Semi-Analytic Estimates of Lyapunov Exponents in Lower-Dimensional Systems

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I. INTRODUCTION

Computing Lyapunov exponents, which measure the average linear stability of chaotic orbits in a $t \to \infty$ limit, entails solving a matrix harmonic oscillator equation with time-dependent frequencies. The differential-geometric analogue is a Jacobi equation (equation of geodesic deviation) on a manifold equipped with the Eisenhart metric. To the extent that aperiodic chaotic orbits can be treated as ‘random,’ this exact equation can be approximated as a stochastic harmonic oscillator equation with ‘randomly varying’ frequencies. The implementation of such a picture, along with more detailed assumptions that would seem reasonable in a thermodynamic limit, has yielded remarkable success in estimating Lyapunov exponents in high-dimensional systems. In lower dimensions, where some of these assumptions are at least questionable, one still derives estimates that are qualitatively correct; but while the general trends of the dynamics tend to be captured, many details are often missed.

The aim of this letter is two-fold, namely (i) to describe how and to what extent this general approach can be improved upon by relaxing some of the underlying assumptions, and (ii) to determine physically why, in lower dimensions, much of the dynamics eludes a statistical description. The analysis will focus on Hamiltonians of the form $H = \sum_{i=1}^{D} p_i^2/2 + V(q_i)$ for two representative potentials, namely the Fermi-Pasta-Ulam (FPU) potential, and a higher-dimensional analogue of the dihedral potential,

$$V(q_1, q_2, ..., q_D) = -\sum_{i=1}^{D} q_i^2 + \frac{1}{4} \left( \sum_{i=1}^{D} q_i^2 \right)^2 - \frac{1}{4} \sum_{i<j}^{D} q_i^2 q_j^2.$$  

(2)

II. RELAXING UNDERLYING ASSUMPTIONS

The key physical assumption underlying the entire analysis is that the exact Jacobi equation can be approximated by a matrix stochastic oscillator equation in which the curvature, which determines the frequencies, varies ‘randomly’ along a chaotic orbit, i.e., that the ‘true’ dynamical equation can be replaced by an approximate statistical equation. Given this assumption, what remains is to specify the statistics of the random process. Basically this has involved three additional assumptions:

1. An assumption of isotropy, which reduces the $D$-dimensional matrix equation to a one-dimensional oscillator equation.
2. An assumption that the curvature fluctuations acting at any given instant are Gaussian-distributed.
3. An assumption regarding the form of the autocorrelation function and an associated correlation time $\tau_c$, which characterise changes in the curvature fluctuations along a chaotic orbit.

Mathematically, the reduction from a $D$-dimensional matrix equation to a one-dimensional stochastic oscillator follows from the assumption that the configuration space can be approximated as quasi-isotropic, i.e., that if the Riemann tensor be viewed as the sum of a Ricci curvature $K$ and a non-isotropic Weyl projective tensor, the latter may be assumed to vanish. Physically, this is equivalent to assuming that there are no preferred directions in space, so that the matrix equation reduces to $D$ identical one-dimensional equations. At least for potentials in which different degrees of freedom enter iden-
tically, it might seem that this assumption becomes increasingly justified in higher dimensions. Earlier investigations found that, for some potentials, the analytic estimate $\chi_{ana}$ converges quite rapidly towards the value $\chi_{num}$ computed numerically, but that for other potentials it does not \[4\]. This suggests that quasi-isotropy is likely not the principal source of error.

It remains, therefore, to consider the form of the curvature fluctuations both at a fixed instant and as a function of time. To the extent that the entire phase space is chaotic, the form of the curvature fluctuations at a fixed instant can be addressed either analytically, given an assumption of ergodicity, or numerically, by evaluating the statistical properties of representative orbit ensembles. However, it would appear that dynamical issues involving the auto-correlation function and the correlation time must be addressed numerically.

### A. Approximating curvature fluctuation as Gaussian-distributed

The assumption is that curvature fluctuations in different directions can be approximated as nearly independent and, at any given instant, Gaussian-distributed. For potentials investigated in \[4\], this approximation was completely unjustified in systems with two degrees of freedom (dof), and questionable in slightly higher-dimensional systems. To determine the accuracy of such an approximation, we compare the Gaussian constructed from numerical estimates of the first two moments of the curvature to the exact curvature distribution function $N[K]$, which can be computed analytically for potentials in which the radius $r$ can be expressed in terms of the Ricci curvature $K$.

