Standard fluctuation-dissipation process from a deterministic mapping

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(Received 21 April 1992; revised manuscript received 7 October 1992)

We illustrate a derivation of a standard fluctuation-dissipation process from a discrete deterministic dynamical model. This model is a three-dimensional mapping, driving the motion of three variables, w, ξ, and π. We show that for suitable values of the parameters of this mapping, the motion of the variable w is indistinguishable from that of a stochastic variable described by a Fokker-Planck equation with well-defined friction γ and diffusion D. This result can be explained as follows. The bidimensional system of the two variables ξ and π is a nonlinear, deterministic, and chaotic system, with the key property of resulting in a finite correlation time for the variable ξ and in a linear response of ξ to an external perturbation. Both properties are traced back to the fully chaotic nature of this system. When this subsystem is coupled to the variable w, via a very weak coupling guaranteeing a large-time-scale separation between the two systems, the variable w is proven to be driven by a standard fluctuation-dissipation process. We call the subsystem a booster whose chaotic nature triggers the standard fluctuation-dissipation process exhibited by the variable w. The diffusion process is a trivial consequence of the central-limit theorem, whose validity is assured by the finite time scale of the correlation function of ξ. The dissipation affecting the variable w is traced back to the linear response of the booster, which is evaluated adopting a geometrical procedure based on the properties of chaos rather than the conventional perturbation approach.

PACS number(s): 05.70.Ln, 05.45.+b, 05.40.+j

I. INTRODUCTION

It is well known that diffusion can be derived from a deterministic picture without recourse to the influence of a stochastic force [1,2]. It has indeed been shown that in the chaotic regime, the time evolution of the momentum of the standard map is well described by the standard diffusion equation and the dependence of the diffusion coefficient on the perturbation strength can be described remarkably well in terms of an analytical expression derived by Rechester and White [2]. Grossmann and Fujisaka [3] have studied diffusive processes in one-dimensional systems and found a drift, as well as diffusion, and an anomalous diffusion has been discovered by Geisel and Thomae [4].

It must be stressed that all the research carried out to date to derive the fluctuation-dissipation relation from a deterministic picture seems to have highlighted the deep differences between chaotic processes and regular fluctuation-dissipation processes associated with standard Brownian motion [5]. For instance, Fujisaka, Grossmann, and Thomae [6] have found that chaos-induced diffusion is analogous to a nonlinear Fokker-Planck equation, and Grossmann [7], who studied the linear response of a mapping, found that "There is *no* simple fluctuation-dissipation theorem, which tells a universal proportionality of correlation and response of the *same* variable." Of course, this is distinctly different from standard Brownian motion described by the Langevin equation

$$\dot{w}(t) = -\gamma w(t) + \xi(t) , \tag{1.1}$$

where $\xi(t)$ is Gaussian white noise, with vanishing mean value, and correlation function

$$\langle \xi(0)\xi(t) \rangle_{eq} = 2D\delta(t) , \tag{1.2}$$

where the brackets denote an ensemble average and the

subscript indicates the equilibrium ensemble. The temperature of the Brownian particle, whose motion is described by (1.1), is defined by the well-known fluctuation-dissipation relation

$$D=\gamma\langle w^2\rangle_{\rm eq}=\gamma k_B T\ , \tag{1.3}$$

the mass of the particle being conventionally set equal to unity. Under these assumptions the process described by (1.1) turns out [5] to have an equivalent description in terms of the evolution of a probability density $\sigma(w;t)$ using the Fokker-Planck equation (FPE):

$$\frac{\partial}{\partial t}\sigma(w;t)=\left[\gamma\frac{\partial}{\partial w}w+D\frac{\partial^2}{\partial w^2}\right]\sigma(w;t)\ . \tag{1.4}$$

It is well known that in this case the response of the variable w to an applied perturbation can be expressed in terms of the unperturbed two-time correlation function of the velocity w. More recently some authors [8–10] have studied the diffusion process resulting from a deterministic picture corresponding to Eq. (1.1), with ξ replaced by a deterministic dynamical process which is a simple mapping. However, in this case, the equivalence in the long-time region between the deterministic process and the standard Brownian motion is the result of the *ad hoc* introduction of a deterministic damping term.

In summary, it is not yet clear under what general conditions a low-dimensional mapping shall have a response that is expressed in terms of an equilibrium correlation function. This would correspond to a conventional description of a susceptibility for the mapping based on the standard linear-response theory. Herein we establish that if a variable w is weakly coupled to a system, of any dimension, provided that this latter system is chaotic and ergodic, then resulting deterministic motion of the variable w conforms to that of a standard fluctuation-dissipation process. The irregularities of the deterministic statistics are, so to speak, washed out, by the large-time-scale separation between the system of interest and the chaotic subsystem. In other words, we find that the influence exerted by the chaotic and ergodic system on the variable w is indistinguishable from that produced by a standard bath with infinitely many degrees of freedom. We call this non-standard bath a *booster*.

For the present approach to the standard fluctuation-dissipation process to apply to the variable of interest, the booster has to satisfy the basic condition of responding linearly to a constant external perturbation. If we adopt a mapping as a booster, then we need to understand the intriguing problem of the linear response of a mapping to an external perturbation [7,11,12]. This problem was previously addressed by van Velsen [11] with models that produced a susceptibility that increased linearly with time. Grossmann [7], on the other hand, was able to find chaotic systems with a more convenient response, one that reaches a stationary value asymptotically. For this reason, the systems studied by Grossmann might be profitable used as boosters.

Our computer calculations, carried out to support the predictions of our theoretical approach, utilize a two-dimensional booster, rather than the one-dimensional one studied by Grossmann. The adoption of a two-dimensional booster allows us to approach the linear-response problem with a method different from that of Grossmann, one based on physical intuition as well as on the mathematical properties of chaos. This is, so to speak, a mathematical realization of the Galton-billiard argument of van Kampen [13], in other words, the description of a chaotic system with a well-defined phase space is given by a microcanonical distribution. As a result of an external perturbation the phase space is modified, and the distribution is accordingly deformed, thereby making it possible to derive an analytical expression for the corresponding stationary susceptibility. This method has some weaknesses compared to that of Grossmann [7], since we have to rely on the ergodic property of a chaotic system, which is not rigorously proved, but only numerically checked.

