Linear response of the Lorenz system

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The present numerical study provides strong evidence that at standard parameters the response of the Lorenz system to small perturbations of the control parameter r is linear. This evidence is obtained not only directly by determining the response in the observable $A(\mathbf{x})=z$, but also indirectly by validating various implications of the assumption of a linear response, like a quadratic response at twice the perturbation frequency, a vanishing response in $A(\mathbf{x})=x$, the Kramers-Kronig relations, and relations between different response functions. Since the Lorenz system is nonhyperbolic, the present results indicate that in contrast to a recent speculation the large system limit (thermodynamic limit) need not be invoked to obtain a linear response for chaotic systems of this type.

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I. INTRODUCTION

Linear response theory is concerned with the reaction of a dynamical system to small external perturbations. For equilibrium systems this reaction can be computed by the Kubo theory [1], starting from the microscopic Hamiltonian of the considered system. This theory is extremely successful in predicting electric conductivities, magnetic susceptibilities, dielectric functions, polarizabilty, and other ''generalized'' susceptibilities [2]. Its most famous result is the fluctuation-dissipation theorem that relates the response of a system to its equilibrium fluctuations.

From the viewpoint of dynamical systems theory the dynamics underlying statistical mechanics is chaotic. For a subclass of these systems, uniformly hyperbolic diffeomorphisms, Ruelle recently presented a rigorous derivation of the Kubo theory [3] and formally generalized this derivation to hyperbolic chaotic flows [4], which include beside equilibrium systems also dissipative systems, i.e., systems far from equilibrium. Although hyperbolic flows are too narrow a class to be physically relevant (compare Gallavotti's discussion of his ''chaotic hypothesis'' [5]), Ruelle argues that if a system shows a linear response, it is appropriately described by the Kubo theory [4].

But not all systems react linearly to small external perturbations. Examples where a linear response fails to exist are phase transitions with a diverging or discontinuous (generalized) susceptibility (the magnetic susceptibility at the Curie point; the specific heat at the transition to superconductivity), or systems with hysteretic behavior, such as ferromagnets. Also systems whose dynamics can essentially be represented by chaotic one-dimensional (1D)-maps will generically not react linearly to external perturbations. This follows from a study by Ershov [6] who showed that the invariant densities of chaotic 1D maps can typically not be expanded in a perturbation parameter. An example is chaotic systems in the inverse period-doubling cascade, whose ''sensitive dependence on parameters'' has been studied by Farmer [7]. For a two-dimensional nonintegrable Hamiltonian system this type of problem has been discussed by Takahashi *et al.* [8].

In view of these examples the question arises how the class of systems showing a linear response can be characterized. As already mentioned, this class should be much wider than the hyperbolic systems considered by Ruelle. But considering nonhyperbolic systems leads to the general problem that such systems are typically infinitesimally close to bifurcations that on parameter changes may destroy the differentiability of the invariant density with respect to parameters—an important ingredient of the Kubo theory—and may render observables to behave discontinuously. Guckenheimer and Holmes call this the failure of the ''dogma of structural stability'' in dynamical systems theory (p. 255f of Ref. [9]). Abraham and Marsden argue that a physically more appropriate notion of stability may be ''downright statistical'' (p. 595 of Ref. [10]), while Ruelle speculates that this problem may only be solved by invoking the thermodynamic limit (p. 410 of Ref. [11]).

As a preparation for future investigations on how a linear response may arise in nonhyperbolic chaotic systems, the present study provides a specific example, where despite of nonhyperbolicity a linear response appears to exist: the Lorenz system at standard parameters [12]. This example indicates that there might be another solution to the stability problem of dynamical systems theory, namely, that there exist bifurcations across which observables behave continuously differentiable so that the thermodynamic limit need not be invoked. That the Lorenz system is nonhyperbolic is especially known from the investigations of Sparrow, who showed that at standard parameters perturbations of the control parameter (usually called r) induce homoclinic bifurcations, whatever small the perturbation might be [13]. The present approach to the linear response of the Lorenz system is numerical, i.e., nonrigorous. Hence the main task of the present paper is to make the evidence for the existence of a linear response as safe as possible. This is done not only by checking the linearity of the response directly, but also by testing various implications of the assumption of a linear response, as the prediction of a quadratic response at twice the perturbation frequency, a vanishing linear response in an antisymmetric observable, the validity of a particular relation between two different response functions, and the Kramers-Kronig relations. The results of these investigations turn out to be in full agreement with the existence of a linear response of the Lorenz system, despite its nonhyperbolicity.

The present study differs from most other studies of the linear response of chaotic systems by the nature of the perturbation considered here: it drives the system through bifurcations so that in view of the considerations from above the existence of a linear response stands in question. For nonhyperbolic systems (as the Lorenz system) almost every perturbation would do so. Nevertheless, there are two types of perturbations to which the response can be guaranteed to be linear, even if the system is nonhyperbolic. One is a perturbation that is equivalent to a coordinate transformation. The examples Grossmann constructs for his linear response theory of 1D maps are of this type [14] (compare Ref. [15]). For 2D maps this type of perturbations was studied in Ref. [16]. The situation for such perturbations parallels the case of hyperbolic systems, for which it is guaranteed that upon sufficiently small perturbations the system is still topologically conjugate to the unperturbed system [3,11]. The other type of perturbations for which a linear response can generally be expected, are perturbations that can be represented as changes in the initial conditions. This is the case, e.g., for the response to a (down-)step-function or delta-function type perturbation. In such situations the response is simply a relaxation in the unperturbed system towards its invariant density (as long as it is unique, as in mixing systems) so that the behavior of the observables depends smoothly on the perturbation. Such perturbations were considered in Refs. [17,18], mainly in search for a fluctuation-response relation for nonequilibrium systems.

Apparently the first discussion of the relationship between a nonlinear dynamics and linear response was van Kampen's critique of the Kubo theory [19] (which essentially applies also to Ruelle's approach). His point is that a macroscopically linear response is only possible because of microscopic randomness, i.e., because of the nonlinearity of the microscopic evolution equations. But in Kubo's theory, according to van Kampen, macroscopic linearity is derived from microcopic linearity, which should be physically wrong; Kubo's answer is found in Ref. [20]. This objection has inspired quite a number of studies of the linear response of chaotic systems, aiming at a better understanding of the relationship between nonlinear dynamics and linear response [21]. With van Kampen's objection the kinetic approach to statistical mechanics stands against that of Gibb's. Therefore Suhl compared for a simple chaotic 2D map, response calculations from a kind of kinetic approach with those from the Kubo approach and obtained different values for the static response [22]—a result that should be further scrutinized. Saito and Matsunaga demonstrated how coarse graining can be invoked to reconcile chaotic dynamics with linear response theory [23].

The idea of the following investigation is to start from the definition of a response function and compare numerical experiments with this definition and its theoretical consequences. Therefore, first the considered response problem is specified and a numerical method to compute dynamical response functions is developed (Sec. II). (Without further proof a short account of this method has already been given in Ref. [24].) In the following sections, the various aspects of a linear response are considered: the linearity itself (Sec. III), the quadratic response at twice the perturbation frequency (Sec. IV), the Kramers-Kronig relations (Sec. V), relations between different response functions (Sec. VI), and finally the vanishing of the linear response in particular observables due to the symmetry of the Lorenz system (Sec. VII). Additional, especially technical aspects are discussed in the appendices.

