Fluctuation-diffusion relationship in chaotic dynamics

Shanta Chaudhuri, Gautam Gangopadhyay, and Deb Shankar Ray
Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700032, India
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We consider the fully developed chaos in a class of driven one-degree-of-freedom nonlinear systems. In analogy to Kubo relations in statistical mechanics, we have quantitatively related the maximal positive Lyapunov exponent, which is characteristic of divergence of trajectories, to the spectral density of fluctuations of the appropriate dynamical variable. A numerical experiment is carried out to confirm the qualitative validity of the theoretical prediction. A generalization of the relationship for N-dimensional Hamiltonian system has been given.

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I. INTRODUCTION

The driven one-degree-of-freedom nonintegrable systems have been the standard paradigms in nonlinear dynamics which exhibit classical chaos [1]. The essential hallmark of chaotic behavior is the positivity of the largest Lyapunov exponent [2] (while its negative or zero value indicates the periodicity or the marginal stability, respectively) which characterizes the exponential divergence of two initially nearby trajectories. Obviously this divergence is related to deterministic stochasticity and the associated fluctuations of the dynamical variables. The question is whether one can relate this divergence of trajectories, which in turn results in diffusion in phase space, to these fluctuations. The object of the present paper is to address this point. We show that (i) the equation describing the separation of two initially nearby trajectories assumes the form of a simple harmonic oscillator with a stochastic frequency while the source of this stochasticity is the Hamilton equation of motion for trajectories and (ii) the maximal positive Lyapunov exponent can be quantitatively related to the special density of the fluctuations. This is analogous to Kubo relations [3] in nonequilibrium statistical mechanics. A numerical experiment is carried out which confirms the theoretical relationship. A generalization of the relationship between the Lyapunov exponents in $2N$ directions and the fluctuations in an N-degree-of-freedom Hamiltonian system has been pointed out. The relation that we derive here shows that the theory of stochastic differential equation with multiplicative noise [4] can provide a very natural description for the present and also other related issues in both conservative and dissipative chaotic dynamics.

The rest of the paper is organized as follows. In Sec. II we derive the fluctuation-diffusion relationship for a driven one-degree-of-freedom system. In the next section we verify the proposed relationship numerically on a system with a double-well potential. In Sec. IV we generalize the relationship for N-degree-of-freedom Hamiltonian systems. The paper is concluded in Sec. V with some critical remarks.

II. THE FLUCTUATION-DIFFUSION RELATIONSHIP

To start with, let us consider the following Hamiltonian for the driven one-degree-of-freedom systems described by the coordinate Q and the momentum P:

$$H=P^2/2+V(Q)-gQ\cos(\omega t) . \tag{1}$$

The first, second, and third terms represent the kinetic energy, potential energy, and the driving term, respectively. g and ω are the coupling constant and the frequency of the external driving force. $V(Q)$ is assumed to be nonlinear such that nonlinearity renders the overall Hamiltonian nonintegrable. Throughout this present work we consider g much above the critical threshold for stochasticity [1] so that full chaos sets in. It is in such a situation one can treat the dynamical variables Q and P as stochastic variables.

The Hamilton equation of motion corresponding to (1) is given by

$$\ddot{Q}=-V'(Q)+g\cos\omega t \tag{2}$$

where the overdot and the prime denote the differentiation with respect to time t and space coordinate Q, respectively.

We now consider two nearby trajectories $Q,\dot{Q},\phi$ and $Q+\Delta Q$, $\dot{Q}+\Delta\dot{Q}$, $\phi+\Delta\phi$ at the same time t [where ϕ is the additional degree of freedom due to the driving term expressed through $\dot{\phi}=\omega$ with initial condition $\phi(t=0)=0$] in a three-dimensional phase space. The time evolution of the separation of these trajectories is then determined by

$$\Delta\ddot{Q}=-V''(Q)\Delta Q \tag{3}$$

in the separation coordinate space ΔQ, $\Delta\dot{Q}$, and $\Delta\phi$ [if we set the initial condition $\Delta\phi(t=0)=0$, then $\Delta\phi(t)=0$ for all $t>0$].

The standard prescription [1,2,5] for calculation of the largest Lyapunov exponent is to solve the trajectory (2) and the separation equations of motion (3) simultaneously for ΔQ and $\Delta\dot{Q}$ as functions of time t. This is then given by

$$\lambda = \lim_{\substack{t\to\infty \\ d(0)\to 0}} \frac{\ln\|d(t)\|/\|d(0)\|}{t} , \tag{4}$$

where the norm $\|d(t)\|$ is defined as $\|d(t)\| = [\Delta\dot{Q}^2 + \Delta Q^2]^{1/2}$. λ is a direct measure of two initially nearby trajectories. Some authors [6] have defined λ with additional trajectory averaging.