Given the assumption of a microcanonical distribution, moments of $K$ satisfy

$$
\langle K^n \rangle = \frac{\int_{V(q)=E} dq \ [E - V(q)]^{(D-2)/2} K^n(q)}{\int_{V(q)=E} dq \ [E - V(q)]^{(D-2)/2}}, \tag{3}
$$

where $D$ is the dimensionality. If one can transform from the coordinates $(q_1, q_2, ..., q_D)$ to $(K, \theta_1, \theta_2, ..., \theta_{D-1})$, where $K$ labels surfaces of constant curvature (density), eq. \[3\] becomes

$$
\langle K^n \rangle = \frac{\int K^n dK \int d\theta_1 d\theta_2 ... d\theta_{D-1} \left| \frac{\partial q}{\partial (K, \theta)} \right| [E - V]^{D-2}}{\int dK \int d\theta_1 d\theta_2 ... d\theta_{D-1} \left| \frac{\partial q}{\partial (K, \theta)} \right| [E - V]^{D-2}}, \tag{4}
$$

and the distribution function

$$
N[K] = \int d\theta_1 d\theta_2 ... d\theta_{D-1} \left| \frac{\partial q}{\partial (K, \theta)} \right| [E - V]^{D-2}, \tag{5}
$$

where the dependence of $\left| \frac{\partial q}{\partial (K, \theta)} \right|$ and $V$ on the transformed coordinates is omitted for brevity. For compact isoenergy surfaces, the integration extends over the entire range of angles $\theta_i$. For a $D$-dimensional potential, a natural choice for the $\theta_i$ are the angles $\psi_i$ of generalized polar coordinates $(r, \psi_1, ..., \psi_{D-1})$, with $0 < \psi_1, \psi_2, ..., \psi_{D-2} < \pi$ and $0 < \psi_{D-1} < 2\pi$, in terms of which the distribution of curvatures becomes

$$
N[K] = \frac{2\pi}{r^{D-1}} \int_0^\pi \int_0^{2\pi} \int_0^{2\pi} \psi_1 \sin^{D-3} \psi_2 \sin \psi_D \left[ E - V \right]^{D-2} \frac{\partial r}{\partial K} \sqrt{ \left( \frac{\partial K}{\partial r} \right)^2 - D} \tag{6}
$$

The results of the direct numerical evaluation of this $(D - 1)$-dimensional integral for the dihedral potential are shown in Fig. \[iii\] (thick lines).

If the shape of the curvature distribution does not deviate significantly from a Gaussian, i.e., if the higher moments of the curvature are non-vanishing but small compared to unity, a better estimate can be obtained through the asymptotic cumulant expansion \[\text{[iv]}\]

$$
C_m(x) = \bar{Z}(x) - \left[ \frac{\gamma_1}{6} \bar{Z}(x)^3 \right] + \left[ \frac{\gamma_2}{24} \bar{Z}(x)^4 + \frac{\gamma_3}{72} \bar{Z}(x)^6 \right] - \left[ \frac{\gamma_1^2}{144} \bar{Z}(x)^7 + \frac{\gamma_1 \gamma_3}{144} \bar{Z}(x)^9 \right] + \left[ \frac{\gamma_2^2}{1152} \bar{Z}(x)^8 + \frac{\gamma_1^2 \gamma_2}{1728} \bar{Z}(x)^{10} + \frac{\gamma_1^4}{31104} \bar{Z}(x)^{12} \right] + ... \equiv p_m(x)Z(x), \tag{7}
$$

where

$$
\bar{Z}(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}}, \tag{8}
$$

$$
Z(x) = \frac{1}{\sigma} Z \left( \frac{x - \langle K \rangle}{\sigma} \right), \tag{9}
$$

$$
\mu_n = \langle (K - \langle K \rangle)^n \rangle, \quad \sigma = \sqrt{\mu_2}, \quad \gamma_1 = \mu_3 / \sigma^3, \quad \gamma_2 = \mu_4 / \sigma^4 - 3. \tag{9}
$$

$p_m(x)$ is a polynomial of degree $m$, where $m$ is the highest derivative of $Z(x)$ kept in the expansion \[\text{[iv]}\]. $\gamma_1$ is the skewness coefficient and $\gamma_2$ the kurtosis.