II. DEFINITIONS AND NUMERICAL PROCEDURE

In the following the response of the Lorenz system to time dependent perturbations of its control parameter r is studied. This system is given by

$$\dot{x}=\sigma(y-x),$$
$$\dot{y}=[r+\epsilon(t)]x-y-xz, \tag{2.1}$$
$$\dot{z}=xy-bz.$$

As Lorenz [12] we take $\sigma=10$, $b=8/3$, and $r=28$ [25]. The perturbation $\epsilon(t)$ of r will be specified below. At these parameters the Lorenz system is known to be chaotic and also nonhyperbolic: any finite change of r results in sequences of homoclinic bifurcations by which the topology of the chaotic attractor is changed [13]. The response to the perturbation is investigated by studying the behavior of an observable $A(\mathbf{x})$, which will be taken as x,z, or x^2.

In Kubo-type response theories, to which Ruelle's approach also belongs, response functions $\chi_A(\tau)$, also called "susceptibility," are defined by

$$\langle\langle \delta A(t)\rangle\rangle=\int_{-\infty}^{t} ds\, \chi_A(t-s)\epsilon(s)+O(\epsilon^2), \tag{2.2}$$

where $\langle\langle \delta A(t)\rangle\rangle$ is an ensemble average defined by

$$\langle\langle \delta A(t)\rangle\rangle=\int d\mathbf{x}\, \delta A(t)\rho_0(\mathbf{x}), \tag{2.3}$$

with $\delta A(t)$ being the deviation from the ensemble average $\langle\langle A\rangle\rangle$ in the unperturbed system,

$$\delta A(t)=A(\mathbf{\Phi}_\epsilon(t,t_0;\mathbf{x}))-\langle\langle A\rangle\rangle. \tag{2.4}$$

Here $\mathbf{\Phi}_\epsilon(t,t_0;\mathbf{x})$ denotes the flow of the perturbed system, i.e., the flow of Eq. (2.1), with the initial condition $\mathbf{\Phi}_\epsilon(t_0,t_0;\mathbf{x})=\mathbf{x}$. The initial density $\rho_0(\mathbf{x})$ is chosen here as the invariant density ρ_0 of the unperturbed system, i.e., for $t<t_0$ it is assumed $\epsilon(t)=0$. Alternatively, one could take an initial density different from ρ_0. Thereby one could study relaxation phenomena, but this is not intended here. The upper limit t of the integral in Eq. (2.2) expresses causality: the response at time t is determined only by perturbations from the past. Accordingly, one can set

$$\chi_A(\tau)=0 \quad \text{for} \quad \tau<0 \tag{2.5}$$

and extend the integral to infinity. It should be noted that by Eq. (2.3) a linear relationship between $\epsilon()$ and $\langle\langle \delta A()\rangle\rangle$ is claimed, but whether such a relationship exists is *a priori* not clear and will depend on the considered system, the type of perturbation $\epsilon()$ and also the chosen observable $A()$.

In order to verify numerically the validity of Eq. (2.2) for a particular system one has to specify the perturbation $\epsilon(t)$. For example, one could take $\epsilon(t)=\epsilon\delta(t-t_0)$, where $\delta()$ is the Dirac delta function. This gives $\chi_A(\tau)=\epsilon^{-1}\langle\langle\delta A(t_0+\tau)\rangle\rangle$. So χ_A could be computed by studying the time development of A after the pulse at t_0 for an ensemble of starting points from the chaotic attractor. This was done in Ref. [17] for the Lorenz system and other systems.

Such a singular perturbation is equivalent to a change in the initial conditions. So using this procedure the susceptibility is computed by starting with a nonequilibrium ensemble and following the subsequent relaxation of the *unperturbed* system. But in view of the problem of nonhyperbolicity the present investigation is concerned with the question, whether the reaction of a system to real *deformations* can be described in terms of a susceptibility. So here persisting perturbations, which change the system and not only the initial conditions, will be considered. To this end the perturbation is chosen as

$$\epsilon(t)=\epsilon\Theta(t)\cos(\Omega t), \tag{2.6}$$

where $\Theta(t)$ is the unit step function so that implicitely $t_0=0$ has been chosen.

This perturbation allows, if χ exists, a very simple procedure to compute numerically the dynamic susceptibility

$$\chi_A(\omega)=\int_{-\infty}^{\infty}d\tau e^{i\omega\tau}\chi_A(\tau), \tag{2.7}$$

the Fourier transform of $\chi_A(\tau)$. Under mild assumptions one can show (see Appendix A) that for the perturbation (2.6) $\chi_A(\omega)$ is given by

$$\chi_A(\Omega)=\lim_{\epsilon\to 0}\frac{2}{\epsilon}\lim_{T\to\infty}\frac{1}{T}\int_0^T dte^{i\Omega t}\delta A(t)=2\lim_{\epsilon\to 0}\frac{1}{\epsilon}\langle e^{i\Omega t}\delta A(t)\rangle, \tag{2.8}$$

where the single angular brackets $\langle\cdots\rangle$ denote the temporal mean (in contrast to the double angular brackets introduced before, which denote the ensemble mean). This is the basic formula used in the following numerical investigation. It states that to compute $\chi_A(\omega=\Omega)$ one has to perturb the considered system by Eq. (2.6) at the very frequency $\omega=\Omega$, compute a time series $\{\delta A(t)\}_t$ from it, and evaluate the right-hand side of Eq. (2.8). To get χ_A as a function of ω one has to repeat this for different driving frequencies $\omega=\Omega$. The linearity of the response is reflected in Eq. (2.8) by the fact that the limit $T\to\infty$ on the right-hand side should be proportional to ϵ in order for $\chi_A(\omega)$ to be independent of ϵ. [The factor 2 arises in Eq. (2.8) because a cosine has been chosen for the perturbation instead of a complex exponential.]

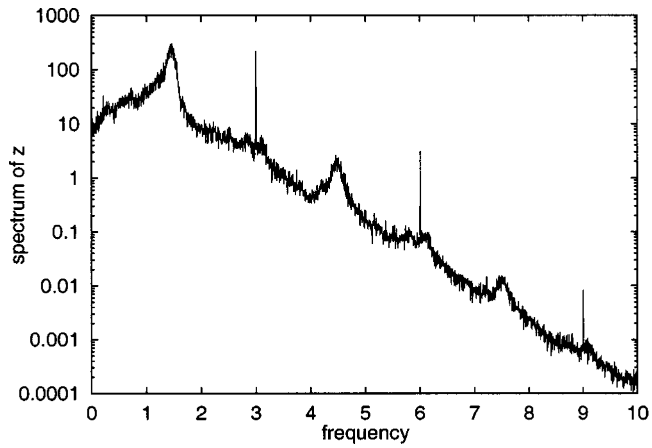

FIG. 1. Autocorrelation spectrum of the observable z for the strongly perturbed Lorenz system ($\epsilon=5.0, f=3$).