In this paper we present the derivation of a standard fluctuation-dissipation process from the following three-dimensional mapping:

$$\begin{aligned} w_{n+1}&=w_n+\xi_{n-k}\ ,\\ \xi_{n+1}&=\xi_n+f(\xi_n,\pi_n,-\Delta^2 w_n)\ ,\\ \pi_{n+1}&=\pi_n+g(\xi_n,\pi_n,-\Delta^2 w_n)\ . \end{aligned} \tag{1.5}$$

We shall discuss both the case where the first equation of this set has $k=-1$ and the case with k equal to unity or larger. The values w_n are to be regarded as being the values taken at discrete times by a continuous variable w, the same symbol as that used in (1.1) to denote the velocity of a Brownian particle. This choice is made because, as we shall see, (1.5) leads to a dynamics for w_n that is virtually indistinguishable from the conventional picture of (1.1). Thus we shall refer to w as the velocity of the Brownian particle regardless of whether we are using (1.1) or (1.5). The functions f and g of this mapping are obtained as follows. A microscopic system with two degrees of freedom is assumed to have the Hamiltonian equations of motion

$$\begin{aligned} \dot\xi&=\pi\ ,\\ \dot\pi&=-\frac{1}{m_1}\frac{\partial U}{\partial\xi}(\xi,\zeta,K)\ ,\\ \dot\zeta&=v\ ,\\ \dot v&=-\frac{1}{m_2}\frac{\partial U}{\partial\zeta}(\xi,\zeta,K)\ , \end{aligned} \tag{1.6}$$

where the Hamiltonian for the unperturbed system is given by $H=m_1\pi^2/2+m_2v^2/2+U(\xi,\zeta)$. These two particle have masses m_1 and m_2 and are coupled to each other via the interaction

$$U=\frac{\xi^2}{2}+\frac{\zeta^2}{2}+\xi\zeta^2-\frac{\xi^3\zeta}{3}+\xi^4\zeta^4-K\xi\ , \tag{1.7}$$

where $K=0$ gives the unperturbed potential. The Hamiltonian represents an oscillator with coordinate ξ and velocity π interacting via a nonlinear interaction with another oscillator, with coordinate ζ and velocity v. The first oscillator is perturbed by a constant field K, acting as

the contribution to the potential $-K\xi$. Notice that the intersection of the solution trajectories with the plane $\zeta=0$ results in a harmonic potential, thereby simplifying the subsequent calculations. We make the choice $m_1=1$, $m_2=0.54$. We shall refer to (1.6) as the microscopic booster for our numerical example.

The connection between the continuous equations (1.6) and the mapping (1.5) is obtained by following the trajectory determined by (1.6) from the pair (ξ_n,π_n) on the plane $\zeta=0$, to the next intersection of that plane at (ξ_{n+1},π_{n+1}). Throughout this motion the value of the perturbation field K is kept fixed at $K=-\Delta^2 w_n$. The subsequent crossing determines the new pair (ξ_{n+1},π_{n+1}) and through the first equation (1.5) the new velocity w_{n+1}. In conclusion, the values (ξ_n,π_n) are obtained from the Poincaré surface of section of (1.6) at $\zeta=0$, with K undergoing an abrupt change at any crossing of this surface. The interval of time between the two subsequent crossings is set equal to unity for convenience.

We would like to draw the attention of the reader to the fact that the time evolution of the variable w, as driven by this three-dimensional map, looks impressively similar to a Brownian motion process. With the numerical calculation of the mapping (1.5) we evaluate the equilibrium correlation function of the velocity,

$$\Psi(t)=\frac{\langle w(0)w(t)\rangle_{\rm eq}}{\langle w^2\rangle_{\rm eq}}, \tag{1.8}$$

and show that, as in Brownian motion, it is an exponential with damping γ. Then let us consider the equilibrium correlation function of the variable

$$A\equiv w^2-\langle w^2\rangle_{\rm eq}, \tag{1.9}$$

$$\Xi(t)\equiv\frac{\langle A(0)A(t)\rangle_{\rm eq}}{\langle A^2\rangle_{\rm eq}} \tag{1.10}$$

In the dynamically Gaussian case [6], the condition

$$\Xi(t)=\Psi^2(t) \tag{1.11}$$

must be fulfilled. Figure 1 shows that this condition is satisfied. Of course, to ensure the Gaussian character of the random variable $w(t)$ one should study all the higher-order correlation functions [14], and a computational calculation of them becomes increasingly difficult upon increase of the order of the correlation function considered. Thus we cannot rigorously state that w is Gaussian on the basis of (1.11). However, we believe that it is plausible that w is Gaussian. Since the decay of the correlation function is exponential, we would be led to conclude on the basis of Doob's theorem [15] that w is also Markovian. On the other hand, a Markovian and Gaussian process is known to evolve by means of a Fokker-Planck equation [14]. The damping γ of the Fokker-Planck equation is determined by the damping of the correlation function $\Psi(t)$. The diffusion coefficient D, according to (1.3), is determined by the width of the equilibrium Gaussian distribution. We see numerically that the mapping of (1.6) leads any initial condition to the same equilibrium distribution, and precisely that given by the Gaussian function of Fig. 2. The width of this "experimental" function turns out to be $(\langle w^2\rangle_{\rm eq})_{\rm fit}=38.5$, compared with the theoretical value $\langle w^2\rangle_{\rm eq}=32.0$ attained later on in this paper. Thus, on the basis of our numerical calculations, and within the specific limits set by them on the determination of the higher-order moments, we can consider the system (1.5) to be equivalent to the Langevin equation (1.1).

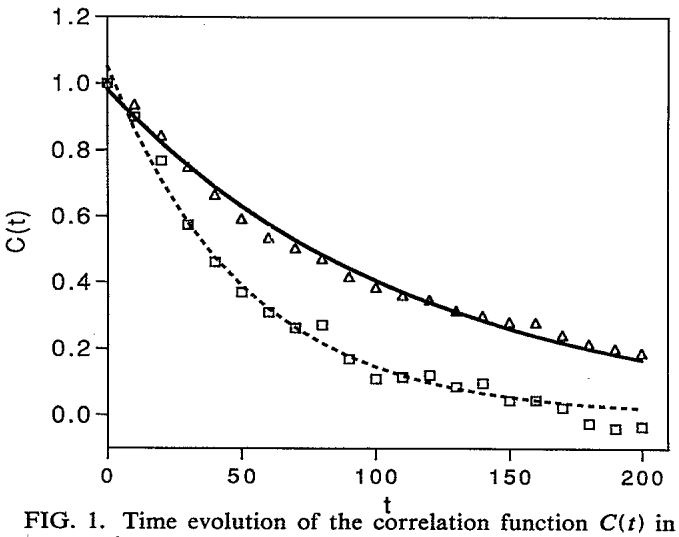

FIG. 1. Time evolution of the correlation function $C(t)$ in the case $\Delta^2=0.01$. The triangles refer to $C(t)=\Psi(t)$, namely, the equilibrium correlation function of the variable w. The squares refer to $C(t)=\Xi$, namely, the equilibrium correlation function of $A\equiv w^2-\langle w^2\rangle_{\rm eq}$. The full line is a fitting exponential with the damping $\gamma_{\rm fit}=0.0111$. The dashed line is an exponential with the damping $2\gamma_{\rm fit}$. The theoretical prediction of Sec. I supplemented with the results of Sec. III of this paper give a damping $\gamma=0.01$.

