Nonlinear fluctuations: The problem of deterministic limit and reconstruction of stochastic dynamics

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(Received 26 January 1981)

The paper discusses the connection between the deterministic and stochastic description of nonlinear, generally nonequilibrium systems. The fluctuations are treated in terms of a Markov process (master equation or Fokker-Planck equation). For processes obeying the symmetry of generalized detailed balance (GDB), the deterministic flow is cast into a form exhibiting the maximum amount of information about the stochastic dynamics. The deterministic flow contains information about Kramers-Moyal moments of order $n \geq 2$. A semipositive definite, symmetric transport matrix is introduced which satisfies generalized Onsager relations. In terms of this transport matrix the deterministic flow of processes obeying GDB can be cast into the standard form of thermodynamics. Some of the results are elucidated using a nonlinear birth and death master equation with nearest-neighbor transitions. Given the deterministic flow, the focus is on the problem of reconstruction of the original stochastic dynamics. The information contained in the deterministic flow of processes obeying GDB is not sufficient for a reconstruction of the stochastic dynamics. Given only the information of both, the stationary probability and deterministic flow, we identify a class of Fokker-Planck processes for which the stochastic dynamics can be uniquely reconstructed.

I. INTRODUCTION

An important problem of statistical mechanics is the derivation of the macroscopic evolution of a many-body system. From the viewpoint of statistical mechanics, the macroscopic evolution is governed by a stochastic process rather than a deterministic flow. However, in many situations the influence of the fluctuations plays a rather minor role. The common approach then is to study the evolution in terms of deterministic, generally nonlinear flow equations. It should be understood, however, that these flow equations are generally *not* identical with the mean value equations of the stochastic process. As has been emphasized for example, by Green[1] and Van Kampen,[2] the deterministic flow should emerge from the stochastic flow. Throughout this paper it is assumed that the macroscopic process can be modeled by a Markov process. Starting from a general master equation, the question of the corresponding deterministic limit has been clarified, about twenty years ago, by Van Kampen.[2] The deterministic limit emerges as a by-product in his fundamental work on the expansion of the master equation. Near critical points his original approach needs to be suitably modified.

From a physical point of view, there is usually good confidence in the form of the deterministic equations. A scientist interested in the role of fluctuations faces then the following crucial question—how does one account for the fluctuations? Statistical mechanics offers two basic approaches: the microscopic and the phenomenological approach. For obvious reasons most scientists do not choose the first very ambitious path. Making no approximations, the first path can clarify only the relevant structures and symmetries, but generally does not allow an explicit calculation of the stochastic expressions. Being left with a phenomenological approach, there are two extreme cases. If the system is subject to "external" noise, i.e., noise which can be arbitrarily structured by the experimentalist, the answer to the above question is usually quite transparent. Our focus here is more on those systems with "internal" noise, i.e., the fluctuations which emerge from the huge number of microscopic degrees of freedom. Generally the stochastic system will be of a mixed type. For the case of internal noise there is considerable argument and confusion about the relationship between the deterministic flow and the phenomenological modeling of the macroscopic process.[2,4-7] The origin of the confusion is that often "reasonable" assumptions are made either tacitly or explicitly, but are not always consistent.

Let us first discuss the situations for which all parties agree. For macroscopic linear systems describing thermal equilibrium the connection between stochastic and deterministic theory has been clarified by Onsager.[8,9] The form of the deterministic flow completely determines the linear stochastic process. General agreement also holds for the class of nonlinear Fokker-Planck equilibrium systems in which the dissipative part of the dynamics is governed by a linear law (linear damping). In the latter case the nonlinear stochastics are modeled by a time-dependent Ginzburg-Landau approach. The initial element of the stochastic modeling is the linear fluctuation-dissipation theorem (FDT) of the form of an Einstein relation.[10] For nonlinear systems which *do* contain a nonlinear irreversible deterministic part, a phenomenological stochastic modeling is much less obvious. In a first approximation one might describe *only the small fluctuations* about the time-dependent nonlinear deterministic flow. Such an approach corresponds to a quasi-linearization of the nonlinear stochastic equations in the sense discussed by Van Kampen,[3] Kubo *et al.*,[11] and Grabert.[12] We will not consider this case further but rather will focus on the connection between deterministic flow and a stochastic flow, which accounts for the large (may be rare) nonlinear fluctuations. Such a theory is necessary because those large fluctuations describe the deviations from a Gaussian behavior as it is reflected in higher-order cumulants. Because the deterministic flow cannot completely determine the stochastic dynamics, one is forced to provide a "prescription" for the modeling of the nonlinear macroscopic process. For nonlinear processes several such prescriptions have been proposed.[6,7,13,14] Most recently, a rather detailed and interesting stochastic modeling prescription for nonlinear thermal Fokker-Planck processes has been put forward by Grabert *et al.*[15,16]

