Fluctuation-dissipation relationship in chaotic dynamics

Bidhan Chandra Bag and Deb Shankar Ray*
Indian Association for the Cultivation of Science, Jadavpur, Calcutta 700032, India
(Received 7 January 2000)

We consider a general N-degree-of-freedom dissipative system that exhibits chaotic behavior. Based on a Fokker-Planck description associated with the dynamics, we establish that the drift and the diffusion coefficients can be related through a set of stochastic parameters that characterize the steady state of the dynamical system in a way similar to the fluctuation-dissipation relation in nonequilibrium statistical mechanics. The proposed relationship is verified by numerical experiments on a driven double-well system.

PACS number(s): 05.45.−a, 05.70.Ln, 05.20.−y

I. INTRODUCTION

Although deterministic in principle, classically chaotic motion is stochastic in nature. Ever since the early numerical study of Chirikov *et al.*, mapping [1] revealed that the motion of a phase-space variable can be characterized by a simple random-walk diffusion equation, attempts have been made to describe the chaotic motion in terms of Langevin or Fokker-Planck equations [1,2]. It is therefore easy to comprehend a close connection between classical chaos and statistical mechanics. Two distinct situations arise in this context. The first one concerns whether classical chaos may serve as a basis for classical statistical mechanics since the ultimate justification of the postulates of statistical mechanics like Boltzmann hypothesis of molecular chaos, ergodicity, or the postulate of equal *a priori* probability rests on the dynamics of each particle [3–5]. The second one concerns the following: Given that the classical chaotic motion is stochastic, how and to what extent one can realize the formulation of statistical mechanics for useful description of classical chaos [6–21] keeping in mind that one essentially deals here with a few-degrees-of-freedom system. The present paper addresses the second issue.

The emergence of stochastic behavior of the classically chaotic system is due to the loss of correlation of initially nearby trajectories. This is reflected in the nature of the largest Lyapunov exponent [22] whose calculation rests on the linear equation-of-motion for the separation of these trajectories. When chaos has fully set in, the time dependence of the linear stability matrix or Jacobian of the system [23] in the equation-of-motion in the tangent space can be described as a stochastic process since the phase-space variables behave as stochastic variables. In a number of recent studies we have shown [17–21] that this fluctuation of the Jacobian is amenable to a theoretical description in terms of the theory of multiplicative noise. This allows us to realize a number of important results of nonequilibrium statistical mechanics, like Kubo relation [17], fluctuation-decoherence relation [18], exponential divergence of quantum fluctuations [19–21], thermodynamically inspired quantities, e.g., entropy production in chaotic dynamics. Based on a Fokker-Planck description in the tangent space where the drift and the diffusion coefficients explicitly depend on the phase-space variables or dynamical properties of the system, we show that a connection between the two moments in terms of the stochastic parameters that characterize the long-time limit of the dynamical system can be established in the spirit of the fluctuation-dissipation relation. We verify the theoretical proposition by numerical experiments on a simple dissipative system.

The rest of the paper is organized as follows: In Sec. II we introduce a Fokker-Planck description of the dynamical system in the tangent space and identify the drift and diffusion coefficients that are the functions of fluctuations of the phase-space variables. This is followed by solving the Fokker-Planck equation for the steady-state distribution required for the calculation of long-time averages in Sec III. In Sec. IV the dynamical stochastic parameters that characterize the long-time behavior of the system are introduced. The first one of them is a well-known stochastic parameter closely related to Kolmogorov entropy. With the help of these stochastic parameters we establish a connection between the drift and diffusion coefficients of the Fokker-Planck equation in the spirit of fluctuation-dissipation relation in nonequilibrium statistical mechanics. In Sec. V we illustrate the general method by an explicit numerical example to verify the theoretical proposition. The paper is concluded in Sec. VI.

II. A FOKKER-PLANCK EQUATION FOR DISSIPATIVE CHAOTIC DYNAMICS

We are concerned here with a general N-degree-of-freedom system whose Hamiltonian is given by

$$H=\sum_{i=1}^{N}\frac{p_i^2}{2m_i}+V(\{q_i\},t),\quad i=1,\ldots,N, \tag{1}$$

where $\{q_i,p_i\}$ are the coordinate and momentum of the ith degree of freedom, respectively, which satisfy the generic form of equations

$$\dot{q}_i=\frac{\partial H}{\partial p_i}\ \text{ and }\ \dot{p}_i=-\frac{\partial H}{\partial q_i}. \tag{2}$$

We now make the Hamiltonian system dissipative by introducing $-\gamma p_i$ on the right-hand side of the second of Eqs.

*Email address: pcdsr@mahendra.iacs.res.in

(2). For simplicity we assume γ to be the same for all the N degrees of freedom. By invoking the symplectic structure of the Hamiltonian dynamics as

$$z_i=\begin{cases} q_i & \text{for} \quad i=1,\ldots,N, \\ p_{i-N} & \text{for} \quad i=N+1,\ldots,2N. \end{cases}$$

and defining I as

$$I=\begin{bmatrix} 0 & E \\ -E & -\gamma E \end{bmatrix},$$

where E is an $N\times N$ unit matrix, and 0 is an $N\times N$ null matrix, the equation-of-motion for the dissipative system can be written as

$$\dot{z}_i=\sum_{j=1}^{2N} I_{ij}\frac{\partial H}{\partial z_j}. \tag{3}$$

We now consider two nearby trajectories, $z_i,\dot{z}_i$ and $z_i+X_i,\dot{z}_i+\dot{X}_i$ at the same time t in $2N$-dimensional phase space. The time evolution of separation of these trajectories is then determined by