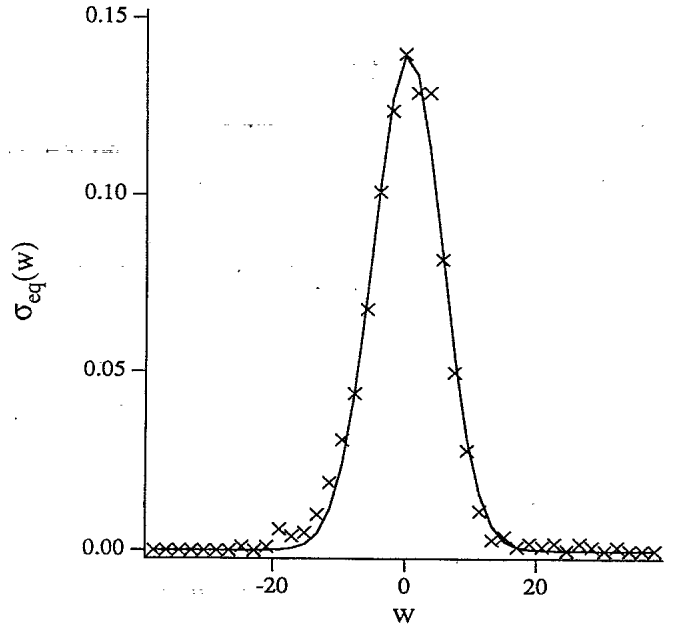

FIG. 2. Equilibrium distribution function of the variable w for $\Delta^2=0.01$. The crosses denote the result of the computer calculation of the mapping of Eq. (1.5). The full line is a Gaussian function with the width $(\langle w^2\rangle_{\rm eq})_{\rm fit}=38.5$, which has to be compared to the theoretical prediction $\langle w^2\rangle_{\rm eq}=32.0$ resulting from the theory of Sec. II.

The purpose of this paper is to establish the theoretical reasons for such an equivalence. This paper is organized as follows. In Sec. II and the corresponding Appendix, we give a short illustration of the linear-response-theory (LRT) approach to the Fokker-Planck equation in the context of a booster rather than a thermal bath. Section III illustrates our approach to calculating the linear response of a chaotic system (the booster) to an external perturbation. Here the susceptibility is determined using a geometrical argument on the Poincaré surface of section. The concluding remarks of Sec. IV point out the elements of novelty of this paper, and the advantages and limitations of our theoretical approach.

II. THE LINEAR-RESPONSE APPROACH TO THE FOKKER-PLANCK EQUATION

We shall explain here with simple and intuitive arguments why the weak coupling between w and a booster, with the properties which are summarized at the end of this section, allows us to obtain a resulting deterministic picture, namely, Eq. (1.5), with the variable w exhibiting the conventional fluctuation-dissipation process. The same result is recovered in the Appendix with more formal arguments.

We plan to show that the system (1.5) can be described by

$$\frac{\partial}{\partial t}\sigma(w;t)=\left[\chi\Delta^2\frac{\partial}{\partial w}w+\tau\langle\xi^2\rangle_0\frac{\partial^2}{\partial w^2}\right]\sigma(w;t)\ . \tag{2.1}$$

This equation has precisely the same structure as the Fokker-Planck equation (1.4). It consists of the linear superposition of a diffusion term and a friction term. The diffusion term has the diffusion coefficient

$$D=\langle\xi^2\rangle_0\tau\ , \tag{2.2}$$

where $\langle\xi^2\rangle_0$ denotes the mean quadratic value of the "force" evaluated in terms of the dynamics of the unperturbed booster. The parameter τ is the time scale of the unperturbed booster and it is defined by

$$\tau=\int_0^\infty\Phi(t)dt\ , \tag{2.3}$$

where again the normalized correlation function

$$\Phi(t)=\frac{\langle\xi\xi(t)\rangle_0}{\langle\xi^2\rangle_0} \tag{2.4}$$

refers to the unperturbed booster. The dynamics of the unperturbed booster is obtained from the map (1.5) by simply setting the interaction strength Δ^2 equal to zero, i.e., making the action of the Brownian particle on its bath, the so-called back-reaction term, equal to zero. If we take into account the mapping nature of the booster, then the time scale of the booster reads

$$\tau=\frac{\sum_n\langle\xi_0\xi_n\rangle_0}{\langle\xi_0^2\rangle_0}\ . \tag{2.5}$$

Note that $\langle\xi^2\rangle_0$ can be evaluated numerically from the dynamics of the unperturbed booster. It is possible to derive this value by adopting the analytical arguments of Sec. III A. Both ways lead to the same result and yield $\langle\xi^2\rangle_0=0.40$. The numerator of the expression of (2.5) is then evaluated numerically from the unperturbed map of (1.5) and the final result is $\tau=0.8$. With the parameters we use for the map of (1.5), the resulting diffusion coefficient turns out to have the value $D=0.32$ from which we obtain a "temperature" $\langle w^2\rangle_{\rm eq}=D/\gamma=32$, which has to be compared to the value $(\langle w^2\rangle_{\rm eq})_{\rm fit}=38.5$ used in Sec. I to define the Brownian motion "equivalent" to the map under study.

In the special case where $\Delta=0$, the motion of the variable w is only driven by the fluctuation process, and our theoretical result coincides with that already found by Grossmann and Fujisaka [3], who indeed remarked on the Kubo-like structure of the formula defining the diffusion coefficient (see also [16]). Actually, there is a still more direct avenue to this result. This is given by the central-limit theorem [17]. When $\Delta=0$, upon increase of time the variable w becomes a sum of infinitely many values of ξ, $w_n=\xi_1+\xi_2+\ldots\xi_n$. Under the basic condition that the variable ξ has a finite time correlation, the central-limit theorem leads immediately to the diffusion coefficient of (2.2). This is therefore a well-assessed result, resting on the work of Grossmann and Fujisaka [3], and still more importantly, on the rigorous foundation of the central-limit theorem [17].