The outline of this paper is as follows. In Sec. II we give a critical discussion of the commonly used prescription[4,7,13,14] that identifies the *deterministic* flow with the conditioned stochastic flow. If not stated explicitly otherwise, the results in this paper always refer to the case of a Markov process satisfying the master equation (integro-operator). Section III contains the main results. We discuss the deterministic limit of generally nonequilibrium processes satisfying the symmetry of generalized detailed balance.[17] We extract explicitly the maximum amount of information about the stochastic dynamics which is contained in the deterministic flow. Without additional assumptions on the physical nature of the stochastic process, there exists no unique stochastic modeling prescription. This is so, because the nontrivial information contained in the deterministic flow is not sufficient for the reconstruction of the original stochastic dynamics. In Sec. III C we identify a class of Fokker-Planck processes for which the information contained in the deterministic flow together with the *a priori* known stationary probability is sufficient for the reconstruction of the stochastic dynamics.

II. DETERMINISTIC FLOW-STOCHASTIC FLOW MODELING

We consider a system described by a set of macrovariables $a=(a_1, a_2, \ldots, a_N)$. The deterministic flow of the nonlinear (dissipative) system is written in the form

$$\frac{da}{dt}=f(a). \tag{2.1}$$

The macroscopic stochastic process will be denoted by $x(t)=(x_1(t), \ldots, x_N(t))$. Then the stochastic flow is given in terms of a stochastic differential equation (SDE) for the Markov process $x(t)$:

$$\frac{dx}{dt}=\beta(x)+\xi(t). \tag{2.2}$$

$\xi(t)$ is a vector of stochastic noise sources. These random perturbations may generally depend on the macroscopic process $x(t)$. A first problem of a stochastic modeling is the establishment of a relationship between (2.1) and (2.2). A stochastic modeling prescription, which is widely used in radio engineering[14] and physics,[7,13] is given by the following requirement: The stochastic flow $A(x)$

$$A(x)=\beta(x)+\langle\xi(t)|x(t)=x\rangle \tag{2.3}$$

given by the conditional averaging of (2.2) with $x(t)=x$, equals the deterministic flow $A(x)=f(x)$. In the case that $x(t)$ refers to a Fokker-Planck process the modeling prescription is completed by providing a prescription for the choice of the diffusion matrix $D(x)$. This is usually accomplished by postulating a nonlinear FDT.[4-7,13,14]

Here the following comments should be noted. If the macroscopic process $x(t)$ is physically defined on a *bounded* domain, the resulting structure of the Fokker-Planck equation does not generally correspond to natural boundary conditions, i.e., additional boundary conditions must generally be supplied. A particularly disturbing feature is given by the following observation. Using a nonlinear state transformation, $x\to x'$, the deterministic flow transforms like a vector (a summation over equal indices is always implied):

$$f_i'(x)=\frac{\partial x_i'}{\partial x_j}f_j(x). \tag{2.4}$$

On the other hand, for a Fokker-Planck process the transformed stochastic flow $A'(x)$ is given by

$$A_i'(x)=\frac{\partial x_i'}{\partial x_j}A_j(x)+\tfrac{1}{2}D_{mn}(x)\frac{\partial^2 x_i'}{\partial x_m\partial x_n}. \tag{2.5}$$

Thus, the postulate in (2.3), valid in one system of coordinates, is generally not valid in a different system of coordinates. This disturbing effect is not present in the prescription of Grabert *et al.*[15,16]

Although the postulate in (2.3) does not necessarily lead to a "wrong" macroscopic process, it does not represent a convincing prescription scheme for the treatment of nonlinear fluctuations.