Actually, Eq. (2.8) will be computed for finite time T and finite perturbation strength ϵ only. So it is important to see how the right-hand side without limits behaves as a function of T and ϵ. Let

$$\chi_A^T(\Omega)=\frac{2}{\epsilon T}\int_0^T dte^{i\Omega t}\delta A(t) \tag{2.9}$$

denote the finite time approximation of $\chi_A(\Omega)$. Now it is assumed that the time series $\{\delta A(t)\}_t$ consists of two parts: a periodic part resulting from the periodic perturbation, and a chaotic part $a(t)$. Such a decomposition is suggested by a glance at the spectra of the perturbed system. As an example in Fig. 1 the autocorrelation spectrum of z is shown for the Lorenz system perturbed at frequency $f=\Omega/2\pi=3$ [26]. Clearly visible is a continuous part with superimposed δ peaks at harmonics $\omega=n\Omega$. This decomposition in a chaotic part and a periodic part gives for sufficiently large T and sufficiently small ϵ,

$$\chi_A^T(\Omega)\approx\frac{a(\Omega)}{\epsilon T}+\chi_A^*(\Omega)e^{i\Omega T}\frac{\sin\Omega T}{\Omega T}+\chi_A(\Omega) \tag{2.10}$$

(see Appendix B). So the condition to obtain accurate numerical results for $\chi_A(\Omega)$ is

$$\epsilon\Omega T\gg 1 \tag{2.11}$$

because then the first and second term are negligible.

III. LINEARITY OF RESPONSE IN $A(\mathbf{x})=z$

In this section the linearity of the response is demonstrated for the observable $A(\mathbf{x})=z$ by direct evaluation of Eq. (2.8). Results of such computations are plotted in Fig. 2. The upper part shows the modulus $|\chi_z^T(\omega)|$ of the finite time approximation χ_z^T for driving frequency $f=\Omega/2\pi=20$ and $T=1000$ as a function of ϵ. For small ϵ the $1/\epsilon$ decrease predicted by Eq. (2.10) is present; it stems from the chaotic background in the time series of $\delta z(t)$. The true value of $|\chi_z(\omega)|$ is reached at $\epsilon\approx 10^{-3}$, where the value of $|\chi_z^T(\omega)|$

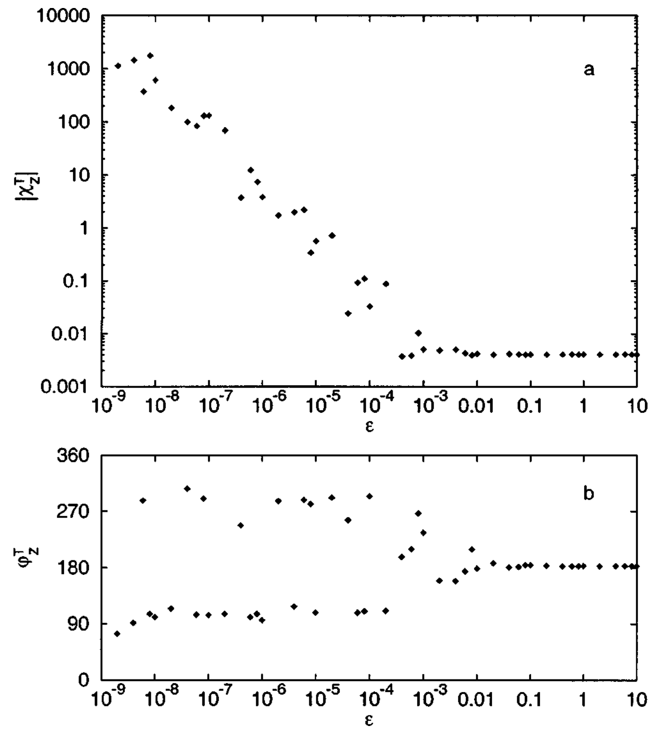

FIG. 2. ϵ dependence of $\chi_z^T = |\chi_z^T| e^{-i\varphi_z^T}$ for $f=20.0$ and $T=1000$. (a) Modulus $|\chi_z^T|$; (b) phase φ_z.

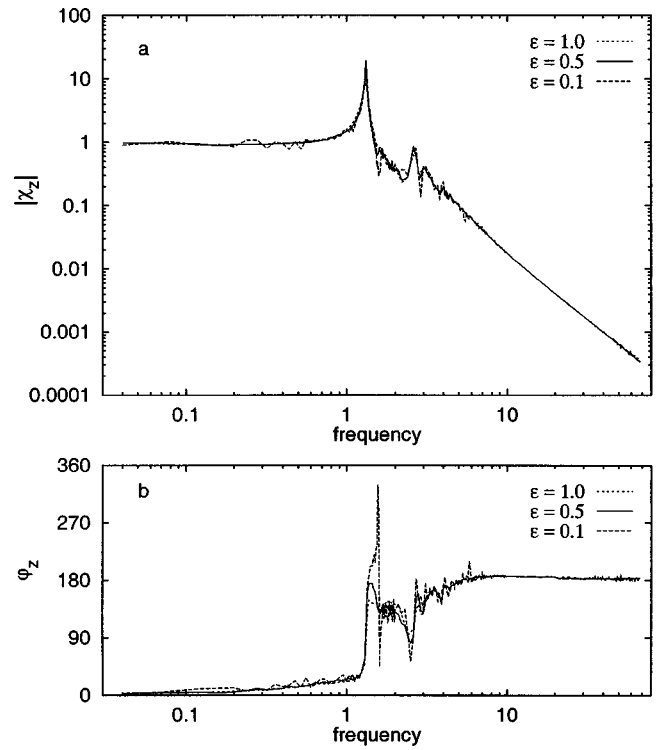

FIG. 3. The response function $\chi_z = |\chi_z| e^{-i\varphi_z}$. To indicate the numerical accuracy the computations from three different ϵ values are shown ($T=4000$). (a) Modulus; (b) phase. (a) is reprinted from [24] with permission from Elsevier.

gets independent of ϵ. Similar computations have been performed for other frequencies and always a plateau in $|\chi_z^T(\omega)|$ could be identified [27]. Computations of the phase φ_z of $\chi_z = |\chi_z| e^{-i\varphi_z}$ give also reliable results [Fig. 2(b)] [28]. These results indicate that the response in z is indeed linear and the response function $\chi_z(\omega)$ exists.

Putting together results from similar computations at other forcing frequencies Ω gives the response function $\chi_z(\omega)$, plotted in Fig. 3 for the range of frequencies $f=0.004$ to $f=68.0$. In the upper part of the figure once more the modulus is shown, whereas the lower part depicts the phase $\varphi_z(\omega)$. In order to indicate the reliability of the results, computations for different values of ϵ have been superimposed.

The behavior of $\chi_z(\omega)$ at low and high frequency is very regular. It is found $\lim_{\omega\to 0}\chi_z(\omega)\approx 1$ and $\lim_{\omega\to\infty}|\chi_z(\omega)| \sim \omega^{-2}$; the latter result can also be obtained from a Kubo-type theory by a moment expansion of $\chi_z(\omega)$ (see Ref. [24]). In the intermediate frequency range the response function shows typical resonance behavior.

