

Time correlation functions in low-dimensional conservative chaotic systems: A memory function approach

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(Received 6 February 1998; accepted 24 July 1998)

Time correlation functions are studied for some conservative chaotic systems with both discrete and continuous time dynamics. For low-dimensional systems a memory function formalism on a microcanonical ensemble turns out to be able to yield useful information on the time correlation function and its energy dependence. © 1998 American Institute of Physics.

[S0021-9606(98)51740-0]

I. INTRODUCTION

Equilibrium time correlation function (TCF) has been playing a fundamental role in statistical mechanics of many-body systems. The linear response theory¹ or more generally the fluctuation-dissipation theorems² show that how various observed quantities such as transport coefficients and the spectra measured by spectroscopic techniques are expressed in terms of the TCFs.

Recently the TCF gathers new interest in connection with *chaos* dynamics, especially in systems with a few degrees of freedom. It is observed for many nonlinear Hamiltonian systems that dynamics becomes more chaotic and the power spectra of the TCFs change from sharp line spectra to grassy or continuous ones³⁻⁷ as the (total) energy and/or strength of nonlinearity increase. A projection operator method^{8,9} clearly shows that effects of a system as a heat bath is concisely represented in terms of the appropriate TCF of the system and from this viewpoint also, the TCF and its dependence on energy are an interesting object to study theoretically.¹⁰

The TCF, which is defined below by Eq. (3) for map dynamics and by Eq. (13) for continuous-time dynamics, is usually calculated in computer experiments from a long time trajectory of system dynamics which is obtained by solving equation of motion. When the system is not ergodic,^{4,5} one has to solve the equation of motion under many initial conditions (with the same energy if we are to calculate the TCF based on a microcanonical ensemble) and the TCF is obtained as the average of the TCF calculated for each trajectory. As expected this is a rather tedious step to calculate the TCF.^{4,5}

In order to calculate the TCF of low-dimensional conservative systems, we apply the memory function formalism⁸ with use of a newly developed algorithm, which enables us to compute higher order memory coefficients. Here we note that the memory function formalism is originally developed for the TCF for many-body condensed matters^{2,8,9} and the

memory coefficients with some lowest orders (up to third or at most fourth) have been used. This is because the N th order coefficient usually (roughly speaking) requires the knowledge of the N -body equilibrium correlations which are not known even approximately for N larger than 3.² In our few-body or low-dimensional systems we can calculate higher order coefficients relatively easily especially when the energy of the system or the nonlinearity parameter is small and the integration in the phase space does not demand heavy computations.

After some general discussions on the relation between the TCF and the memory function,^{8,11,12} we consider explicitly the standard map³ and the Nelson system¹³ as examples of discrete-time and continuous-time dynamical systems, respectively. Numerical results for the TCF show that the memory function approach together with our method to calculate the moments in the microcanonical ensemble can yield useful information on dynamical properties of low-dimensional nonlinear systems.

II. TCF FOR DISCRETE-TIME DYNAMICS

First we consider conservative map dynamics governed by

$$\mathbf{x}_{n+1} = \mathbf{G}(\mathbf{x}_n), \quad (1)$$

where \mathbf{x}_n denotes the phase point at time $t=n$ ($n=0,1,2,\dots$) and \mathbf{G} satisfies $|\partial\mathbf{G}(\mathbf{x})/\partial\mathbf{x}|=1$. Equation of motion (1) is equivalent to the following Frobenius-Peron equation for the distribution function $p(\mathbf{x};n)$,³

$$p(\mathbf{x};n+1) = \int d\mathbf{x}' p(\mathbf{x}';n) \delta(\mathbf{x} - \mathbf{G}(\mathbf{x}')) \equiv L^\dagger p(\mathbf{x};n). \quad (2)$$

The TCF $\phi_A(n)$ of the dynamical variable $A(\mathbf{x})$ is defined by

$$\phi_A(n) = \int d\mathbf{x}_0 p_{\text{eq}}(\mathbf{x}_0) A(\mathbf{x}_0) A(n|\mathbf{x}_0) \equiv \langle A(0)A(n) \rangle, \quad (3)$$

where $p_{\text{eq}}(\mathbf{x}_0)$ denotes the equilibrium distribution for the initial phase \mathbf{x}_0 and

$$A(n|\mathbf{x}_0) \equiv A(\mathbf{G}(\mathbf{G}(\dots(\mathbf{G}(\mathbf{x}_0))\dots)) \equiv L^n A(\mathbf{x}_0), \quad (4)$$

with \mathbf{G} appearing n times. The operators L^\dagger in Eq. (2) and L in Eq. (4) are seen to satisfy

$$\int d\mathbf{x} f(\mathbf{x}) L^\dagger g(\mathbf{x}) = \int d\mathbf{x} g(\mathbf{x}) L f(\mathbf{x}), \quad (5)$$

for arbitrary functions $f(\mathbf{x})$ and $g(\mathbf{x})$.¹¹ The stationarity of the TCF, $\langle A(m)A(n+m) \rangle = \langle A(0)A(n) \rangle$ readily follows from the relation $L^\dagger p_{\text{eq}}(\mathbf{x}) = p_{\text{eq}}(\mathbf{x})$ satisfied by an equilibrium distribution.

