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Positive Lyapunov Exponents in the Kramers Oscillator

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The maximum Lyapunov exponent is computed numerically for the double-well oscillator in a heat bath. Positive exponents are found in a wide range of friction coefficients in the low-damping regime.

KEY WORDS: Stochastic nonlinear systems; Lyapunov exponents.

1. INTRODUCTION

The paper is devoted to the effect of noise on the celebrated double-well-oscillator which is the standard model for studying thermal activation between two stable states (Kramers problem).[1,2]

The concept of Lyapunov exponents is applied to the model. In the framework of a linear stability analysis, Lyapunov exponents measure the mean stability properties of orbits. These exponents play an essential role in the theory of deterministic chaos. In deterministic systems Lyapunov exponents may be regarded as a definition of chaos, and they are intimately related to attractor dimensions and the Kolmogorov entropy.[3] Lyapunov exponents can be understood as weighted sums of unstable and stable motions. Since noise may influence the corresponding weights, it will lead to nontrivial behavior[4,5] as demonstrated below.

Several investigations have reported positive Lyapunov exponents for stochastic discrete maps and complex nonlinear systems.[5-14] It has been shown that small noise may destabilize periodic orbits, leading to seemingly chaotic behavior.[5-10] In these cases we have deterministically a chaotic repeller (termed also a chaotic transient) and a periodic attractor.

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Since the transients are more robust against fluctuations, the noisy trajectories resemble truly chaotic orbits at adjacent parameter values. These effects might be termed "noise-induced chaos" since the resulting dynamics exhibits many features of chaos. We will claim that positive Lyapunov exponents in the Kramers oscillator have a different meaning. Otherwise it is worth mentioning that fluctuations may stabilize chaotic dynamics.[11–13] In these cases noise strengthens the regular aspects of the dynamics.

The new point is the investigation of Lyapunov exponents in a nonlinear oscillator which is well investigated and physically well understood. The double-well oscillator is characterized by stable regions near the bottoms of the potential valleys and unstable dynamics in the vicinity of the saddle point and its separatrix. Consequently, averaging over the local divergence rate may lead to positive Lyapunov exponents, which means that the dynamics on average is diverging. We have found numerically positive values in the low-damping regime and will give an interpretation of this observation in the discussion. Therefore, the Kramers oscillator could serve also as a standard example for the investigation of the meaning of positive Lyapunov exponents in stochastic systems.

2. LYAPUNOV EXPONENTS

We study the bistable oscillator proposed by Kramers[1]

$$\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= -\gamma x_2 - \frac{dU}{dx_1} + (2\varepsilon\gamma)^{1/2}\,\xi(t) \end{aligned} \tag{2.1}$$

with

$$\langle \xi(t) \rangle = 0, \qquad \langle \xi(t)\,\xi(t') \rangle = \delta(t-t') \tag{2.2}$$

and

$$U(x_1) = -\frac{a}{2}x_1^2 + \frac{b}{4}x_1^4 \qquad (a, b > 0) \tag{2.3}$$

These equations describe the stochastic motion within a bistable potential. The model was proposed by Kramers[1] to study rate coefficient of chemical reactions. The noise is scaled in such a way that ε stands for the temperature of a heat bath. Hence, the stationary probability distribution density does not depend on the friction coefficient γ. The stationary density is just the canonical distribution

$$P(x_1, x_2) = N^{-1} \exp\left\{ -\frac{1}{\varepsilon}\left[\frac{x_2^2}{2} + U(x_1)\right]\right\} \tag{2.4}$$

To characterize the dynamics of the trajectories, usually the mean transition rates between the valleys are investigated. This concept, introduced by Kramers,[1] was studied extensively and several approximative representations for arbitrary γ were given.[2] We point out that positive Lyapunov exponents will be found in the low-damping regime where the Kramers rate is increasing linearly with the friction coefficient.

This Lyapunov exponent as an additional characterization of the dynamics will be introduced now. In order to analyze the stability properties of orbits, we compute the evolution of infinitesimal deviations $\mathbf{q}$ from the stochastic trajectories $\mathbf{x}(t)$. The vector $\mathbf{q}$ is governed by the linearized version of Eq. (2.1):

$$\begin{aligned} \dot{q}_1 &= q_2 \\ \dot{q}_2 &= -\gamma q_2 - \left(\frac{d^2U}{dx_1^2}\right) q_1 \end{aligned} \tag{2.5}$$

Equations (2.1) and (2.5) constitute a coupled system of stochastic equations, since the second derivative of $U(x_1)$ depends on the coordinate x_1. Equation (2.1) describes the motion in phase space, whereas Eq. (2.5) describes the evolution of perturbations $\mathbf{q}$ in tangent space.