IV. QUADRATIC RESPONSE AT 2Ω

Another important feature of linear response can be checked numerically. A Fourier transform of the defining relation (2.2) gives $\langle\langle \delta A(\omega)\rangle\rangle = \chi_A(\omega)\epsilon(\omega) + O(\epsilon^2)$. If one now specializes to a periodic perturbation at frequency $\omega=\Omega$, one sees that the definition (2.2) assumes a response only at that very driving frequency Ω. But usually (compare Fig. 1) a response is also observed at harmonics of Ω. So in order for the relation (2.2) to be valid, this response at harmonics should be at least of order ϵ^2. This has been checked numerically by computing

$$\Psi_A(\Omega) = \lim_{\epsilon\to 0}\frac{2}{\epsilon^2}\lim_{T\to\infty}\frac{1}{T}\int_0^T dt e^{i2\Omega t}\delta A(t)$$

$$= 2\lim_{\epsilon\to 0}\frac{1}{\epsilon^2}\langle e^{2i\Omega t}\delta A(t)\rangle. \qquad (4.1)$$

This relation defines in analogy to Eq. (2.8) a response function that describes in order ϵ^2 the response at 2Ω to a perturbation at frequency Ω. The results for the observable $A(\mathbf{x})=z$ at driving frequency $f=20$ and finite T are displayed for different ϵ in Fig. 4. For small ϵ the usual drop off is seen. This is followed by a plateau where $|\Psi_z(\Omega)|$ is independent of ϵ. This shows that indeed the response at two times the driving frequency is proportional to ϵ^2. So once more agreement with the definition (2.2) is found.

V. KRAMERS-KRONIG RELATIONS

Another implication of the definition (2.2) is the Kramers-Kronig relations. Let χ_A' and χ_A'' denote the real and imaginary part of χ_A. Then one can derive from Eq. (2.2) together with the assumed causality of χ_A the Kramers-Kronig relations [2]

$$\chi_A'(\Omega) = +\frac{1}{\pi}P\int_{-\infty}^{\infty} d\omega \frac{\chi_A''(\omega)}{\omega-\Omega}, \qquad (5.1)$$

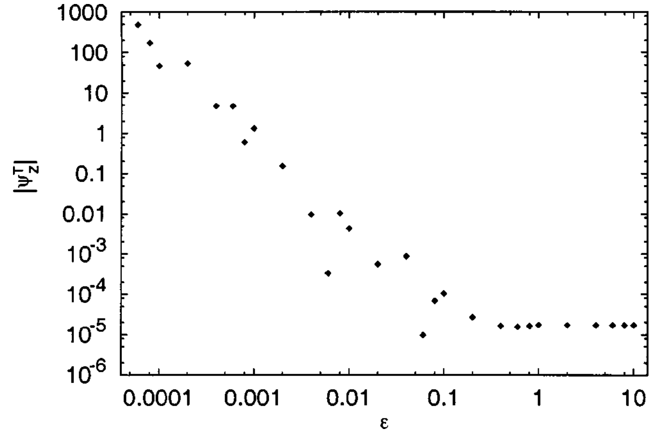

FIG. 4. Quadratic response at the first harmonic. Shown is $|\Psi_z^T|$. The system is perturbed at frequency $f=10.0$ but the response is observed at frequency $2f=20.0$. ($T=400$).

$$\chi_A''(\Omega)=-\frac{1}{\pi}P\int_{-\infty}^{\infty}d\omega\frac{\chi_A'(\omega)}{\omega-\Omega}. \tag{5.2}$$

Here P indicates that the principle value of the integral has to be taken. Figure 5(a) [Fig. 5(b)] compares the direct result for χ_z' [χ_z''] on the left-hand side of Eq. (5.1) [Eq. (5.2)] with its computation through χ_z'' [χ_z'] on the right-hand side, where the integrals have been evaluated by the trapezoidal rule. The curves are in good agreement. This verifies another important signature of response functions, namely, their causality. It should be noted that numerically the response function $\chi_z(\omega)$ considered here is obtained from a large number of independent numerical experiments at different frequencies.

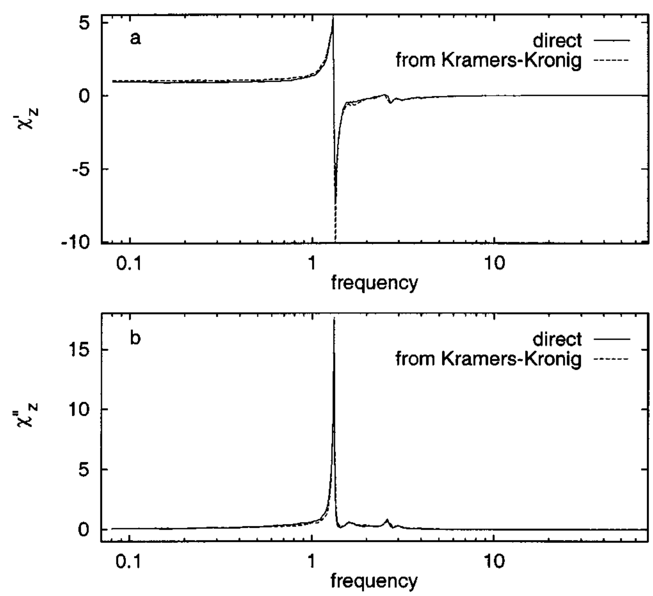

FIG. 5. Check of the Kramers-Kronig relations for the response function $\chi_z=\chi_z'+i\chi_z''$ ($\epsilon=0.5,T=4000$). (a) Comparison of direct numerical data for χ_z' with a computation of χ_z' through χ_z'' by the first Kramers-Kronig relation. (b) Analogous computations for χ_z''.

Hence, the confirmed causality is a gross feature of $\chi_z(\omega)$ and not a consequence of the individual experiments. Therefore the good agreements in Fig. 5 also indicate the validity and accuracy of the employed numerical method by which $\chi_z(\omega)$ was computed.

VI. RELATIONS BETWEEN RESPONSE FUNCTIONS

From Eq. (2.8) one can derive a general relation between the response functions $\chi_A(\Omega)$ and $\chi_{\dot{A}}(\Omega)$, where $\dot{A}(t)=(d/dt)A[\Phi_\epsilon(t,t_0;\mathbf{x})]$,

$$\begin{aligned}\chi_{\dot{A}}(\Omega)&=\lim_{\epsilon\to0}\frac{2}{\epsilon}\lim_{T\to\infty}\frac{1}{T}\int_0^T dte^{i\Omega t}\frac{d}{dt}\delta A(t)\\&=\lim_{\epsilon\to0}\frac{2}{\epsilon}\lim_{T\to\infty}\frac{(-i\Omega)}{T}\int_0^T dte^{i\Omega t}\delta A(t)\\&=-i\Omega\chi_A(\Omega),\end{aligned} \tag{6.1}$$

where it has been assumed that for physically relevant states $A(t)$ is bounded so that the border terms of the partial integration vanish. This relationship is also obtained by a Kubo-type theory (see Appendix D.) Considering for the Lorenz system the observables $A(\mathbf{x})=z$ and $A(\mathbf{x})=x^2$, one obtains from Eq. (6.1) by invoking the first and third equation of Eq. (2.1)

$$\begin{aligned}-i\Omega\chi_{x^2}(\Omega)&=\chi_{\dot{x}^2}(\Omega)=2\sigma[\chi_{xy}(\Omega)-\chi_{x^2}(\Omega)],\\-i\Omega\chi_z(\Omega)&=\chi_{\dot{z}}(\Omega)=\chi_{xy}(\Omega)-b\chi_z(\Omega),\end{aligned} \tag{6.2}$$

so that after the elimination of χ_{xy} one finds that the response in x^2 is completely determined by the response in z,

$$\chi_{x^2}(\Omega)=2\sigma\frac{b-i\Omega}{2\sigma-i\Omega}\chi_z(\Omega). \tag{6.3}$$

Numerically this relation is confirmed in Fig. 6 by comparing χ_{x^2}, computed directly from the perturbed Lorenz system, with χ_{x^2}, computed by Eq. (6.3) from χ_z. A host of other relations between response functions can be derived from Eq. (6.1), as shown in Appendix C.