$$\dot{X}_i=\sum_{j=1}^{2N} J_{ij}(t)X_j \tag{4}$$

in the tangent space $\{X_i\}$, where

$$J_{ij}=\sum_k I_{ik}\frac{\partial^2 H}{\partial z_k \partial z_j}. \tag{5}$$

Therefore, the $2N\times 2N$ linear stability matrix $\boldsymbol{J}$ assumes the following form:

$$\mathbf{J}=\begin{bmatrix} 0 & E \\ \mathbf{M}(\mathbf{t}) & -\gamma E \end{bmatrix}, \tag{6}$$

where $\mathbf{M}$ is an $N\times N$ matrix. Note that the time dependence of stability matrix $\mathbf{J}(t)$ is due to the second derivative $\partial^2 H/\partial z_k \partial z_j$, which is determined [23] by the equation-of-motion (3). The procedure for calculation of X_i and the related quantities is to solve the trajectory equation (3) simultaneously with Eq. (4). Thus when the dissipative system described by Eq. (3) is chaotic, $\mathbf{J}(t)$ becomes (deterministically) stochastic due to the fact that z_i's behave as stochastic variables and the equation-of-motion (4) in the tangent space can be interpreted as a stochastic equation [17–21].

In the next step we shall be concerned with a stochastic description of $\mathbf{J}(t)$ or $\mathbf{M}(\mathbf{t})$. For convenience we split up $\mathbf{M}$ into two parts as

$$\mathbf{M}=\mathbf{M}_0+\mathbf{M}_1(\mathbf{t}), \tag{7}$$

where $\mathbf{M}_0$ is independent of variables $\{z_i\}$ and therefore behaves as a sure or constant part and $\mathbf{M}_1$ is determined by the variables $\{z_i\}$ for $i=1,\ldots,2N$. $\mathbf{M}_1$ refers to the fluctuating part. We now rewrite the equation-of-motion, (4) in tangent space as

$$\begin{aligned}\dot{X}&=\mathbf{JX}\\ &=\mathbf{L}(\{X_i\},\{z_i\}),\end{aligned} \tag{8}$$

where $\mathbf{X}$ and $\mathbf{L}$ are the vectors with $2N$ components. Corresponding to Eq. (7), L in Eq. (8) can be split up again to yield

$$\dot{X}=\mathbf{L}^0(X)+\mathbf{L}^1(X,\{z_i(t)\}), \quad i=1,\ldots,2N. \tag{9}$$

Equation (4) indicates that Eq. (8) is linear in $\{X_i\}$. Equations (4), (5), and (6) express the fact the first N components of L^1 are zero and the last N components of L^1 are the functions of $\{X_i\}$ for $i=1,\ldots,N$. The fluctuation in L_i^1 is caused by the chaotic variables $\{z_i\}$'s. This allows us to write the following relation (which will be used later on),

$$\boldsymbol{\nabla}_X\cdot L^1\phi(\{X_i\})=L^1\cdot\boldsymbol{\nabla}_X\phi(\{X_i\}), \tag{10}$$

where $\phi(\{X_i\})$ is any function of $\{X_i\}$. $\boldsymbol{\nabla}_X$ refers to differentiation with respect to components $\{X_i\}$ (explicitly $X_i=\boldsymbol{\Delta}q_i$ for $i=1,\ldots,N$ and $X_i=\boldsymbol{\Delta}p_i$ for $i=N+1,\ldots,2N$).

Note that Eq. (9) by virtue of Eq. (8) is a linear stochastic differential equation with multiplicative noise where the noise is due to $\{z_i\}$ determined by equation-of-motion (3). This is the starting point of our further analysis.

Equation (9) determines a stochastic process with some given initial conditions $\{X_i(0)\}$. We now consider the motion of a representative point X in $2N$-dimensional tangent space $(X_1,\ldots,X_{2N})$ as governed by Eq. (9). The equation of continuity, which expresses the conservation of points determines the variation of density function $\phi(X,t)$ in time as given by

$$\frac{\partial\phi(X,t)}{\partial t}=-\boldsymbol{\nabla}_X\cdot L(t)\phi(X,t). \tag{11}$$

Expressing A_0 and A_1 as

$$A_0=-\boldsymbol{\nabla}_X\cdot L^0 \quad \text{and} \quad A_1=-\boldsymbol{\nabla}_X\cdot L^1, \tag{12}$$

we may rewrite the equation of continuity as

$$\frac{\partial\phi(X,t)}{\partial t}=[A_0+\alpha A_1(t)]\phi(X,t). \tag{13}$$

It is easy to recognize that while A_0 denotes the sure part, A_1 contains the multiplicative fluctuations through $\{z_i(t)\}$. α is a parameter introduced from outside to keep track of the order of fluctuations in the calculations. At the end we put $\alpha=1$.

One of the main results for the linear equations of the form with multiplicative noise may now be in order [25]. The average equation of $\langle\phi\rangle$ obeys $[P(x,t)\equiv\langle\phi\rangle]$,

$$\dot{P}=\left\{A_0+\alpha\langle A_1\rangle+\alpha^2\int_0^\infty d\tau\langle\langle A_1(t)\exp(\tau A_0)\right.$$
$$\left.\times A_1(t-\tau)\rangle\rangle\exp(-\tau A_0)\right\}P(x,t). \tag{14}$$

The above result is based on second-order cumulant expansion and is valid when fluctuations are small but rapid and the correlation time τ_c is short but finite or more precisely

$$\langle\langle A_1(t)A_1(t')\rangle\rangle=0 \quad \text{for} \quad |t-t'|>\tau_c. \tag{15}$$

We have, in general, $\langle A_1\rangle\neq 0$. Here $\langle\langle\cdots\rangle\rangle$ implies $\langle\langle\zeta_i\zeta_j\rangle\rangle=\langle\zeta_i\zeta_j\rangle-\langle\zeta_i\rangle\langle\zeta_j\rangle$.

