Gaussian Model for Chaotic Instability of Hamiltonian Flows

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A general method to describe Hamiltonian chaos in the thermodynamic limit is presented which is based on a model equation independent of the dynamics. This equation is derived from a geometric approach to Hamiltonian chaos recently proposed, and provides an analytic estimate of the largest Lyapunov exponent λ. The particular case of the Fermi-Pasta-Ulam β-model Hamiltonian is considered, showing an excellent agreement between the values of λ predicted by the model and those obtained with computer simulations of the tangent dynamics.

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Many problems and applications ranging from the general theory of dynamical systems to plasma and condensed matter physics are represented in terms of many degrees of freedom Hamiltonian systems of the form

$$\mathcal{H}(\mathbf{q},\mathbf{p}) = \sum_{i=1}^{N} \frac{p_i^2}{2m} + V(\mathbf{q}), \qquad (1)$$

where $V(\mathbf{q})$ is a nonlinear interaction potential among N particles with mass m, positions $\mathbf{q} = q^1,\ldots,q^N$, and momenta $\mathbf{p} = p^1,\ldots,p^N$.

For most of the interesting choices of $V(\mathbf{q})$—apart from some remarkable exceptions, like the Toda lattice model—Hamiltonian (1) is nonintegrable and the corresponding equations of motion

$$m\frac{d^2q^i}{dt^2} = -\frac{\partial V}{\partial q_i}, \qquad i = 1,\ldots,N, \qquad (2)$$

exhibit chaotic, i.e., unpredictable, behavior despite their deterministic nature. One of the most interesting features of these Hamiltonian models is the presence of a transition from a weakly to a strongly chaotic regime when the energy per particle is increased, and numerical results suggest that this transition is stable in the thermodynamic limit $N \to \infty$ [1]. The degree of chaoticity of Eqs. (2) can be quantified by the largest Lyapunov exponent $\lambda_{\max}$, which, roughly speaking, is a measure of the mean rate of exponential divergence between nearby orbits. The rigorous definition of Lyapunov exponents can be found elsewhere [2]. Here we rather deal with an estimate λ of $\lambda_{\max}$ which, for Hamiltonian systems of the form (1), is defined as follows: First the equations of motion (2) are linearized along a generic trajectory yielding the evolution equations

$$\frac{d^2\xi^i}{dt^2} + \frac{\partial^2 V}{\partial q_i \partial q^j}\xi^j = 0, \qquad i = 1,\ldots,N, \qquad (3)$$

for the variations $\boldsymbol{\xi} = \xi^1,\ldots,\xi^N$ of the coordinates (summation over repeated indices is understood throughout the paper and $m = 1$ is also assumed); then λ is given by

$$\lambda = \lim_{t\to\infty} \frac{1}{t} \ln \frac{\|\boldsymbol{\xi}(t)\|}{\|\boldsymbol{\xi}(0)\|}, \qquad (4)$$

where $\|\boldsymbol{\xi}\|$ is the Euclidean norm of $\boldsymbol{\xi}$.

An algorithm to compute λ was developed by Benettin, Galgani, and Strelcyn [3]. Numerical analysis based on this algorithm shows that the transition between weak and strong chaos can be detected by a scaling crossover of λ as a function of the energy per degree of freedom $\epsilon = E/N$ [1].

Simple algebraic manipulations of Eqs. (3) lead to the equation

$$\frac{1}{2}\frac{d^2\|\boldsymbol{\xi}\|^2}{dt^2} + \frac{\partial^2 V}{\partial q^i \partial q^j}\xi^i\xi^j - \left(\frac{d\|\boldsymbol{\xi}\|}{dt}\right)^2 - \|\boldsymbol{\xi}\|^2 \left\| \frac{d\boldsymbol{\mu}}{dt} \right\|^2 = 0, \qquad (5)$$

where $\boldsymbol{\mu} = \boldsymbol{\xi}/\|\boldsymbol{\xi}\|$. The term containing $d\boldsymbol{\mu}/dt$ can be neglected [4], and by standard substitutions [5] we arrive at an evolution equation for the norm $\|\boldsymbol{\xi}\|$ having the form of a generalized Hill equation

$$\frac{d^2\psi}{dt^2} + Q(t)\,\psi = 0, \qquad (6a)$$

$$Q(t) = \frac{\partial^2 V}{\partial q^i \partial q^j}\frac{\xi^i}{\|\boldsymbol{\xi}\|}\frac{\xi^j}{\|\boldsymbol{\xi}\|}, \qquad (6b)$$

where $|\psi|$ is proportional to $\|\boldsymbol{\xi}\|$.