VII. VANISHING RESPONSE IN $A(x)=x$

For the Lorenz system another implication of Eq. (2.2) is the vanishing of the linear response in the observable $A(\mathbf{x})=x$. This can be seen as follows.

The Lorenz system is invariant under the transformation $S(x,y,z)=(-x,-y,z)$. Accordingly, a mapping $h(\mathbf{x})$ will be called symmetric if $h\circ S=h$ and antisymmetric if $h\circ S=-h$. At standard parameters the attractor of the Lorenz system has the same symmetry as the system itself [13] so that time and ensemble averages of antisymmetric observables vanish. The perturbation $\epsilon(t)$ in the perturbed Lorenz system (2.1) conserves the symmetry so that one can expect that also for small but finite ϵ time averages of antisymmetric observ-

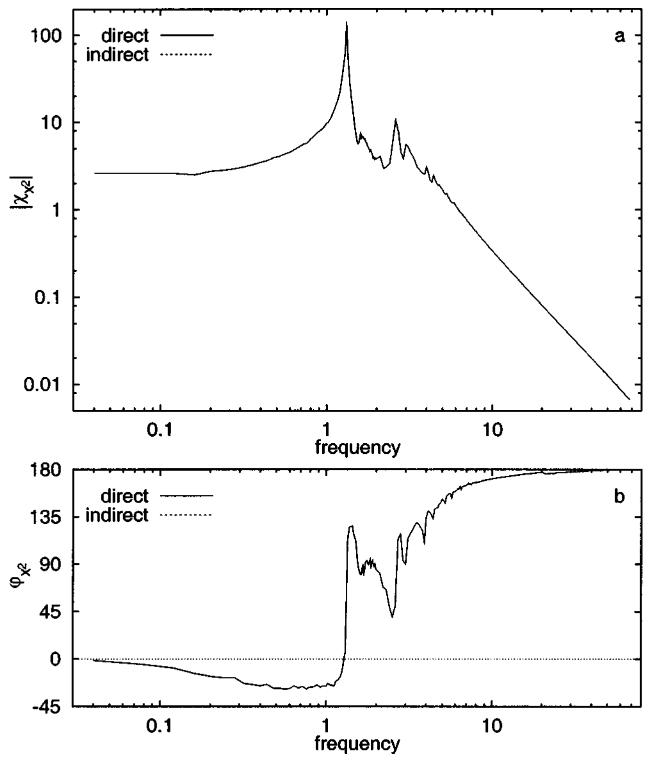

FIG. 6. The susceptibility $\chi_{x^2}=|\chi_{x^2}|e^{-i\varphi_{x^2}}$, computed directly from Eq. (2.8) and indirectly from χ_z via Eq. (6.3). Differences are so small that they are invisible in the plot ($\epsilon=0.5,T=4000$). (a) Modulus; (b) phase.

ables vanish. With this observation a time average of the second equation in Eq. (2.1) gives

$$\langle\cos(\Omega t)x\rangle_\epsilon=0, \tag{7.1}$$

where an index ϵ has been attached to the angular bracket to stress that it denotes a time average over the perturbed dynamics. Now, since $\langle x\rangle_0=0$, the response function related to $A(\mathbf{x})=x$ is according to Eq. (2.8) given by

$$\chi_x(\Omega)=\lim_{\epsilon\to 0}\frac{2}{\epsilon}\langle e^{i\Omega t}x\rangle_\epsilon, \tag{7.2}$$

so that with Eq. (7.1) the real part of $\chi_x(\Omega)$ vanishes. But according to the second of the Kramers-Kronig relations (5.1) this implies that also the imaginary part is zero so that

$$\chi_x(\Omega)=0. \tag{7.3}$$

This result can also be derived from a Kubo-type theory; see Appendix D.

A numerical analysis confirms this expectation: Figure 7 shows the dependence of χ_x^T at frequency $f=20$ on ϵ. The curve shows the typical $1/\epsilon$ behavior always present for finite T. For large values of ϵ the data seem to saturate at a very small level, but two orders below the plateau found for the response in $A(\mathbf{x})=z$ (compare Fig. 2). In contrast to the case of the response in z, the plateau here is strongly fluctuating.

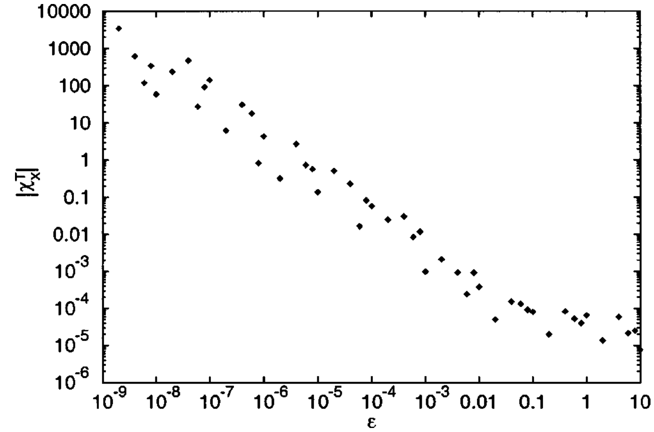

FIG. 7. ϵ dependence of $|\chi_x^T|$ for $f=20.0$ ($T=1000$).

Such a fluctuating plateau is in accordance with a vanishing susceptibility: it can be explained by an additional contribution to Eq. (2.10), which arises from fluctuations in the height of the periodic component of the system, always present for finite length T of the time series (see Appendix B). Moreover, this plateau seems not to stabilize, even for very long time series. All these findings indicate that $\chi_x(\omega)$ is indeed zero. The same conclusion can be drawn from Fig. 8, where the autocorrelation spectrum of the observable x in the presence of strong perturbations is shown. Although the spectrum is deformed as compared to the unperturbed case (not shown), no δ peaks at f or its harmonics are present, but such peaks would be expected for a linear response. A numerical analysis for the observable $A(\mathbf{x})=y$, whose response should also vanish [use the first of Eqs. (2.1)], gives similar results.

VIII. DISCUSSION

The foregoing considerations have shown that for the Lorenz system at standard parameters the various implications of the definition (2.2) of a response function are consistent with numerical results. Accordingly, there is strong evidence

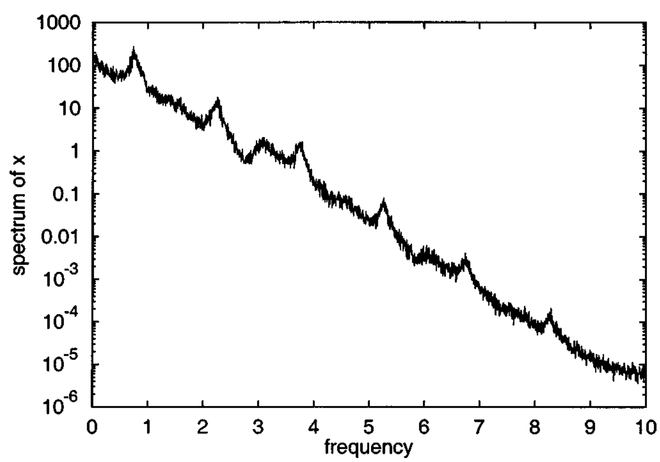

FIG. 8. Autocorrelation spectrum of the observable x for the strongly perturbed Lorenz system ($\epsilon=5.0,f=3.0$).

that for the Lorenz system a linear response exists. This is insofar interesting, as Ruelle's rigorous foundation of linear response theory applies only to hyperbolic systems. So, according to the numerical results presented here, the Lorenz system provides an example where despite nonhyperbolicity a linear response exists.