In particular, one generally would expect that the dissipative, nonlinear stochastic flow $A(x)$ depends on a parameter ϵ measuring the strength of the fluctuations. Following Van Kampen,[3] the deterministic flow is then given by

$$f(a)=A(a,\epsilon=0) \tag{2.6}$$

III. SYSTEMS OBEYING GENERALIZED DETAILED BALANCE

A. Derivation of the deterministic flow

In this subsection we study the relationship between the deterministics and the stochastics of nonlinear, generally nonequilibrium macroscopic Markov processes satisfying a generalized detailed balance symmetry (GDB);[17,18] i.e., in terms of a state transformation θ we have for the joint probability $p^{(2)}$ the symmetry

$$p^{(2)}(x,\tau;y,0)=p^{(2)}(\theta y,\tau;\theta x,0). \tag{3.1}$$

In the following we restrict the discussion to state transformations θ satisfying

$$\theta^2=\underline{1}. \tag{3.2}$$

For the sake of convenience only we also choose an adapted coordinate system, i.e.,

$$\theta x_i=\theta_i x_i,\quad \theta_i=\pm 1 \tag{3.3}$$

for all components x_i. Let ϵ denote the parameter measuring the strength of the fluctuations. In chemical reactions ϵ is likely to be identified with the inverse of a reacting volume, in thermal diffusion problems an obvious choice will be the temperature $\epsilon=kT$ (k: Boltzmann constant), whereas in open quantum optical systems ϵ^{-1} is proportional to the number of atoms which can be excited. This parameter is generally not identical with the parameter describing the limiting approach of a non-Markov process to a Markov process. Our starting point is the master equation written in "intensive" variables x. In terms of the parameter ϵ the transition probabilities $W(Y\to X)=W(X,Y)$ of the "extensive" variables $X=x/\epsilon$ generally obey a scaling[3,11]

$$W(X,Y)=c(\epsilon)[\varphi_0(y;X-Y)+\epsilon\varphi_1(y;X-Y)+\cdots]\geq 0. \tag{3.4}$$

The form in (3.4) is likely to hold for most stochastic processes. The factor $c(\epsilon)$ can always be absorbed in a redefinition of the time variable. Without loss of generality we set $c(\epsilon)$ equal to ϵ^{-1}. In terms of the symmetric Kramers-Moyal moments $K_{i_1\ldots i_n}$, $i_s=1,\ldots,N$:

$$\begin{aligned}K_{i_1\ldots i_n}(x,\epsilon)&=\int U_{i_1}U_{i_2}\cdots U_{i_n}[\varphi_0(x,U)+\epsilon\varphi_1(x,U)+\cdots]\,dU\\&=K^0_{i_1\ldots i_n}(x)+\epsilon K^1_{i_1\ldots i_n}(x)+\cdots.\end{aligned} \tag{3.5}$$

The master equation has the form (summation convention over equal indices)

$$\begin{aligned}\dot p_t(x,\epsilon)&=\Gamma p_t(x,\epsilon)\\&=\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}\epsilon^{n-1}\left(\frac{\partial^n K_{i_1\ldots i_n}(x,\epsilon)p_t(x,\epsilon)}{\partial x_{i_1}\cdots\partial x_{i_n}}\right).\end{aligned} \tag{3.6}$$

If $\bar p(x,\epsilon)$ is the stationary probability of (3.6) the necessary and sufficient condition for GDB reads[17]

$$\bar p(x,\epsilon)=\bar p(\theta x,\epsilon) \tag{3.7a}$$

and with the operator $\bar\Gamma=\bar p^{-1/2}\Gamma\bar p^{1/2}$

$$\bar\Gamma=O_\theta^{-1}\bar\Gamma^* O_\theta. \tag{3.7b}$$

The superscript (*) denotes the transpose and O_θ is the transformation (operator) in probability space induced by the state transformation θ. Inserting the Kramers-Moyal expansion into (3.7b) we obtain a useful relationship among the moments (no summation convention over indices of $\{\theta_i\}$):

$$\begin{aligned}&\bar p(x,\epsilon)K_{i_1\ldots i_n}(\theta x,\epsilon)\\&=[(-\theta_{i_1})\cdots(-\theta_{i_n})]\\&\quad\times\sum_{m=0}^{\infty}\frac{(-\epsilon)^m}{m!}\left(\frac{\partial^m K_{i_1\ldots i_n\ldots i_{n+m}}(x,\epsilon)\bar p(x,\epsilon)}{\partial x_{i_{n+1}},\cdots,\partial x_{i_{n+m}}}\right)\end{aligned} \tag{3.8}$$