The projection operator technique leads to the exact Langevin-type equation¹¹

$$A(n|\mathbf{x}_0) = \sum_{m=0}^{n-1} \psi_A(m) A(n-1-m|\mathbf{x}_0) + f(n|\mathbf{x}_0) \quad (n \geq 1), \quad (6)$$

where the memory function $\psi_A(m)$ and the random force $f(n|\mathbf{x}_0)$ are defined by

$$\psi_A(m) = \langle (L f(m|\mathbf{x}_0)) A(\mathbf{x}_0) \rangle / \langle A^2 \rangle, \quad (7)$$

$$f(n|\mathbf{x}_0) = (Q_A L)^n A(\mathbf{x}_0), \quad (8)$$

with $P_A \equiv 1 - Q_A$ denoting the projection operator onto the variable A , $P_A B \equiv \langle B A \rangle A / \langle A^2 \rangle$. Since the random force $f(n|\mathbf{x}_0)$ is orthogonal to $A(\mathbf{x}_0)$, that is, $\langle A(\mathbf{x}_0) f(n|\mathbf{x}_0) \rangle = 0$ due to the projection operator Q_A in Eq. (8), we immediately obtain from Eqs. (3) and (6),

$$\phi_A(n) = \sum_{m=0}^{n-1} \psi_A(m) \phi_A(n-1-m). \quad (9)$$

If we introduce a generating function $\tilde{\phi}_A(z) \equiv \int_{n=0}^{\infty} \phi_A(n) z^n$ and a similarly defined $\tilde{\psi}_A(z)$, Eq. (9) is expressed as^{8,11}

$$\tilde{\phi}_A(z) = \phi_A(0) / [1 - z \tilde{\psi}_A(z)]. \quad (10)$$

The memory function $\psi_A(n)$ provides us with a simple picture on how the TCF $\phi_A(n)$ behaves as a function of (discrete) time $t=n$. That is, if the memory is short-lived and we have $\psi_A(n) = 0$ for $n \geq 1$, the TCF becomes a simple exponential function $\phi_A(n) = \alpha^n \phi_A(0)$ with $\alpha = \psi_A(0)$.¹⁴ It is easily confirmed from the inverse relation $\phi_A(n) = (2\pi i)^{-1} \int dz \tilde{\phi}_A(z) / z^{n+1}$ that the TCF is generally expressed as the sum of M exponential functions when the memory $\psi_A(m)$ is (nearly) zero for $m \geq M$. We notice however from Eq. (10) that the TCF does not decay to zero, due to the presence of the pole at $z=1$ in the inverse formula above, when the nonzero part of the memory function satisfies $\int_{m=0}^{M-1} \psi_A(m) = 1$. We will see some examples of this later for the standard map.

III. TCF FOR CONTINUOUS-TIME DYNAMICS

Next we consider dynamics governed by a differential equation

$$d\mathbf{x}/dt = \mathbf{V}(\mathbf{x}), \quad (11)$$

where $\mathbf{x}(t)$ denotes the phase point at time t and \mathbf{V} satisfies $\nabla \cdot \mathbf{V}(\mathbf{x}) = 0$ since we consider a conservative system. The distribution function $p(\mathbf{x};t)$ evolves in time according to

$$\partial p(\mathbf{x};t) / \partial t = -\nabla \cdot [\mathbf{V}(\mathbf{x}) p(\mathbf{x};t)] \equiv L^\dagger p(\mathbf{x};t). \quad (12)$$

As in the case of the discrete-time dynamics, the TCF $\phi_A(t)$ of the dynamical variable $A(\mathbf{x}(t))$ is defined by

$$\phi_A(t) = \int d\mathbf{x}_0 p_{\text{eq}}(\mathbf{x}_0) A(\mathbf{x}_0) A(t|\mathbf{x}_0) \equiv \langle A(0)A(t) \rangle, \quad (13)$$

where $p_{\text{eq}}(\mathbf{x}_0)$ denotes the equilibrium distribution for the initial phase \mathbf{x}_0 and

$$A(t|\mathbf{x}_0) \equiv \int d\mathbf{x} A(\mathbf{x}) \exp(L^\dagger t) \delta(\mathbf{x} - \mathbf{x}_0) = \exp(Lt) A(\mathbf{x}_0). \quad (14)$$