But why this linear response exists is currently not understood. Nevertheless, it is clear that its existence is related to the nature of the bifurcations that arise from the perturbation, because one can easily think of bifurcations that prevent a linear response. In the present case changes of the control parameter induce homoclinic bifurcations that newly introduce or destroy unstable periodic orbits [13]. One could speculate that (for some unknown reason) the effect of these bifurcations on the differentiability of the invariant measure with respect to the perturbation parameter is exactly zero. But it could also be that the differentiability is only approximate. This might happen if the newly created or just destroyed orbits are much longer than the decorrelation time of the chaotic dynamics. In that case the contribution of these orbits to the invariant measure would be negligible, so that in any practical sense these topological changes would not affect the invariant measure and it remains differentiable. It would be interesting to check this idea numerically.

Previous studies of the linear response of chaotic systems considered the response in the time domain. Instead, in the present study the response was analyzed in the frequency domain. This was made possible by showing that dynamic response functions $\chi_A(\omega)$, originally defined by ensemble averages, can as well be obtained from particular time averages of the system periodically perturbed at that very frequency $\Omega=\omega$ [see Eqs. (2.2) and (2.8)]. This relationship is of quite general nature. Its derivation was based mainly on the physically plausible assumption that response functions have a finite decay time. Moreover, in Appendix D it has been shown that under this assumption several implications of this time series approach to linear response can as well be obtained by a Kubo-type theory so that it is in various aspects equivalent to a Kubo formalism.

In principle, from the computed response function χ_z, shown in Fig. 3, Ruelle's prediction, that for dissipative systems no fluctuation-dissipation relationship exists [3,4], could be checked: If a fluctuation-dissipation relationship holds, then response functions $\chi_A(\tau)$ could be represented as $\chi(\tau)=\Theta(\tau)C(\tau)$, where $C(\tau)$ is a correlation function. In that case the dynamic susceptibility $\chi(\omega)$ would have in the lower complex plane the same poles as the spectral function $C(\omega)$. But since the poles of the latter are identical to the resonances of the considered system, the poles of $\chi(\omega)$ would then also represent resonances. Hence, to disprove the existence of a fluctuation-dissipation relationship, it would be sufficient to show that $\chi(\omega)$ contains poles outside the set of resonances. Since the first few resonances of the Lorenz system are known from a periodic orbit analysis by Eckhardt and Ott [29], such a comparison should in principle be possible here by locating the poles of the numerically known susceptibility $\chi_z(\omega)$. I tried this by computing Padé approximants to $\chi_z(\omega)$. Some of the poles obtained in this way approximately reproduced the resonances from Eckhardt and Ott. But unfortunately the locations of the other poles could not be trusted, since they turned out to vary erratically with the order of the approximants. Hence it could not be decided whether $\chi_z(\omega)$ shows poles outside the spectrum of resonances. This "noisy" behavior of the poles is probably a result of the extremely peaked nature of $\chi_z(\omega)$ (in Fig. 3 this is obscured by the logarithmic plotting) that arises mainly from the first few resonances so that the contribution of other poles cannot be resolved.

Finally it should be noted that the Lorenz equations describe in a certain approximation the dynamics of NH_3 lasers [30,31]. Hence, similar computations of χ_{x^2} as those presented here, but for somewhat different system parameters, could predict the intensity response to pump-parameter perturbations.

APPENDIX A

In this appendix the basic relation (2.8) is derived on the basis of three assumptions: First, it is assumed that $\chi(\omega)$ is meromorphic in the lower complex plane without poles at infinity. This assumption is reasonable because then the usual physical interpretation of $\chi(\omega)$ is possible: Poles of $\chi(\omega)$ represent resonances. Second, it is assumed that the response functions decay with finite memory so that all poles lie off the real axis. And finally it is assumed that the time series $\{e^{i\Omega t}\delta A(t)\}_t$ is ergodic, so that

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\, e^{i\Omega t}\langle\langle\delta A(t)\rangle\rangle=\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\, e^{i\Omega t}\delta A(t)$$
$$=\langle e^{i\Omega t}\delta A(t)\rangle. \tag{A1}$$

Equation (2.8) can now be derived as follows. With Eq. (A1) one gets from the definition (2.2) with the periodic perturbation (2.6)

$$\langle e^{i\Omega t}\delta A(t)\rangle=\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\, e^{i\Omega t}$$
$$\times\int_{-\infty}^{\infty} ds\, \chi_A(t-s)\epsilon\Theta(s)\cos(\Omega s). \tag{A2}$$

It is convenient to introduce the following representation for the unit-step function $\Theta(t)$:

$$\Theta(t)=\lim_{\kappa\to 0}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}\frac{i}{\omega+i\kappa},\quad \kappa>0. \tag{A3}$$

This, together with the Fourier representation $\chi_A(\tau)=\int(d\omega/2\pi)e^{-i\omega\tau}\chi(\omega)$, gives

$$\langle e^{i\Omega t}\delta A(t)\rangle = \lim_{T\to\infty}\lim_{\kappa\to 0}\frac{\epsilon}{(2\pi)^2 T}\int_{-\infty}^{\infty}d\omega\chi(\omega)\int_{-\infty}^{\infty}d\omega'\frac{i}{\omega'+i\kappa}\int_0^T dt e^{i(\Omega-\omega)t}\int_{-\infty}^{\infty}ds e^{i(\omega-\omega')s}\cos\Omega s$$
$$=\lim_{T\to\infty}\lim_{\kappa\to 0}\frac{\epsilon}{2(2\pi)T}\int_{-\infty}^{\infty}d\omega\chi(\omega)\int_{-\infty}^{\infty}d\omega'\frac{i}{\omega'+i\kappa}\,\frac{e^{i(\Omega-\omega)T}-1}{i(\Omega-\omega)}[\delta(\omega-\omega'+\Omega)+\delta(\omega-\omega'-\Omega)]$$
$$=\lim_{T\to\infty}\lim_{\kappa\to 0}\frac{\epsilon}{2(2\pi)}\int_{-\infty}^{\infty}d\omega\chi(\omega)\exp\left(-i(\omega-\Omega)\frac{T}{2}\right)\frac{\sin\left((\omega-\Omega)\frac{T}{2}\right)}{(\omega-\Omega)\frac{T}{2}}\left[\frac{i}{\omega-\Omega+i\kappa}+\frac{i}{\omega+\Omega+i\kappa}\right]. \quad \text{(A4)}$$

Because $\chi(\omega)$ is assumed to be meromorphic without poles at infinity $\chi(\omega)$ is finite on the infinite demicircle in the lower complex plane,

$$\lim_{R\to\infty}|\chi(Re^{i\varphi})|<M, \qquad \varphi\in[\pi,2\pi]. \quad \text{(A5)}$$

