Lyapunov exponents from unstable periodic orbits

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We propose a method that allows us to analytically compute the largest Lyapunov exponent of a Hamiltonian chaotic system from the knowledge of a few unstable periodic orbits (UPOs). In the framework of a recently developed theory for Hamiltonian chaos, by computing the time averages of the metric tensor curvature and of its fluctuations along analytically known UPOs, we have re-derived the analytic value of the largest Lyapunov exponent for the Fermi-Pasta-Ulam–β (FPU-β) model. The agreement between our results and the Lyapunov exponents obtained by means of standard numerical simulations confirms the point of view which attributes to UPOs the special role of efficient probes of general dynamical properties, among them chaotic instability.

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I. INTRODUCTION

Unstable periodic orbits are widely studied in the field of classical nonlinear dynamical systems [1], since they form the "skeleton" [2] of the phase space of these systems and are very sensitive to local characteristic features of the dynamics. There is a vast literature about UPOs and their applications, We just mention a few of them: characterization of dynamical systems [3], control of classical chaos, semiclassical quantization [4], statistical properties of turbulence [5], and characterization of complex systems [6]. Furthermore, they are useful for a characterization of quantum chaos and for the description of some thermodynamic properties of dynamical systems with many degrees of freedom [7].

In the present paper, we lend further credit to the common wisdom of the relevance of UPOs for the study of chaotic dynamics. Furthermore, a remarkable outcome of our present work is that a very few UPOs are sufficient to achieve the final result, thus confirming similar and somewhat surprising outcomes reported in recent literature [5,8], where it is shown that just one UPO is enough to derive relevant statistical properties of chaotic and turbulent systems. The method that we propose to link in a new way UPOs and chaos is based on a combination of an already existing Riemannian geometric theory of Hamiltonian chaos with the analytic knowledge of some UPOs, and leads to the analytic computation of the largest Lyapunov exponents of Hamiltonian systems.

It is well known that the degree of chaoticity of a dynamical system is measured by the largest Lyapunov exponent λ_1 which provides a measure of the dynamical instability in terms of the local growth rate of the distance of nearby trajectories, averaged along a sufficiently long reference trajectory. The largest Lyapunov exponent λ_1 for standard Hamiltonian systems, described by Hamiltonian functions of the form $H=\Sigma_{i=1}^{N}\frac{1}{2}p_i^2+V(q_1,\ldots,q_N)$, is computed by numerically integrating the tangent dynamics equation

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

along a reference trajectory $q(t)=(q_1(t),\ldots,q_N(t))$, and then $\lambda_1=\lim_{t\to\infty}(1/2t)\log\{\Sigma_{i=1}^{N}[\dot{\xi}_i^2(t)+\xi_i^2(t)]/\Sigma_{i=1}^{N}[\dot{\xi}_i^2(0)+\xi_i^2(0)]\}$. In the conventional theory of chaos, dynamical instability is caused by homoclinic intersections of perturbed separatrices, but this theory seems in adequate to treat chaos in Hamiltonian systems with many degrees of freedom. In this case, direct numerical simulation is the only way to compute λ_1.

Recently, it has been proposed by Pettini [9] 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. [10], 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

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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 *bona fide* ergodic and mixing.

Therefore, the analytic computation of the largest Lyapunov exponent can be done whenever the simplifying hypotheses of Ref. [10] are justified and the microcanonical averages of the mentioned geometric quantities are analytically computable. This is just the case of the FPU-β model which has been considered in Ref. [10]. Nevertheless, whenever exact dynamical solutions are known, an alternative method is possible: to compute the averages of the required geometric quantities as time averages along these trajectories.

The purpose of the present work is to show that, whenever the *time averages* of the Ricci curvature and of its fluctuations are analytically computable along some unstable periodic orbits, the above-mentioned replacement of time averages with microcanonical ones can be avoided, and a reasonable analytic estimate of the values of λ_1 can be obtained. 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 λ_1. A similar problem was already addressed in [13], where the authors gave an analytical estimate of the largest Lyapunov exponent at high energy density for the Fermi-Pasta-Ulam-β model by computing the average of the modulational instability growth rates associated to unstable modes.