Our next task is to interpret Eq. (3) as a stochastic differential equation with multiplicative noise where the source of noise is the deterministic stochasticity in Eq. (2). To this end we now define the fixed points Q_e which satisfy $V'(Q_e)=0$. Since $V(Q)$ is nonlinear, Q_e are, in general, multivalued. We choose the stable equilibrium Q_e^s for which $V''(Q_e^s)>0$ as the reference state and define fluctuation $\xi(t)$ of $V''(Q)$ as

$$\xi(t) = V''(Q) - V''(Q_e^s) . \tag{5}$$

[Instead of $V''(Q_e^s)$ we could have chosen the average $\langle V''(Q)\rangle$ as the reference state and defined fluctuations as $\xi(t) = V''(Q) - \langle V''(Q)\rangle$ for which $\langle \xi(t)\rangle = 0$.]

Insertion of (5) in (3) leads to the following equation:

$$\Delta\ddot{Q} + [V''(Q_e^s) + \xi(t)]\Delta Q = 0 . \tag{6}$$

In terms of scaled time τ defined as $\tau = [V''(Q_e^s)]^{1/2} t$ and $\alpha = [V''(Q_e^s)]^{-1}$, where α is the strength of fluctuations we rewrite (6) as

$$\frac{d^2\Delta Q}{d\tau^2} + \omega^2(\tau)\Delta Q = 0 , \tag{7}$$

with

$$\omega^2(\tau) = 1 + \alpha\xi(\tau) . \tag{8}$$

Rescaled noise source equation (2) is given by

$$\frac{d^2 Q}{d\tau^2} + \overline{V'(Q)} = \kappa \cos\Omega\tau , \tag{9}$$

where $\overline{V'(\xi)} = V'(Q)/[V''(Q_e^s)]$, $\Omega = \omega/[V''(Q_e^s)]^{1/2}$, and $\kappa = g/[V''(Q_e^s)]$.

Equation (9) is the exact Hamilton equation of motion. For κ much beyond the stochastic threshold κ_e when chaos has fully set in one can treat $Q(\tau)$ or $\xi(\tau)$ as a stochastic process. The frequency ω^2 of the harmonic oscillator (7) then becomes stochastic [9].

We must emphasize two points at this stage. First we must consider $\kappa \gg \kappa_e$ for a complete stochasticity [7] (or in other words the measure of regular region is overwhelmingly small). Second, to calculate $\xi(t)$ from (9) and (5) we make no approximation. So the stochastic process $\xi(t)$ is exact.

We have thus established that the time evolution of the separation of two initially nearby trajectories follows the equation of a harmonic oscillator with fluctuating frequency. Over the last several decades many authors have studied this system [4,8] to illustrate the effect of random coefficients in differential equations in connection with wave propagation, mechanical system, line broadening, lasers, etc. We see here that chaotic dynamics also offers a similar situation. A classic comprehensive treatment has been given by van Kampen [4]. What follows next is that we use a standard result [4] to the present problem and show how the fluctuation in frequency leads to divergence of initially close trajectories. Essentially one constructs the equation of motion for the second moments from (7) and (8). These are

$$\frac{d}{d\tau}\begin{bmatrix}\Delta Q^2\\ \Delta\dot{Q}^2\\ \Delta Q\Delta\dot{Q}\end{bmatrix} = \underline{A}\begin{bmatrix}\Delta Q^2\\ \Delta\dot{Q}^2\\ \Delta Q\Delta\dot{Q}\end{bmatrix} , \tag{10}$$

where the matrix $\underline{A}$ is the sum [4] of a sure part $\underline{A}_0$ and a stochastic part $\underline{A}_1$ with

$$\underline{A}_1 = \alpha\xi(t)\underline{B} . \tag{11}$$

$\underline{B}$ represents the matrix

$$\begin{bmatrix}0 & 0 & 0\\ 0 & 0 & -2\\ -1 & 0 & 0\end{bmatrix} .$$

The equation of motion for the averages [4] is given by

$$\frac{d}{d\tau}\begin{bmatrix}\langle\Delta Q^2\rangle\\ \langle\Delta\dot{Q}^2\rangle\\ \langle\Delta Q\Delta\dot{Q}\rangle\end{bmatrix} = \begin{bmatrix}0 & 0 & 2\\ \alpha^2 c_3 & -\alpha^2 c_2 & -2-2\alpha c\\ -1-\alpha c+\alpha c_1 & 1 & -\alpha^2 c_2\end{bmatrix}\begin{bmatrix}\langle\Delta Q^2\rangle\\ \langle\Delta\dot{Q}^2\rangle\\ \langle\Delta Q\Delta\dot{Q}\rangle\end{bmatrix} , \tag{12}$$