The present work aims at obtaining an analytic expression for λ in the limit $N \to \infty$. At first sight this goal hits against a major obstacle: $Q(t)$ has to be computed along a dynamical trajectory [Eqs. (6) are coupled to Eqs. (2) and (3)]. Hence Eq. (6a) can be useful to compute λ only if we are able to model $Q(t)$ by a function which is independent of the dynamics. The main point of this Letter is to show how such a model can be actually formulated using the differential geometric structure underlying dynamics.

The dynamics described by Eqs. (2) is equivalent to a geodesic flow on a Riemannian manifold. In fact, both the dynamical trajectories and the geodesics of a Riemannian manifold are derived from a variational principle. The variational principle for dynamics is Hamilton's (or Maupertuis's) least action principle stating that the trajectories are the extrema of the action functional. The geodesics of a Riemannian manifold are defined as the extrema of the arclength functional $\ell_{AB} = \int_A^B ds$, where $ds^2 = g_{\mu\nu} dq^\mu dq^\nu$ is the Riemannian metric. Hence a suitable choice of the ambient manifold and of its metric tensor g makes a correspondence between action and arclength such that the geodesics are identified with the dynamical trajectories [6]. In this geometric framework, the natural tool to tackle dynamical chaos is the Jacobi equation for geodesic spread [7]

$$\frac{\nabla}{ds}\frac{\nabla}{ds} J^\mu + R^\mu_{\nu\eta\lambda} \frac{dq^\nu}{ds} J^\eta \frac{dq^\lambda}{ds} = 0, \tag{7}$$

describing the evolution of geodesic deviation vector field $\mathbf{J}$, often referred to as the Jacobi field. This is a local stability equation for the geodesics. Here ∇/ds is the covariant derivative along the geodesic and R is the Riemann curvature tensor. Throughout the paper, Greek indices run from 1 to $\mathcal{N}$, where $\mathcal{N}$ is the dimension of the Riemannian manifold, and Latin indices from 1 to N which is the dimension of the configuration space (in general $\mathcal{N} \geq N$). The vector field $\mathbf{J}$ plays for the geodesic flow the same role that the variation vector $\boldsymbol{\xi}$ plays for the dynamical trajectories. In previous papers [8,9] it has been shown that for a particular choice of the metric g, due to Eisenhart [10], the dynamics (2) can be interpreted as a geodesic flow in an $(N+2)$-dimensional manifold with local coordinates $q^0, q^1, \ldots, q^N, q^{N+1}$: q^0 is a time coordinate, $q^1, \ldots, q^N$ belong to configuration space, and q^{N+1} is related to the action. Direct computation of Eq. (7) for Eisenhart metric leads exactly to Eq. (3) after renaming $J^1, \ldots, J^N$ as $\xi^1, \ldots, \xi^N$. An equation describing the evolution of the norm $\|\mathbf{J}\| = \sqrt{g_{\mu\nu} J^\mu J^\nu}$ naturally follows from Eq. (7) and can be cast in the form of a generalized Hill equation as in the case of Eq. (6):

$$\frac{d^2\psi}{ds^2} + K(s)\,\psi = 0, \tag{8a}$$

$$K(s) = R_{\mu\nu\eta\lambda} \frac{J^\mu}{\|\mathbf{J}\|} \frac{dq^\nu}{ds} \frac{J^\eta}{\|\mathbf{J}\|} \frac{dq^\lambda}{ds}, \tag{8b}$$

where $|\psi|$ is proportional to $\|\mathbf{J}\|$. Here $K(s)$ is the sectional curvature relative to the plane spanned by $\mathbf{J}$ and $d\mathbf{q}/ds$ [11]; $K(s)$ is the generalization to high-dimensional manifolds of the usual Gaussian curvature of two-dimensional surfaces. In the case of Eisenhart metric the arclength parametrization is affine, i.e., $ds^2 = C^2 dt^2$ with C a constant, and the only nonvanishing components of the curvature tensor are $R_{0i0j} = \partial^2 V/\partial q^i \partial q^j$. Hence $K(s) \equiv Q(t)/C^2$, with Q given by Eq. (6b), $\|\mathbf{J}\| \equiv \|\boldsymbol{\xi}\|$, and Eq. (8a) gives just Eq. (6a). The solutions of Eq. (8) can be exponentially growing—thus implying chaos—under two circumstances: Either the sectional curvature K is negative along the geodesics, or it oscillates, fulfilling the conditions for parametric instability. The former case is considered in ergodic theory: Following the geometric approach it is possible to obtain rigorous proofs of ergodicity and mixing for abstract dynamical systems for which all the sectional curvatures are negative. This is the case of Anosov flows [2]. On the other hand, it is found that curvatures are mostly positive for generic Hamiltonians of the form (1), provided that V is a binding potential with minimum, therefore parametric instability plays a crucial role to make chaos in conservative dynamical systems of physical interest [8,9].