It can be verified that the norm of the deviation $\mathbf{q}$ obeys

$$\frac{d}{dt} \|\mathbf{q}\| = \frac{q_i J_{ij}(\mathbf{x}) q_j}{\|\mathbf{q}\|^2} \|\mathbf{q}\| = L(\mathbf{x}, \mathbf{q}) \|\mathbf{q}\| \tag{2.6}$$

where $J_{ij}(\mathbf{x})$ is the Jacobian of the considered dynamical system. Integrating formally Eq. (2.6) gives

$$\|\mathbf{q}(t)\| = \|\mathbf{q}(0)\| \exp\left\{\int_0^t L(\mathbf{x}, \mathbf{q})\, dt'\right\} \tag{2.7}$$

The quantity $L(\mathbf{x}, \mathbf{q})$ is the local divergence rate depending on the phase space coordinates x_1 and x_2 and also on the direction of the perturbation $\mathbf{q}$.

The maximum Lyapunov exponent will be obtained as the long-time average of the local divergence rate,[4, 8] i.e.,

$$\lambda_1 = \lim_{t\to\infty} \frac{1}{t} \int_0^t L(\mathbf{x}, \mathbf{q})\, dt' = \lim_{t\to\infty} \frac{1}{t} \ln \left\{\frac{\|\mathbf{q}(t)\|}{\|\mathbf{q}(0)\|}\right\} \tag{2.8}$$

If ergodicity is assumed, the long-time average in Eq. (2.8) might be replaced by an average over a stationary probability distribution density. However, the canonical distribution in Eq. (2.4) is not sufficient, since the value of the rate $L(\mathbf{x}, \mathbf{q})$ depends also on the direction of the deviation $\mathbf{q}$, hence, the joint density of $\mathbf{x}$ and the angle of $\mathbf{q}$ will be necessary for an analytical calculation of λ_1.

Since this density is unknown, we estimate the Lyapunov exponent numerically via long runs of the stochastic trajectory. The local divergence rate $L(\mathbf{x}, \mathbf{q})$ is interpreted as a stochastic variable depending on the actual samples generated by Eqs. (2.1) and (2.5). Therefore, Eq. (2.8) represents the time average over a stochastic variable.

Results are shown in Fig. 1 for two different values of the noise intensity as a function of the friction coefficient. Every point represents the mean

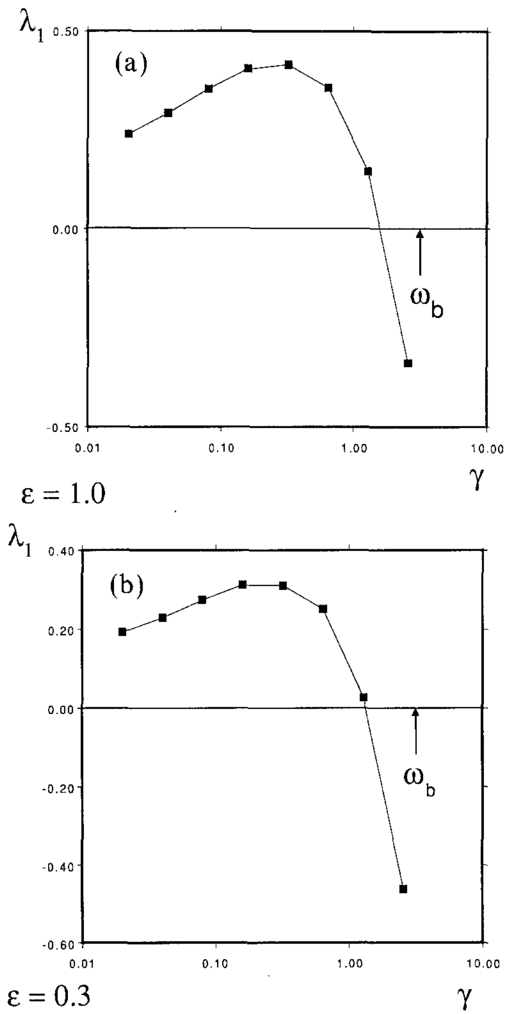

Fig. 1. Maximum Lyapunov exponent in the Kramers oscillator versus friction coefficient. The arrow indicates the value of the barrier frequency. $a = 10$, $b = 100$, and (a) $\varepsilon = 1$, (b) $\varepsilon = 0.3$.

