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Extension of Statistical Replacement to Systems with Time-Correlated Fluctuations

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Nonlinear systems with correlated stochastic parameters are approximated by simpler systems. This method is an extension of an earlier version of statistical replacement and statistical linearization. The extended method is applicable to systems with correlated fluctuations. We show how this general method reduces to the earlier methods in special cases.

KEY WORDS: Statistical replacement; statistical linearization; Gaussian representation; additive fluctuations; multiplicative fluctuations; correlated noise.

1. INTRODUCTION

Stochastic differential equations (SDEs) play an important role in the theoretical study of physical and chemical phenomena. Difficulties often arise in solving these equations for at least two reasons. First, almost all realistic equations are nonlinear, thereby preventing an exact closed solution. A related point is that the equations involve nonadditive fluctuations, i.e., the fluctuating terms in general depend (often multiplicatively) on the dynamical variables under consideration. Second, the random noise is invariably correlated at different times. Although the correlation times of these fluctuations are often (but not always) small, the finite correlation times can often have an important effect on the behavior of observables and should therefore be included for quantitative analysis.

In the past few years a great deal of work has been done[1-3] on nonlinear SDEs with colored multiplicative fluctuations. Particular attention

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has been devoted to the development of methods (approximate and exact) to handle the colored noise in these systems. On the other hand, little has been done to develop methods to deal with the nonlinearities in the equations. Often nonlinear differential equations are solved numerically. However, in the case of stochastic equations the Monte Carlo numerical method involves the calculation of the trajectory corresponding to each realization of a large (ideally infinite) ensemble of the random functions. The significant quantities are obtained by averaging over the ensemble of realizations. To avoid the high cost of such simulation procedures, it is desirable to develop approximation techniques for studying selected moments of the equilibrium and time-dependent distributions that are associated with the nonlinear SDEs.

A technique used for this purpose is called statistical linearization.[4–6] Since a linear SDE can be solved in closed form, the tactic is to find the most suitable linear equation that reproduces the essential features of the nonlinear equation as closely as possible. The linear equation is parametrized by the coefficients of the zeroth and first powers of the dynamical variables. These parameters are adjusted by the linearization scheme in such a way that the mean square difference between the linear and nonlinear equations is the minimum possible. In a recent paper[7] we extended this method in several ways and the extended method was called statistical replacement. First of all, we noted that unlike statistical linearization, the replacement equation need not be linear. It can be any SDE that is exactly soluble. We used a thermodynamic criterion to choose this replacement equation so that certain important qualitative features are shared by the original and replacement equations. Statistical replacement is applicable to systems with any number of degrees of freedom, provided the replacement equation also contains the same number of degrees of freedom. The most significant extension is for equations with multiplicative fluctuations. All previous authors had used statistical linearization for single Langevin equations with additive noise delta-correlated in time. Despite the extension provided by our statistical replacement technique, the restriction to delta-correlated fluctuations remains. Moreover, the scheme was based on a separate treatment of drift and diffusion contributions. This separation was based on heuristic arguments. That scheme reproduces the lowest few moment equations exactly. We also reported some numerical examples in which the agreement between the approximate and exact results was excellent.

Here we extend statistical replacement to a more general class of SDEs [involving at most a first-degree polynomial in the noise; see Eq. (2.1) below]. We first develop a method for equations with *correlated* noise. We find that in the white noise limit the new scheme differs from the one repor-

ted earlier. Since the new scheme is based on more general considerations and lacks the heuristic separation of drift and diffusion contributions, it is an improvement over the previous one. However, practical use of both schemes usually involves only the lowest moment equations and both schemes reproduce these moment equations exactly.

In Section 2 we present a general derivation of formal equations for the variational parameters and show how the exact moment equations immediately follow from the scheme. In Section 3 we take the white noise limit of the new scheme and obtain practical expressions for the parameters. Sections 4 and 5 are comparisons of the new white noise limit with our earlier scheme. There we also rederive some of the conclusions arrived at earlier in the light of the new approach. In Section 6 we show how to make practical use of the method for the linearization of equations with exponentially correlated noise. The Gaussian property of the solution of the linearized equation is used to close the moment equations. Finally, we show a numerical example in Section 7, and Section 8 contains some final remarks.

2. A GENERAL SCHEME FOR STATISTICAL REPLACEMENT

Our goal in this paper is to reduce to a tractable form equations of the general type

$$\dot{\mathbf{x}} = \mathbf{F}(\mathbf{x}) + \mathbf{g}(\mathbf{x})\,\boldsymbol{\eta}(t) \tag{2.1}$$

where $\boldsymbol{\eta}(t)$ is taken as a vector random function of time with as yet unspecified statistical properties. Following the theme of the traditional method of statistical linearization, we propose to replace Eq. (2.1) with a linear equation of the form

$$\dot{\mathbf{x}} = \boldsymbol{\alpha}(t) + \boldsymbol{\beta}(t)\,\mathbf{x} + \boldsymbol{\gamma}(t)\,\boldsymbol{\eta}(t) \tag{2.2}$$