Now we are going to exploit the fact that using Eisenhart metric Eqs. (8) lead to Eqs. (6) up to a time reparametrization $ds^2 = C^2 dt^2$. In particular, we can take advantage of the fact that $Q(t)$ in Eq. (6b) is the sectional curvature $K(s)$ in Eq. (8b) to find a model equation for $\|\boldsymbol{\xi}\|(t)$ independent of the details of the dynamics (i.e., of computer generated trajectories). First of all, at large N and with generic, i.e., random, initial conditions, we assume that—for a nonintegrable system—$K(s)$ is well represented by a random process of the form

$$K(s) \simeq \langle K \rangle_s + \langle \delta^2 K \rangle_s^{1/2}\, \eta(s), \tag{9}$$

where the averages are taken along a geodesic, $\eta(s)$ is a normalized Gaussian noise with zero mean, and $\langle \delta^2 K \rangle^{1/2}$ is the rms fluctuation of K. The next step is a suitable estimate of mean and variance of the random process (9): Here the geometric nature of $Q(t)$, i.e., $Q(t) \equiv C^2 K(s)$, comes in to help. With the aid of an elementary result in Riemannian geometry, a rough estimate of K can be obtained. This involves Ricci curvature K_R which is defined by [7]

$$K_R \equiv R_{\mu\nu} \frac{dq^\mu}{ds} \frac{dq^\nu}{ds}, \tag{10}$$

where $R_{\mu\nu}$ is the Ricci tensor. At each point of the manifold the mentioned estimate gives [8] $K \simeq K_R/(\mathcal{N} - 1) \simeq K_R/N$ at large N. Such a replacement is a pointwise average of the sectional curvatures that can be independently defined at each point. The replacement would be exact for a class of manifolds called isotropic—or constant curvature—manifolds. Therefore, in order to get rid of the dependence of $K(s)$ upon the evolution of $\mathbf{J}/\|\mathbf{J}\|$, we replace K by K_R/N; this is the "zeroth order" approximation of $K(s)$. Then to account for the fluctuations described by the second term on the right-hand side of Eq. (9) it is natural to use the fluctuations of Ricci curvature and to replace Eq. (9) by

$$K(s) \simeq \frac{1}{N}\langle K_R \rangle_s + \frac{1}{N}\langle \delta^2 K_R \rangle_s^{1/2}\, \eta(s), \tag{11}$$

which is now independent of $\mathbf{J}$; nevertheless, it still depends on the dynamics because the averages are taken along a geodesic. Now, since we want to estimate the largest Lyapunov exponent, i.e., a time-asymptotic quantity which should not be affected by the details of the dynamics, we replace the averages $\langle\cdot\rangle_s$ over a generic geodesic with statistical averages over a microcanonical measure $\langle\cdot\rangle_E$. Our estimate of the sectional curvature K is thus rewritten as

$$K(s) \simeq \frac{1}{N}\langle K_R\rangle_E + \frac{1}{N}\langle \delta^2 K_R\rangle_E^{1/2}\,\eta(s)\,. \tag{12}$$

For many models of physical interest $K_R > 0$, hence a major source of chaos in this picture is parametric instability.

Now, inserting Eq. (12) into Eq. (8a) and using the arclength parametrization $ds^2 = C^2 dt^2$, from Eq. (6) we obtain a model equation for ψ in the form of a random oscillator

$$\frac{d^2\psi}{dt^2} + \gamma(t)\,\psi = 0\,, \tag{13}$$

where $\gamma(t)$ is no longer a dynamical observable as $Q(t)$ is, but a Gaussian random process—$\gamma(t) \equiv C^2 K(t)$—whose mean γ_0 and variance σ_γ are

$$\gamma_0 = \langle k_R\rangle_E = \frac{C^2}{N}\langle K_R\rangle_E\,, \tag{14a}$$

$$\sigma_\gamma^2 = \langle \delta^2 k_R\rangle_E = \frac{C^2}{N}\langle (K_R - \langle K_R\rangle)^2\rangle_E\,, \tag{14b}$$

