) q^i \dot{q}^k - V(q) ,
\]

where \(a_{ik}\) is the kinetic energy tensor that in terms of the total energy \(E\) and kinetic energy, reads

\[
\sum_{ik} a_{ik} q^i \dot{q}^k = 2(E - V) = 2W ,
\]

Following the method due to Eisenhart [3], the differentiable \(N\)-dimensional configuration space \(\mathcal{M}\), on which the lagrangian coordinates \((q^1, \ldots, q^N)\) can be used as local coordinates, is enlarged. The ambient space thus introduced embodies the time coordinate and is given as \(\mathcal{M} \times \mathbb{R}^2\), with local coordinates \((q^0, q^1, \ldots, q^N, q^{N+1})\), where \((q^1, \ldots, q^N) \in \mathcal{M}\), \(q^0 \in \mathbb{R}\) is the time coordinate, and \(q^{N+1} \in \mathbb{R}\) is a coordinate closely related to Hamilton action. With Eisenhart we define a pseudo-Riemannian non-degenerate metric \(g_E\) on \(\mathcal{M} \times \mathbb{R}^2\) as

\[
ds_E^2 = \sum_{\mu \nu} g_{\mu \nu} dq^\mu \otimes dq^\nu = dq^0 \otimes dq^{N+1} + dq^{N+1} \otimes dq^0 + \sum_{ij} a_{ij} dq^i \otimes dq^j - 2V(q) dq^0 \otimes dq^0 .
\]

\[
(4)
\]

Natural motions are now given by the canonical projection \(\pi\) of the geodesics of \((\mathcal{M} \times \mathbb{R}^2, g_E)\) on the configuration space-time: \(\pi : \mathcal{M} \times \mathbb{R}^2 \rightarrow \mathcal{M} \times \mathbb{R}\). However, among all the geodesics of \(g_E\) the natural motions belong to the subset of those geodesics along which the arclength is positive definite

\[
ds^2 = \sum_{\mu \nu} g_{\mu \nu} dq^\mu dq^\nu = 2C^2 dt^2 > 0 ,
\]

\[
(5)
\]

where \(C\) is a real arbitrary constant. More details can be found in Ref. [3].

The stability of a geodesic flow is studied by means of the Jacobi–Levi-Civita (JLC) equation for geodesic spread. In local coordinates and in terms of proper time \(s\) the JLC equation reads as

\[
\frac{\nabla^2 J^k}{ds^2} + \sum_{ijr} R^k_{ijr} \frac{dq^i}{ds} \frac{J^j}{ds} \frac{dq^r}{ds} = 0 ,
\]

\[
(6)
\]

where \(J\) is the Jacobi vector field of geodesic separation, \(\nabla\) the covariant derivative is given by \(\nabla J^k / ds = dJ^k / ds + \sum_{ij} \Gamma^k_{ij} dq^i / ds J^j\), and \(R^k_{ijr}\) are the components of the Riemann-Christoffel curvature tensor which, in terms of the Christoffel coefficients \(\Gamma^i_{jk}\), are

\[
R^k_{ijr} = \partial_j \Gamma^k_{ir} - \partial_r \Gamma^k_{ij} + \sum_t \Gamma^t_{ir} \Gamma^k_{jt} - \Gamma^t_{ij} \Gamma^k_{rt} ,
\]

\[
(7)
\]

where \(\partial_j = \partial / \partial q^j\). The Christoffel coefficients, in turn, are defined as

\[
\Gamma^i_{jk} = \frac{1}{2} \sum_m g^{im} \left( \partial_j g_{km} + \partial_r g_{mj} - \partial_m g_{jk} \right) .
\]

\[
(8)
\]

In Ref. [2] it has been shown that the Jacobi equation (10), written for the Eisenhart metric of the enlarged configuration space, nicely yields the standard tangent dynamics equation (11). Moreover, under suitable simplifying hypotheses, mainly of geometric type, in Ref. [9] it has been shown that Eq.(15) can be replaced by a scalar effective equation

\[
\frac{d^2 \psi}{ds^2} + (k_R) s \psi + \frac{1}{\sqrt{N - 1}} (\delta^2 K_R)^{1/2} \eta(s) \psi = 0 ,
\]

\[
(9)
\]

where \(\psi\) stands for any of the components \(J^i\) of the Jacobi field, since in this effective picture all of them obey the same equation. Moreover, \(K_R = \sum_{ijk} g^{ij} R^k_{ikj}\) is the
Ricci curvature and $k_R = K_R/(N-1)$ which, for the Eisenhart metric, takes the simple form

$$k_R(q) = \frac{\Delta V}{(N-1)} \approx \frac{1}{N} \sum_{i=1}^{N} \frac{\partial^2 V(q)}{\partial q_i^2}. \quad (10)$$