The L^\dagger in Eq. (12) and L in Eq. (14) are related with each other through Eq. (5) as before. The stationarity of the TCF, $\langle A(t')A(t+t') \rangle = \langle A(0)A(t) \rangle$ readily follows from the relation $L^\dagger p_{\text{eq}}(\mathbf{x}) = 0$ for an equilibrium distribution. By putting $t' = -t$, we see that the TCF is even in t , $\phi_A(t) = \phi_A(-t)$.

The short-time or Taylor expansion of the TCF is obtained from Eqs. (13) and (14) as

$$\phi_A(t) = \sum_{n=0}^{\infty} c_n t^{2n} / (2n)!, \quad (15)$$

with the coefficient $c_n = (-1)^n \int d\mathbf{x}_0 p_{\text{eq}}(\mathbf{x}_0) [L^n A(\mathbf{x}_0)]^2$. For continuous-time dynamics we use, instead of the z -transformation, the Laplace transformation

$$\tilde{\phi}_A(s) = \int_0^{\infty} dt \phi_A(t) e^{-st} = \sum_0^{\infty} c_n / s^{2n+1}. \quad (16)$$

By iteratively employing the memory function formalism, we can express $\tilde{\phi}_A(s)$ in the continued fraction expansion (CFE) of the infinite order

$$\tilde{\phi}_A(s) = B_0 / \{s + \{B_1 / \{s + \{B_2 / \{s + \{B_3 / \{s + \dots\} \dots\} \dots\} \dots\} \dots\} \}, \quad (17)$$

where the n th order coefficient B_n can be expressed in terms of $\{c_0, \dots, c_n\}$.¹²

Let us suppose that we could calculate the coefficients $\{B_n\}$ up to $n=M$. First we rewrite Eq. (17) as

$$\tilde{\phi}_A(s) = B_0 / \{s + \{B_1 / \{s + \dots + \{B_{M-2} / \{s + \tilde{\Omega}(s)\} \dots\} \dots\} \} \quad (18)$$

by introducing the $(M-1)$ th order memory function

$$\tilde{\Omega}(s) \equiv B_{M-1} / \{s + B_M / \{s + \dots\} \dots\}. \quad (19)$$

Our M th order Gaussian approximation in the time space consists of

$$\Omega(t) \simeq \Omega_G(t) \equiv B_{M-1} \exp[-B_M t^2 / 2], \quad (20)$$

or in the s -space,

$$\tilde{\Omega}_G(s) = B_{M-1} [2\pi / B_M]^{1/2} \times \exp[s^2 / (2B_M)] \text{erfc}[s / (2B_M)^{(1/2)}]. \quad (21)$$

It is noted that Eq. (20) gives the correct short-time expansion of $\Omega(t)$ up to t^2 . Since the Gaussian approximation (20)