where we have also defined the symbols $\langle k_R\rangle_E$ and $\langle\delta^2 k_R\rangle_E$. In the case of Eisenhart metric the only nonvanishing component of the Ricci tensor is $R_{00} = \triangle V$, where $\triangle$ stands for the Euclidean Laplacian, thus $C^2 K_R = \triangle V$. In the above definitions the probability measure is, as previously stated, a microcanonical distribution so that for any observable A

$$\langle A\rangle_E = \frac{\int d^N\mathbf{q}\, d^N\dot{\mathbf{q}} A\,\delta(\mathcal{H} - E)}{\int d^N\mathbf{q}\, d^N\dot{\mathbf{q}}\,\delta(\mathcal{H} - E)}\,. \tag{15}$$

Thus the quantities (14) can be computed independently of the dynamics.

The process $\gamma(t)$ is not completely defined unless its time correlation function $\Gamma_\gamma(t_1,t_2)$ is given. The simplest choice is to assume that γ is a stationary δ-correlated process, i.e.,

$$\Gamma_\gamma(t_1,t_2) = \Gamma_\gamma(|t_1 - t_2|) = \tau\,\sigma_\gamma^2\,\delta(|t_1 - t_2|)\,, \tag{16}$$

where τ is a characteristic time which we estimate with the aid of geometry. On a curved surface a typical length scale is the curvature radius ρ, which is related to the curvature K by $\rho^2 = 2/K$; on a constant curvature $\mathcal{N}$-dimensional manifold (e.g., an $\mathcal{N}$ sphere) $\rho^2 = 2(\mathcal{N} - 1)/K_R$. According to our Gaussian model (14), an average curvature radius is $\rho_1^2 = 2C^2/\gamma_0$ and another length scale, related with fluctuations, is $\rho_2^2 = \gamma_0 C^2/2\sigma_\gamma^2$. Hence, using $ds^2 = C^2 dt^2$, two characteristic time scales are given by $\tau_{1,2} = \rho_{1,2}/C$, and we obtain a characteristic time as $\tau^{-1} = \tau_1^{-1} + \tau_2^{-1}$, i.e.,

$$\tau = \left[\sigma_\gamma\left(\sqrt{\frac{2}{\gamma_0}} + \sqrt{\frac{\gamma_0}{2\sigma_\gamma^2}}\right)\right]^{-1}\,. \tag{17}$$

Equation (13) admits exponentially unstable solutions whenever $\gamma(t)$ has a nonvanishing random component [12]. The asymptotic rate of exponential growth of the solutions will provide our estimate of λ. Thus we put

$$\lambda = \lim_{t\to\infty}\frac{1}{t}\ln\frac{|\psi(t)|}{|\psi(0)|}\,, \tag{18}$$

where ψ is the solution of the stochastic differential equation (13), and $|\psi(t)|/|\psi(0)|$ can be computed through the evolution of the second moments of ψ. Such evolution is readily obtained by means of a method due to Van Kampen [12] and yields—through Eq. (18)—the following expression for λ:

$$\lambda\,(\gamma_0,\sigma_\gamma,\tau) = \frac{1}{2}\left(\Lambda - \frac{4\gamma_0}{3\Lambda}\right)\,, \tag{19a}$$

$$\Lambda = \left(\sigma_\gamma^2\tau + \sqrt{\frac{64\gamma_0^3}{27} + \sigma_\gamma^4\tau^2}\right)^{1/3}\,. \tag{19b}$$

Let us now apply our Gaussian model to a particular case, the Fermi-Pasta-Ulam (FPU) β model defined by the Hamiltonian

$$\mathcal{H} = \sum_{i=1}^{N}\left[\frac{p_i^2}{2} + \frac{1}{2}(q_{i+1} - q_i)^2 + \frac{\mu}{4}(q_{i+1} - q_i)^4\right]\,. \tag{20}$$

The reason for this choice is twofold. First, Hamiltonian (20) allows the analytic computation of all the quantities entering Eqs. (19) in the limit $N \to \infty$, and one can compare the result for λ with numerical estimates obtained by the algorithm of Ref. [3]. Moreover, the FPU model exhibits the transition from weak to strong chaos, which is marked by a scaling crossover in the dependence of λ on the energy density $\epsilon = E/N$. The explicit expression for k_R in the case (20) is