The relation (3.8) imposes severe conditions on the structure of the Kramers-Moyal moments of $x(t)$ satisfying GBD. Further we define

$$\begin{aligned}K_i^-(x,\epsilon)&=\tfrac12[K_i(x,\epsilon)-\theta_iK_i(\theta x,\epsilon)]\\&=-\theta_iK_i^-(\theta x,\epsilon),\\K_i^+(x,\epsilon)&=\tfrac12[K_i(x,\epsilon)+\theta_iK_i(\theta x,\epsilon)]\\&=\theta_iK_i^+(\theta x,\epsilon),\end{aligned} \tag{3.9}$$

and

$$\begin{aligned}S_i^+(x,\epsilon)&=K_i^+(x,\epsilon)\bar p(x,\epsilon)\\&\quad-\tfrac12\epsilon\frac{\partial}{\partial x_j}[K_{ij}(x,\epsilon)\bar p(x,\epsilon)].\end{aligned} \tag{3.10}$$

The first moment $K_i(x,\epsilon)$ can be rewritten as

$$K_i(x,\epsilon)=K_i^-(x,\epsilon)+\frac{\epsilon}{2}\bar{p}^{-1}(x,\epsilon)\frac{\partial}{\partial x_j}[K_{ij}(x,\epsilon)\bar{p}(x,\epsilon)]$$
$$+\bar{p}^{-1}(x,\epsilon)S_i^+(x,\epsilon)\,. \tag{3.11}$$

With $K_{i_1}\equiv K_i$ we obtain from (3.8) an important relation for $K_i^+(x,\epsilon)$:

$$K_i^+(x,\epsilon)=\tfrac{1}{2}\bar{p}^{-1}(x,\epsilon)\times\sum_{m=1}^{\infty}\frac{\epsilon^m(-1)^{m+1}}{m!}\left(\frac{\partial^m K_{i_1\cdots i_{1+m}}(x,\epsilon)\bar{p}(x,\epsilon)}{\partial x_{i_2}\partial x_{i_3},\ldots,\partial x_{i_{1+m}}}\right). \tag{3.12}$$

Obviously, $K^+(x,\epsilon)$ and thus $S^+(x,\epsilon)$ contain contributions of higher-order Kramers-Moyal moments.

For a Fokker-Planck process ($K_{i_1\cdots i_n}=0, n>2$), the conditions in (3.7) reduce in terms of the quantities (3.9) and (3.10) to the equivalent relations[17]

$$\frac{\partial}{\partial x_i}[K_i^-(x,\epsilon)\bar{p}(x,\epsilon)]=0\,, \tag{3.13a}$$

$$S_i^+(x,\epsilon)=0\,, \tag{3.13b}$$

and

$$K_{ij}(x,\epsilon)=\theta_i\theta_jK_{ji}(\theta x,\epsilon)\,. \tag{3.13c}$$

The relation (3.13c) holds on the support of $\bar{p}$. For the case that θ denotes the usual time-reversal operation, the relations (3.13) reduce to the well-known potential conditions.[19,20] Moreover, the quantities $K_{i_1}^-(x,\epsilon), K_{i_1i_2}(x,\epsilon)$ and the stationary probability $\bar{p}$ completely determine the dynamics of a Fokker-Planck process obeying GDB.

With the relation (3.12) we are now in a position to study the stochastic information contained in the deterministic flow of a master equation process (3.6) obeying GDB. In view of the scaling in (3.6) the stationary probability obeys[11]

$$-\epsilon\ln\bar{p}(x,\epsilon)=\phi_0(x)+\epsilon\phi_1(x)+\cdots\,. \tag{3.14}$$