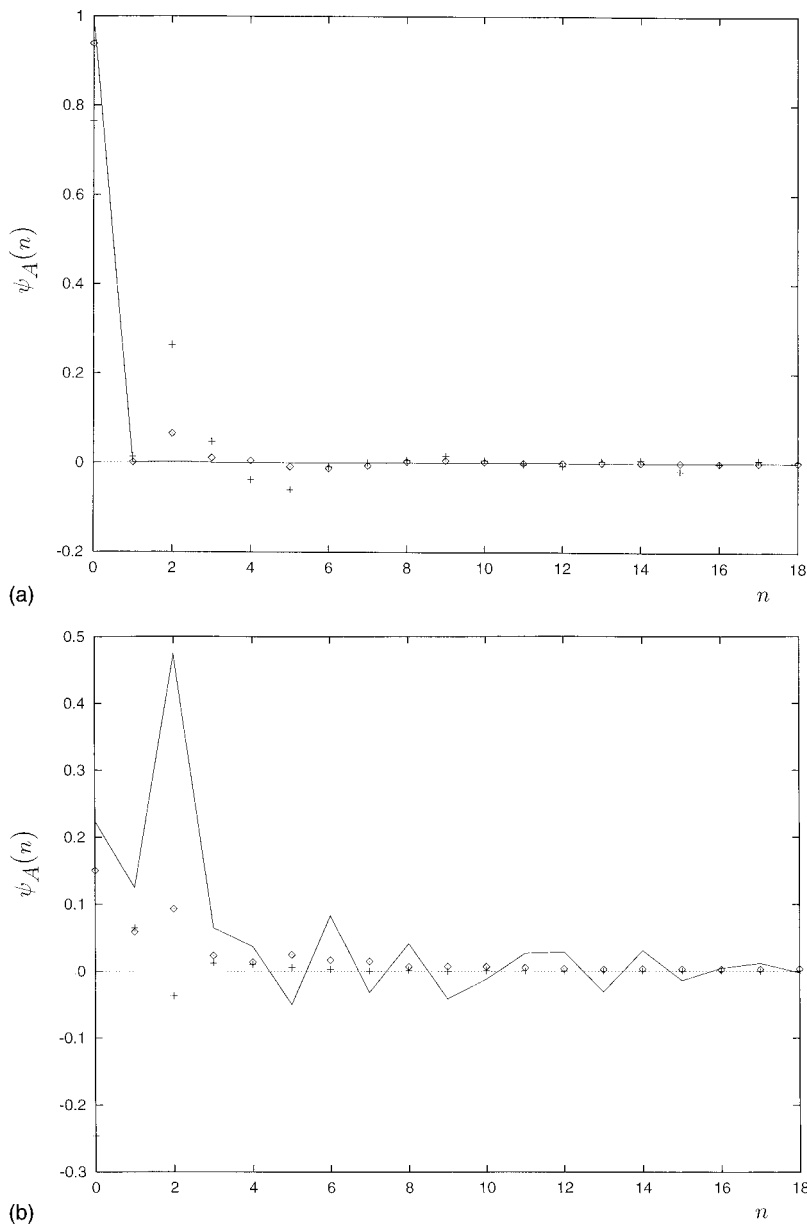


FIG. 1. (a) The memory function $\psi_A(n)$ for $A = \cos(p)$ for $K=0.1$ (denoted by a solid line), 0.5 (denoted by \diamond), and 0.9 (denoted by $+$). We note that $\psi_A(n)$ is defined for zero and positive integer n with the line for guide of the eyes. (b) The same as (a) for $K = 2.0$ (denoted by a solid line), 6.0 (denoted by \diamond), and 10.0 (denoted by $+$).

or (21) formally takes into account effects of higher order terms ($n > M$), it is considered to be better than simply setting $B_n = 0$ for $n > M$.²

IV. NUMERICAL RESULTS

To illustrate how the formalism developed above may be applied to the TCF of low-dimensional nonlinear systems, we consider the standard map^{3,15} (the Nelson system¹³) as a typical model in discrete (continuous)-time dynamics.

A. TCF for the standard map

As a conservative discrete-time system we consider the standard map

$$\theta_{n+1} = \theta_n + p_n, \quad p_{n+1} = p_n + K \sin(\theta_{n+1}). \quad (22)$$

It is well-known that as the nonlinearity parameter K becomes large the system behaves more and more chaotically with the last KAM torus disappearing around $K = 1$.¹⁵ Here we consider the variables $\{\theta_n, p_n\}$ to be in the range $(0, 2\pi)$

and the equilibrium distribution is taken to be uniform in this region. We can easily calculate the TCF $\phi_A(n)$ up to n (≈ 20), by numerically performing the integration in Eq. (3). It is noted however that as K becomes large $A(n|\mathbf{x}_0)$ depends on the initial phase \mathbf{x}_0 rather sensitively and this tendency is enhanced as the order n becomes large. Thus in order to numerically calculate $\phi_A(n)$ precisely, we must choose the mesh size $\Delta \mathbf{x}_0 = (\Delta \theta_0, \Delta p_0)$ for discretization of the integral in Eq. (3) small enough ($\leq 2\pi/10^4$ for $n \leq 20$).

The memory function (7) with $A(\mathbf{x}_0) = \cos(p_0)$ is shown for small and large values of K in Figs. 1(a) and 1(b), respectively. The $\psi_A(n)$ seems to decay to zero for large n irrespective of the K values. From Fig. 2(a) it is seen that the TCF $\phi_A(n)$, corresponding to $\psi_A(n)$, does not necessarily go to zero for large n when the nonlinearity parameter K is small and chaotic or mixing effects are small accordingly. Asymptotic behavior is generally rather difficult to ascertain from numerical analyses. However from Figs. 3(a) and 3(b), which depict $\Psi_A(n) \equiv \sum_{m=0}^n \psi_A(m)$, we clearly see that