The friction term is expressed by

$$\gamma=\Delta^2\chi\ . \tag{2.6}$$

The symbol χ denotes the susceptibility of the booster, i.e., its linear response to the application of a constant external field K to the booster. This subject has been studied by some authors [11,7] and the results which seem to have the closest relevance with our project are those of Grossmann [7]. The theory developed by Grossmann [7] would apparently allow us to use a one-dimensional mapping as a booster. The adoption of the two-dimensional booster described in Sec. I allows us, however, to determine the key parameter χ by means of geometrical arguments. This is described in detail in the next section. The reader must keep in mind, however, that our purpose is not that of providing original results on the linear response of a simple mapping to an external perturbation. Rather, we plan to establish that the response of the variable w of the composite system (1.5), namely, w plus booster, obeys a standard linear-response theory, i.e., we show that w is driven by a standard fluctuation-dissipation process.

For this purpose, it is necessary for us to demonstrate that the friction of Eq. (2.6) stems from the same interaction which generates the diffusion process and the corresponding diffusion coefficient of (2.2). This can be shown by using the wide time-scale separation between w and booster (which can be controlled by decreasing the intensity of the interaction strength Δ^2). Let us assume that the variable w is given an initial value so large as to make it possible to neglect the fluctuations resulting from the chaotic motion of ξ. Notice furthermore that if the variable w moves very slowly, then its rate of change is deter-

mined by the mean value reached by ξ at a fixed w (imagined as being constant). In other words, the first equation of (1.5) is equivalent to

$$\dot{w}=\langle\xi\rangle_w \ , \tag{2.7}$$

where with $\langle\xi\rangle_w$ we denote the mean value of ξ reached in the presence of the external field $K=-\Delta^2 w$. Here is where we use the LRT which, as shown in the next section, after abrupt application of an external field K, shows that the variable w reaches the mean value $\langle\xi\rangle_K$,

$$\langle\xi\rangle_K=\chi K \ . \tag{2.8}$$

The next section is devoted to the evaluation of the susceptibility χ. Here we limit ourselves to remarking that if we replace K with $-\Delta^2 w$ in (2.8) and we plug the resulting expression into (2.7), the phenomenological damping equation

$$\dot{w}=-\gamma w \tag{2.9}$$

is recovered, with the friction γ given by (2.6).

Finally, to derive the Fokker-Planck equation (2.1) we must make the assumption that friction and diffusion can be linearly superimposed upon one another. In the Appendix we derive this property, with more rigorous arguments, as a natural outcome of a perturbation-projection method.

Let us summarize the properties of the booster which are necessary to derive the Fokker-Planck equation of (2.1).

(i) The booster has an asymptotic invariant measure. We have seen that we can select a stochastic (completely chaotic) system for the booster that is also ergodic and inhabits any small volume in phase space for a limited time. This enabled us to define an equilibrium probability density (invariant measure), in terms of which the mean quadratic value

$$\langle\xi^2\rangle_0=\int_\Omega \xi^2\rho_{\rm eq}(\xi,\pi)d\xi d\pi \ , \tag{2.10}$$

where Ω is the domain of the phase space over which the variables are defined, is a well-defined positive definite quantity (without loss of generality we focus on the condition $\langle\xi\rangle_0=0$).

(ii) The booster has a finite time scale. The characteristic time of the booster, τ, is defined by (2.3).

(iii) The booster responds linearly to an external perturbation. When we apply an external perturbation K to the booster, we find that within a very short time, characteristically $\sim\tau$, the booster reaches a new equilibrium distribution with a mean value given by (2.8).

(iv) Coarse graining in time. The microscopic booster is studied on a time scale much greater than its intrinsic time scale. This is the reason why it turned out to be possible to adopt the master-equation approach discussed in the Appendix. The detailed structure of the master equation to be used is not known, nor is it necessary to know it. It is only necessary to set the constraint that this master equation must satisfy and still lead to the same equilibrium correlation function and the same susceptibility as the true booster.

III. CHAOS AND FRICTION

Within this section we will illustrate an approach to determining the linear response of a booster which the reader should compare to that used by Grossmann [7]. Thus the derivation of a stationary value for the susceptibility of a mapping illustrated here is not a novel result, but it is different from that used by Grossmann and it is a crucial step in deriving our final result on the conventional fluctuation-dissipation process driving the variable w. Here we show that the chaotic properties of the booster, which prevent us from using the conventional LRT of Kubo [18], nevertheless lead us to an analytical determination of χ, and this analytical result is made possible by the chaotic properties of the booster and its consequent ergodicity.

A. Definition of the map dominion

Let us consider the system described by the equation of motion (1.6), i.e., the system with the Hamiltonian

$$H=\frac{m_1\pi^2}{2}+\frac{m_2+v^2}{2}+U(\xi,\zeta,K) \ . \tag{3.1}$$

We study the behavior of this system at a fixed value E of its mechanical energy and look for appropriate parameter values that give rise to a chaotic motion. Since the energy E is a constant of motion, the four variables ξ, ζ, π, and v are not independent. The velocity variable v can be considered as a function of the other variables and of the energy E:

$$v=\left[\frac{2}{m_2}\left[E-\frac{m_1\pi^2}{2}-U(\xi,\zeta,K)\right]\right]^{1/2} \ . \tag{3.2}$$

In the three-dimensional space ξ,ζ,π the trajectories of the system lie inside a domain $\Omega(E)$, defined by the condition

$$v^2\geq 0 \ , \tag{3.3}$$

imposed by energy conservation. This domain is surrounded by the surface $S(E)$ defined by the region of the phase space where $v=0$, namely,

$$E-\frac{m_1\pi^2}{2}-U(\xi,\zeta,K)=0 \ . \tag{3.4}$$

The surface $S(E)$ is shown schematically in Fig. 3.

The "thermal bath" of our Brownian particle w is a booster obtained as a Poincaré map of the generating system (1.6). Let us consider the Poincaré map corresponding to the intersection of the trajectories inside the dominion $\Omega(E)$ with the plane defined by $\zeta=\zeta^*$; ζ^* will denote a generic fixed value of the variable ζ. The points of the Poincaré map lie within a manifold Σ given by the intersection of the domain $\Omega(E)$ with the plane $\zeta=\zeta^*$. The manifold Σ is formally defined by the condition

$$E-\frac{m_1\pi^2}{2}-U(\xi,\zeta^*,K)\geq 0 \ . \tag{3.5}$$

The manifold Σ is illustrated in Fig. 4 for the case $K=0$. The Poincaré map is area preserving; then the invariant

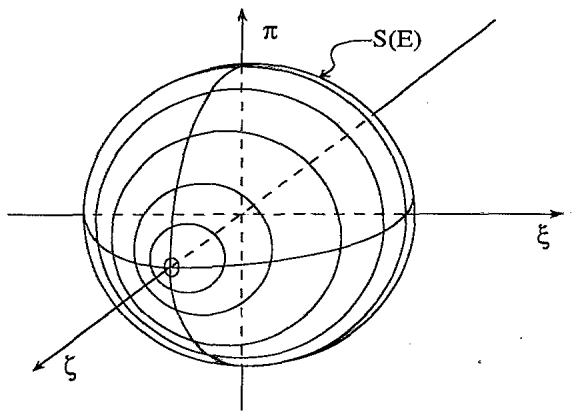

FIG. 3. A schematic illustration of the dominion $\Omega(E)$ with the surface $S(E)$.

measure is the Lebesgue (or flat) measure $d\mu = d\xi\, dv$, where ξ and v are the coordinates on the plane $\zeta = \zeta^*$, i.e., the variables of the booster.