This allows one to show by some simple estimates that the last integral in Eq. (A4), evaluated over the infinite demicircle in the negative complex plane, vanishes so that the integral in Eq. (A4) can be extended by the infinite demicircle to the closed loop Γ around the negative complex plane. Once more, using that $\chi(\omega)$ is meromorphic in the lower complex plane, i.e., the only singularities in that part of the plane are poles, one is now able to evaluate Eq. (A4) by the method of residues. Let ω_k denote the locations of the poles of $\chi(\omega)$ and r_k their respective residues. Then one has

$$\langle e^{i\Omega t}\delta A(t)\rangle = \lim_{T\to\infty}\lim_{\kappa\to 0}\frac{\epsilon}{2(2\pi)}\oint_\Gamma d\omega\chi(\omega)\exp\left(-i(\omega-\Omega)\frac{T}{2}\right)\frac{\sin\left((\omega-\Omega)\frac{T}{2}\right)}{(\omega-\Omega)\frac{T}{2}}\left[\frac{i}{\omega-\Omega+i\kappa}+\frac{i}{\omega+\Omega+i\kappa}\right]$$
$$=\frac{\epsilon}{2}\lim_{T\to\infty}\left\{\chi(\Omega)+\chi(-\Omega)e^{i\Omega T}\frac{\sin\Omega T}{\Omega T}+\sum_{k=0}^{\infty}r_k\exp\left(-i(\omega_k-\Omega)\frac{T}{2}\right)\frac{\sin(\omega_k-\Omega)\frac{T}{2}}{(\omega_k-\Omega)\frac{T}{2}}\left[\frac{1}{\omega_k-\Omega}+\frac{1}{\omega_k+\Omega}\right]\right\}$$
$$=\frac{\epsilon}{2}\chi(\Omega), \quad \text{(A6)}$$

where in the last line the assumption that all poles ω_k lie off the real axis was used. Besides a missing limit $\epsilon\to 0$, which should be inserted into Eq. (A6) to stress the fact that mathematically χ_A is only defined in this limit, this is the desired relationship (2.8).

APPENDIX B

In this appendix the effect of a finite integration time T on the accuracy of the numerical computation of $\chi_A(\Omega)$ by Eq. (2.8) is discussed; especially Eq. (2.10) will be derived.

As discussed in Sec. II it is assumed that the time series $\delta A(t)$ consists of two parts, a chaotic part $a(t)$ and a periodic part oscillating at driving frequency Ω and its harmonics $n\Omega$,

$$\delta A(t)=a(t)+\sum_{n=1}^{\infty}b_n\cos(n\Omega t-\phi_n). \quad \text{(B1)}$$

In order to specify $a(t)$ as chaotic, assume that its Fourier transform is continous. Then

$$\frac{1}{T}\int_0^T dt\, e^{i\Omega t}a(t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}d\omega\, a(\omega)\exp\left(i(\Omega-\omega)\frac{T}{2}\right)\times\frac{\sin(\Omega-\omega)\frac{T}{2}}{(\Omega-\omega)\frac{T}{2}}\approx\frac{a(\Omega)}{2T}, \quad \text{(B2)}$$

where in the last step use has been made of the fact that $\sin[(\Omega-\omega)T/2]/[(\Omega-\omega)T/2]$ is heavily peaked at $\omega=\Omega$ for sufficiently large T, and thus the continous function $a(\omega)$ is mainly evaluated around $\omega=\Omega$ and can be drawn before the integral.

Together with similar computations for the periodic part one obtains with Eq. (2.9),

$$\chi_A^T(\Omega)=\frac{a(\Omega)}{\epsilon T}+\chi_A^*(\Omega)e^{i\Omega T}\frac{\sin\Omega T}{\Omega T}+\chi_A(\Omega)+\frac{1}{\epsilon}\sum_{n=2}^{\infty}b_n\left[e^{-i\phi_n}\exp\left(i(n+1)\Omega\frac{T}{2}\right)\frac{\sin(n+1)\Omega\frac{T}{2}}{(n+1)\Omega\frac{T}{2}}+e^{i\phi_n}\exp\left(-i(n-1)\Omega\frac{T}{2}\right)\frac{\sin(n-1)\Omega\frac{T}{2}}{(n-1)\Omega\frac{T}{2}}\right], \tag{B3}$$

where the identity $b_1e^{i\phi_1}=\epsilon\chi_A(\Omega)$ has been used, which can be verified from the limit $T\to\infty$. To obtain χ_A numerically for finite T all other terms in Eq. (B3) have to be small. This is the case for the first term if ϵT is sufficiently large and the second term is negligible if $\Omega T\gg 1$. The terms in the infinite sum are small if $\epsilon\Omega T\gg 1$. (Actually numerical computations show that $b_n\sim\epsilon^2$ for $n>1$ (as expected in linear response theory) so that the sum is negligible if the much weaker condition $\Omega T/\epsilon\gg 1$ is fulfilled.) Since one is interested here only in the case $\epsilon\ll 1$, these conditions can be condensed to $\epsilon\Omega T\gg 1$, as claimed in Eq. (2.11).

To explain the fluctuating plateau observed in the response in x (see Fig. 7) one has to go a step further. In computations of spectra of time series of periodically perturbed chaotic systems one observes that the height of the periodic peaks depends on the particular interval of the infinite time series used to compute the spectrum. So the amplitude of the periodic contribution in Eq. (B1) is not a constant but may depend on time. For simplicity we neglect harmonics and concentrate on the fundamental frequency Ω only. Accordingly, assume that in addition to b_1 there is a time dependent chaotic contribution $c_1(t)$ (with zero mean) modulating the periodic part around b_1. So Eq. (B1) assumes the form

$$\delta A(t)=a(t)+[b_1+c_1(t)]\cos(\Omega t-\phi_1). \tag{B4}$$

The same procedure as above gives

$$\frac{1}{T}\int_0^T dt\, e^{i\Omega t}c_1(t)\cos(\Omega t-\phi_1)\approx\frac{1}{4T}c_1(\omega=-2\Omega)e^{-i\phi_1} \tag{B5}$$

[where $c_1(\omega=0)=0$ was used]. So one gets another contribution to Eq. (B3),

$$\frac{1}{\epsilon T}c_1(2\Omega)e^{-i\phi_1}. \tag{B6}$$

Assuming $c_1(t)$ to be proportional to ϵ, because it is a result of the external perturbation, this contribution is independent of ϵ but vanishes for $T\to\infty$. So if the response function χ_A vanishes, this contribution produces in a plot of χ_A^T against ϵ (like in Fig. 7) a plateau around which the fluctuations of different runs can be seen.