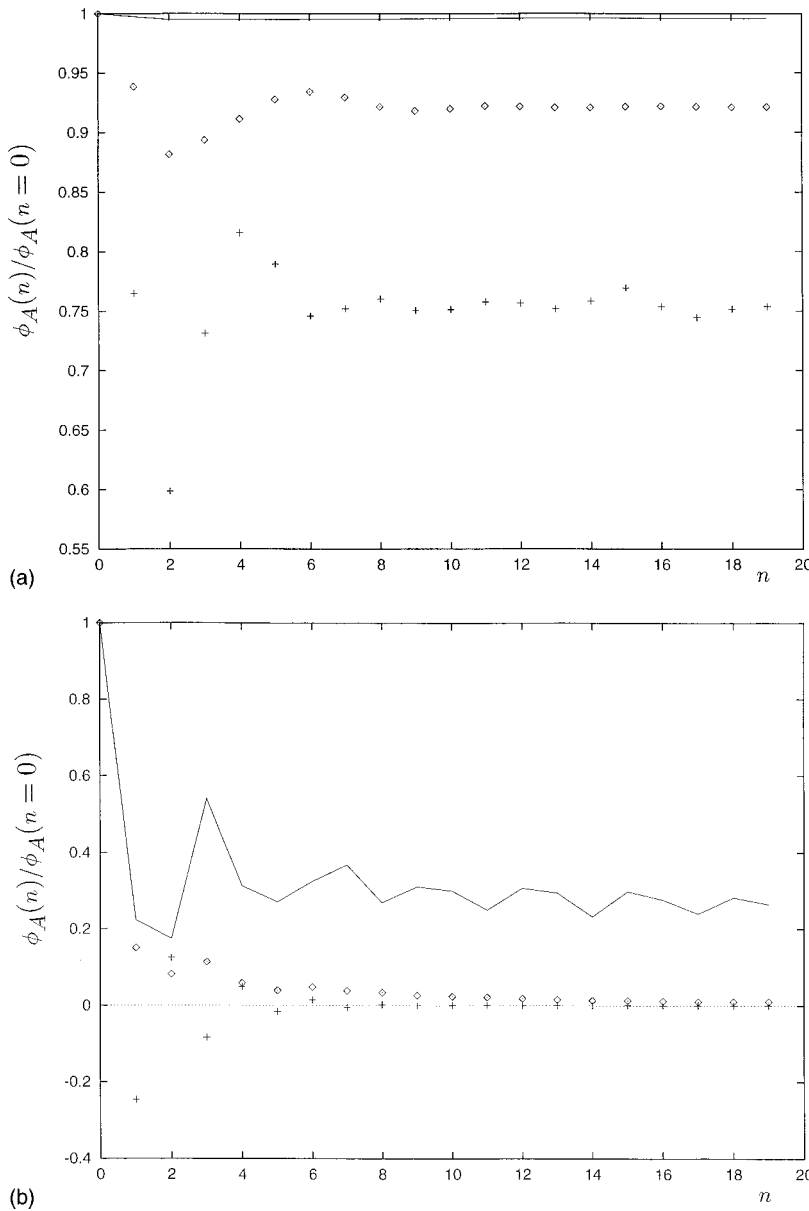


FIG. 2. (a) The normalized TCF $\phi_A(n)/\phi_A(n=0)$ for $A = \cos(p)$ for $K = 0.1$ (denoted by a solid line), 0.5 (denoted by \diamond), and 0.9 (denoted by $+$). (b) The same as (a) for $K = 2.0$ (denoted by a solid line), 6.0 (denoted by \diamond), and 10.0 (denoted by $+$).

$\Psi_A(n)$ approaches 1 for small values of K and this means the nondecaying or nonergodic behavior of the TCF as explained below the line of Eq. (10). For $K \leq K_c \approx 4$ it is expected from numerical calculations that the TCF does not decay with the asymptotic value $\phi_A(n=\infty)$ monotonically decreasing to zero as K approaches K_c .

B. TCF for the Nelson model

As a conservative continuous-time system we consider a Nelson model with Hamiltonian

$$H(\mathbf{x}) = (p_1^2 + p_2^2)/2 + (y_2 - y_1^2/2)^2 + 0.05y_1^2 \equiv K_E + V_E, \tag{23}$$

where the first term K_E on the right-hand side of Eq. (23) denotes the kinetic part of the total energy. As the equilibrium distribution $p_{eq}(\mathbf{x}) (\mathbf{x} = \{p_1, p_2, y_1, y_2\})$, we take a microcanonical ensemble

$$p_{eq}(\mathbf{x}) = \delta(H(\mathbf{x}) - E), \tag{24}$$

and our main interest is centered on how the TCF of the Nelson system changes as the energy E of the system is changed. It is known from numerical experiments that for $E > 0.3$ dynamics is wholly chaotic and gradually it crosses over to fairly irregular to harmonic (regular) as E decreases.¹³ Due to the presence of the Dirac δ -function in the integral in Eq. (13) we need to perform integration in a three (not four) dimensional space.¹⁶