In Sec. II, we briefly summarize the geometrical theory for Hamiltonian chaos of Ref. [9]. In Sec. III, we derive the explicit form of some unstable periodic orbits, we work out the time averages of the Ricci curvature and of its fluctuations along these analytically known trajectories, and we compute the largest Lyapunov exponents. Finally, in Sec. IV, we give some concluding remarks.

II. GEOMETRY AND DYNAMICS

Let us summarize the geometrization of Newtonian dynamics tackled in [9]. It applies to standard autonomous systems described by the Lagrangian function (all the indices run from 1 to N degrees of freedom)

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

where a_{ik} is the kinetic energy tensor and $V(q)$ is the potential. From

$$2W = \sum_{ik} a_{ik}\dot{q}^i\dot{q}^k = 2(E - V), \qquad (3)$$

where E is the total energy and W the kinetic energy, and from Maupertuis' least action principle,

$$\delta\int 2W dt = \delta\int \sqrt{2[E - V(q)]a_{ik}\dot{q}^i\dot{q}^k}dt = 0,$$

the natural motions can be seen as geodesics $(\delta\int ds = 0)$ of the configuration space endowed with the Jacobi metric whose line element is

$$ds^2 = 2[E - V(q)]a_{ik}dq^i dq^k. \qquad (4)$$

This is a well known way of rephrasing Newtonian dynamics in the Riemannian geometric language. Another geometrization of Newtonian dynamics is obtained by following the method due to Eisenhart [14], where 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 nondegenerate metric g_E on $\mathcal{M}\times\mathbb{R}^2$ as

$$\begin{aligned} ds_E^2 &= \sum_{\mu\nu} g_{\mu\nu}dq^\mu \otimes dq^\nu \\ &= dq^0\otimes dq^{N+1} + dq^{N+1}\otimes dq^0 \\ &\quad + \sum_{ij} a_{ij}dq^i\otimes dq^j - 2V(q)dq^0\otimes dq^0. \end{aligned} \qquad (5)$$

Natural motions are now given by the canonical projection π of the geodesics of $(\mathcal{M}\times\mathbb{R}^2, g_E)$ on the configuration space-time: $\pi: \mathcal{M}\times\mathbb{R}^2 \to \mathcal{M}\times\mathbb{R}$. 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,

$$ds^2 = \sum_{\mu\nu} g_{\mu\nu}dq^\mu dq^\nu = 2C^2dt^2 > 0, \qquad (6)$$

where C is a real arbitrary constant. More details can be found in [9].

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

$$\frac{\nabla^2 J^k}{ds^2} + \sum_{ijr} R^k{}_{ijr}\frac{dq^i}{ds}J^j\frac{dq^r}{ds} = 0, \qquad (7)$$

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

$$R^k{}_{ijr} = \partial_j\Gamma^k_{ri} - \partial_r\Gamma^k_{ji} + \sum_t \Gamma^t_{ri}\Gamma^k_{jt} - \Gamma^t_{ji}\Gamma^k_{rt}, \qquad (8)$$

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

$$\Gamma^i_{jk} = \frac{1}{2}\sum_m g^{im}(\partial_j g_{km} + \partial_k g_{mj} - \partial_m g_{jk}). \tag{9}$$

In [9], it has been shown that the Jacobi equation (7), written for the Eisenhart metric of the enlarged configuration space, nicely yields the standard tangent dynamics equation (1). In Refs. [11,12], the direct numerical computation of the solutions of Eq. (7), worked out for both Jacobi and Eisenhart metrics, shows that the quantitative information on chaos, given by the largest Lyapunov exponent, is encoded in the geometry underlying dynamics.