We assume a noncritical behavior and set

$$x(t)=a(t)+\epsilon^{1/2}\xi(t)\,. \tag{3.15}$$

Following Van Kampen[3] we readily transform the master equation to the new stochastic process $\xi(t)$. Collecting the lowest-order terms (singular terms proportional $\epsilon^{-1/2}$) we find the deterministic flow

$$\frac{da_i}{dt}=K_i(a,\epsilon=0)=f_i(a) \tag{3.16a}$$

$$=K_i^-(a,\epsilon=0)+\tfrac{1}{2}\tilde{K}_{ij}(a)\chi_j^0(a) \tag{3.16b}$$

with $\tilde{K}$ being a symmetric effective transport matrix

$$\tilde{K}_{ij}(a)=K_{ij}(a,\epsilon=0)+\sum_{m=2}^{\infty}\frac{(-1)^{m+1}}{m!}K_{ijn_1\cdots n_{m-1}}(a,\epsilon=0)\times\chi_{n_1}^0(a)\cdots\chi_{n_{m-1}}^0(a)=\tilde{K}_{ji}(a) \tag{3.17}$$

and

$$\chi_i^0(a)=\lim_{\epsilon\to 0}\left(\epsilon\frac{\partial\ln\bar{p}(a,\epsilon)}{\partial a_i}\right)=-\frac{\partial\phi_0(a)}{\partial a_i}\,. \tag{3.18}$$

Equation (3.16b) is the *macroscopic deterministic flow of the process in (3.6) obeying* GDB *with* $\theta^2=\underline{1}$. In terms of the transport matrix $\tilde{K}$ the deterministic flow *does contain* information of Kramers-Moyal moments of order $n\geq 2$. However, except in an *a priori* Fokker-Planck case, it is generally not possible to disentangle information about the higher Kramers-Moyal moments from the effective transport matrix $\tilde{K}$. The deterministic flow contains two contributions; a "reversible" part f^-, and an "irreversible" part, f^+:

$$f_i^-(a)=K_i^-(a,\epsilon=0)=-\theta_if_i^-(\theta a)\,, \tag{3.19}$$

$$f_i^+(a)=\tfrac{1}{2}\tilde{K}_{ij}(a)\chi_j^0(a)=\theta_if_i^+(\theta a)\,. \tag{3.20}$$

The quantities f^+ and f^- possess specific transformation properties under θ. As a result, the "circulation" $r(x)=f(x)-f^+(x)$ can never contain "irreversible" components if the system obeys a GDB symmetry. In virtue of (3.20) and (3.7a) and the symmetry of $\tilde{K}$, we obtain that $\tilde{K}$ satisfies generalized Onsager relations:

$$\tilde{K}_{ij}(a)=\theta_i\theta_j\tilde{K}_{ji}(\theta a)\,. \tag{3.21}$$

Observing $\phi_0(a)=\phi_0(\theta a)$ and the transformation property of $K^-(a,\epsilon=0)$ we obtain

$$K_i^-(a,\epsilon=0)\chi_i^0(a)=0 \tag{3.22a}$$

and

$$\frac{d\phi_0}{dt}=-\tfrac{1}{2}\chi_i^0(a(t))\tilde{K}_{ij}(a(t))\chi_j^0(a(t))=-\chi_i^0(a(t))f_i^+(a(t))\leq 0\,. \tag{3.22b}$$

The inequality in (3.22b) follows from the result that the matrix $\tilde{K}$ is semipositive definite (see Appendix A). Because ϕ_0 is bounded from below, (3.22b) shows that ϕ_0 is a Liapunoff function for the deterministic flow in (3.16b) of the master equation process in (3.6) obeying GDB. The Liapunoff function is of a type as constructed by Graham[21] for Fokker-Planck processes [$\tilde{K}_{ij}(a)=K_{ij}(a,\epsilon=0)$].

B. Example

A birth and death master equation with nearest-neighbor transitions has useful application in a variety of nonequilibrium problems as, e.g., in quantum optics, electronic transport, chemical reactions, etc.[22] In terms of the transition rates $W(N\to N+1)=W^+(N)$ and $W(N\to N-1)=W^-(N)$ the master equation reads

$$\dot{p}_t(N)=W^+(N-1)p_t(N-1)+W^-(N+1)p_t(N+1) - [W^+(N)+W^-(N)]p_t(N)\,,\quad N=0,1,\ldots\,. \tag{3.23}$$