Numerically we calculate the coefficients $\{B_n\}$ in Eq. (17) up to $n = M (= 20)$, based on the well-known formula $B_n = \langle (f_n)^2 \rangle / \langle (f_{n-1})^2 \rangle$ with f_n the n th order random force,¹² and employ the M th order Gaussian approximation Eqs. (20) or (21). We now briefly comment on how the n th order random force f_n can be obtained by solving a difference equation. Since Hamiltonian (23) consists of polynomials only, the equations of motion are also of polynomial forms. From this fact the random forces $\{f_n\}$ is expressed as the sum of polynomials, that is, $f_n = \sum_{l_1, l_2, l_3, l_4} C_{l_1, l_2, l_3, l_4}^{(n)} p_1^{l_1} p_2^{l_2} y_1^{l_3} y_2^{l_4}$ with $l_i \geq 0$. We consider the case $A(\mathbf{x}) = y_1$, for which f_1

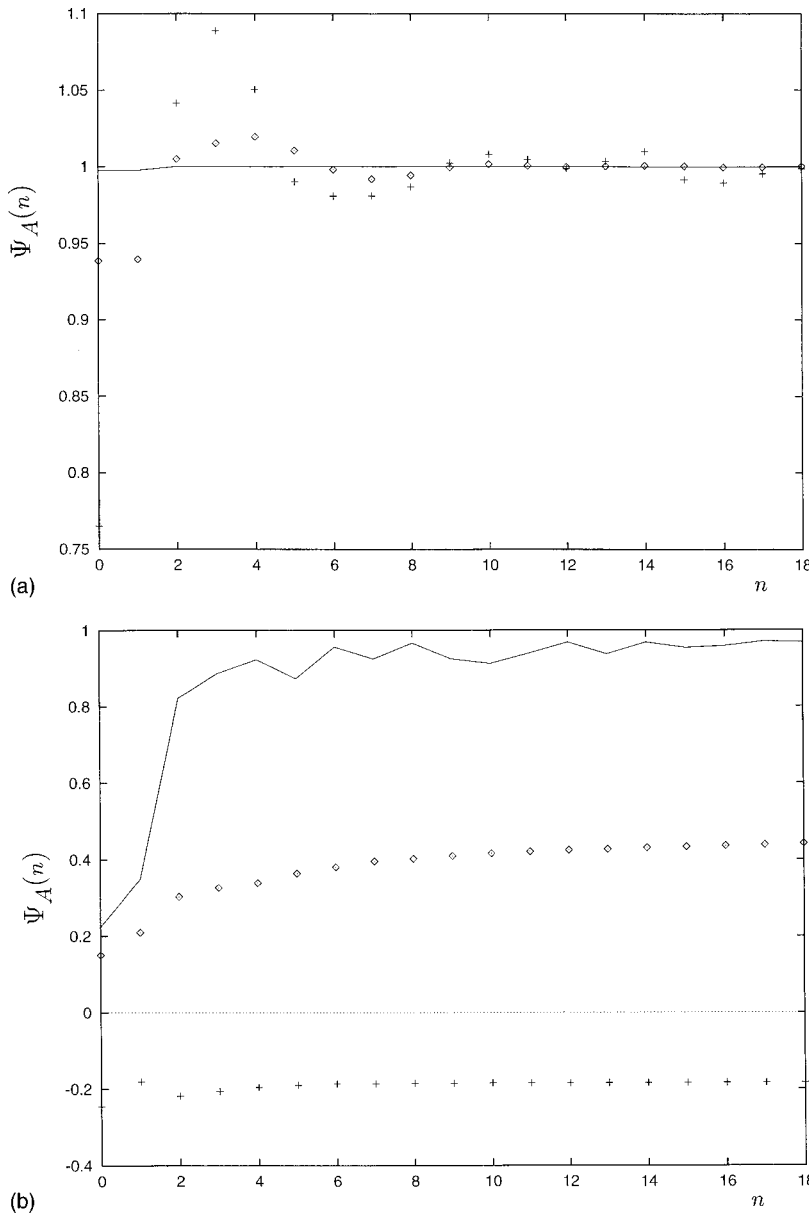


FIG. 3. (a) The partial sum $\Psi_A(n) \equiv \sum_{m=0}^n \psi_A(m)$ for $K=0.1$ (denoted by a solid line), 0.5 (denoted by \diamond), and 0.9 (denoted by $+$). (b) The same as (a) for $K=2.0$ (denoted by a solid line), 6.0 (denoted by \diamond), and 10.0 (denoted by $+$).