Under suitable simplifying hypotheses, mainly of geometric type, in Ref. [10] it has been shown that Eq. (7) can be replaced by a scalar effective equation

$$\frac{d^2\psi}{ds^2} + \langle k_R\rangle_s \psi + \frac{1}{\sqrt{N-1}}\langle \delta^2 K_R\rangle_s^{1/2}\eta(s)\psi = 0, \tag{10}$$

where ψ 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, $K_R = \Sigma_{ijk} g^{ij} R^k_{\ ikj}$ is the Ricci curvature and $k_R = K_R/(N-1)$, which, for the Eisenhart metric, takes the simple form

$$k_R(q) = \frac{\Delta V}{(N-1)} \simeq \frac{1}{N}\sum_{i=1}^N \frac{\partial^2 V(q)}{\partial q_i^2}. \tag{11}$$

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 $\langle\delta^2 K_R\rangle_s$ of Ricci curvature and of its second moment, respectively, cannot be known analytically for a chaotic orbit, hence the need for an assumption of ergodicity allowing the replacement of time averages by microcanonical averages on a constant energy surface Σ_E, corresponding to the energy value E of interest. At variance with time averages along chaotic orbits, microcanonical averages can be computed analytically for some models. It is worth remarking that, after the replacement of time averages by means of static microcanonical averages $\langle k_R\rangle_{\mu_E}$ and $\langle\delta^2 K_R\rangle_{\mu_E}$, the scalar equation (10) is independent of the numerical knowledge of the dynamics.

Then the largest Lyapunov exponent for the effective model given by Eq. (10), defined as

$$\lambda_1 = \lim_{t\to\infty}\frac{1}{2t}\log\frac{\psi^2(t)+\dot{\psi}^2(t)}{\psi^2(0)+\dot{\psi}^2(0)}, \tag{12}$$

is obtained by solving this stochastic differential equation by means of a standard method due to van Kampen [10]. The final analytic expression for λ_1 reads

$$\lambda_1(\Omega_0,\sigma_\Omega,\tau) = \frac{1}{2}\left(\Lambda - \frac{4\Omega_0}{3\Lambda}\right), \tag{13}$$

where $\Omega_0 = \langle k_R\rangle_{\mu_E}$, $\sigma_\Omega^2 = N\langle\delta^2 k_R\rangle_{\mu_E}$,

$$\Lambda = \left[2\sigma_\Omega^2\tau + \sqrt{\left(\frac{4\Omega_0}{3}\right)^3 + (2\sigma_\Omega^2\tau)^2}\right]^{1/3}, \tag{14}$$

and

$$2\tau = \frac{\pi\sqrt{\Omega_0}}{2\sqrt{\Omega_0(\Omega_0+\sigma_\Omega)} + \pi\sigma_\Omega}. \tag{15}$$

III. 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

$$H(p,q) = \sum_{i=1}^N \frac{1}{2}p_i^2 + \sum_{i=1}^N\left[\frac{1}{2}(q_{i+1}-q_i)^2 + \frac{\beta}{4}(q_{i+1}-q_i)^4\right], \tag{16}$$

with periodic boundary conditions $q_{N+1} \equiv q_1$. This system has been introduced by Fermi, Pasta, and Ulam in their celebrated work [15] on the equipartition properties of the dynamics of many nonlinearly coupled oscillators. Since then, a huge number of papers have been devoted to the study of the link between microscopic dynamical properties and macroscopic thermodynamic and statistical properties of classical many-body systems.

The linear terms in Hamiltonian (16) can be diagonalized by introducing suitable harmonic normal coordinates. The latter are obtained by means of a canonical linear transformation [16]. Denoting the normal coordinates and momenta by Q_k and P_k for $k=0,\ldots,N-1$, the transformation is given by

$$Q_k(t) = \sum_{n=1}^N S_{kn}q_k(t), \quad P_k(t) = \sum_{n=1}^N S_{kn}p_k(t), \tag{17}$$

where $k=0,\ldots,N-1$, and S_{kn} is the orthogonal matrix [16] whose elements are

$$S_{kn} = \frac{1}{\sqrt{N}}\left[\sin\left(\frac{2\pi kn}{N}\right) + \cos\left(\frac{2\pi kn}{N}\right)\right], \tag{18}$$

$n=1,\ldots,N$ and $k=0,\ldots,N-1$. The full Hamiltonian (16) in the new coordinates reads

$$H(\boldsymbol{Q},\boldsymbol{P}) = \frac{1}{2}P_0^2 + \frac{1}{2}\sum_{i=1}^{N-1}(P_i^2 + \omega_i^2 Q_i^2) + H_1(\boldsymbol{Q}), \tag{19}$$

where the anharmonic term is

$$H_1(\boldsymbol{Q}) = \frac{\beta}{8N}\sum_{i,j,k,l=1}^{N-1}\omega_i\omega_j\omega_k\omega_l C_{ijkl}Q_iQ_jQ_kQ_l. \tag{20}$$

