Spectral Analysis of Conservative Dynamical Systems

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The distribution of local Lyapunov exponents is used to analyze power spectra of conservative dynamical systems. It is shown that sharp and broad peaks in the spectra can be related to well defined regions in phase space, associated with algebraic and exponential stretching of distances, respectively.

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Spectra of highly excited atomic and molecular systems have been measured in some detail in the past years. Examples are the quadratic Zeeman effect (QZE) for the hydrogen atom in a strong magnetic field,[1] the photodissociation spectrum of the H_3^+ molecular ion,[2] and the stimulated emission pumping spectra of acetylene[3] and Na_3.[4] In all cases, coarse graining of the experimental high-resolution spectrum yields a low-resolution spectrum with distinct regularities such as equally spaced broadened peaks. The classical dynamics of these systems is mostly chaotic. A detailed quantum-mechanical analysis of the QZE has shown[1(b)] that many features of the low-resolution spectrum can be related to unstable classical periodic orbits. A full quantum-mechanical investigation of molecules such as H_3^+ or Na_3 is prohibitive. Studies of the classical-mechanical spectra of these systems have shown structures which are in close agreement with experimental observations. There are numerical indications that the peaks are associated with the presence of "quasiregular" (laminar) motion in the chaotic signals.[1(c),4] Here we mention a recent study[5] on Ar_3 clusters where a qualitative correlation, in a high-dimensional system, is made between a drop in the K entropy (as energy is increased) and an enlarged fraction of quasiregular and chaotic motion. However, a general theory does not exist.

Power spectra or correlation functions have been investigated for simple dissipative systems, such as one-dimensional piecewise-linear maps, or in connection with particular phenomena such as period doubling, intermittency, and "periodic chaos" (see Refs. 6 and 7 and references therein). The analysis of conservative systems has mainly focused on the long-time behavior of correlation functions[8] which exhibit, in many cases, a power-law decay[9] (corresponding to low-frequency noise of the $1/f$ type in the spectra[10]). The asymptotic behavior of correlation functions for a certain class of hyperbolic dynamical systems (either dissipative or conservative) has been recently explained in terms of generalized Lyapunov exponents.[7] In general, however, very few results are available about relations between the "ordered" part of power spectra (i.e., the resonances) and dynamical invariants such as Lyapunov exponents or metric entropies.

It is known that the power spectrum of hyperbolic (axiom A) dynamical systems is a meromorphic function in a strip of the complex plane.[11] The position of the poles (resonance) depends on the system under consideration and, according to it, the asymptotic decay of the correlation function $C(t)$ may be exponential or not. Moreover, $C(t)$ is modulated if the poles are not purely imaginary: In Ref. 12 this effect has been related to the possibility of dividing the time signal $x(t)$ into consecutive time intervals with approximately independent behavior. This approach was especially effective in describing systems exhibiting type-I intermittency, where an alternation of laminar phases and chaotic bursts occurs. The trajectory almost locks on a period for a long time, thus contributing a well defined frequency to the spectrum; then it enters a shorter, highly chaotic, phase before being reinjected into the regular one. The mean rejection time is related to a second, low-frequency, component.

In the present work we provide a method for the decomposition of power spectra in conservative dynamical systems, based on the analysis of local (effective) Lyapunov exponents.[13] The spectra are shown to consist of a "regular" part, characterized by very sharp peaks, corresponding to the motion in the vicinity of the invariant tori, where the divergency of nearby orbits is algebraic, and a "purely chaotic" one, exhibiting broadened peaks on a smooth background, corresponding to regions where the divergence is predominantly exponential. The decomposition is achieved by evaluating the probability distribution of local Lyapunov exponents[14] which, because of the presence of islands, displays a power-law correction to the usual exponential behavior.

We consider the standard map[15] in the form

$$x_{k+1} = x_k + K \sin y_k \pmod{2\pi},$$
$$y_{k+1} = x_{k+1} + y_k \pmod{2\pi}, \tag{1}$$

as a model of the Poincaré section of a typical nonhyperbolic Hamiltonian system with two degrees of freedom, whose phase space is the torus $0 \le x, y \le 2\pi$. For $K > K_c \approx 0.97$, the mapping generates chaotic trajectories that encircle the torus in both directions[16] and regular invariant curves that appear as "islands" in phase space. In Fig. 1 we show the numerically converged