Equation (14) is exact in the limit $\tau_c\rightarrow 0$. Making use of relation (12) in Eq. (14) we obtain

$$\frac{\partial P}{\partial t}=\left\{-\boldsymbol{\nabla}\cdot L^0-\alpha\langle\boldsymbol{\nabla}\cdot L^1\rangle+\alpha^2\int_0^\infty d\tau\langle\langle\boldsymbol{\nabla}\cdot L^1(t)\right.$$
$$\left.\times\exp(-\tau\boldsymbol{\nabla}\cdot L^0)\boldsymbol{\nabla}\cdot L^1(t-\tau)\rangle\rangle\exp(\tau\boldsymbol{\nabla}\cdot L^0)\right\}P. \tag{16}$$

The above equation can be transformed into the following Fokker-Planck equation ($\alpha=1$) for probability density function $P(X,t)$, (the details are given in the Appendix):

$$\frac{\partial P(X,t)}{\partial t}=-\boldsymbol{\nabla}\cdot\mathbf{F}P(X,t)+\sum_{i,j}\mathcal{D}_{ij}\frac{\partial^2 P}{\partial X_i\partial X_j}, \tag{17}$$

where

$$\mathbf{F}=L^0+\langle L^1\rangle+\mathbf{Q} \tag{18}$$

and $\mathbf{Q}$ is a $2N$-dimensional vector whose components are defined by

$$Q_j=-\int_0^\infty\langle\langle R_j'\rangle\rangle d\tau d_1(\tau)d_2(\tau). \tag{19}$$

Here the determinants $\det_1(\tau)$, $\det_2(\tau)$ and R_j' are given by

$$\det{}_1(\tau)=\left|\frac{dX^{-\tau}}{dX}\right|,$$

$$\det{}_2(\tau)=\left|\frac{dX}{dX^{-\tau}}\right|$$

and

$$R_j'=\sum_i L_i^1(X,t)\frac{\partial}{\partial X_i}\sum_k L_k^1(X^{-\tau},t-\tau)\frac{\partial X_j}{\partial X_k^{-\tau}}. \tag{20}$$

It is easy to recognize F as an evolution operator. Because of the dissipative perturbation we note that div $F<0$.

The diffusion coefficient $\mathcal{D}_{ij}$ in Eq. (17) is defined as

$$\mathcal{D}_{ij}=\int_0^\infty\sum_k\langle\langle L_i^1(X,t)L_k^1(X^{-\tau},t-\tau)\frac{dX_j}{dX_k^{-\tau}}\rangle\rangle$$
$$\times\det{}_1(\tau)\det{}_2(\tau)d\tau \tag{21}$$

We have followed closely van Kampen's approach [25] a to generalized Fokker-Planck equation (17). Before concluding this section several critical remarks regarding this derivation need attention:

First, the stochastic process $\mathbf{M}_1(\mathbf{t})$ determined by $\{z_i\}$ is obtained *exactly* by solving equations-of-motion (3) for the chaotic motion of the system. It is therefore necessary to emphasize that we have *not assumed* any special property of noise, such as, $\mathbf{M}_1(\mathbf{t})$ is Gaussian or δ correlated. We reiterate Van Kampen's emphasis in this approach.

Second, the only assumption made about the noise is that its correlation time τ_c is short but finite compared to the coarse-grained time scale over which the average quantities evolve.

Third, we take care of fluctuations up to second order, which implies that the deterministic noise is not too strong.

Equation (17) is the required Fokker-Planck equation in the tangent space $\{X_i\}$. Note that the drift and diffusion coefficients are determined by the phase-space $\{z_i\}$ properties of the chaotic system and directly depend on the correlation functions of the fluctuations of the second derivatives of the Hamiltonian (5).

III. THE STEADY-STATE DISTRIBUTION AND THE CALCULATION OF AVERAGES

In what follows we shall be concerned with the long-time limit of the dynamical system. Thus the steady-state distribution of the tangent space coordinates $X_i (i=1,\ldots,2N)$ are especially relevant for the present purpose. To make all these coordinates dimensionless we use the following transformations in Eq. (17):

$$\tau'=\omega' t,$$

$$y_i=\frac{X_i}{d_0} \quad \text{for} \quad i=1,\ldots,N, \tag{22}$$

$$y_i=\frac{X_i}{\omega' d_0} \quad \text{for} \quad i=N+1,\ldots,2N,$$

where ω' is a scaling constant having dimension of reciprocal of time (a possible choice is the linearized frequency of the dynamical system) and τ' becomes a dimensionless variable. d_0 is a constant (to be specified later) having the dimension of length. The resulting Fokker-Planck equation (17) reduces to

$$\frac{\partial P(y,\tau')}{\partial\tau'}=-\boldsymbol{\nabla}\cdot F'(y)P+\sum_{i,j}\mathcal{D}_{ij}'(y)\frac{\partial^2 P}{\partial y_i\partial y_j}. \tag{23}$$

Note that Eq. (23) is independent of d_0 since $F(X)$ is linear in $\{X_i\}$ and $\mathcal{D}(X)$ is quadratic in $\{X_i\}$. Next we consider the stationary state of the system ($\partial P/\partial \tau' = 0$) and make use of the following linear transformation (with $\alpha_{2N} = 1$)

$$U = \sum_{i=1}^{2N} \alpha_i y_i \tag{24}$$

in Eq. (23) to obtain the equation for steady-state probability distribution $P_s(U)$:

$$\frac{\partial}{\partial U} \lambda U P_s(U) + \mathcal{D}_s \frac{\partial^2 P_s}{\partial U^2} = 0. \tag{25}$$

α_i-s ($i = 1, \ldots, 2N-1$) are the constants to be determined. Here

$$\lambda U = -\sum_i \alpha_i F_i'(y) \tag{26}$$

and

$$\mathcal{D}_s = \sum_{i,j} \mathcal{D}_{ij}' \alpha_i \alpha_j , \tag{27}$$

and we disregard the time dependence of $\mathcal{D}'$ under weak noise approximation, to treat $\mathcal{D}'$ as a constant in the usual way.