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

$$\Delta_r = \begin{cases}(-1)^m & \text{for } r = mN \text{ with } m\in\mathbb{Z}\\ 0 & \text{otherwise,}\end{cases} \tag{21}$$

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

$$C_{ijkl} = -\Delta_{i+j+k+l} + \Delta_{i+j-k-l} + \Delta_{i-j+k-l} + \Delta_{i-j-k+l}. \qquad (22)$$

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

$$\ddot{Q}_r = -\omega_r^2 Q_r - \frac{\beta\omega_r}{2N}\sum_{j,k,l=1}^{N-1}\omega_j\omega_k\omega_l C_{rjkl}Q_jQ_kQ_l \qquad (23)$$

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

As is shown in Ref. [16], the equations of motion (23) admit some exact, periodic solutions that can be explicitly expressed in closed analytical form. The simplest 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 $C_{reee}=0\,\forall\, r\in\{1,\ldots,N-1\}$ with $r\neq e$; it is easily verified that this condition is satisfied for

$$e = \frac{N}{4};\frac{N}{3};\frac{N}{2};\frac{2N}{3};\frac{3N}{4}. \qquad (24)$$

Thus, for solutions with initial conditions $Q_j=0$ and $\dot{Q}_j=0$ for $j\neq e$, the whole system (23) reduces to a one degree of freedom (and thus integrable) system described by the equation of motion

$$\ddot{Q}_e = -\omega_e^2 Q_e - \frac{\beta\omega_e^4 C_{eeee}}{2N}Q_e^3, \qquad (25)$$

where $C_{eeee}=4,4,3,3,2$ for $e=N/4$, $3N/4$, $N/3$, $2N/3$, and $N/2$, respectively. The harmonic frequencies of the modes (24) are $\omega_e=\sqrt{2}$, $\sqrt{2}$, $\sqrt{3}$, $\sqrt{3}$, and 2 for $e=N/4$, $3N/4$, $N/3$, $2N/3$, and $N/2$, respectively. In order to simplify the notation, in the following, let us set $\hat{C}_e=C_{eeee}$.

The general solution of Eq. (25) is a Jacobi elliptic cosine,

$$Q_e(t) = A\,\mathrm{cn}(\Omega_e(t-t_0),k), \qquad (26)$$

where the free parameters (modal) amplitude A and time origin t_0 are fixed by the initial conditions. The frequency Ω_e and the modulus k of Jacobi elliptic cosine function [17] depend on A as follows:

$$\Omega_e = \omega_e\sqrt{1+\delta_e A^2}, \quad k = \sqrt{\frac{\delta_e A^2}{2(1+\delta_e A^2)}}, \qquad (27)$$

with $\delta_e=\beta\omega_e^2\hat{C}_e/(2N)$. 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 $\mathbf{K}(k)$ and in terms of Ω_e by

$$T_e = \frac{4\mathbf{K}(k)}{\Omega_e}. \qquad (28)$$

The modal amplitude A is one-to-one related to the energy density $\epsilon=E/N$. In fact, computing the total energy (19) on the OM solution $Q_j(t)\equiv\delta_{je}Q_e(t)$, one finds

$$\epsilon N = \frac{1}{2}(P_e^2+\omega_e^2Q_e^2) + \frac{\beta}{8N}\omega_e^4\hat{C}_eQ_e^4. \qquad (29)$$

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

$$A = \left[2N\left(\frac{\sqrt{1+2\beta\epsilon\hat{C}_e}-1}{\beta\omega_e^2\hat{C}_e}\right)\right]^{1/2}. \qquad (30)$$

This relation allows us to express all the parameters of the solution (26) in terms of the more physically relevant parameter ϵ. The period T_e is

$$T_e = \frac{4\mathbf{K}(k)}{\omega_e(1+2\beta\epsilon\hat{C}_e)^{1/4}}, \qquad (31)$$

where $k=k(\epsilon)$ can be found from Eqs. (27) and (30).