In Eq. (10), $\eta(s)$ is a gaussian white noise with zero mean and unit variance, and $\langle \cdot \rangle_s$ stands for time averaging along a reference geodesic. Time averages $\langle k_R \rangle_s$ and $\langle \partial^2 K_R \rangle_s$ of Ricci curvature and of its fluctuations along some analytically unstable periodic orbits of the system described by the Hamiltonian $H(p, q)$.

$$H(p, q) = \sum_{i=1}^{N} \frac{1}{2} p_i^2 + \sum_{i=1}^{N} \left[ \frac{1}{2} (q_{i+1} - q_i)^2 + \frac{\beta}{4} (q_{i+1} - q_i)^4 \right], \quad (15)$$

with periodic boundary conditions $q_{N+1} \equiv q_1$. This system has been introduced by Fermi, Pasta and Ulam in their celebrated work on the equipartition properties of the dynamics of many non-linearly coupled oscillators. Since then, a huge amount of papers have been devoted to the study of the link between microscopic dynamical properties and macroscopic thermodynamical and statistical properties of classical many body systems.

The linear terms in Hamiltonian (15) can be diagonalized by introducing suitable harmonic normal coordinates. The latters are obtained by means of a canonical linear transformation $\mathbf{T}$. Denoting the normal coordinates and momenta by $Q_k$ and $P_k$ for $k = 0, \ldots, N-1$, the transformation is given by

$$Q_k(t) = \sum_{n=1}^{N} S_{kn} q_n(t), \quad P_k(t) = \sum_{n=1}^{N} S_{kn} p_n(t), \quad (16)$$

where $k = 0, \ldots, N-1$, and $S_{kn}$ is the orthogonal matrix whose elements are

$$S_{kn} = \frac{1}{\sqrt{N}} \left[ \sin \left( \frac{2 \pi k n}{N} \right) + \cos \left( \frac{2 \pi k n}{N} \right) \right], \quad (17)$$

$n = 1, \ldots, N$ and $k = 0, \ldots, N-1$. The full Hamiltonian in the new coordinates reads

$$H(Q, P) = \frac{1}{2} P_i^2 + \frac{1}{2} \sum_{i=1}^{N-1} \left( P_i^2 + \omega_i^2 Q_i^2 \right) + H_1(Q), \quad (18)$$

where the anharmonic term is

$$H_1(Q) = \frac{\beta}{8N} \sum_{i,j,k,l=1}^{N-1} \omega_i \omega_j \omega_k \omega_l C_{ijkl} Q_i Q_j Q_k Q_l. \quad (19)$$

The $\omega_k = 2 \sin (\pi k / N)$, for $k \in \{1, \ldots, N-1\}$, are the normal frequencies for the harmonic case ($\mu = 0$), being $\omega_k = \omega_{N-k}$. By defining

$$\Delta_r = \left\{ \begin{array}{ll} (-1)^m & \text{for } r = mN \text{ with } m \in \mathbb{Z} \\ 0 & \text{otherwise} \end{array} \right., \quad (20)$$

the integer-valued coupling coefficients $C_{ijkl}$ are explicitly given by

$$C_{ijkl} = -\Delta_{i+j+k+l} + \Delta_{i+j+k+l} + \Delta_{i-j+k-l} + \Delta_{i+j+k-l}. \quad (21)$$

By eliminating the motion of the center of mass (which corresponds to the zero index), we now easily get the equations of motion for the remaining $N-1$ degrees of freedom, which, at the second order, read as

$$\ddot{Q}_r = -\omega_r^2 Q_r - \frac{\beta \omega_r}{2N} \sum_{j,k,l=1}^{N-1} \omega_j \omega_k \omega_l C_{ijkl} Q_j Q_k Q_l, \quad (22)$$

for $r = 1, \ldots, N-1$.

As is shown in Ref. [10], the equations of motion (22) admit some exact, periodic solutions that can be explicitly expressed in closed analytical form. The simplest

3. ANALYTIC COMPUTATION OF LYAPUNOV EXPONENTS

In the following, we work out time averages of the Ricci curvature and of its fluctuations along some analytically known unstable periodic orbits of the system described by the Hamiltonian $H(p, q)$.