local divergence rate of runs with 500 transitions between the two valleys which were averaged over 50 initial conditions. For both noise intensities the second moment $\langle \Delta\lambda^2 \rangle$ obtained from the ensemble of initial conditions is of the order 10^{-4}. Thus we obtained positive values of λ_1 over a wide range of friction coefficients. For the results shown we have $\gamma < \omega_b = a^{1/2}$, where ω_b is the barrier frequency of $U(x)$ and, therefore, we found $\lambda_1 > 0$ in the low-damping regime.

3. DISCUSSION

In deterministic systems a positive Lyapunov exponent may serve as a definition of chaos. In our system of consideration, however, the terminus "chaos" seems to be not appropriate, since no other features of chaotic dynamics, such as strange attractors or homoclinic orbits, are present.

However, even though our observation of a positive Lyapunov exponent should not be termed chaos, the quantity λ_1 is of considerable relevance for the characterization of the dynamics. There is a vast mathematical literature of Lyapunov exponents in various stochastic system (see, e.g., Arnold and Wikstütz[14] and references therein).

The origin of a positive Lyapunov exponent can be understood from inspection of Fig. 2. Oscillations within a valley are compatible with a linear decrease of ln $\|q\|$ with a slope of about $-\gamma/2$, which is just the

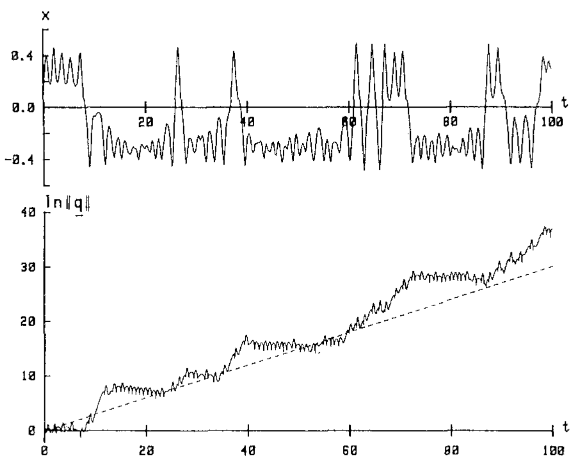

Fig. 2. Realization of the process (2.1) and the corresponding evolution of ln $\|\mathbf{q}(t)\|$. Note the decrease of $\|q\|$ during the motion within the potential valleys and the increase during transitions. The slope of the dashed line gives the Lyapunov exponent λ_1. (Adapted from Herzel *et al.*[8])

real part of the eigenvalue of the Jacobian in the stable foci. In contrast, transitions to the other valley are accompanied by an increase of ln $\|q\|$.

We note that the separatrix in the low-damping regime twirls several times around the saddle point (see Fig. 8 in ref. 2) and the stable foci in a region with finite values of probability. Therefore, during the transition the trajectory crosses several times the separatrix and spends a lot of time in this instable region.

The superposition of these regimes, unstable and stable ones, leads to a mean exponential increase of $\|\mathbf{q}\|$ which corresponds to a positive exponent λ_1. This accumulation of instability can be interpreted as a succession of coin tossing to choose one of the two valleys. That means that the crossing of the separatrix by noise is the essential mechanism to get a positive exponent.

Obviously, even if a positive Lyapunov exponent cannot be identified with chaos, the fact itself contains additional information on the dynamics of the Kramers oscillator. In order to understand the implications of a positive exponent, we discuss the dynamics of a cloud of initially nearby points. The separation of these points due to noise is a diffusionlike process with a power-law growth of distances. In contrast, a positive Lyapunov exponent implies that there is an exponential separation of orbits in one direction. The cloud of points will be stretched out exponentially. It is a question of time scales whether or not exponential separation dominates over the diffusive separation. It was shown in Ebeling *et al.*[15] that for small time scales a diffusion law was applicable, whereas on a large time scale nearby orbits separate exponentially. In other words, a positive Lyapunov exponent indicates a "mixing flow" of the stochastic trajectories which is not reflected by the stationary probability distribution density and the mean transition rates.

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