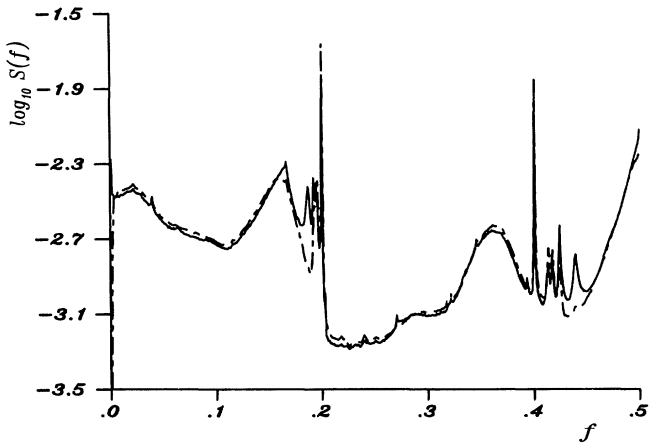

FIG. 1. Average power spectrum (solid line) of the standard map, for $K=2$, compared with the reconstructed spectrum (dashed line), obtained from the two Λ intervals $I_1^{(n)}=[0,0.06]$ and $I_2^{(n)}=[0.44,0.52]$. The averages are computed over 120 runs of 262144 iterates each, with $n=256$. The spectra are then compressed by a factor of 512 in frequency and normalized to unit area.

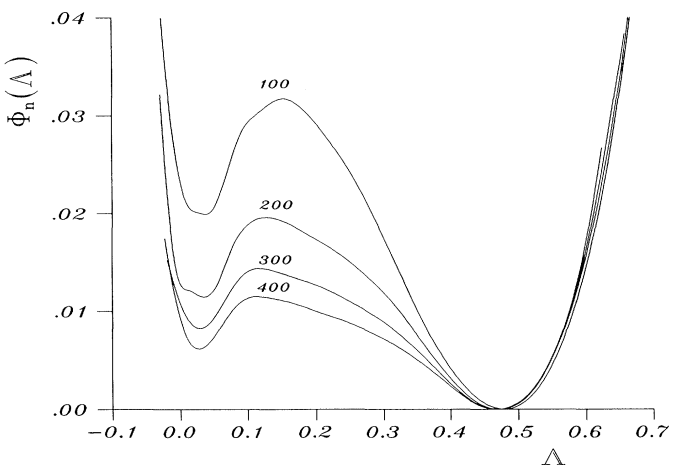

FIG. 2. Spectrum $\Phi_n(\Lambda)$ of (approximate) effective Lyapunov exponents Λ, for $K=2$ and $n=100$, 200, 300, and 400. A histogram, based on 10^8 runs, with bin size 2.4×10^{-2}, 1.7×10^{-2}, 1.6×10^{-2}, and 1.5×10^{-2}, respectively, was smoothed using a standard routine. The values of $P_{\max}(n)$ are 0.106, 0.114, 0.124, and 0.129 for $n=100$ to 400, respectively, found at $\Lambda=0.479$, 0.475, 0.473, and 0.461, respectively.

average power spectrum for the x coordinate at $K=2$. A number of very narrow peaks emerge from a smooth background which seems to present some broadened peaks. The width of the latter ones is much smaller than the average Lyapunov exponent of the system (equal to 0.45, for $K=2$). These features resemble those of highly excited systems such as the H_3^+ or the Na_3 molecules. The purpose of this Letter is to provide a method which allows one to distinguish the dynamical origin of this structure. Our analysis, although illustrated for a simple case, is general in form and is not limited to two-dimensional maps or to Hamiltonian systems with two degrees of freedom.

The first step is to divide a "long" trajectory[17] into intervals of length n and evaluate the (first) local Lyapunov exponent λ_n for each of them. Indicating that $d(n)$ the (infinitesimal) distance between two trajectories at time n, λ_n is defined by the asymptotic relation $\mu(n)\equiv d(n)/d(0)\sim n^{\gamma_n}e^{n\lambda_n}$, for $n\gg1$. In the limit $n\rightarrow\infty$, λ_n equals the average Lyapunov exponent $\langle\lambda\rangle$, for almost all initial conditions. Chaotic trajectories are generally characterized by positive values of λ_n. When, however, the orbit is close to a regular region, the local Lyapunov exponent will be very small for long times and the divergence of nearby points will be described by the algebraic exponent γ_n. The two kinds of behavior can be efficiently distinguished by computing the approximate local Lyapunov exponent $\Lambda_n\equiv n^{-1}\ln\mu(n)$ ($\approx\lambda_n$, for large n). When power-law corrections are not important, the probability distribution $P(\Lambda;n)$ of local Lyapunov exponents scales as $P(\Lambda;n)\sim e^{-n\Phi(\Lambda)}$, for $n\rightarrow\infty$.[14] In this case the asymptotic function $\Phi(\Lambda)$ has been named the spectrum of (effective) Lyapunov exponents by Grassberger, Badii, and Politi.[14] It has a minimum (equal to zero) at $\Lambda=\langle\lambda\rangle$ and is positive and finite for $\Lambda\leq\Lambda_{\max}$ (where $\Lambda_{\max}$ is the Lyapunov exponent of the most unstable periodic orbit). In Fig. 2 we plot the finite-n approximation $\Phi_n(\Lambda)=-n^{-1}\ln[P(\Lambda;n)/P_{\max}(n)]$, for $K=2$ and $n=100$, 200, 300, and 400 [$P_{\max}(n)$ is the maximum value of $P(\Lambda;n)$]. From the figure, one can clearly distinguish two qualitatively different scaling regions of $P(\Lambda;n)$ with n. The exponential scaling law is evident for $\Lambda\geq0.35$ and the minimum of $\Phi_n(\Lambda)$ is close to $\langle\lambda\rangle$. The power-law scaling is more appropriate for $\Lambda\approx0$, while a superposition of the two behaviors occurs at intermediate Λ values.