In terms of the standard coordinates, the OM solutions result,

$$q_n(t) = \frac{1}{\sqrt{N}}Q_e(t)\left[\sin\left(\frac{2\pi ne}{N}\right)+\cos\left(\frac{2\pi ne}{N}\right)\right], \qquad (32)$$

where e is one of the values listed in Eq. (24).

The Ricci curvature along a periodic trajectory, obtained by substituting Eq. (32) into Eq. (11), is

$$k_R(t) = 2 + \frac{6\beta}{N}\omega_e^2Q_e^2(t), \qquad (33)$$

and we can compute its time average $\overline{k_R}$ as

$$\overline{k_R} = 2 + \frac{6\beta}{N}\omega_e^2\overline{Q^2}_e. \qquad (34)$$

After simple algebra, using standard properties of the elliptic functions, we find

$$\overline{Q^2}_e = \frac{1}{T_e}\int_{t_0}^{T_e+t_0}dt\,Q_e^2 = \frac{A^2}{\mathbf{K}k^2}[\mathbf{E}+(k^2-1)\mathbf{K}]. \qquad (35)$$

The time-averaged Ricci curvature results

$$\overline{k_R} = 2 + \frac{12}{\mathbf{K}k^2\hat{C}_e}[\sqrt{1+2\beta\epsilon\hat{C}_e}-1][\mathbf{E}+(k^2-1)\mathbf{K}], \qquad (36)$$

where $\mathbf{K}$ and $\mathbf{E}$ are the complete elliptic integrals of the first and second kind, respectively, both depending on the modulus k which, from Eqs. (27) and (30), is determined by the energy density ϵ,

$$k^2 = \frac{1}{2}\left(1-\frac{1}{\sqrt{1+2\beta\epsilon\hat{C}_e}}\right). \qquad (37)$$

Now, using Eqs. (36) and (37), and the tabulated values for $\mathbf{E}$ and $\mathbf{K}$, $\overline{k_R}$ is given as a function of the energy density ϵ. In Fig. 1, a comparison is made between $\overline{k_R}$ versus ϵ, worked out for the OM solutions under consideration, and $\langle k_R\rangle_{\mu_E}$ versus ϵ, the average Ricci curvature analytically computed in Ref. [10].

By definition, the average of the curvature fluctuations is

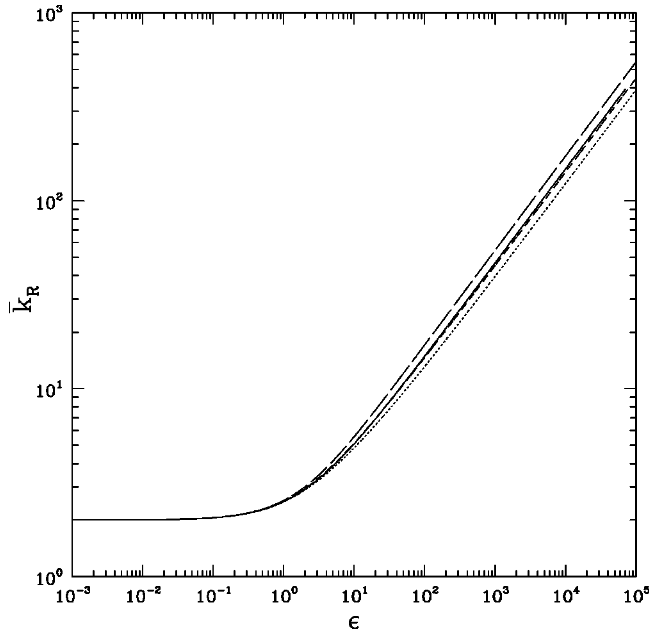

FIG. 1. $\overline{k_R}$ vs ϵ, worked out by means of the three single-mode solutions identified by the values of e listed in Eq. (24) (dotted, dashed, and long-dashed lines refer to $e=N/4,3N/4$, $e=N/3,2N/3$, and $e=N/2$, respectively), is compared with $\langle k_R\rangle_{\mu_E}$ computed in [10] (continuous line). The agreement is very good on a broad range of values of energy density ϵ.