Due to the chaotic and ergodic dynamics of the generating system given by Eq. (1.6), the dynamics of this Poincaré map is mixing; then μ is the unique invariant measure on Σ and almost any distribution function relaxes to the flat distribution. Thus the mean value and the mean square value of the booster variable ξ are respectively given by the following expressions:

$$\langle \xi \rangle = \frac{\int\int_\Sigma \xi\, d\xi\, d\pi}{\int\int_\Sigma d\xi\, d\pi} \tag{3.6}$$

and

$$\langle \xi^2 \rangle = \frac{\int\int_\Sigma \xi^2 d\xi\, d\pi}{\int\int_\Sigma d\xi\, d\pi} . \tag{3.7}$$

B. Response to a weak external perturbation

Let us now consider the unperturbed Hamiltonian H_0 given by

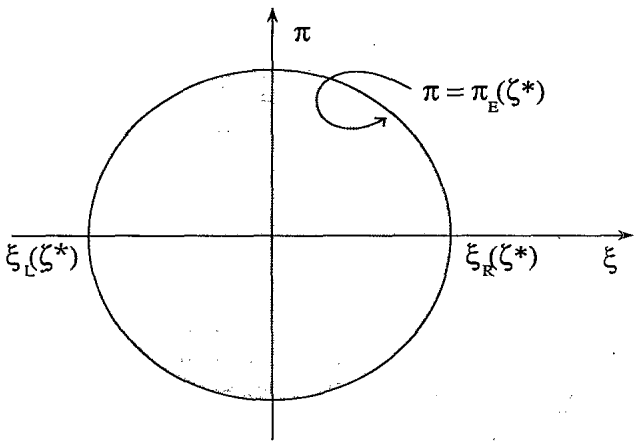

FIG. 4. Schematic illustration of the intersection between the dominion $\Omega(E)$ and the plane $\zeta = \zeta^*$ (Poincaré plane), i.e., the Σ domain.

$$H_0 = \frac{m_1 \pi^2}{2} + \frac{m_2 v^2}{2} + U_0(\xi,\zeta) , \tag{3.8}$$

where $U_0(\xi,\zeta) \equiv U(\xi,\zeta,K=0)$. We will denote quantities referring to the unperturbed system ($K=0$) with the subscript 0. However, for the sake of notational simplicity, we will use the definition

$$V(\xi,\zeta) \equiv U_0(\xi,\zeta) , \tag{3.9}$$

which, using the explicit expression in (1.7) for the potential, yields

$$V(\xi,\zeta) = \frac{\xi^2}{2} + \frac{\zeta^2}{2} + \xi\zeta^2 - \frac{\xi^3\zeta}{3} + \xi^4\zeta^4 . \tag{3.10}$$

Let us assume that the perturbation $H_1 = K\xi$ is switched on at $t=0$. Thus the resulting total Hamiltonian reads:

$$\begin{aligned} H &= \frac{m_1\pi^2}{2} + \frac{m_2 v^2}{2} + U(\xi,\zeta,K) \\ &\equiv \frac{m_1\pi^2}{2} + \frac{m_2 v^2}{2} + V(\xi,\zeta) + \Theta(t)K\xi \\ &\equiv H_0 + H_1 , \end{aligned} \tag{3.11}$$

where $\Theta(t)$ is the unit step function, namely $\Theta(t)=0$ for $t<0$ and $\Theta(t)=1$ for $t \geq 0$.

Let us imagine that we are dealing with an ensemble of systems. Suppose that an individual unperturbed system of the ensemble has coordinates $\xi(0),\zeta(0),\pi(0)$ and energy $E(0^-)=E$. Immediately after the abrupt application of the perturbation, the system behaves as if it has "felt" the influence of the additional potential $K\xi$. If $t=0$ is the time when the external perturbation is applied, that individual system of the ensemble will have the new energy,

$$\begin{aligned} E(0^+) &= \frac{m_1\pi(0)^2}{2} + \frac{m_2 v(0)^2}{2} + U(\xi(0),\zeta(0),K) \\ &= E + K\xi(0) . \end{aligned} \tag{3.12}$$

In the following time evolution the system will have an energy $E(0^+)$ fixed, with obviously

$$E(0^+) = H_0(\xi,\zeta,\pi,v) + K\xi . \tag{3.13}$$

From (3.12) and (3.13) follows that

$$E = H_0(\xi,\zeta,\pi,v) + K(\xi - \xi(0)) \equiv H_0 + \tilde{H}_1 . \tag{3.14}$$

From now on E in (3.14) will be a quantity constant in time, while the resulting interaction term will change in time with the motion of ξ, according to the definition (3.14) and to the specific value $\xi(0)$ that ξ has at the time the external perturbation is abruptly switched on.

It is important to note that if the interaction term $\tilde{H}_1$ is small enough the domain $\Omega(E)$ is slightly modified from the unperturbed one. By contrast the individual trajectories are sensibly dependent on the perturbation, whatever its intensity due to the assumption that the unperturbed system is in the chaotic regime. This is a central property, on which our LRT treatment rests. As pointed out by van Kampen [13], LRT is not applicable

to the single trajectories, i.e., at the microscopic level, but it can be recovered in a statistical sense.