where

$$c_1 = \int_0^\infty \langle\langle \xi(\tau)\xi(\tau-\tau')\rangle\rangle \sin 2\tau' d\tau' ,$$

$$c_2 = \int_0^\infty \langle\langle \xi(\tau)\xi(\tau-\tau')\rangle\rangle (1-\cos 2\tau') d\tau' ,$$

$$c_3 = \int_0^\infty \langle\langle \xi(\tau)\xi(\tau-\tau')\rangle\rangle (1+\cos 2\tau') d\tau' ,$$

$$c = \langle \xi(t)\rangle , \quad \text{and} \quad \langle\langle x_i x_j\rangle\rangle = \langle x_i x_j\rangle - \langle x_i\rangle\langle x_j\rangle .$$

The dynamics of separation of nearby trajectories is then determined by the following relevant eigenvalue obtained up to second order in α:

$$\lambda_0 = \alpha^2(c_3 - c_2)/2 .$$

What is immediately apparent is that the positivity of λ_0 leads to instability or divergence of $\langle \Delta Q^2 + \Delta\dot{Q}^2\rangle$. We then identify $\lambda_0/2$ as λ, the largest positive Lyapunov exponent as defined from a purely dynamical point of view in Eq. (4), and obtain

$$\lambda=\tfrac{1}{4}\alpha^2(c_3-c_2)\ .$$

Rewriting (c_3-c_2) in terms of spectral density of fluctuations one obtains the desired relation (scaled) as follows;

$$\lambda=\frac{\alpha^2}{2}\int_0^\infty \langle\langle \xi(\tau)\xi(\tau-\tau')\rangle\rangle \cos 2\tau' d\tau'\ . \tag{13}$$

This relation becomes more simple if $\langle V''(Q)\rangle$ is used as the reference state instead of $V''(Q_e^s)$ and define $\xi(t)=V''(Q)-\langle V''(Q)\rangle$. The unscaled equation assumes the following form and we have (since $\langle \xi \rangle=0$)

$$\lambda=\frac{\int_0^\infty \langle \xi(t)\xi(t-t')\rangle \cos[2\{\langle V''(Q)\rangle\}^{1/2}t']dt'}{2\{\langle V''(Q)\rangle\}}\ . \tag{13a}$$

Equation (13) relates the maximal positive Lyapunov exponent to the spectral density of fluctuations at twice the frequency of the "unperturbed" ($\alpha=0$) oscillator. This is the central result of the paper.

The above result associates the largest Lyapunov exponent with the correlation time of a multiplicative stochastic process. More precisely, the maximal Lyapunov exponent is related to the cosine transform of the correlation function of the curvature of the potential $V(Q)$. The appearance of curvature of the potential in the above relationship is also indicative of the fact that it basically concerns the stability of the motion since it was pointed out by Toda [11] that the stability of the motion is determined largely by the curvature of the potential, at least locally. It is also important to note that the Lyapunov exponent is a measure of rate of divergence of initially nearby trajectories, as a consequence of which the diffusive motion in phase space takes place. The relation thus may be interpreted as a fluctuation-diffusion relationship. The divergence of the second moments in the present discussion is a consequence of the linear treatment of the nonlinear potential $V(Q)$.

Correlation function expressions are available for a number of other properties. For example, a transport coefficient, such as electrical conductivity, σ, can be expressed as a Fourier transform of the current correlation function $\langle J(0)J(\tau)\rangle$ as follows:

$$\sigma(\omega)=\frac{1}{kT}\int_0^\infty e^{-i\omega\tau}\langle J(0)J(\tau)\rangle d\tau\ , \tag{13b}$$

where k is the Boltzmann constant and T is the absolute temperature. The formal similarity of the expressions 13(a) and 13(b) cannot be overlooked and this carries the message that our proposed relationship can be viewed as an analog of Kubo relation in chaotic dynamics, where we relate a maximal Lyapunov exponent, a transport coefficient for Hamiltonian system to the appropriate correlation functions.