Putting Eq. (24) in Eq. (26) and comparing the coefficients of y_i on both sides we obtain the $2N$ algebraic equation (for $\alpha_i, \ldots, \alpha_{2N-1}$ and λ). The set $\{\alpha_i\}$ and λ are therefore known.

The exact steady-state solution, P_s has the well-known Gaussian form that is given by

$$P_s(\{y_i\}) = N \exp\left(-\frac{\lambda}{2\mathcal{D}_s} \sum_{i,j} \alpha_i \alpha_j y_i y_j \right), \tag{28}$$

where N is the normalization constant. Equation (28) expresses the probability distribution of tangent space coordinates of the dynamical system in the long-time limit. The important relevant quantity that measures the separation of initially nearby trajectories when the system has attained the stationary state can be computed by calculating the average of

$$\sum_{i=1}^{2N} y_i^2$$

Making use of the distribution (28) we obtain

$$\left\langle \sum_{i=1}^{2N} y_i^2 \right\rangle = \frac{\mathcal{D}_s}{\lambda} \sum_{i=1}^{2N} \frac{1}{\alpha_i^2}. \tag{29}$$

Note that the average as calculated above is a function of $\mathcal{D}_s$, λ, and α_i-s, which are dependent on the phase-space properties of the dynamical system.

IV. STOCHASTIC PARAMETERS, CONNECTION BETWEEN $\mathcal{D}_s$ AND λ; FLUCTUATION-DISSIPATION RELATION

Equation (25) is a steady-state Fokker-Planck equation in tangent space with linear drift and constant diffusion coefficients where the coordinates have been expressed as dimensionless variables $\{y_i\}$. λ and $\mathcal{D}_s$ are the first and second moments, respectively, of the underlying stochastic process. Our objective here is seek a connection between the two moments. In standard nonequilibrium statistical mechanics this connection is expressed by the fluctuation-dissipation relation through temperature, an equilibrium parameter characterizing the equilibrium state. Our approach here is to follow a somewhat similar procedure. This implies that we search for the stochastic parameters that characterize the long-time limit of the nonlinear dynamical system. We show that an appropriate relation between $\mathcal{D}_s$ and λ can be established through these parameters.

An important parameter proposed many years ago by Casartelli *et al.* [24] (a precursor for the largest Lyapunov exponent used as a measure of regularity or chaoticity of a nonlinear dynamical system) is the long-time average of $\ln d(t)/d_0$, where d_0 is the separation of the two initially nearby trajectories and $d(t)$ is the corresponding separation at some time *t*. To express $d(t)$ (having dimension of length) we write

$$d(t) = \left[\sum_{i=1}^{N} (X_i)^2 + \sum_{i=N+1}^{2N} \left(\frac{X_i}{\omega'} \right)^2 \right]^{1/2}.$$

$d(t)$ is determined by solving numerically Eqs. (3) and (4) simultaneously or their appropriately transformed version for the initial condition z_0 corresponding to Eq. (3). In going from the jth to the $j+1$th step of the iteration in course of time evolution, any of the components of X say X_i has to be initialized as $X_i^{j0} = (X_i^j/d_j) d_0$. This initialization implies that at each step, the iteration starts with same magnitude of d_0 but the direction of d_0 for step $j+1$ is that of $d(t)$ for the jth step (considered in terms of the ratio X_i^j/d_j). For a pictorial illustration we refer to Fig. 1 of Ref. [22]. The jth time of iteration implies $t = jT (j = 1,2, \ldots, \infty)$ and T is the characteristic time that corresponds to the shortest ensemble-averaged period of a nonlinear dynamical system. Thus following Casartelli *et al.* [24] a stochastic parameter can be defined by the following time average of $\ln d_j/d_0$ as

$$\sigma_n(t, z_0, d_0) = \frac{1}{n} \sum_j^n \ln \frac{d_j}{d_0}. \tag{30}$$

It has been shown [24] that as $n \to \infty, \sigma_n$ has a definite value. For the disordered system it is positive and for the regular system it is zero. The difference of σ_n from the largest Lyapunov exponent is also noteworthy. Our object here is to generalize Eq. (30) by defining the other higher-order moments (higher than the first $\sigma_{n\to\infty}$). To express these quantities we define first

$$\sigma' = \ln \frac{d(t)}{d_0}. \tag{31}$$

We now make use of the transformation (22) to express $d(t)$ as a dimensionless quantity in terms of σ' as follows:

$$\ln \sum_{i=1}^{2N} y^2 = 2\sigma'. \tag{32}$$

The method of cumulant expansion on the other hand tells us that the average of the sum of y_i^2 can be written as

$$\left\langle \sum_{i=1}^{2N} y_i^2 \right\rangle = \exp\left(\sum_m A_m \right), \quad m=1,2,3, \ldots, \tag{33}$$

where A_m's result from cumulants of the stochastic quantity $2\sigma'$. A_m's are calculated dynamically from the following relations:

$$A_1 = m_1, \quad A_2 = \frac{1}{2!}[m_2 - m_1^2],$$

$$A_3 = \frac{1}{3!}[m_3 - 3m_1 m_2 + 2m_1^3], \tag{34}$$

$$A_4 = \frac{1}{4!}[m_4 - 3m_2^2 - 4m_1 m_3 + 12 m_1^2 m_2 - 6m_1^4], \quad \text{etc.},$$

where

$$m_k = \frac{2^k}{n} \sum_{j=1}^{n} \left(\ln \frac{d_j}{d_0} \right)^k \quad [k=1,2,3,4, \ldots].$$