Fig. \[iv\] shows three representations $N_i(K)$ of the curvature distribution for the dihedral potential: the Gaussian approximation, the cumulant expansion, and the exact value computed from the eq. \[iv\], along with the difference between them as measured by $\Delta(N_i, N_j) = \left[ \int \left( N_i(K) - N_j(K) \right)^2 dK \right]^{1/2}$. Given that all the approximations are normalized, i.e. that they enclose unit
FIG. 1: The distribution of curvatures, $N[K]$, approximated by a Gaussian $Z(K)$ (thin solid line), cumulant expansion $C_{12}(K)$ (dashed line) and exact (thick solid line), as computed by eq. (6), for the dihedral potential with dimensionality $D = 3, 4, 5, 6$ and energy levels $E = 1, 3, 6$. The last column shows the absolute difference between the exact value of $N[K]$ and the purely Gaussian approximation $Z(K)$ (squares), exact value and the cumulant expansion $C_{12}(K)$ (diamonds) and the Gaussian approximation and the cumulant expansion (triangles). A function of the form $(a/\sqrt{D}) + b$ is fit through data points (dashed lines).

surface, $\Delta$ represents the relative difference between the approximations. It is apparent that, as the dimensionality $D$ is increased, the convergence of the exact distribution towards a Gaussian distribution is of order $1/\sqrt{D}$, which is the usual thermodynamical behavior. The cumulant expansion provides slightly more accurate estimates to the curvature distribution than the Gaussian approximation, but also converges as $1/\sqrt{D}$.

B. Auto-correlation function $\Gamma(t) \equiv \langle K(0)K(t) \rangle$

The stochastic oscillator equation can be solved analytically using a method developed by van Kampen [7] if one assumes that the correlation time $\tau_c$, defined such that the auto-correlation function $\Gamma(t) \equiv \langle K(0)K(t) \rangle \approx 0$ for $t > \tau_c$, is short compared with the duration of the stochastic process. When the correlation time scaled in terms of the the average orbital time at that energy is short, typically less than $\bar{t} = 2$, which is the case for the 3-dimensional dihedral potential at low energies and the FPU potential for all dimensions and energies, accurate estimates of the Lyapunov exponents are found (Fig. 2). It is also evident that, for the dihedral potential, the correlation time grows with energy, which renders van Kampen’s analytic solution increasingly inaccurate. Because of the long tail of the auto-correlation function, even in higher dimensions the agreement between the numerical results and the geometric estimates does not improve. Empirically, it appears that the threshold at which van Kampen’s method yields accurate estimates is $\tau_c = \bar{t}/2 \lesssim 1$. This is consistent with the fact that van Kampen’s solution is the first term in a power series expansion in $\tau_c$, with error $\propto \tau_c^2$.

In point of fact, estimating Lyapunov exponents as outlined in [2, 3, 4] assumes that the stochastic process is delta-correlated, i.e., $\Gamma(t) = \tau^2 \delta(t)$, where $\tau$ represents a characteristic time scale. However, that assumption
FIG. 2: Auto-correlation function \( \Gamma \) in units of dynamical times for the 3-, 6- and 9-dimensional dihedral potential with energies \( E = 0, 4, 8, 12 \), (top three rows, respectively), and 4-, 5- and 6-dimensional FPU potential with energies \( \log_{10} E = 1, 1.6, 2.8, 3.4 \) (bottom three rows, respectively), along with the analytic (dashed lines) and numerical estimates (solid lines) of the Lyapunov exponents (rightmost column).

was introduced purely on grounds of computational convenience, and does not accurately reflect the shape of the actual correlation function. Rather, analysis of data such as those exhibited in Fig. 2 for both the dihedral and FPU potentials, reveals that the auto-correlation function is well fit by the functional form

\[
\Gamma(t) = Ae^{-pt} \sin \omega t, \tag{10}
\]

where \( \omega^{-1} \) is comparable to, and strongly correlates with, a typical orbital time scale (Fig. 3). The damping rate \( p \) appears to correlate with the rate \( \lambda \) at which an initially localized ensemble of orbits would evolve towards a microcanonical equilibrium [8], which implies that it is comparable to, but somewhat smaller than, the value of the largest Lyapunov exponent – typically \( \lambda \sim 0.2 - 0.65\chi \).