$$\langle \delta^2 K_R\rangle_\mu = \langle (K_R - \langle K_R\rangle_\mu)^2\rangle_\mu = (N-1)^2[\langle (k_R)^2\rangle_\mu - (\langle k_R\rangle_\mu)^2]. \tag{38}$$

Again, by replacing the microcanonical averages with time averages, from Eq. (34) and after some trivial algebra, we get

$$\overline{\delta^2 k_R} = \frac{36\beta^2\omega_e^4}{N^2}[\overline{Q^4}_e - \overline{Q^2}_e\overline{Q^2}_e]. \tag{39}$$

The new term

$$\overline{Q_e^4} = \frac{A^4}{T_e}\int_0^{T_e} dt\, \mathrm{cn}^4(\Omega_e t,k) = \frac{A^4}{4\mathbf{K}}\int_0^{4\mathbf{K}} d\theta\, \mathrm{cn}^4(\theta,k)$$

can be computed by resorting to standard properties of the elliptic functions, and the result is

$$\overline{Q_e^4} = \frac{A^4}{3\mathbf{K}k^4}[\mathbf{K}(2-5k^2+3k^4) + 2\mathbf{E}(2k^2-1)]. \tag{40}$$

Finally, Eqs. (40) and (35) in Eq. (39) yield

$$\overline{\delta^2 k_R} = \frac{192\left[(k^2-1) + 2(2-k^2)\dfrac{\mathbf{E}}{\mathbf{K}} - 3\left(\dfrac{\mathbf{E}}{\mathbf{K}}\right)^2\right]}{(1-2k^2)^2\hat{C}_e^2}. \tag{41}$$

From Eq. (37) and making use of the tabulated values for **E** and **K**, Eq. (41) provides the mean fluctuations of curvature as a function of ϵ.

In Fig. 2, a comparison is made between the time average of the Ricci curvature fluctuations $\overline{\delta^2 k_R}$ as a function of the energy density ϵ, worked out along the OM solution that we

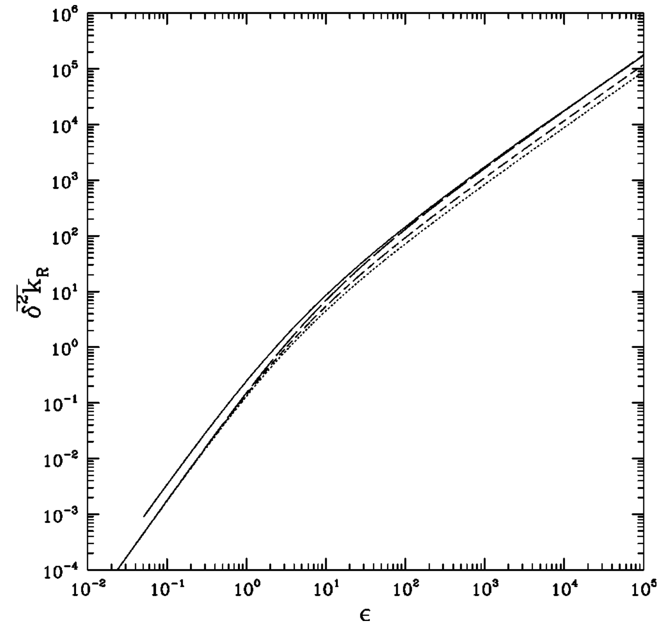

FIG. 2. In this figure, we report three curves for $\overline{\delta^2 k_R}$ vs ϵ computed by integrating the curvature fluctuations along the three single-mode solutions considered in the present paper (dotted, dashed, and long-dashed lines refer to $e=N/4,3N/4$, $e=N/3,2N/3$, and $e=N/2$, respectively), and a comparison is made with the same quantity computed in [10] (continuous line). Also in this case the agreement is very good.