In the spirit of Ref. [24] we inquire, whether these moments/cumulants reach their steady-state values in the long-time limit. We have numerically examined the dependence of m_k's on various parameters. The parameters are n, the time, d_0, the measure of initial separation, the characteristic time T (jth time of iteration implies $t = jT, j = 1,2, \ldots, \infty$). Our observation is that the limit m_k or limit A_m as $n \to \infty$ seems to exist in all cases. We have examined [26] these limits for a number of test cases, e.g., for Lorentz system, Henon-Heiles system, and others. In Fig. 1 we exhibit a typical representative long-time behavior of the cumulants A_m ($m = 1$ to 4) for a driven double-well potential system discussed in the next section. It is apparent that they attain their long-time limits as $n \to \infty$. Second, the first two cumulants are much higher compared to others The first moment is the stochastic parameter defined by Casartelli *et al.* [24] as a quantity closely related to Kolmogorov entropy. We are therefore led to believe that the quantities A_m's characterize the long-time limit or the steady state of a dynamical system.

The relations (33) and (29) can now be combined to give

$$\mathcal{D}_s = \frac{\lambda}{\sum_{i=1}^{2N}} \frac{1}{\alpha_i^2} \exp\left(\sum_m A_m \right). \tag{35}$$

The above relation is the central result of this paper. This establishes a connection between the drift and the diffusion coefficients of the Fokker-Planck equation (25) through the stochastic parameters characterizing long-time behavior of the nonlinear dynamical system. It must be emphasized that both the drift λ and the diffusion $\mathcal{D}_s$ coefficients arise from the deterministic stochasticity implied in the dynamical equation-of-motion (3). The relation (35) is therefore reminiscent of the familiar fluctuation-dissipation relation.

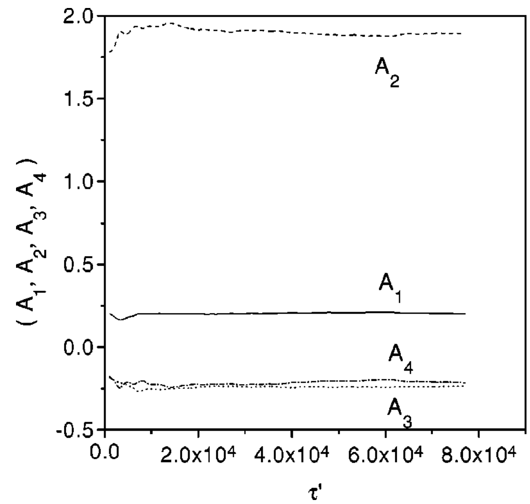

FIG. 1. The first four dimentionless cumulants A_1, A_2, A_3, and A_4 are plotted against dimentionless time for the dynamical system described by Eq. (39).

A few points regarding the relation (35) are in order. It is important to note that the fluctuation-dissipation relation in conventional nonequilibrium statistical mechanics is valid for a stochastic system for which the noise is internal. The spiritual root of this relation lies at the dynamic balance between the input of energy into the system from the fluctuations of the surrounding and the output of energy from the system due to its dissipation into the surrounding. The system-reservoir model [27,28] developed over the last few decades suggests that the coupling between the system and the reservoir is responsible for a common origin of drift and diffusion. In the present theory this common mechanism is the fluctuations of the phase-space variables (or second derivative of the Hamiltonian) inherent in both the drift λ and the diffusion $\mathcal{D}_s$ coefficients of the Fokker-Planck equation. We point out that the relation is still valid for the pure Hamiltonian system ($\gamma = 0$). For this reason the relation (35) is somewhat formal in contrast to the standard fluctuation-dissipation relation.

V. AN EXAMPLE AND NUMERICAL VERIFICATION

To illustrate the theory developed above, we now choose a driven double-well oscillator system with Hamiltonian

$$H = \frac{p_1^2}{2} + a q_1^4 - b q_1^2 + \epsilon q_1 \cos \Omega t, \tag{36}$$

where p_1 and q_1 are the momentum and position variables of the system, a and b are the constants characterizing the potential, and ϵ includes the effect of coupling constant and the driving strength of the external field with frequency Ω. This model has been extensively used in recent years for the study of chaotic dynamics [17,18,29].

The dissipative equations-of-motion for the tangent space variables X_1 and X_2 corresponding to q_1 and p_1 [Eq. (8)] read as follows:

$$\frac{d}{dt}\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \mathbf{J}\begin{bmatrix} X_1 \\ X_2 \end{bmatrix}, \quad \begin{Bmatrix} \mathbf{\Delta} q_1 = X_1 \\ \mathbf{\Delta} p_1 = X_2 \end{Bmatrix}, \tag{37}$$

where $\mathbf{J}$ as expressed in our earlier notation $z_1 = q_1$ and $z_2 = p_1$ is given by

$$\begin{pmatrix} 0 & 1 \\ \zeta(t) + 2b & -\gamma \end{pmatrix},$$

where $\zeta(t) = -12az_1^2$. Equation (37) is thus rewritten as

$$\frac{d}{dt}\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} = L^0 + L^1 \tag{38}$$

with

$$L^0 = \begin{pmatrix} X_2 \\ 2bX_1 - \gamma X_2 \end{pmatrix} \quad \text{and} \quad L^1 = \begin{pmatrix} 0 \\ \zeta(t) X_1 \end{pmatrix},$$

where L^0 and L^1 are the constant and the fluctuating parts (vectors), respectively. The fluctuation in L^1, i.e., in $\zeta(t)$, is due to stochasticity of the following chaotic dissipative dynamical equations-of-motion;

$$\dot{z}_1 = z_2 \quad \text{and} \quad \dot{z}_2 = -az_1^3 + 2bz_1 - \epsilon \cos \Omega t - \gamma z_2 . \tag{39}$$