III. THE NUMERICAL EXPERIMENT

To verify the basic proposition (13) we have carried out a numerical experiment on a driven one-degree-of-freedom system described by a double-well potential $V(Q)=aQ^4-bQ^2$ and the equations of motion (2) and (6). To define the fluctuation $\xi(t)$ we adopt $\langle V''(Q)\rangle$ as the reference state. The parameters chosen [7] are as follows: $a=0.5$, $b=10.0$, and $\omega=6.07$. The driving field amplitude g is varied from 9 to 12. A direct numerical calculation of the maximal Lyapunov exponent using the well-known method of Benettin, Galgani, and Strelcyn [2,5] yields the values varying from 0.0477 to 0.0532 as tabulated in Table I, whereas the eigenvalues obtained by a numerical evaluation of the exponentially fitted correlation function are compared side by side. It is apparent that for $g=12$ the discrepancy is $\approx 25\%$. Keeping in view the fact that our perturbation calculation is correct up to $\approx O(\alpha^2\tau_c)$ the order-of-magnitude agreement roughly demonstrates the qualitative validity of the proposed relationship. A typical plot of decay of correlation function (which is characteristic of chaos) is depicted in Fig. 1 for a single trajectory.

TABLE I. Computed values of maximal Lyapunov exponents [Eq. (13a)] for different values of g compared to dynamically calculated values.

g	λ (theory)	λ (dynamical)
9.0	0.0585	0.0496
10.0	0.0489	0.0502
10.5	0.0502	0.0495
11.0	0.0479	0.0502
11.5	0.0440	0.0532
12.0	0.0385	0.0477

IV. GENERALIZATION OF THE RELATIONSHIP FOR A HAMILTONIAN SYSTEM

The basic proposition Eq. (13) derived for a driven one-degree-of-freedom Hamiltonian system, however, is generalizable to N-degree-of-freedom Hamiltonian systems.

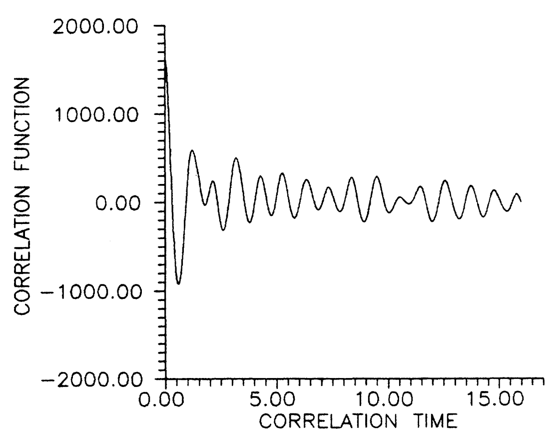

FIG. 1. A correlation function $\langle \xi(t)\xi(t-\tau)\rangle_t$ is plotted as a function of time τ for the parameters mentioned in the text. [$g=10.0$, initial conditions $Q(0)=0.05$, $P(0)=0.0$. Both the units are arbitrary.]

To this end we consider a Hamiltonian

$$H(\mathbf{p},\mathbf{q})=\tfrac{1}{2}(\mathbf{p}\cdot\mathbf{p})+V(\mathbf{q}) , \tag{14}$$

where $\mathbf{p}$ and $\mathbf{q}$ are the N-dimensional vectors of momenta and coordinates, respectively. The equations of motion are

$$\begin{aligned}\dot{\mathbf{q}}&=\nabla_{\mathbf{p}}H(\mathbf{p},\mathbf{q})=\mathbf{p} ,\\ \dot{\mathbf{p}}&=-\nabla_{\mathbf{q}}H(\mathbf{p},\mathbf{q})=-\nabla_{\mathbf{q}}V(\mathbf{q}) .\end{aligned} \tag{15}$$

We then introduce the variables $\Delta\mathbf{q}$ and $\Delta\mathbf{p}$ which measure the separation of two trajectories in coordinate and momentum space, respectively, for which the linearized equation of motion is

$$\Delta\dot{\mathbf{q}}=-\underline{V}(t)\cdot\Delta\mathbf{q} , \tag{16}$$

where $\underline{V}(t)$ is the $N\times N$ matrix of the second derivative of the potential $V(\mathbf{q})$. Defining an $N\times N$ fluctuation matrix $\underline{\xi}(t)$ as

$$\underline{V}(t)=v\underline{1}+\underline{\xi}(t) ,$$

where v is the (scalar) modulus of the largest element of the matrix $\underline{V}(t)$ evaluated at the stable fixed point of the system [decomposition of $\underline{V}$ could also be made as $\underline{V}=\mathrm{diag}(\underline{w})+\underline{\xi}$, so that in each direction there is a different time scale $(\omega_i)^{1/2}$; in fact all that we need is a suitable reference state], we may rewrite Eq. (16) as a rescaled equation

$$\Delta\ddot{\mathbf{q}}=[\underline{1}+\alpha\underline{\xi}(t)]\Delta\mathbf{q} .$$

Here t refers to scaled time $v^{1/2}t$ and $\alpha=1/v$. $\underline{1}$ is the $N\times N$ unit matrix. Equation (15) should be similarly rescaled.