$\hat{H}(p, q) = \sum_{i=1}^{N} \frac{1}{2} \ddot{q}_i^2 + \sum_{i=1}^{N} \left[ \frac{1}{2} (q_{i+1} - q_i)^2 + \frac{\beta}{4} (q_{i+1} - q_i)^4 \right], \quad (15)$
ones, consisting of one mode (OM), have only one excited mode, which we denote by the index \( e \), and thus are characterized by \( Q_j(t) \equiv 0 \) for \( j \neq e \). The solitary modes are found by setting \( C_{ee} = 0 \) \( \forall r \in \{1, \ldots, N-1\} \) with \( r \neq e \); it is easily verified that this condition is satisfied for
\[
e\frac{N}{4}, \frac{N}{3}, \frac{2N}{3}, \frac{3N}{4}.
\]
(23)

Thus, for solutions with initial conditions \( Q_j = 0 \) and \( \dot{Q}_j = 0 \) for \( j \neq e \), the whole system (22) reduces to a one degree of freedom (and thus integrable) system described by the equation of motion
\[
\ddot{Q}_e - \omega_e^2 Q_e = \frac{\beta \omega_e^4 C_{ee}}{2N} Q_e^3,
\]
where \( C_{ee} = 4, 4, 3, 3, 2 \) for \( e = N/4, 3N/4, N/3, 2N/3, N/2 \), respectively. The harmonic frequencies of the modes (22) are \( \omega_e = \sqrt{2}, \sqrt{3}, \sqrt{3}, 2 \) for \( e = N/4, 3N/4, N/3, 2N/3, N/2 \), respectively. In order to simplify the notation, in the following, let us set \( \dot{C}_e = C_{ee} \).

The general solution of (22) is a Jacobi elliptic cosine
\[
Q_e(t) = A \text{cn} [\Omega_e(t - t_0), k],
\]
where the free parameters (modal) amplitude \( A \) and time origin \( t_0 \) are fixed by the initial conditions. The frequency \( \Omega_e \) and the modulus \( k \) of Jacobi elliptic cosine function (11) depend on \( \Omega_e \) as follows
\[
\Omega_e = \omega_e \sqrt{1 + \delta_e A^2}, \quad k = \sqrt{\frac{\delta_e A^2}{2(1 + \delta_e A^2)}},
\]
(26)

with \( \delta_e = \beta \omega_e^2 \dot{C}_e/(2N) \). This kind of solution is periodic, and its oscillation period \( T_e \) depends on the amplitude \( A \), since it is given in terms of the complete elliptic integral of the first kind \( K(k) \) and in terms of \( \Omega_e \) by
\[
T_e = \frac{4K(k)}{\Omega_e}.
\]
(27)

The modal amplitude \( A \) is one-to-one related to the energy density \( \epsilon = E/N \). In fact, computing the total energy (23) on the OM solution \( Q_j(t) \equiv \delta_j \dot{Q}_e(t) \), one finds
\[
\epsilon N = \frac{1}{2} \left( P_e^2 + \omega_e^2 Q_e^2 \right) + \frac{\beta}{8N} \omega_e^4 \dot{C}_e Q_e^4.
\]
(28)

Since at \( t = t_0 \) the coordinates result \( (Q_e(t_0), P_e(t_0)) = (A, 0) \), by solving the previous equation for \( A \) we get
\[
A = \left[ 2N \left( \frac{1 + 2\beta \dot{C}_e}{\beta \omega_e^2 C_e} - 1 \right) \right]^{1/4}.
\]
(29)

This relation allows to express all the parameters of the solution (22) in terms of the more physically relevant parameter \( \epsilon \). The period \( T_e \) is
\[
T_e = \frac{4K(k)}{\omega_e(1 + 2\beta \dot{C}_e)^{1/4}}.
\]
(30)

where \( k = k(\epsilon) \) can be found from (24) and (29).

In terms of the standard coordinates, the OM solutions result
\[
q_n(t) = \frac{1}{\sqrt{N}} Q_e(t) \left[ \sin \left( \frac{2\pi n}{N} + \cos \left( \frac{2\pi n}{N} \right) \right) \right], \quad (31)
\]
where \( e \) is one of the values listed in (26).

The Ricci curvature along a periodic trajectory, obtained by substituting Eq. (31) into Eq. (10), is
\[
k_R(t) = 2 + \frac{6\beta}{N} \omega_e^2 Q_e^2(t),
\]
and we can compute its time average \( \overline{k}_R \) as
\[
\overline{k}_R = 2 + \frac{6\beta}{N} \omega_e^2 \overline{Q}_e^2.
\]
(33)

After simple algebra, using standard properties of the elliptic functions, we find
\[
\overline{Q}_e^2 = \frac{1}{T_e} \int_{t_0}^{t_0 + T_e} dt Q_e^2 = A^2 \frac{K(k)}{K^2} (E + (k^2 - 1)K).
\]
(34)