The result of Eq. (A5) can then be applied and after some algebra the Fokker-Planck equation (17) for the dissipative driven double-well oscillator assumes the following form:

$$\frac{\partial P}{\partial t} = -X_2 \frac{\partial P}{\partial X_1} - \omega^2 X_1 \frac{\partial P}{\partial X_2} + \gamma \frac{\partial}{\partial X_2}(X_2 P) + \mathcal{D}_{21} \frac{\partial^2 P}{\partial X_2 \partial X_1} + \mathcal{D}_{22} \frac{\partial^2 P}{\partial X_2^2}, \tag{40}$$

where

$$\mathcal{D}_{21} = X_1^2 \int_0^\infty \langle\langle \zeta(t)\zeta(t-\tau)\rangle\rangle \tau e^{-\gamma\tau} d\tau$$

and

$$\mathcal{D}_{22} = X_1^2 \int_0^\infty \langle\langle \zeta(t)\zeta(t-\tau)\rangle\rangle e^{-\gamma\tau} d\tau - X_1 X_2 \times \int_0^\infty \langle\langle \zeta(t)\zeta(t-\tau)\rangle\rangle \tau e^{-\gamma\tau} d\tau \tag{41}$$

with

$$\omega^2 = 2b + c + c_2, \quad c_2 = \int_0^\infty \langle\langle \zeta(t)\zeta(t-\tau)\rangle\rangle \tau e^{-\gamma\tau} d\tau, \quad \text{and} \quad c = \langle \zeta \rangle. \tag{42}$$

The similarity of Eq. (40) to generalized Kramers' equation cannot be overlooked. This suggests a clear interplay of chaotic diffusive motion and dissipation in the dynamics.

Using the transformation (22), Eq. (40) can be written as

$$\frac{\partial P}{\partial \tau'} = -y_2 \frac{\partial P}{\partial y_1} - \overline{\omega}^2 y_1 \frac{\partial P}{\partial y_2} + \overline{\gamma} \frac{\partial}{\partial y_2}(y_2 P) + \mathcal{D}'_{21} \frac{\partial^2 P}{\partial y_2 \partial y_1} + \mathcal{D}'_{22} \frac{\partial^2 P}{\partial y_2^2}, \tag{43}$$

where

$$\overline{\omega}^2 = \frac{\omega^2}{\omega'^2}, \quad \overline{\gamma} = \frac{\gamma}{\omega'},$$

$$\mathcal{D}'_{21} = \frac{y_1^2(0)}{\omega'^2} \int_0^\infty \langle\langle \zeta(\tau')\zeta(\tau'-\tau)\rangle\rangle \tau e^{-\gamma\tau} d\tau$$

and

$$\mathcal{D}'_{22} = \frac{y_1^2(0)}{\omega'^2} \int_0^\infty \langle\langle \zeta(\tau')\zeta(\tau'-\tau)\rangle\rangle e^{-\gamma\tau} d\tau - \frac{y_1(0) y_2(0)}{\omega'} \int_0^\infty \langle\langle \zeta(\tau')\zeta(\tau'-\tau)\rangle\rangle \tau e^{-\gamma\tau} d\tau \tag{44}$$

and the time dependence of y_1 and y_2 in the diffusion coefficients have been frozen under weak noise approximation.

Now using the linear transformation (24) in Eq. (43) we obtain in the stationary state

$$\frac{\partial}{\partial U} \lambda U P_s + \mathcal{D}_s \frac{\partial^2 P_s}{\partial U^2} = 0, \tag{45}$$

where

$$U = \alpha_1 y_1 + y_2, \quad \lambda U = -\alpha_1 y_2 - \overline{\omega}^2 y_1 + \overline{\gamma} y_2, \tag{46}$$

and

$$\mathcal{D}_s = \mathcal{D}'_{22}, \tag{47}$$

where for simplicity it has been assumed that $\mathcal{D}'_{21}$ is much smaller compared to the Markovian contribution $\mathcal{D}'_{22}$.

Comparing the coefficients of y_1 and y_2 on both sides of Eq. (46) we obtain

$$\lambda \alpha_1 = -\overline{\omega}^2 \quad \text{and} \quad \lambda = -\alpha_1 + \overline{\gamma}.$$

Therefore we have

$$\alpha_1 = \frac{-\overline{\gamma} - \sqrt{\overline{\gamma}^2 + 4\overline{\omega}^2}}{2} \quad \text{and} \quad \lambda = \frac{\overline{\gamma} + \sqrt{\overline{\gamma}^2 + 4\overline{\omega}^2}}{2}. \tag{48}$$

Here the negative value of α_1 is taken to make λ positive for a physically allowed solution of the steady-state distribution (49). The solution of Eq. (45) is given by

$$P_s = N \exp\left(-\frac{\lambda}{2\mathcal{D}_s}(\alpha_1^2 y_1^2 + 2\alpha_1 y_1 y_2 + y_2^2) \right). \tag{49}$$

With the help of above distribution the average quantities in tangent space can be calculated. Thus we have

$$\langle y_1^2 + y_2^2 \rangle = \frac{\mathcal{D}_s}{\lambda}\left(\frac{1}{\alpha_1^2} + 1 \right). \tag{50}$$

The fluctuation dissipation relation (35) can then be obtained by combining Eq. (50) with Eq. (33) as follows:

$$\mathcal{D}_s = \frac{\lambda}{\left(\frac{1}{\alpha_1^2} + 1 \right)} \exp\left(\sum_m A_m \right). \tag{51}$$