Thus from the geometric deformation of this dominion we easily derive the corresponding change of the mean value of the variable ξ of the Poincaré map, thereby determining the susceptibility χ of the booster. The additional potential $K(\xi-\xi(0))$ moves the extrema $\xi_R(\zeta^*)$ and $\xi_L(\zeta^*)$ of the Poincaré map domain towards the right (with $K<0$) or the left (with $K>0$) in a continuous way. This is equivalent to saying that, although the linear response in the sense of Kubo is not justified [18], the system admits linear response in the sense of van Kampen [13]. For enough small values of K, Eq. (2.8) applies, and from Eqs. (2.8) and (3.6) we obtain

$$\chi=\left[\frac{\partial}{\partial K}\left[\frac{\int\int_{\Sigma}\xi\, d\xi\, d\pi}{\int\int_{\Sigma} d\xi\, d\pi}\right]\right]_{K=0} . \tag{3.15}$$

With the choice $\zeta^*=0$, the condition (3.5) becomes particularly simple: using the Hamiltonian (3.14) with the unperturbed potential given by (3.10) and $\zeta^*=0$, we obtain the following expression for the manifold Σ:

$$E-m_1\frac{\pi^2}{2}-\frac{\xi^2}{2}-K(\xi-\xi(0))\geq 0 , \tag{3.16a}$$

which can be rewritten as

$$m_1\pi^2+(\xi-K)^2-[2E+2K\xi(0)+K^2]\leq 0 . \tag{3.16b}$$

The points that satisfy the inequality (3.16) are those that lie within the region of the $\zeta=0$ plane surrounded by an ellipse centered on $\xi_c=K$, $\pi_c=0$. It follows that the mean value $\langle\xi\rangle$ of the booster variable ξ, calculated from Eq. (3.6), is equal to K, and it is independent of the value $\xi(0)$. From Eq. (3.15) we get immediately that

$$\chi=1 . \tag{3.17}$$

C. The transport coefficients of FPE

We are now in a position to complete the derivation of the transport coefficients of (1.4), namely the diffusion coefficient D of (2.2) and the friction γ of (2.6). The unperturbed energy of the booster is set at $E=0.8$. With this choice of the energy value the booster is in a very chaotic regime, and the intersections of the chaotic trajectories with the plane $\zeta=0$ are randomly distributed over the accessible Poincaré phase space (see Fig. 5). Furthermore, the numerical calculation shows that the modulus of the greatest Lyapunov exponent is larger than 4. The system is proved to a very good approximation to be ergodic since the numerical calculation shows that the distribution of the points on the Poincaré map is a flat function. Therefore to obtain the transport coefficient we can use the results of Secs. III A and III B.

According to the theory of Sec. II and the Appendix, the derivation of the diffusion coefficient D rests on the properties of the Poincaré map of the unperturbed booster; more precisely, D is obtained by multiplying τ defined in (2.3) by $\langle\xi^2\rangle_0$. This latter quantity is given by (3.7) supplemented with (3.16). As far as the friction γ is concerned, we have to use the susceptibility χ of the booster; thus from (3.17) we have $\chi=1$, i.e., from (2.6) $\gamma=\Delta^2$. Thus in the physical condition of Fig. 1, we get $\gamma=0.01$ and $\langle w^2\rangle_{eq}=D/\gamma=32$, which are precisely the values pointed out in Sec. I to be in remarkably good agreement with the numerical result. Of course, the theory we have been using implies a large time-scale separation between system and bath. This means low values of the coupling strength Δ^2. How low the values must be for the LRT to hold true can be illustrated by making a comparison between the numerical and the theoretical predictions of $\langle w^2\rangle_{eq}$ for different values of the coupling strength Δ^2.

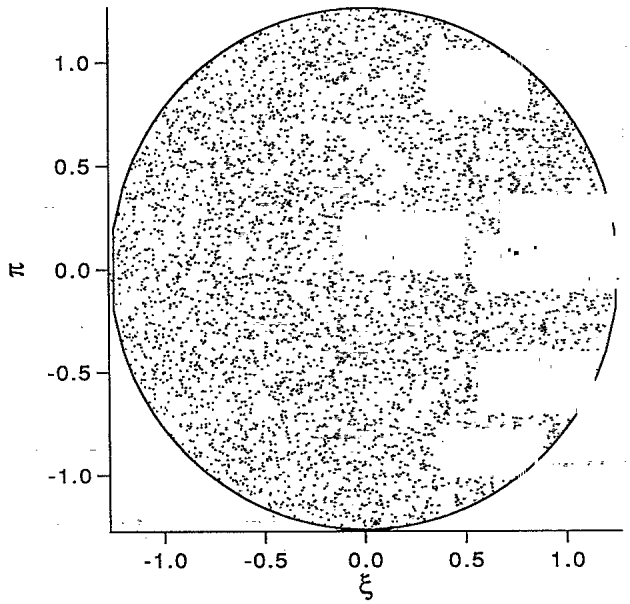

FIG. 5. Distribution of the intersection of the trajectories of Eq. (1.6) with the plane $\zeta=0$ in the chaotic case corresponding to $E=0.8$.

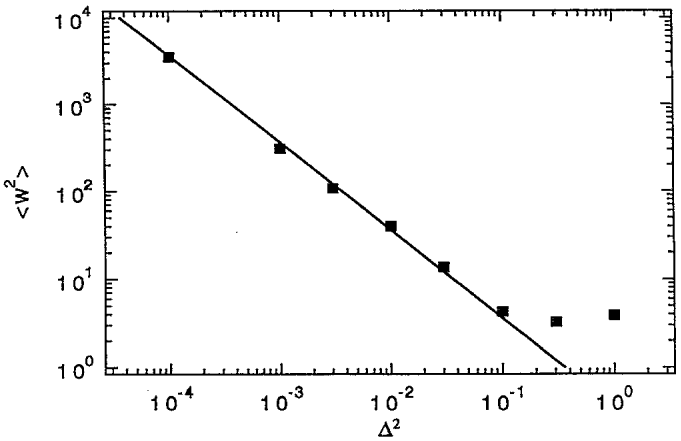

FIG. 6. The equilibrium mean square velocity as a function of Δ^2. The black squares denote the result of the numerical solution of the mapping (1.5). The solid line refers to the theoretical prediction of Eq. (3.18). Note that $\langle\xi^2\rangle_0=0.53$, derived with both numerical calculations on the unperturbed booster and analytical calculations and $\tau=0.8$ (as a result of a numerical calculation on the unperturbed booster) and $\chi=1$, according to the analytical prediction of (3.17).

This quantity is the ratio of the diffusion D to the friction γ. Thus from (2.2) and (2.6) we get the theoretical prediction

$$\langle w^2 \rangle_{eq} = \frac{\langle \xi^2 \rangle_0 \tau}{\Delta^2 \chi} . \tag{3.18}$$

Figure 6 shows that the accuracy of the theoretical prediction is fairly good in the region of extremely weak coupling strengths. As expected, in the region of higher coupling strengths the departure from the FPE prediction becomes increasingly large upon an increase of the coupling strength. The physical effects of the deviation from the linear condition shall be the object of investigation of future papers.