The structure in (3.23) implies that the process $N(t)$ satisfies generalized detailed balance with $\theta N=N$. The stationary probability $\bar{p}(N)$ is well known to be given by

$$\bar{p}(N)=\bar{p}(N=0)\prod_{i=0}^{N-1}\frac{W^+(i)}{W^-(i+1)} \simeq \bar{p}(N=0)\left(\frac{W^+(0)W^-(0)}{W^+(N)W^-(N)}\right)^{1/2}\exp\int_0^N dM\ln\left(\frac{W^+(M)}{W^-(M)}\right). \tag{3.24}$$

We further assume the scaling

$$W^\pm(N)=\epsilon^{-1}\gamma^\pm(x) \tag{3.25}$$

with x denoting the "intensive" variable

$$x=\epsilon N\,. \tag{3.26}$$

The Kramers-Moyal moments $K_n(x,\epsilon=0)$ (index $n=1,\ldots$ denotes the order), are readily evaluated:

$$K_n(x,\epsilon=0)=\gamma^+(x)+(-1)^n\gamma^-(x)\,. \tag{3.27}$$

From (3.24) and (3.26) we obtain for the potential $\phi_0(x)$ the result

$$\phi_0(x)=-\int_0^x\ln\left(\frac{\gamma^+(y)}{\gamma^-(y)}\right)dy\,, \tag{3.28a}$$

or in terms of the "force" $\chi^0(x)$

$$\chi^0(x)=\ln\gamma^+(x)-\ln\gamma^-(x)\,. \tag{3.28b}$$

For the calculation of $\tilde{K}(x)$, (3.17), we introduce

$$\alpha=\ln\gamma^+(x)\,,\quad \beta=\ln\gamma^-(x)\,. \tag{3.29}$$

Inserting the Kramers-Moyal moments into the expression (3.17) we have

$$\begin{aligned}\tilde{K}(x)&=e^\alpha+e^\beta-\tfrac{1}{2}(e^\alpha-e^\beta)(\alpha-\beta)+\frac{1}{3!}(e^\alpha+e^\beta)(\alpha-\beta)^2-+\cdots\\&=e^\beta\left(1+\frac{(\alpha-\beta)}{2}+\frac{(\alpha-\beta)^2}{3!}+\cdots\right)-e^\alpha\left(-1+\frac{(\alpha-\beta)}{2}-\frac{(\alpha-\beta)^2}{3!}+-\cdots\right)\\&=\frac{e^\beta}{(\alpha-\beta)}(e^{(\alpha-\beta)}-1)-\frac{e^\alpha}{(\alpha-\beta)}(e^{-(\alpha-\beta)}-1)\\&=2\frac{e^\alpha-e^\beta}{\alpha-\beta}=2\frac{\gamma^+(x)-\gamma^-(x)}{\ln\gamma^+(x)-\ln\gamma^-(x)}\geq 0\,.\end{aligned} \tag{3.30}$$

In terms of the *nonequilibrium* transport coefficient $\tilde{K}(x)$ the deterministic flow consequently reads

$$\frac{da}{dt}=\tfrac{1}{2}\tilde{K}(a)\chi^0(a)=\gamma^+(a)-\gamma^-(a)\,, \tag{3.31}$$

which equals the expected result.

C. Problem of reconstruction of the stochastic dynamics—Fokker-Planck case

The structure of the deterministic flow (3.16b) exhibits several interesting facts: Without further information about the stochastic functions of the process $x(t)$, i.e., information about the macroscopic transition probabilities, the information contained in (3.16b) is *not* sufficient for the reconstruction of the macroscopic process $x(t)$. Any reconstruction procedure must involve additional information on the physical nature of the process. It often happens that the stationary probability is known *a priori*; but that information with the information contained in (3.16b) is generally not sufficient for a unique reconstruction of the original stochastic dynamics.