λ and α_1 are to be calculated using Eq. (48). For these we require explicit numerical evaluation of $\overline{\omega^2}$ as defined in Eqs. (43) and (44). The dissipative chaotic motion is governed by Eqs. (37) and (39). We choose the following values of the parameters [29] $a = 0.5, b = 10, \epsilon = 10, \Omega = 6.07,$ and $\gamma = 0.001$. The coupling-cum-field strength ϵ has been varied from set to set. We choose the initial conditions $z_1(0) = -3.5$ and $z_2(0) = 0$, which ensures strong global chaos. Note that c_2 as expressed in Eq. (42) and in the diffusion coefficients are the integrals over the correlations of $\zeta(t)$ $\zeta(t)$ is the fluctuating part of the second derivative of the potential $V(z)$ and is given by $\zeta(t) = -12az_1^2$. To calculate the correlation function $\langle\langle \zeta(t)\zeta(t-\tau) \rangle\rangle$ and the average $\langle \zeta(t) \rangle$ it is necessary to determine long-time series in $\zeta(t)$ by numerically solving the classical equation-of-motion (39). The next step is to carry out the averaging over the time series. For further details of the numerical procedure we refer to the earlier work [19–21]. On the other hand the cumulants $A_m (m = 1,2,3,4)$ [as defined in Eqs. (34) and (35)] are calculated from Eqs. (37) and (39) directly. The method has already been outlined in Sec. IV and in Ref. [24]. We then plot the theoretically calculated values of $\mathcal{D}_s$ from the evaluation of λ, α_1 and the cumulants for several values of the coupling constant ϵ [Eq. (36)] and compare them with the diffusion coefficients obtained from the direct numerical integration of Eqs. (39) and (37) with the appropriate transformation (22) for the corresponding values of ϵ. The result is shown in Fig. 2. It may be noted that the theoretical and numerical results are in good agreement. The validity of the fluctuation-dissipation relation as proposed in Eq. (35) is therefore reasonably satisfactory.

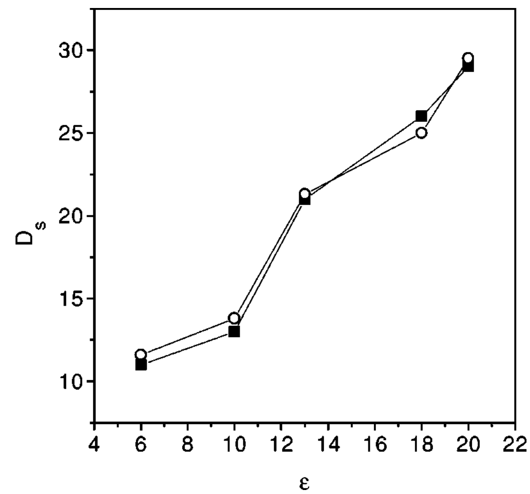

FIG. 2. The diffusion coefficients calculated numerically (marked as dark squares) using Eqs. (38) and (39) after transformation (22) are compared with theoretically obtained values (marked as circles) using Eq. (51) for several values of the coupling-cum-external field strength ϵ (units are arbitrary).

VI. CONCLUSIONS

The crucial question of instability of classical motion essentially rests on the linear stability matrix or Jacobian matrix associated with the equations-of-motion. While the linear stability analysis around the fixed points is based on the assumption of constancy of this matrix we take full account of the time dependence of the quantity in the chaotic regime by considering it to be a stochastic process, since the phase variables behave stochastically. Based on a Fokker-Planck description in the tangent space we trace the origin of chaotic diffusion and drift in the correlation of fluctuations of the linear stability matrix.

The main conclusions of this study are the following :

(i) We show that a class of dynamical stochastic parameters that attain their steady-state values in the long-time limit of the dynamical system may be used to characterize the dynamical steady state of the system. The first one of them that was proposed by Casartelli *et al.* [24] several years ago as a measure of the chaoticity of the system, is closely related to Kolmogorov entropy.

(ii) We establish a connection between the drift and the diffusion coefficients of the Fokker-Planck equation and the dynamical stochastic parameters in the spirit of fluctuation-dissipation relation. The realization of this relation in chaotic dynamics therefore carries the message that although comprising a few degrees of freedom, a chaotic system may behave as a statistical-mechanical system (although in a somewhat different sense).

The theoretical relations proposed here are generic for *N*-degree-of-freedom chaotic Hamiltonian system with or without dissipation and have been verified by numerical analysis of a driven nonlinear dissipative system. We hope that the present approach will find useful application in searching for the related thermodynamically inspired quantities in few-degrees-of-freedom systems.

ACKNOWLEDGMENT

B. C. Bag is indebted to the Council of Scientific and Industrial Research (CSIR), Government of India, for financial support.

APPENDIX: THE DERIVATION OF THE FOKKER-PLANCK EQUATION

We first note that the operator $e(-\tau \nabla \cdot L^0)$ provides the solution of the equation [Eq. (13), $\alpha = 0$]

$$\frac{\partial f(X,t)}{\partial t} = -\nabla_X \cdot L^0 f(X,t). \tag{A1}$$

f signifies the "unperturbed" part of P which can be found explicitly in terms of characteristic curves. The equation

$$\dot{X} = L^0(X) \tag{A2}$$

determines for a fixed t a mapping from $X(\tau=0)$ to $X(\tau)$, i.e., $X \to X^\tau$ with inverse $(X^\tau)^{-\tau} = X$. The solution of Eq. (A1) is

$$f(X,t) = f(X^{-t},0)\left|\frac{dX^{-t}}{dX}\right| = e[-t\nabla \cdot F_0]f(X,0), \tag{A3}$$

$|d(X^{-t})/d(X)|$ being a Jacobian determinant. The effect of $e(-t\nabla \cdot L^0)$ on $f(X)$ is as

$$e(-t\nabla \cdot L^0)f(X,0) = f(X^{-t},0)\left|\frac{dX^{-t}}{dX}\right|. \tag{A4}$$