IV. CONCLUDING REMARKS

This paper shows that the mapping (1.5) can be used as the generator of Brownian motion with finite friction. The elements of novelty of the present analysis compared to the preceding approaches [1–10] are evident. We have derived a standard fluctuation-dissipation process by coupling our system to a booster. This means that the velocity w should respond to external perturbation according to the standard predictions of the Kubo LRT. This is obtained without invoking the chaotic and ergodic condition on the whole system, but only on a subsystem of it (the booster). The statistics of the booster can be distinctly different from the Gaussian statistics and its response does not need to adhere to the predictions of the conventional LRT. Then, the chaotic dynamics of the booster is filtered and perceived as regular Gaussian statistics by the system of interest. However, the booster must respond linearly to an external perturbation acting on it, and this technical aspect, subsidiary to the major purpose of deriving a conventional fluctuation-dissipation process out of a deterministic picture, is here approached with a method inspired by physical intuition, which makes transparent why linear response (not necessarily in the form of the conventional one predicted by the Kubo LRT) can be derived in spite of the highly nonlinear response of the single trajectories. We adhere to the spirit of the arguments raised by van Kampen, and derive the linear response of the booster without adopting a perturbation approach. We do not address the problem of whether or not the resulting susceptibility can be written in terms of the equilibrium correlation function of the variable ξ. Further, the possibility of expressing the response in terms of an equilibrium correlation function is not completely ruled out by the results of Sec. III. The central result of this paper is not affected by the resolution of this problem, whatever it might be: This is so because for the demonstration that w obeys a standard fluctuation-dissipation process, it is only necessary that, after a perturbation, the booster very quickly reaches a state with a stationary susceptibility.

The ergodicity of the booster is assumed in our analysis rather than being mathematically proven. This might have raised difficulties, due to the fact that, as shown by Dahlqvist and Russberg [20], small stability islands can escape the numerical investigation. However, it is easy to show that these stability islands when they exist produce a breakdown of the LRT at such small values of the perturbation $-\Delta^2 w$ that the process is dominated at that stage by diffusion, thereby remaining totally unaffected by an extremely weak nonlinear drift.

The mapping studied in this paper has a physical origin which does not fulfill the Hamiltonian constraints on the interaction between the Brownian particle and booster even when the unperturbed booster is Hamiltonian as it is here. It must be noticed that the change in the energy of the booster at the $(n+1)$th "collision" with the Brownian particle is

$$(\Delta E)_{n+1} = \Delta^2 \xi_{n-k} \xi_{n+k} , \tag{4.1}$$

and with the choice adopted, i.e., $k \geq 1$, due to the fact that ξ_{n-k} does not have any significant correlation with ξ_{n+1} the mean energy of the booster remains virtually unchanged, thereby mimicking the behavior of ideal thermal baths. We also took into consideration the case $k=-1$, a value of k which makes the whole system area preserving. In this case the mean change in the energy of the booster at any collision does not vanish. Instead the relative value of the mean energy change is given by

$$(\Delta E/E) = \Delta^2 \langle \xi^2 \rangle / E \approx \Delta^2 = \gamma / \chi . \tag{4.2}$$

This implies that in a time scale of the order of the macroscopic relaxation time the energy of the booster changes by 100%. In this situation the conditions under which the Fokker-Planck equation (2.1) is obtained, with time-independent transport parameters, are violated. The change of the energy of the booster in the case in which $k=-1$ is not surprising, even if the LRT developed in this paper does not predict this. In fact the LRT is a perturbative theory, thus it holds on a "mesoscopic" time scale, i.e., on a time scale much larger than the microscopic one but not necessarily larger than the macroscopic relaxation time $1/\gamma$. This does not invalidate our LRT treatment, but only implies a slight modification of the theory so as to take nonstationary conditions into account. We divide the macroscopic time region explored into many time intervals, each of which is much larger than the microscopic time scale but still much shorter than the macroscopic one. In each interval the conditions for the Fokker-Planck equation (2.1), with a time-independent friction, are fulfilled. Thus in the macroscopic time scale we obtain a Fokker-Planck equation with a time-dependent friction, and no stationary condition. With the choice $k \geq 1$ we bypass this problem, thereby making the booster mimic very well the influence of a thermal bath with an infinite number of degrees of freedom.

ACKNOWLEDGMENTS

We thank the Texas Higher Education Coordinating Board (TARP Grant No. 003594-038) for partial support of this research. R.M. thanks Istituto di Fisica della Materia for financial support. The Istituto Nazionale di Fisica Nucleare (Pisa and Pavia Sections), Professor M. Giordano, and the Centro di Calcolo del Dipartimento di Fisica dell'Universitá di Pisa are warmly thanked for ac-

cessing their computer facilities. X.F. thanks the National Science Foundation and The Pittsburgh Supercomputing Center for providing him with access to a Cray YMP supercomputer under Contract No. PHY910031P.

APPENDIX

Let us write the system to study in the continuous time representation

$$\dot{w}=\xi \ , \qquad \dot{\xi}=R(\xi,\pi,-\Delta^2 w) \ . \tag{A1}$$

Let us study this system in a Liouville-like representation [21]. This reads

$$\frac{\partial}{\partial t}\rho(w,\xi,\pi;t)=(\mathcal{L}_a+\mathcal{L}_{\rm int}+\mathcal{L}_b)\rho(w,\xi,\pi;t) \ , \tag{A2}$$

where $\rho(w,\xi,\pi;t)$ is the Liouville-like density function at time t of all the variables defining the system of Eq. (1.8). Here the Liouville-like operators are those for the system dynamics $\mathcal{L}_a$, the bath dynamics $\mathcal{L}_b$, and the system-bath interaction $\mathcal{L}_{\rm int}$. From (A1) we conclude that the Brownian particle does not move without the bath

$$\mathcal{L}_a=0 \tag{A3}$$

and

$$\mathcal{L}_{\rm int}\equiv\mathcal{L}_{\rm RF}-\xi\frac{\partial}{\partial w} \ . \tag{A4}$$

$\mathcal{L}_{\rm RF}$ expresses the action of the reaction field on the bath. This is hard to define when, as we must do, explicitly referring to the discrete time representation of (1.5). This difficulty is bypassed by having recourse to the time-scale separation between system and booster. The booster is studied in a time scale much more extended than its own time scale. Thus rather than to its exact Liouville-like equation for its Liouville-like function, we use a master-equation approach driving the probability distribution of it. In other words, we make the following replacement:

$$\mathcal{L}_{\rm RF}+\mathcal{L}_b\rightarrow\Gamma(-\Delta^2 w,\xi,\pi) \ , \tag{A5}$$

where $\Gamma(-\Delta^2 w,\xi,\pi)$ is a master-equation operator describing in the coarse graining representation the dynamics of the booster under the action of the field $K=-\Delta^2 w$. Therefore this operator also takes into account the effect of the interaction contribution which refers to the action exerted by the system of interest on the booster.