In the following we *restrict* the discussion to Fokker-Planck processes obeying GDB. The deterministic flow in (3.16b) contains valuable information about Fokker-Planck drift and diffusion coefficients: $K^-(x,\epsilon=0)$, $\tilde{K}_{ij}(x)=K_{ij}(x,\epsilon=0)$. Next we introduce the *class* (H) of Fokker-Planck processes $x(t)$ defined by the following constraints: (1) $x(t)$ is a Fokker-Planck process obeying a scaling (3.4) and satisfying GDB with $\theta^2=\underline{1}$. (2) The (scaled) diffusion coefficients $K_{ij}(x,\epsilon)$ of $x(t)$ are ϵ independent. (3) The "reversible" drift $K^-(x,\epsilon)$ is either identically zero with the stationary probability being $\bar{p}(x,\epsilon)=\bar{p}(\theta x,\epsilon)$, or (4) if $K^-(x,\epsilon)\neq 0$, the reversible drift of $x(t)$ equals the deterministic reversible drift, $K^-(x,\epsilon)=f^-(x)\neq 0$ with $f^-(x)$ being source free, $(\partial/\partial x_i)f_i^-(x)=0$, and $\bar{p}(x,\epsilon)=(1/Z)\exp[-\phi_0(x)/\epsilon]$ [see (3.13a)].

The class (H) processes possess the following useful property. Given only knowledge of $\bar{p}(x,\epsilon)$ together with the information contained in the deterministic flow (3.16b), the stochastic dynamics of class (H) processes can be consistently reconstructed by writing

$$K_i^*(x,\epsilon)=\frac{\epsilon}{2}\bar{p}^{-1}(x,\epsilon)\ \frac{\partial}{\partial x_j}[K_{ij}(x,\epsilon=0)\bar{p}(x,\epsilon)] \tag{3.32}$$

and for $K^-(x,\epsilon)=f^-(x)\neq 0$,

$$K_i(x,\epsilon)=f_i^-(x)-\tfrac{1}{2}K_{ij}(x,\epsilon=0)\frac{\partial\phi_0(x)}{\partial x_j}+\frac{\epsilon}{2}\frac{\partial}{\partial x_j}[K_{ij}(x,\epsilon=0)]\,, \tag{3.33}$$

where

$$K_{ij}(x,\epsilon)=K_{ij}(x,\epsilon=0)=\theta_i\theta_j K_{ji}(\theta x,\epsilon=0) \tag{3.34}$$

satisfies generalized Onsager relations.

Among physical systems which likely can be modeled by a class (H) Fokker-Planck process are Fokker-Planck systems with $\bar{\Gamma}$, (3.7b), being a Hermitian operator (e.g., one-dimensional Fokker-Planck processes). In this case we always have a GDB symmetry with even variables only, i.e., $\theta x_i=x_i$ and $K^-(x,\epsilon)=0$. Examples are Risken's Fokker-Planck treatment[23] of the single-mode laser without detuning, models of absorptive optical bistability,[24,25] or overdamped thermal Brownian motion with nonuniform damping in an external field. Physical class (H) systems which do contain a consistent reversible drift $K^-(x,\epsilon)=f^-(x)$ are various equilibrium problems[16,26] or certain (nonequilibrium) Gauss-Markov processes. Another nontrivial but somewhat mathematical example is presented in Appendix B.

Whereas class (H) Fokker-Planck processes are not restricted to describe thermal equilibrium only, it should also be noted that the class of thermal Fokker-Planck processes with $K_{ij}(x,\epsilon)=K_{ij}(x)$ (Ref. 16) is not fully contained as a subclass of class (H) processes.

In view of the relations in (3.32)–(3.34) a word of caution is appropriate. Given $\bar{p}(x,\epsilon)$ and the deterministic limit (3.16b), one always can write down the Fokker-Planck dynamics in (3.32)–(3.34). However, the physics of the system under consideration is generally *not* consistent with such resulting (approximative) Fokker-Planck dynamics. An interesting problem in this context is the study of the conditions under which the correct physics of a system can be modeled consistently by a class (H) Fokker-Planck process and, in a related way, how and to what extent one can "approximate" master equation dynamics obeying GDB with $K^-(x,\epsilon)=0$ by class (H) Fokker-Planck dynamics. A discussion of this rather delicate problem is beyond the scope of this paper, where we have restricted ourselves to save statements only. We hope to return to this problem in a future communication.