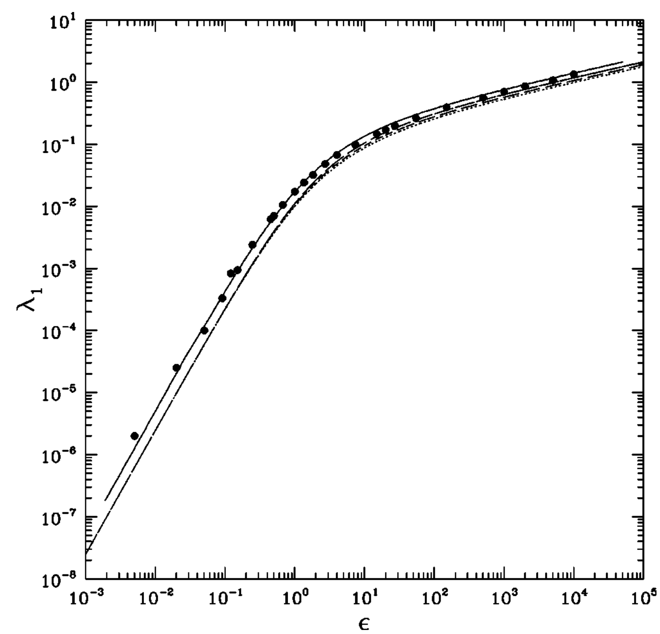

FIG. 3. This figure shows the largest Lyapunov exponent λ_1 obtained by integrating the suitable geometric quantity along the three single-mode solutions considered in the present paper, plotted vs ϵ. Dotted, dashed, and long-dashed lines refer to $e=N/4,3N/4$, $e=N/3,2N/3$, and $e=N/2$, respectively. Continuous line refers to the Lyapunov exponent computed in [10]. The full circles are the values for λ_1 computed by numerical integration. The agreement is again very good on a broad range of ϵ values.

considered, and $\langle \delta^2 k_R \rangle_{\mu_E}$ versus ϵ analytically computed in Ref. [10]. The agreement is very good, thus confirming from a completely new point of view that unstable periodic orbits are special tools for dynamical systems analysis; in this case, certain geometric quantities of configuration space are surprisingly well sampled by UPOs because time averages computed along them are very close to microcanonical averages performed on the whole energy hypersurfaces.

Finally, we can compute the Lyapunov exponents as a function of the energy density ϵ by inserting Eqs. (36), (37), and (41) into the analytic formulas (13) and (14), replacing $\langle k_R \rangle_{\mu_E}$ and $\langle \delta^2 k_R \rangle_{\mu_E}$ by means of the corresponding time averages computed above. Figure 3 shows that the overall agreement between our analytic results, the analytic results from [10], and the results obtained by numerical integration of the tangent dynamics, is very good. The agreement is globally very good because at high energy density our results are really very close to the other mentioned ones, and at low energy density the discrepancy does not exceed—at worst—a factor of 2 on a range of many decades of energy density and with the use of only *one* unstable periodic orbit.

IV. CONCLUDING REMARKS

In conclusion, tackling the FPU-β model, we have found that some global curvature properties of the configuration space manifold—whose geodesics coincide with the trajectories of the system—are efficiently sampled by unstable periodic orbits. This is shown in Figs. 1 and 2 where the analytic energy dependence of the microcanonical averages of Ricci curvature and of its fluctuations is compared to the same quantities obtained by time-averaging along three unstable periodic orbits. Then, since the averages of these geometric quantities enter an analytic formula to compute the largest Lyapunov exponents, unstable periodic orbits can be used to compute them. The results obtained in this work are in very good agreement with those reported in Ref. [10]. Even though we have performed our computations only for one specific model (FPU-β), we surmise that this method can be of general validity. In fact, the computations given in the present work remove an ergodic assumption made in the Riemannian theory of Hamiltonian chaos, where it is assumed that the time averages of the relevant geometric quantities, to be computed along chaotic orbits, can be replaced by static microcanonical averages. While chaotic trajectories cannot be known analytically, UPOs can, and efficiently do the same job.

Finally, let us remark that this impressive efficiency of UPOs in "smartly" sampling of the phase space of Hamiltonian systems, while confirming the special relevance of UPOs among all the possible phase-space trajectories of a nonlinear Hamiltonian system, opens an interesting subject for future investigation: understanding the deep reasons for their peculiarity.

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