This simplification in Eq. (16) yields

$$\frac{\partial P}{\partial t} = \Bigg\{ -\nabla \cdot L^0 - \alpha\langle \nabla \cdot L^1\rangle + \alpha^2 \int_0^\infty d\tau \left|\frac{dX^{-\tau}}{dX}\right| \times \langle\langle \nabla \cdot L^1(X,t)\nabla_{-\tau} \cdot L^1(\mathbf{x}^{-\tau},t-\tau)\rangle\rangle \left|\frac{dX}{dX^{-\tau}}\right| \Bigg\} P. \tag{A5}$$

Now to express the Jacobian, $X^{-\tau}$ and $\nabla_{-\tau}$ in terms of ∇ and X, we solve Eq. (A2) for short time (this is consistent with the assumption that the fluctuations are rapid [25]).

We now write the solution of Eq. (A2) [using Eqs. (4)–(6)] as follows:

$$\begin{pmatrix} X_1^{-\tau} \\ \vdots \\ X_N^{-\tau} \end{pmatrix} = -\tau \begin{pmatrix} X_{N+1} \\ \vdots \\ X_{2N} \end{pmatrix} + \begin{pmatrix} X_1 \\ \vdots \\ X_N \end{pmatrix} = \begin{pmatrix} \overline{G}_1(X) \\ \vdots \\ \overline{G}_N(X) \end{pmatrix} \tag{A6}$$

and

$$\begin{pmatrix} X_{N+1}^{-\tau} \\ \vdots \\ X_{2N}^{-\tau} \end{pmatrix} = e^{\gamma\tau} \begin{pmatrix} X_{N+1} \\ \vdots \\ X_{2N} \end{pmatrix} - \tau \begin{pmatrix} G_{N+1}(X) \\ \vdots \\ G_{2N}(X) \end{pmatrix} = \begin{pmatrix} \overline{G}_{N+1}(X) \\ \vdots \\ \overline{G}_{2N}(X) \end{pmatrix}. \tag{A7}$$

Here the terms of $O(\tau^2)$ are neglected. Since the vector $X^{-\tau}$ is expressible as a function of X we write

$$X^{-\tau} = \overline{G}(X), \tag{A8}$$

and the following simplification holds good:

$$\begin{aligned} L^1(X^{-\tau},t-\tau) \cdot \nabla_{-\tau} &= L^1[\overline{G}(X),t-\tau] \cdot \nabla_{-\tau} \\ &= \sum_k L_k^1[\overline{G}(X),t-\tau]\frac{\partial}{\partial X_k^{-\tau}} \\ &= \sum_j \sum_k L_k^1[\overline{G}(X),t-\tau]g_{jk}\frac{\partial}{\partial X_j}; \\ &\quad j,k=1,\ldots,2N, \end{aligned} \tag{A9}$$

where

$$g_{jk} = \frac{\partial X_j}{\partial X_k^{-\tau}}. \tag{A10}$$

In view of Eqs. (A6) and (A7) we note

$$\begin{aligned} &\text{if } j=k \text{ then } g_{jk}=1, \ k=1,\ldots,N \\ &\qquad\qquad\qquad\quad = e^{-\gamma\tau}, \ k=N+1,\ldots,2N \\ &\text{if } j\neq k \text{ then } g_{jk} \propto -\tau e^{-\gamma\tau} \text{ or } 0. \end{aligned}$$

Thus g_{jk} is a function of τ only. Let

$$\mathbf{R}_j = \sum_k L_k^1[\overline{G}(X),t-\tau]g_{jk}. \tag{A11}$$

From Eqs. (8), (9), and (A8) we write

$$L_i^1(X^{-\tau},t-\tau) = L_i^1[\overline{G}(X),t-\tau] = 0 \quad \text{for} \quad i=1,\ldots,N. \tag{A12}$$

So the conditions (A11), (A12), and (A6) imply that

$$\begin{aligned} R_j(X,t-\tau) &= R_j(X_1,\ldots,X_N,t-\tau) \quad \text{for} \quad j=1,\ldots,N, \\ R_j(X,t-\tau) &= R_j(X_1,\ldots,X_{2N},t-\tau) \\ &\qquad \text{for} \quad j=N+1,\ldots,2N. \end{aligned} \tag{A13}$$

We next carry out the following simplifications of the α^2 term in Eq. (A5). We make use of relation (10) to obtain

$$\begin{aligned} L^1(X,t)\cdot\nabla \sum_j R_j \frac{\partial}{\partial X_j}P(X,t) &= \sum_i L_i^1(X,t)\frac{\partial}{\partial X_i}\sum_j R_j \frac{\partial}{\partial X_j}P(X,t) \\ &= \sum_{i,j} L_i^1(X,t)R_j \frac{\partial^2}{\partial X_i \partial X_j}P(X,t) \\ &\quad + \sum_j \mathbf{R}_j' \frac{\partial}{\partial X_j}P(X,t), \end{aligned} \tag{A14}$$

where

$$R_j' = \sum_i L_i^1(X,t)\frac{\partial}{\partial X_i}R_j. \tag{A15}$$

Conditions (A12) and (A13) imply that

$$R_j' = 0 \quad \text{for} \quad j = 1, \ldots, N,$$

$$R_j' = R_j'(X_1, \ldots, X_N, t - \tau) \neq 0 \quad \text{for} \quad j = N+1, \ldots, 2N. \tag{A16}$$

By Eq. (A16) one has

$$R' \cdot \nabla P(X,t) = \nabla \cdot R' P(X,t). \tag{A17}$$

Making use of Eqs. (10), (A9), (A14), and (A17) in Eq. (A5) we obtain the Fokker-Planck equation (17).

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