C. Characteristic time scale of the process \( \tau \)

In earlier work, the characteristic time scale \( \tau \) was defined in a seemingly ad hoc fashion as the geometric mean of two time scales which were identified using purely geometric considerations, i.e., \( \tau^{-1} = 2(\tau_1^{-1} + \tau_2^{-1}) \), where \( \tau_1 \) represents the typical time between successive conjugate points on the manifold, i.e., points where the Jacobi field of geodesic deviation vanishes, and \( \tau_2 \) corresponds to the length scale on which curvature fluctuations become comparable to the average curvature. In point of fact, however, \( \tau_1 \) and \( \tau_2 \) are closely related to the physically relevant time scales entering into the problem: quite generally, it appears that, to a fair degree of approximation, \( \tau_1 \propto \omega^{-1} \) and, as such, scales as a characteristic orbital time scale, and that \( \tau_2 \propto p^{-1} \) and, as such, scales as the damping time or, equivalently, the time scale associated with chaotic phase mixing as an ensemble evolves.
towards a time-independent equilibrium [8]. If we define these two physical time scales and their geometric mean as

\[ t_1 = \frac{2\pi}{\omega}, \quad t_2 = \frac{1}{p}, \quad t^{-1} = 2(t_1^{-1} + t_2^{-1}), \quad (11) \]

we find a strong correlation between \( \tau \) and \( t \), as well as between \( \tau_1 \) and \( t_1 \) (first and fourth panel in the rightmost column of Fig. 3). The time \( t_2 \) is typically an order of magnitude longer than \( t_1 \), which means that the characteristic time \( t \) is determined primarily by the shorter time scale \( t_1 \), the orbital time scale.

Assuming proportionality constants that are comparable for both scalings the geometric mean would thus involve \( \tau \propto 1/(p+\omega) \). In point of fact, an auto-correlation function of the form (10) implies a characteristic time scale

\[ t_\Gamma = \frac{\int_0^\infty \Gamma(t)dt}{\int_0^\infty \Gamma(t)dt} = \frac{2p}{p^2 + \omega^2}. \quad (12) \]

Although this differs from the preceding formula for \( \tau \), we find an excellent correlation between the time \( t_\Gamma \) and the time scale \( \tau \) defined geometrically (second and fifth row in the rightmost column of Fig. 3).
III. DYNAMICS

Statistical estimates of the largest Lyapunov exponent in lower-dimensional Hamiltonian system entail two types of approximations: (1) time-independent – the space is approximated as isotropic and the curvature fluctuations as Gaussian-distribution, and (ii) time-dependent – stochastic oscillations are approximated as a delta-correlated process with a characteristic time scale $\tau$ derived using ad hoc geometric arguments. The time-independent approximations reduce the dynamics to a one-dimensional stochastic oscillator equation; the time-dependent approximations are used to solve that equation via van Kampen’s method.

At least for the two potentials considered here, the time-independent approximations appear well-justified and are unlikely sources of significant error. However, numerical computations show that the time-dependent approximations are not always justified. The simplifications which reduce the exact integral equation for $K(t)$ to a linear first order differential equation for $\langle K(t) \rangle$ rely entirely on the assumption that the auto-correlation time $t_c$ is short when compared with the duration of the process. As is evident from the slow decay of the auto-correlation function, this assumption typically fails for the dihedral potential, so that van Kampen’s method is strictly speaking inapplicable. The FPU potential has a more rapidly decaying auto-correlation function with a much shorter auto-correlation time. In this case, van Kampen’s method is applicable and, as illustrated in Fig. 2, yields more accurate estimates of the largest Lyapunov exponents. That this approach works much better for the FPU potential than for the dihedral potential may reflect the fact that the FPU system is sparsely coupled in the sense that each coordinate ‘interacts’ only with the neighbouring ones, while in the dihedral potential every coordinate is coupled to every other one. This possibility would seem related to the fact that many properties of dynamical systems appear to depend not simply on the number of degrees of freedom, but on their connectance $4$, a measure of the extent to which these degrees of freedom are directly coupled.

Justifying the time-independent approximations reinforces the idea that chaos in lower-dimensional systems can be modeled by a one-dimensional stochastic oscillator. However, only in some cases, when the auto-correlation function damps sufficiently quickly, can van Kampen’s method be employed to estimate solutions to this stochastic oscillator equation.

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[1] L. P. Eisenhart, Ann. Math. 30, 591 (1929).
[2] M. Pettini, Phys. Rev. E 47, 828 (1993).
[3] L. Casetti, C. Clementi, and M. Pettini, Phys. Rev. E 54, 5969 (1996).
[4] H. E. Kandrup, I. V. Sideris, and C. L. Bohn, Phys. Rev. E 65, 016214 (2002).
[5] G. Ciraolo and M. Pettini, Cel. Mech. and Dyn. Astron. 83, 171 (2002).
[6] M. Abramowitz and I. Stegun, Handbook of Mathematical Functions (Dover, New York, 1974).
[7] N. G. van Kampen, Phys. Rep. 24, 171 (1976).
[8] H. E. Kandrup and S. J. Novotny, astroph/0204019.
[9] C. Froeschlé, Phys. Rev. A 18, 277 (1978).