A more detailed analysis of the local stretching properties of the map would require considering the full two-dimensional distribution $\hat{P}(\lambda,\gamma;n)\sim n^{\psi(\gamma)}e^{-n\phi(\lambda)}$ of algebraic and Lyapunov exponents. The relevant information during the laminar phase is contained in the spectrum $\psi(\gamma)$. In regions of phase space where λ is bounded away from zero only the exponential term $\phi(\lambda)$ survives [and coincides with $\Phi(\Lambda)$], for large n. Accordingly, the distribution $P(\Lambda;n)$ of approximate Lyapunov exponents Λ exhibits the characteristic shape illustrated in Fig. 2. The regions of different scaling behavior can be identified by letting n vary. These observations have been tested for various values of the parameter K, corresponding to largely different numbers of islands in phase space, and are in agreement with the findings of Ref. 10.

To analyze the spectrum we now consider portions of trajectory which have a Λ either in a narrow strip I_1 of width 0.06, around the high-probability peak adjacent to $\Lambda=0$, or in the interval $I_2\equiv[0.44,0.52]$, centered around $\langle\Lambda\rangle$. The width of the two intervals is prescribed by the

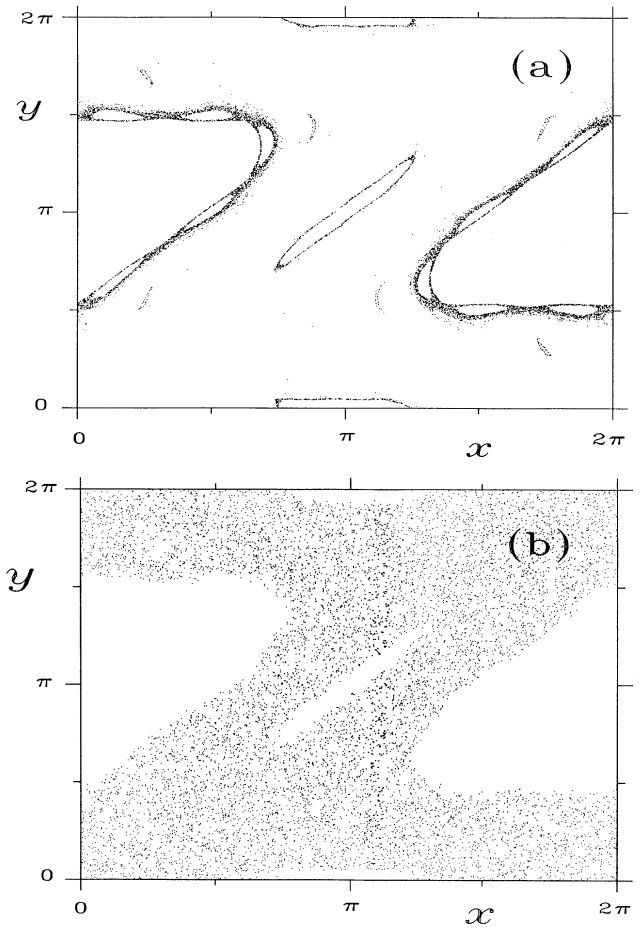

FIG. 3. Decomposition of the phase space of the standard map, for $K=2$. The regions corresponding to $0 \leq \Lambda \leq 0.06$ and $\Lambda \in [0.44,0.52]$ are displayed in (a) and (b), respectively.