$=dy_1/dt=p_1$, thus $C_{l_1, l_2, l_3, l_4}^{(1)} = \delta_{l_1, 1} \delta_{l_2, 0} \delta_{l_3, 0} \delta_{l_4, 0}$ and the higher-order coefficient $C_{l_1, l_2, l_3, l_4}^{(n)}$ ($n \geq 2$) is determined recursively from $C_{l_1, l_2, l_3, l_4}^{(n-1)}$, where effects of the projection operator are to be properly taken into account. The difficulty in the numerical calculations is that as the energy E increases the phase space is extended and at the same time we must use the small mesh sizes for Δp_2 , Δy_1 , and Δy_2 since the higher-order random force consists of higher-order polynomials. This situation is qualitatively similar to what we encountered before for the standard map, Eq. (22), when K became large. Accordingly we had to restrict our calculation of the TCF of the Nelson system to $E \leq 0.01$.

In Fig. 4 we show the power spectrum $G_A(\omega)$ which is obtained from $\tilde{\phi}_A(s)$ by

$$G_A(\omega) = \text{real part of } \tilde{\phi}_A(s=i\omega), \quad (25)$$

for $A=y_1$ for $E=0.001$. In this case dynamics is seen to be rather regular and we observe nearly harmonic oscillation

around $\omega = 1/\sqrt{10} \approx 0.316$, which is obtained from Eq. (23) in the harmonic limit. As expected numerical results are dependent on the M -value we adopt in the M th order Gaussian approximation, Eqs. (18) and (20). In Fig. 5 we show the spectra for $E=0.01$ when we set $M=19$ and $M=20$. It is noted that the two spectra from $M=17$ and $M=19$ Gaussian approximations (also the two spectra from $M=18$ and $M=20$ Gaussian approximations) are almost indistinguishable on the scale of the figure. We see from Fig. 5 that the spectrum for $E=0.01$ has relatively broad peak around $\omega=0.4$ and the TCF, corresponding to the spectrum, shows damped oscillation decaying to zero for $t \geq 60$ in contrast to the TCF for $E=0.001$ which decays to zero for $t \geq 2000$. In leaving this section it is noted that strength of nonlinearity, which can be estimated with the fraction f of chaotic phase-space, is rather weak for the two cases $E=0.001$ and $E=0.01$ studied above. Here we estimate f from the surface of the section and/or with use of a method of Henon-Heiles,¹⁷ in which

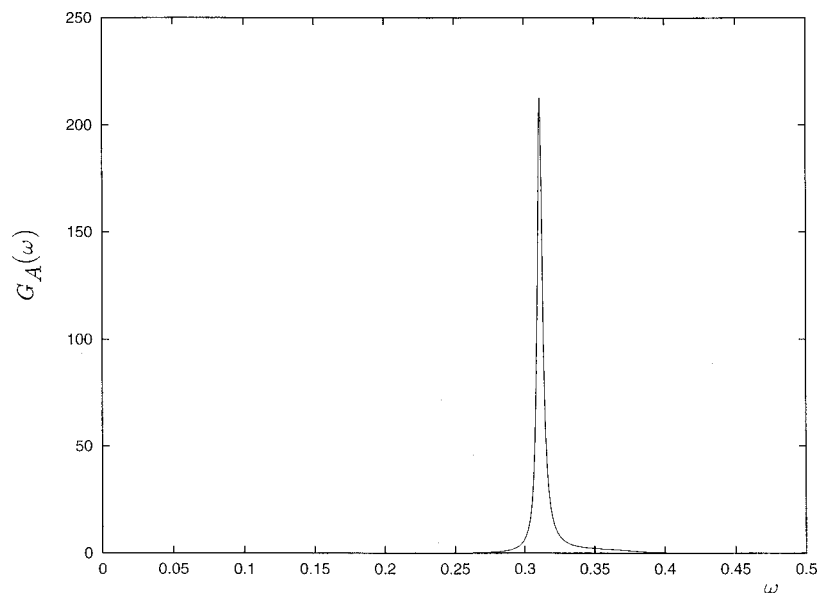


FIG. 4. The power spectrum (25) with $A=y_1$ for $E=0.001$ calculated under the $M=20$ Gaussian approximation.

one takes many phase-point pairs, very close each other initially, and count the fraction of pairs which moves far apart with time. The fraction f is about 70% for $E=0.1$ (strong nonlinearity) but 2% and less than 0.1% for $E=0.01$ and $E=0.001$, respectively. In view of the fact that the TCF could be calculated in a strongly nonlinear region for the standard map, we may say that our approach to the TCF or its spectrum has more severe restrictions for the continuous-time dynamics compared to discrete-time one.