APPENDIX C

From Eq. (6.1) a host of relations between response functions can be derived. Consider for the Lorenz system observables of type

$$A(\mathbf{x})=x^ky^lz^m,\quad k,l,m\in\mathbb{N}. \tag{C1}$$

Related response functions will be denoted by $\chi_{k,l,m}(\Omega)$ and for shortness the dependence on Ω is omitted. From Eqs. (6.1), (2.8), and (2.1) one obtains

$$\begin{aligned}-i\Omega\chi_{k,l,m}&=\lim_{\epsilon\to 0}\frac{2}{\epsilon}\left\langle e^{i\Omega t}\left(\frac{d}{dt}(x^ky^lz^m)-\left\langle\frac{d}{dt}(x^ky^lz^m)\right\rangle_0\right)\right\rangle_\epsilon\\&=k\sigma\chi_{k-1,l+1,m}-(k\sigma+l+bm)\chi_{k,l,m}\\&\quad+lr\chi_{k+1,l-1,m}-l\chi_{k+1,l-1,m+1}+m\chi_{k+1,l+1,m-1}\\&\quad+2l\lim_{\epsilon\to 0}\langle e^{i\Omega t}\cos(\Omega t)x^{k+1}y^{l-1}z^m\rangle_\epsilon\end{aligned} \tag{C2}$$

because $\langle\dot{A}\rangle_0=0$ for bounded $A(\mathbf{x})$. Moreover,

$$2\lim_{\epsilon\to 0}\langle e^{i\Omega t}\cos(\Omega t)x^{k+1}y^{l-1}z^m\rangle_\epsilon=\langle x^{k+1}y^{l-1}z^m\rangle_0, \tag{C3}$$

because, in analogy to the considerations of Sec. IV, $\langle e^{2i\Omega t}x^{k+1}y^{l-1}z^m\rangle\sim\epsilon^2$. Entering these results into Eq. (C2) one finally obtains

$$\begin{aligned}(k\sigma+l+bm-i\Omega)\chi_{k,l,m}&=k\sigma\chi_{k-1,l+1,m}+lr\chi_{k+1,l-1,m}+m\chi_{k+1,l+1,m-1}\\&\quad-l\chi_{k+1,l-1,m+1}+l\langle x^{k+1}y^{l-1}z^m\rangle_0.\end{aligned} \tag{C4}$$

Relations (6.2) are special cases of this result for $(k,l,m)=(0,0,1)$ and $(k,l,m)=(2,0,0)$.

APPENDIX D

Equation (6.1), from which the relations (6.2) and (6.3) between the response functions were derived, and also the vanishing of the linear response in $A(\mathbf{x})=x$ (see Sec. VII) have so far been derived from the time series representation (2.8) of response functions. In this appendix it is shown that a more standard approach by a Kubo-type theory as presented in [4,24] leads to the same results.

Consider a perturbed dynamical system

$$\dot{\mathbf{x}}=\mathbf{F}_0(\mathbf{x})+\epsilon(t)\mathbf{F}_1(\mathbf{x}) \tag{D1}$$

with $\epsilon(t)=0$ for $t<0$. Then the related Liouville equation for the nonequilibrium density $\rho(\mathbf{x},t)$ reads

$$i\frac{\partial\rho}{\partial t}=\mathcal{L}_0\rho+\epsilon(t)\mathcal{L}_1\rho, \tag{D2}$$

where the Liouville operator $\mathcal{L}_0$ and the perturbation operator $\mathcal{L}_1$ are given by

$$\mathcal{L}_k\rho=-i\nabla\cdot[\mathbf{F}_k(\mathbf{x})\rho], \quad k=0,1. \tag{D3}$$

Let $\rho_0(\mathbf{x})$ denote the stationary density of the unperturbed system ($\mathcal{L}_0\rho_0=0$). Then Eq. (D2) has to first order in ϵ the solution

$$\rho(\mathbf{x},t)=\rho_0(\mathbf{x})-i\int_{t_0}^{t}ds\,\epsilon(s)e^{i(s-t)\mathcal{L}_0}\mathcal{L}_1\rho_0(\mathbf{x})+O(\epsilon^2). \tag{D4}$$

Rewriting Eq. (2.3) as

$$\langle\langle\delta A(t)\rangle\rangle=\int d\mathbf{x}\,\delta A(\mathbf{x})\rho(\mathbf{x},t) \tag{D5}$$

and entering Eq. (D4) one finds by a comparison with Eq. (2.2)

$$\chi_A(\tau)=-i\Theta(\tau)\int d\mathbf{x}A(\mathbf{x})e^{-i\tau\mathcal{L}_0}\mathcal{L}_1\rho_0(\mathbf{x}). \tag{D6}$$

From this equation the vanishing response in the observable $A(\mathbf{x})=x$ follows immediately by noting that for the perturbed Lorenz system (2.1) $\mathcal{L}_0$ and $\mathcal{L}_1$ are invariant under the symmetry operation S introduced in Sec. VII so that also $e^{-i\tau\mathcal{L}_0}\mathcal{L}_1\rho_0(\mathbf{x})$ is symmetric, because ρ_0 is symmetric [13]. But the observable $A(\mathbf{x})=x$ is antisymmetric. Accordingly, the integral in Eq. (D6) vanishes so that indeed $\chi_x(\tau)=0$ and thus $\chi_x(\omega)=0$.

To derive Eq. (6.1) consider the observable

$$\dot{A}(\mathbf{x})=\frac{d}{dt}A(\mathbf{x}(t))=\dot{\mathbf{x}}\cdot\nabla A(\mathbf{x})=\mathbf{F}_0\cdot\nabla A+\epsilon(t)\mathbf{F}_1\cdot\nabla A. \tag{D7}$$

Because in the unperturbed system $\langle\langle\dot{A}\rangle\rangle=0$ one gets [from Eqs. (D4) and (D7)]

$$\begin{aligned}\langle\langle\delta\dot{A}(t)\rangle\rangle=\langle\langle\dot{A}(t)\rangle\rangle&=\int d\mathbf{x}\,\rho_0\mathbf{F}_0\cdot\nabla A+\epsilon(t)\int d\mathbf{x}\,\rho_0\mathbf{F}_1\nabla A-i\int_{t_0}^{t}ds\,\epsilon(s)\int d\mathbf{x}(e^{i(s-t)\mathcal{L}_0}\mathcal{L}_1\rho_0)(\mathbf{F}_0\cdot\nabla A)+O(\epsilon^2)\\&=-i\int d\mathbf{x}A(\mathbf{x})\mathcal{L}_0\rho_0-i\int_{-\infty}^{+\infty}ds\,\epsilon(s)\delta(t-s)\int d\mathbf{x}\,A(\mathbf{x})\mathcal{L}_1\rho_0-\int_{-\infty}^{+\infty}ds\,\epsilon(s)\Theta(t-s)\int d\mathbf{x}\,A(\mathbf{x})\mathcal{L}_0e^{i(s-t)\mathcal{L}_0}\mathcal{L}_1\rho_0\\&\quad+O(\epsilon^2).\end{aligned} \tag{D8}$$

Using $\mathcal{L}_0\rho_0=0$, a comparison with Eq. (2.2) finally gives

$$\begin{aligned}\chi_{\dot{A}}(\tau)&=-i\delta(\tau)\int d\mathbf{x}\,A(\mathbf{x})\mathcal{L}_1\rho_0-\Theta(\tau)\int dx\,A(\mathbf{x})\mathcal{L}_0e^{-i\tau\mathcal{L}_0}\mathcal{L}_1\rho_0\\&=-i\delta(\tau)\int d\mathbf{x}\,A(\mathbf{x})\mathcal{L}_1\rho_0-i\Theta(\tau)\frac{d}{d\tau}\int dx\,A(\mathbf{x})e^{-i\tau\mathcal{L}_0}\mathcal{L}_1\rho_0\\&=\frac{d}{d\tau}\chi_A(\tau),\end{aligned} \tag{D9}$$

where in the last line Eq. (D6) and $(d/d\tau)\Theta(\tau)=\delta(\tau)$ have been used. A Fourier transform gives the desired relation (6.1).

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[27] For frequencies around $f=1$ very long integration times T (up to $T=10^5$) are needed to see the beginning of the plateau. The reason for this is that in this range of ''internal frequencies'' the chaotic background $a(\omega)$ is very large so that the first term in Eq. (2.10) gives considerable contributions for smaller T.

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