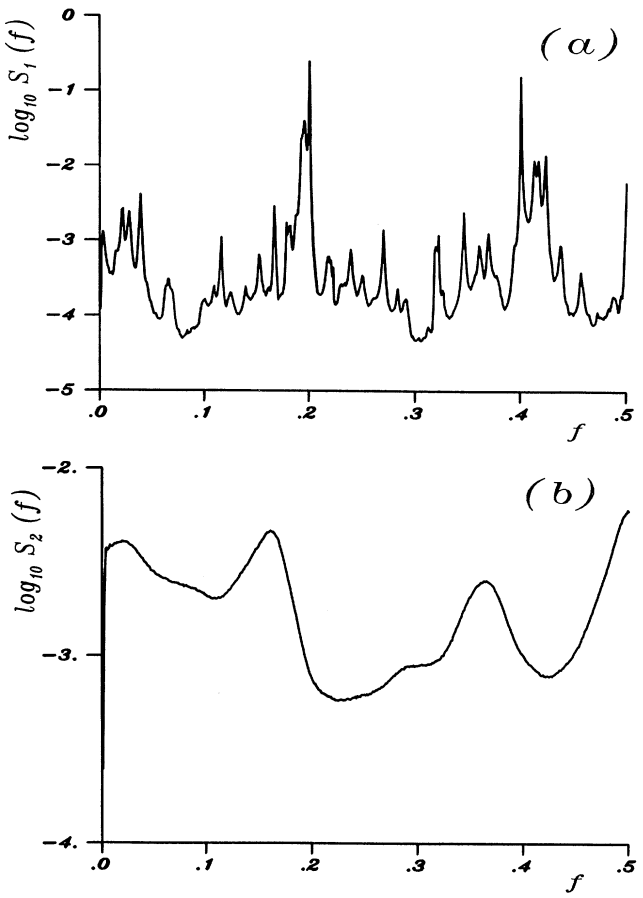

FIG. 4. Decomposition of the power spectrum, for $K=2$: The partial spectra (a) and (b) are computed for Λ values in the same intervals considered in Figs. 3(a) and 3(b). The parameter n and the number of iterations and averages are the same as in Fig. 1.

half-width of the peaks of $P(\Lambda;n)$.[18] We then construct two time series $X_k^{(n)}(I_i)$ $(i=1,2)$ consisting of the variable $x_k-\langle x\rangle$ $(k=m,\ldots,m+n)$ if the corresponding Λ (computed in the time interval $[m,m+n]$) belongs to the interval I_i, and equal to zero otherwise. In Fig. 3, we display the regions of phase space which correspond to (a) $\Lambda \in I_1$ and (b) $\Lambda \in I_2$, for $K=2$ and $n=100$. Chaotic and regular trajectories are clearly identified without need of any geometrical specification (such as the range of laminar behavior in $1-d$ intermittency). The power spectra $S_i(f)$ of the two signals $X_k^{(n)}(I_i)$, evaluated for $n=256$, are displayed in Fig. 4 [the area $\int S_i(f)df$ has been normalized to 1]. The first one contains all the narrow peaks of the full spectrum, while the second one closely resembles the "chaotic" background. Note the dominant peaks in Fig. 4(a) at the frequencies of 0.2, 0.4, and 0.5. The first two frequencies come from the period 5 at the center of the island chain surrounding the large island. The peak at 0.5 comes from the period 2 orbit at the center. A more detailed analysis of the frequencies is presented elsewhere.[19] In Fig. 1, the sum of the two partial spectra (dashed line), weighed according to the respective occurrence probability $[w(I_1)=3.36\times10^{-2}, w(I_2)=0.484]$, is compared with the true spectrum (solid line). Good agreement is obtained, although the first partial signal $X_k^{(n)}(I_1)$, which yields the relevant sharp peaks, has a probability of the order of 10^{-2}.

The method proposed in this paper allows the identification of laminar regions in conservative dynamical systems without need of constructing surfaces of section and of partitioning phase space in an arbitrary way. For highly excited molecular systems, due to their high dimensionality, it is virtually impossible to determine appropriate Poincaré sections. The present method achieves a separation of power spectra into sharp and broadband features by utilizing only the distribution of local Lyapunov exponents. This can be computed with sufficient accuracy also in systems with three or more degrees of freedom.

This analysis has been successfully applied to a model

with two degrees of freedom (the Hénon-Heiles potential)[19] and we are in the process of extracting the regions of laminar flow in the H_3^+ molecular ion. This technique will therefore be very effective for a classical-mechanical interpretation of the coarse-grained spectrum of excited molecular systems. It also applies to any model with orbits close to marginal stability, including dissipative intermittent maps. In such a case, the Lyapunov exponent Λ can be interpreted as the inverse of the laminar time τ and the evaluation of $P(\Lambda;n)$ is equivalent to that of the distribution of τ.[12]

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[17]The reason for choosing a long trajectory is technical; it assures that all segments of length n originate in the irregular region. An alternative procedure is a statistical sampling of phase space in the irregular region with trajectory segments of equal length n.

[18]However, the final result is quite insensitive to the magnitude of the interval. Reducing the interval only necessitates longer samplings but does not noticeably change the final result.

[19]M. A. Sepúlveda, R. Badii, and E. Pollak (to be published).