Following exactly as in the previous case we obtain the equation of motion for averages or the first moments,

$$\frac{d}{dt}\begin{bmatrix}\langle\Delta q\rangle\\ \langle\Delta p\rangle\end{bmatrix}=\begin{bmatrix}\underline{0} & \underline{1}\\ -\underline{1}-\alpha\underline{c}+\frac{1}{2}\alpha^2\underline{c}_1 & -\frac{1}{2}\alpha^2\underline{c}_2\end{bmatrix}\begin{bmatrix}\langle\Delta q\rangle\\ \langle\Delta p\rangle\end{bmatrix} , \tag{17}$$

where $\underline{c}$ is the average of $N\times N$ fluctuation matrix $\underline{\xi}$ and $\underline{c}_1$ and $\underline{c}_2$ are the $N\times N$ spectral density matrices of fluctuations as given by

$$\begin{aligned}\underline{c}_1&=\int_0^{\alpha}\langle\langle\underline{\xi}(t)\underline{\xi}(t-\tau)\rangle\rangle\sin 2\tau d\tau ,\\ \underline{c}_2&=\int_0^{\alpha}\langle\langle\underline{\xi}(t)\underline{\xi}(t-\tau)\rangle\rangle(1-\cos 2\tau)d\tau , \quad \underline{c}=\langle\underline{\xi}(t)\rangle .\end{aligned}$$

The stability of the motion depends on the eigenvalues of the $2N\times 2N$ matrix as given in Eq. (17) which can be identified as the Lyapunov characteristic exponents λ_i for all $2N$ directions from the following relation:

$$\left[\underline{T}\begin{bmatrix}\underline{0} & \underline{1}\\ -\underline{1}-\alpha\underline{c}+\frac{1}{2}\alpha^2\underline{c}_1 & -\frac{1}{2}\alpha^2\underline{c}_2\end{bmatrix}\underline{T}^{-1}\right]_{ij}=\lambda_i\delta_{ij} , \tag{18}$$

where $\underline{T}$ is a $2N\times 2N$ matrix.

Equation (18) may be recognized as the generalized fluctuation-diffusion relationship since it relates the diffusive motion in phase space in terms of Lyapunov exponents for all $2N$ directions to the fluctuations in an N-degree-of-freedom Hamiltonian system [10]. (Note that exponents can be both positive and negative depending on expansion or contraction of the relevant direction.)

V. CONCLUSION

Before concluding, some critical remarks regarding the derivation need attention.

First, the stochastic process $\xi(t)$ is determined *exactly* by solving the Hamilton equation of motion (9) for $\kappa\gg\kappa_e$. The special cases where $\xi(t)$ is a Gaussian, stochastic process or even a δ-correlated process have received so much attention in the literature that it is necessary to emphasize [4] that throughout the present work, these assumptions have *not* been made.

Second, for α, however small but finite, the eigenvalue λ_0 is always positive. This implies that no matter how small the fluctuation is, the trajectory diverges. We therefore believe that this relationship must be very *generic* in classical chaotic dynamics.

Third, we point out [4] that since van Kampen's equation of motion for averages (which is equivalent to the result obtained by second-order cumulant expansion) rests on an expansion in $\alpha\tau_c$ (where τ_c is the correlation time), the stochastic $\xi(t)$ must have a correlation time τ_c which is small but finite compared to the "coarse-grained" time scale over which the average quantities evolve [that τ_c is *small* but *finite* is the only assumption made about the stochastic process $\xi(t)$ [4,7]].

Fourth, in the calculation of eigenvalues we take care of fluctuation strength of the order α^2. Therefore the Lyapunov exponents are *correct up to a leading order* $\approx O(\alpha^2)$.

In conclusion, we have quantitatively related the Lyapunov characteristic exponents to the spectral density of the fluctuations of the dynamical variables. Since Lyapunov exponents characterize the diffusive motion of the system in phase space and mimic the behavior of transport coefficients it is apparent that the relation is analogous to Kubo relations in statistical mechanics, which relate the transport coefficients to the spectral densities of fluctuations in a linearized scheme. We hope that the methods of stochastic differential equation for multiplicative noise as employed in the present treatment will also be useful in similar issues in dissipative chaotic dynamics.

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