Let us leave for a moment the problem of the system coupled to the booster, and focus our attention on the problem of the response of the booster to an external perturbation by means of the master-equation formalism. This means that we have to deal with the following equation of motion:

$$\frac{\partial}{\partial t}p(\xi,\pi;t)=\Gamma(K,\xi,\pi)p(\xi,\pi;t) \ , \tag{A6}$$

where $p(\xi,\pi;t)$ is the coarse-grained probability distribution of the variables ξ and π, rather than the corresponding Liouville-like function. Note that at $K=0$ the operator $\Gamma(K,\xi,\pi)$ must be reduced to Γ_0, which is the master-equation operator describing the unperturbed dynamics of the booster,

$$\frac{\partial}{\partial t}p(\xi,\pi;t)=\Gamma_0 p(\xi,\pi;t) \ . \tag{A7}$$

The equilibrium distribution of this master equation, $p_0(x,\mathbf{p})$, is by definition the probability distribution fulfilling the equation

$$\Gamma_0 p_0(\xi,\pi)=0 \ . \tag{A8}$$

Indicating the averages over the equilibrium solution to the master equation of the unperturbed bath by a zero subscript,

$$\langle A\rangle_0\equiv\int d\xi\, d\pi\, A(\xi,\pi)p_0(\xi,\pi) \ , \tag{A9}$$

we can write the autocorrelation function for the doorway variable as

$$\Phi(t)=\langle\xi\exp(\Gamma_0 t)\xi(0)\rangle_0/\langle\xi^2\rangle_0 \ , \tag{A10}$$

so that we can express the correlation time τ as

$$\tau=\int_0^\infty\Phi(t)dt \ . \tag{A11}$$

The correlation time is the characteristic time scale for the booster process and we assume that the time evolution of the variable ξ driven by the master-equation approach leads to the same time correlation time as that resulting by a numerical treatment of the trajectories of (1.5) with $K=0$. Note that the definition itself of the normalized correlation function of Eq. (A10) implies that the bath is characterized by an equilibrium distribution over which the doorway variable gets a well-defined mean quadratic value, $\langle\xi^2\rangle_0$.

According to the linear-response property (which is made possible by the adoption of the master-equation approach) with K's weak enough we must also have

$$\Gamma=\Gamma_0+K\Gamma_1 \ . \tag{A12}$$

The master-equation operator Γ_1 must be defined in such a way as to fit the result of the linear response outlined above. To do that, let us solve Eq. (A12) with the perturbation method. The first-order perturbation leads us to

$$\frac{\partial}{\partial t}p_1(\xi,\pi;t)=\Gamma_0 p_1(\xi,\pi;t)+K\Gamma_1 p_0(\xi,\pi) \ , \tag{A13}$$

from which we obtain the following time evolution:

$$p_1(\xi,\pi;t)=K\int_0^t dt'\exp[\Gamma_0(t-t')]\Gamma_1 p_0(\xi,\pi) \ . \tag{A14}$$

Using this expression to evaluate the mean value of the doorway variable at the time t we finally get for the response function $\chi(t)$ the following expression in terms of Γ_1:

$$\chi(t)=\int_0^t\langle\xi(t')\Gamma_1\rangle_0 dt' \ . \tag{A15}$$

where, of course, the time evolution of ξ is driven by the operator $\Gamma_0^\dagger$ adjoint to Γ_0. Before proceeding with the foundation of the FPE we must stress that the expression

Eq. (A14) is the result of a first-order treatment of the process statistically, *and only statistically*, equivalent to the original Liouvillian-like problem. In the case of a chaotic microscopic system this might turn out to be remarkably different from a first-order approach within the Liouville space. Actually, the master-equation approach takes explicitly into account the fact that chaos makes a deterministic treatment inadequate. It is quite remarkable that the master-equation approach makes it possible to adopt a perturbation treatment. A possible explanation is that chaos is generated by strong nonlinearities and it is incompatible with the adoption of a perturbative treatment, which is closely related to the assumption of linearity. However, although linearity is incompatible with the behavior of individual trajectories, chaos results in a linear behavior in a statistical sense.

Let us now come back to studying Eq. (A1). Within the theoretical framework of the master-equation approach Eq. (A2) can be replaced by the equation

$$\frac{\partial}{\partial t}\rho_\Gamma(w,\xi,\pi;t)=\left[-\xi\frac{\partial}{\partial w}+\Delta^2 w\Gamma_1+\Gamma_0\right]\times\rho_\Gamma(w,\xi,\pi;t)\ . \tag{A16}$$

Here $\rho_\Gamma(w,\xi,\pi;t)$ is a probability rather than a density [the conventional meaning of $\rho(w,\xi,\pi;t)$]. To be more precise this function is the result of a coarse graining only on the space of the variables ξ and π, and coincides with the density function as far as the variable w is concerned.

The FPE for the contracted probability distribution

$$\sigma(w;t)\equiv\int d\xi\, d\pi\,\rho_\Gamma(w,\xi,\pi;t) \tag{A17}$$

is easily obtained by using the projection-perturbation approach of Ref. [22], at the second order. We obtain

$$\frac{\partial}{\partial t}\sigma(w;t)=\left\{\int_0^t\langle[\exp(\Gamma_0^\dagger t')\xi]\xi\rangle_0\frac{\partial^2}{\partial w^2}+\Delta^2\frac{\partial}{\partial w}w\int_0^t\langle\exp(\Gamma_0^\dagger t')\xi\Gamma_1\rangle_0 dt'\right\}\sigma(w;t), \tag{A18}$$

which can be rewritten as

$$\frac{\partial}{\partial t}\sigma(w;t)=\left\{\langle\xi^2\rangle_0\tau(t)\frac{\partial^2}{\partial w^2}+\Delta^2\frac{\partial}{\partial w}w\chi(t)\right\}\sigma(w;t)\ , \tag{A19}$$

with

$$\tau(t)\equiv\int_0^t\Phi(s)ds \tag{A20}$$

and $\chi(t)$ given by (A15). We remind the reader that $\Phi(s)$ is the unperturbed correlation function of the doorway variable ξ, defined by Eq. (2.4). Note that we use the convention

$$\tau\equiv\tau(\infty)\ . \tag{A21}$$

For t going to infinity Eq. (A20) tends to the standard FPE of Eq. (1.4) with

$$\gamma\equiv\Delta^2\chi\ , \tag{A22}$$

where χ denotes the stationary value of the response $\chi(t)$, given by

$$\chi\equiv\chi(\infty)=\int_0^\infty dt'\langle\xi(t')\Gamma_1\rangle_0=-\left\langle\xi\frac{1}{\Gamma_0}\Gamma_1\right\rangle_0\ . \tag{A23}$$

Thus the central result of Eq. (2.1) is derived.

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