The time averaged Ricci curvature results
\[
\overline{k}_R = 2 + 12 \frac{K(k)}{K^2} \left( \sqrt{1 + 2\beta \dot{C}_e} - 1 \right) \left( \frac{E}{K^2} + (k^2 - 1)K \right),
\]
where \( K \) and \( E \) are the complete elliptic integrals of the first and second kind respectively, both depending on the modulus \( k \) which, from (29) and (32), is determined by the energy density \( \epsilon \)
\[
k^2 = \frac{1}{2} \left( 1 - \frac{1}{1 + 2\beta \dot{C}_e} \right).
\]
(36)

Now, using Eqs. (35) and (36), and the tabulated values for \( E \) and \( K \), \( \overline{k}_R \) is given as a function of the energy density \( \epsilon \). In Fig. 1 a comparison is made between \( \overline{k}_R \) versus \( \epsilon \), worked out for the OM solutions under consideration, and \( \langle k_R \rangle_{\mu \in E} \) versus \( \epsilon \), the average Ricci curvature analytically computed in Ref. (4).

By definition, the average of the curvature fluctuations is
\[
\langle \delta^2 k \rangle_{\mu} = \langle (K_R - \langle K_R \rangle_{\mu})^2 \rangle_{\mu} = (N - 1)^2 \left[ (\langle K_R \rangle_{\mu})^2 - \langle (K_R)_{\mu} \rangle^2 \right].
\]
(37)

Again, by replacing the microcanonical averages with time averages, from Eq. (35) and after some trivial algebra, we get
\[
\overline{\delta^2 k}_R = \frac{36\beta^2 \omega_e^4}{N^2} \left[ \overline{Q}_e^4 - \overline{Q}_e^2 \overline{Q}_e^2 \right].
\]
(38)

The new term
\[
\overline{Q}_e^4 = \frac{A^4}{T_e} \int_0^{T_e} dt \text{cn}^4(\Omega_e t, k) = \frac{A^4}{4K} \int_0^{4K} d\theta \text{cn}^4(\theta, k)
\]
(30)
can be computed by resorting to standard properties of the elliptic functions and the result is

$$\bar{Q}_c^H = \frac{A^4}{3k^4} \left[ K(2 - 5k^2 + 3k^4) + 2E(2k^2 - 1) \right].$$  \hfill (39)

Finally, Eqs. (36) and (38) in (37) yield

$$\bar{\delta^2 k_R} = \frac{192 \left[ (k^2 - 1) + 2(2 - k^2) \frac{E}{K} - 3 \left( \frac{E}{K} \right)^2 \right]}{(1 - 2k^2)^2 C_e^2}.$$  \hfill (40)

From Eq. (38) and making use of the tabulated values for $E$ and $K$, equation (40) provides the mean fluctuations of curvature as a function of $\epsilon$.

In Fig. 2, a comparison is made between the time average of the Ricci curvature fluctuations $\bar{\delta^2 k_R}$ as a function of the energy density $\epsilon$, worked out along the OM solution that we considered, and $\langle \delta^2 k_R \rangle_{\mu E}$ versus $\epsilon$ analytically computed in Ref. 6 (continuous line). The agreement is very good on a broad range of values of energy density $\epsilon$.

FIG. 2: In this figure we report three curves for $\bar{\delta^2 k_R}$ versus $\epsilon$ computed by integrating the curvature fluctuations along the three single mode solutions considered in the present paper (dotted, dashed and long-dashed lines refer to $\epsilon = N/4, 3N/4, e = N/3, 2N/3$ and $\epsilon = N/2$, respectively), and a comparison is made with the same quantity computed in Ref. 6 (continuous line). Also in this case the agreement is very good.

4. CONCLUDING REMARKS

In conclusion, we have found that some global curvature properties of the configuration space manifold – whose geodesics coincide with the trajectories of a Hamiltonian system – are well sampled by unstable periodic orbits. Then, since the averages of these curvature quantities enter an analytic formula to compute the largest Lyapunov exponent, unstable periodic orbits can be used also to compute Lyapunov exponents through the time averages of the same geometric quantities. In the present work, this result has been obtained in the
FIG. 3: This figure shows the largest Lyapunov exponent $\lambda_1$ obtained by integrating the suitable geometric quantity along the three single mode solutions considered in the present paper, plotted vs. $\epsilon$. Dotted, dashed and long-dashed lines refer to $\epsilon = N/4, 3N/4, \epsilon = N/3, 2N/3$ and $\epsilon = N/2$, respectively. Continuous line refers to the Lyapunov exponent computed in [6]. The full circles are the values for $\lambda_1$ computed by numerical integration. The agreement is again very good on a broad range of $\epsilon$ values.

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