IV. SUMMARY

We have examined the deterministic limit of generally nonequilibrium master equation processes obeying GDB symmetry. In terms of a semipositive definite (nonequilibrium) transport matrix $\tilde{K}(a)$, which satisfies generalized Onsager relations, the deterministic flow can be cast into a form exhibiting the maximum amount of information about the stochastic dynamics. The deterministic flow does contain information about Kramers-Moyal moments of order $n\geq 2$. The quantity $\phi_0(x)$, (3.14), which gives in the limit of small noise the probability for steady states, serves as a Liapunoff function for the deterministic flow of master equation processes (3.6), obeying GDB. Given the information of the stationary probability together with the information contained in the deterministic flow, (3.16b), we identified a class of Fokker-Planck processes for which the stochastic dynamics can be reconstructed.

Recently, the question of the deterministic limit of general discrete master equations has attracted attention among the mathematicians.[27,28] Compared with the van Kampen[3] result, (2.6), these papers do not predict a different deterministic flow. However, in those papers the limiting procedures are made more precise. In particular, the question of the type of convergence of stochastic process to deterministic process is clarified on a more rigorous level.

ACKNOWLEDGMENT

The author would like to thank Hermann Grabert for valuable comments.

APPENDIX A

The result that the matrix $\tilde{K}$ is semipositive definite follows from the definition (3.17). It is sufficient to show that $\tilde{K}$ can be recast as a covariance matrix over the semipositive measure $\varphi_0(x,U)$, See (3.4). With

$$\zeta_i=U_i\left(1+\sum_{m=2}^{\infty}\frac{(-1)^{m+1}}{m!}U_{i_1}\cdots U_{i_{m-1}}\chi^0_{i_1}(a)\cdots\chi^0_{i_{m-1}}(a)\right)^{1/2} \tag{A1}$$

$$= U_i \underbrace{\left[\frac{1-e^{-ux}}{ux}\right]^{1/2}}_{\geq 0}$$

we obtain

$$\tilde{K}_{ij}(a)=\langle\zeta_i\zeta_j\rangle_{\varphi_0}$$

$$=\int\varphi_0(a,U)U_iU_j\left(1+\sum_{m=2}^{\infty}\frac{(-1)^{m+1}}{m!}U_{i_1}\cdots U_{i_{m-1}}\chi^0_{i_1}(a)\cdots\chi^0_{i_{m-1}}(a)\right)dU\,. \tag{A2}$$

With z denoting an arbitrary vector we have

$$z_t\bar{K}_{tj}(a)z_j = \langle (z_t\zeta_t)^2\rangle_{\varphi_0} \geq 0\,. \tag{A3}$$

APPENDIX B

The Fokker-Planck process

$$\dot{p}_t(x,y) = -y\frac{\partial}{\partial x}p_t(x,y) + (ax+bx^3)\frac{\partial}{\partial y}p_t(x,y)$$
$$+\frac{\partial}{\partial y}\{[\gamma + \exp-(y+y^2)]yp_t(x,y)\}$$
$$+\epsilon\frac{\partial}{\partial y}\{[1+2y]\exp-(y+y^2)p_t(x,y)\}$$
$$+\epsilon\frac{\partial^2}{\partial y^2}\{[\gamma+\exp-(y+y^2)]p_t(x,y)\}$$
$$\gamma>0,\quad b>0 \tag{B1}$$

possesses the stationary probability $\bar{p}(x,y)$:

$$\bar{p}(x,y) = \frac{1}{Z}\exp\left[-\left(\frac{a}{2}x^2+\frac{b}{4}x^4+\frac{y^2}{2}\right)/\epsilon\right]. \tag{B2}$$

The process in (B1) obeys the conditions (3.13a)–3.13c) with respect to the transformation

$$\theta x = -x\,,$$
$$\theta y = y\,. \tag{B3}$$

Moreover, (B1) is an example for a class (H) process satisfying the conditions (1)–(4) in Sec. IIIC. The reversible drift is evaluated to be

$$\begin{pmatrix} f_x^- \\ f_y^- \end{pmatrix} = \begin{pmatrix} y \\ -ax-bx^3 \end{pmatrix} \tag{B4}$$

and the irreversible deterministic drift reads in terms of the transport matrix $K_{ij}(x,y)$:

$$\begin{pmatrix} f_x^+ \\ f_y^+ \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 0 & 0 \\ 0 & 2[\gamma+\exp-(y+y^2)] \end{pmatrix}\begin{pmatrix} -ax-bx^3 \\ -y \end{pmatrix}. \tag{B5}$$

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