$$k_R = 2 + \frac{6\mu}{N}\sum_{i=1}^{N}(q_{i+1} - q_i)^2\,. \tag{21}$$

The quantities we need are the microcanonical averages $\langle k_R\rangle_E$ and $\langle\delta^2 k_R\rangle_E$. From the computational point of view it is easier to use the Gibbs canonical measure $\langle\cdot\rangle_G$, because the partition function for the FPU one-dimensional chain is known [13] and in the thermodynamic limit the results are equivalent. In fact, $\langle k_R\rangle_E = \langle k_R\rangle_G + \mathcal{O}(1/N)$ and $\langle\delta^2 k_R\rangle_E = \langle\delta^2 k_R\rangle_G + F + \mathcal{O}(1/N)$ where F is a corrective term which does not vanish in the thermodynamic limit and can be computed by means of Gibbsian averages [14]. The results are expressed in terms of the parameter $\theta = \sqrt{\beta/2\mu}$, where β is the inverse temperature, and a relation between the energy density $\epsilon = E/N$ and the parameter θ allows one to obtain the

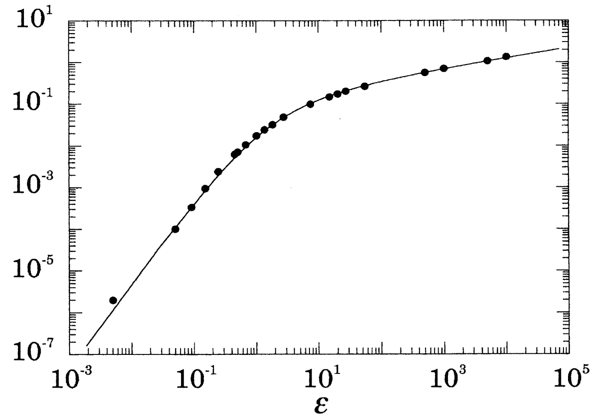

FIG. 1. Largest Lyapunov exponent λ vs energy density $\epsilon = E/N$ for the FPU β model with $\mu = 0.1$. The analytic result obtained from Eq. (19) (solid line) is here compared with the values obtained by computer simulations of the tangent dynamics—Eq. (3)—with $N = 256$ (full circles).

results as functions of ϵ (see Ref. [9] for details). The relation between ϵ and θ is

$$\epsilon(\theta) = \frac{1}{8\mu}\left(\frac{3}{\theta^2} + \frac{1}{\theta}\frac{D_{-3/2}(\theta)}{D_{-1/2}(\theta)}\right), \tag{22}$$

and the formulas for $\langle k_R\rangle_E(\theta)$ and $\langle \delta^2 k_R\rangle_E(\theta)$ are

$$\langle k_R\rangle_E(\theta) = 2 + \frac{3}{\theta}\frac{D_{-3/2}(\theta)}{D_{-1/2}(\theta)}, \tag{23}$$

$$\langle \delta^2 k_R\rangle_E(\theta) = \frac{9}{\theta^2}\left\{2 - 2\theta\frac{D_{-3/2}(\theta)}{D_{-1/2}(\theta)} - \left[\frac{D_{-3/2}(\theta)}{D_{-1/2}(\theta)}\right]^2\right\} + F(\theta), \tag{24}$$

where D_ν are parabolic cylinder functions. According to Ref. [14] we find the correction $F(\theta)$ in the form

$$F(\theta) = \frac{1}{4\mu\theta}\left(\frac{\partial\epsilon(\theta)}{\partial\theta}\right)^{-1}\left(\frac{\partial\langle k_R\rangle(\theta)}{\partial\theta}\right)^2, \tag{25}$$

where $\partial\epsilon/\partial\theta$ and $\partial\langle k_R\rangle/\partial\theta$ are computed from Eqs. (22) and (23). The explicit expression of the time constant τ in the case of the FPU chain is obtained from Eq. (17) by substituting γ_0 with $\langle k_R\rangle_E$ given by Eq. (23) and σ_γ with $\langle \delta^2 k_R\rangle_E^{1/2}$ given by Eq. (24).

Substituting Eqs. (23) and (24) and the expression of τ into Eqs. (19) yields an analytic expression of $\lambda(\epsilon)$ for the FPU model, valid in the $N \to \infty$ limit (see Fig. 1). From this expression one can easily determine the asymptotic behaviors of $\lambda(\epsilon)$, $\lambda(\epsilon) \sim \epsilon^2$ as $\epsilon \to 0$, and $\lambda(\epsilon) \sim \epsilon^{1/4}$ as $\epsilon \to \infty$. The crossover between the two power laws occurs at $\epsilon \sim 0.12/\mu$, thus confirming also in the thermodynamic limit the value of the energy threshold between weak and strong chaoticity already estimated in Refs. [1] and [9].

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