V. REMARKS

In this paper we studied the TCF for low-dimensional systems. From a standpoint of numerical calculations of the TCF, it is usually obtained from a long trajectory of system dynamics. In other words it is necessary to first solve equation of motion for long time in order to calculate the TCF. However, as stressed before,⁵ it is sometimes necessary to consider ensemble of trajectories and the TCF should be ob-

tained as the average over this ensemble. In this case it is not realistic to rely on trajectories in order to obtain the TCF. The motivation to apply the memory function formalism to calculate the TCF stemmed from our needs to avoid the use of many long-time-solutions of differential (or difference) equations. Our approach enables us to calculate the TCF exactly in the short-time region and approximately in the long-time one.

The final remark is concerned with the autoregressive moving-average (ARMA) model for the time-series prediction¹⁸

$$A_n = \sum_{i=0}^p \Psi_i A_{n-1-i} + \sum_{i=0}^q \Theta_i \xi_{n-i} \equiv \sum_{i=0}^p \Psi_i A_{n-1-i} + F_n, \quad (26)$$

where $\{\Psi_i\}$ ($0 \leq i \leq p$) and $\{\Theta_j\}$ ($0 \leq j \leq q$) together with p and q are parameters of the model and ξ_i denotes the Gaussian white noise with zero mean and unit variance. First we

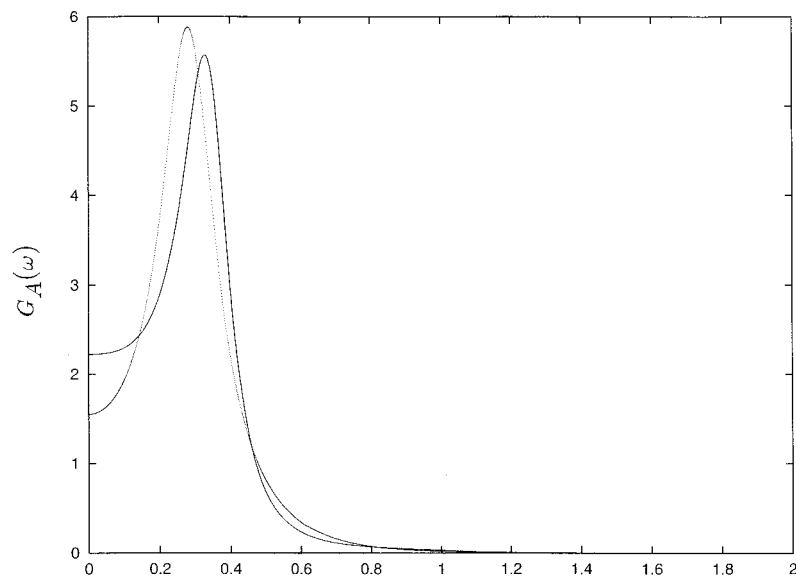


FIG. 5. The same as Fig. 4 for $E=0.01$ calculated under the $M=20$ (denoted by a solid line) and $M=19$ (denoted by a dotted line) Gaussian approximations.

note the similarity of Eq. (6) to Eq. (26). Actually if the memory $\psi_A(m)$ vanishes when $m > p$, we can show that the random force $f(n|\mathbf{x}_0)(n > p)$ is expressed as F_n in Eq. (26) with $q = p$. This means that the ARMA model with the special condition $p = q$ can be derived from a dynamical model (1) as a generalized Langevin equation when the memory is short lived (up to p). This point will be discussed separately in the near future.

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¹⁰We cannot know whether a system of interest is ergodic before detailed numerical simulations are performed. So the TCF should be calculated in itself based on the definition (3) or (13).

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¹⁶From $dH = dp_1 \partial H / \partial p_1 = p_1 dp_1$ we have $\int dp_1 dp_2 dy_1 dy_2 f(\mathbf{x}) \delta(H - E) = \sum_{p_1} \int dp_2 dy_1 dy_2 f(\mathbf{x}) / |p_1|$, where the sum over p_1 means the summation over the two solutions of equation $H(\mathbf{x}) - E = 0$, namely $p_1 = \pm [2(E - V - p_2^2/2)]^{1/2}$.

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