The coefficients $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, and $\boldsymbol{\gamma}$ are to be determined by an appropriate error minimization technique. In Ref. 7, we showed in the case of white noise that it is easy to extend these methods to cases where the replacement equation can also be a tractable nonlinear equation instead of Eq. (2.2). However, since most replacements are linear in practice, let us confine ourselves to linearization for our present purposes. We will briefly discuss a nonlinear replacement in Section 5. As noted in Ref. 7, the replacement (2.2) is appropriate only if the process $\mathbf{x}(t)$ has finite first- and second-order moments, and we therefore confine ourselves to such processes. Systems with low-order instabilities should be replaced with simpler

systems that exhibit similar instabilities. Proceeding formally, the error made in the replacement is obtained as

$$\boldsymbol{\varepsilon}(t) = \boldsymbol{\alpha}(t) + \boldsymbol{\beta}(t)\,\mathbf{x} - \mathbf{F}(\mathbf{x}) + [\boldsymbol{\gamma}(t) - \mathbf{g}(\mathbf{x})]\,\boldsymbol{\eta}(t) \tag{2.3}$$

When $\mathbf{g}(\mathbf{x})$ is independent of $\mathbf{x}$, it is customary to leave the noise term undisturbed. In this case $\boldsymbol{\gamma}(t) - \mathbf{g}(\mathbf{x})$ in Eq. (2.3) would vanish and thus $\boldsymbol{\varepsilon}$ would not involve the noise $\boldsymbol{\eta}(t)$ explicitly. Here we do wish to replace the functional dependence of $\mathbf{g}$ on $\mathbf{x}$ with an $\mathbf{x}$-independent $\boldsymbol{\gamma}(t)$ and therefore $\boldsymbol{\eta}(t)$ is present in $\boldsymbol{\varepsilon}$. The parameters α_i, β_{ij}, and γ_{ij} at a given time are selected in order to minimize the mean square error $\langle \varepsilon_i \varepsilon_j \rangle$ at that instant of time, where the brackets $\langle \cdot \rangle$ denote an average over an ensemble of the fluctuations $\boldsymbol{\eta}(t)$. Hence we obtain variational equations for these parameters at each time. They are

$$\boldsymbol{\alpha} + \boldsymbol{\beta}\langle \mathbf{x} \rangle + \boldsymbol{\gamma}\langle \boldsymbol{\eta} \rangle = \langle \mathbf{F} \rangle + \langle \mathbf{g}\boldsymbol{\eta} \rangle \tag{2.4}$$

$$\boldsymbol{\alpha}\langle \mathbf{x}^T \rangle + \boldsymbol{\beta}\langle \mathbf{x}\mathbf{x}^T \rangle + \boldsymbol{\gamma}\langle \boldsymbol{\eta}\mathbf{x}^T \rangle = \langle \mathbf{F}\mathbf{x}^T \rangle + \langle \mathbf{g}\boldsymbol{\eta}\mathbf{x}^T \rangle \tag{2.5}$$

$$\boldsymbol{\alpha}\langle \boldsymbol{\eta}^T \rangle + \boldsymbol{\beta}\langle \mathbf{x}\boldsymbol{\eta}^T \rangle + \boldsymbol{\gamma}\langle \boldsymbol{\eta}\boldsymbol{\eta}^T \rangle = \langle \mathbf{F}\boldsymbol{\eta}^T \rangle + \langle \mathbf{g}\boldsymbol{\eta}\boldsymbol{\eta}^T \rangle \tag{2.6}$$

where T denotes the transpose.

The parameters are to be fixed by solving these equations. We do this in later sections. Here we note that these formal equations are sufficient to show that Eq. (2.2) exactly reproduces the first and second moment equations corresponding to Eq. (2.1). The moment equations from Eq. (2.1) are

$$\frac{d}{dt}\langle \mathbf{x} \rangle = \langle \mathbf{F} \rangle + \langle \mathbf{g}\boldsymbol{\eta} \rangle \tag{2.7}$$

$$\frac{d}{dt}\langle \mathbf{x}\mathbf{x}^T \rangle = \langle \mathbf{x}\mathbf{F}^T \rangle + \langle \mathbf{F}\mathbf{x}^T \rangle + \langle \mathbf{x}\boldsymbol{\eta}^T\mathbf{g}^T \rangle + \langle \mathbf{g}\boldsymbol{\eta}\mathbf{x}^T \rangle \tag{2.8}$$

Those obtained from Eq. (2.2) are

$$\frac{d}{dt}\langle \mathbf{x} \rangle = \boldsymbol{\alpha} + \boldsymbol{\beta}\langle \mathbf{x} \rangle + \boldsymbol{\gamma}\langle \boldsymbol{\eta} \rangle \tag{2.9}$$

$$\frac{d}{dt}\langle \mathbf{x}\mathbf{x}^T \rangle = \boldsymbol{\alpha}\langle \mathbf{x}^T \rangle + \langle \mathbf{x} \rangle \boldsymbol{\alpha}^T + \boldsymbol{\beta}\langle \mathbf{x}\mathbf{x}^T \rangle + \langle \mathbf{x}\mathbf{x}^T \rangle \boldsymbol{\beta}^T + \boldsymbol{\gamma}\langle \boldsymbol{\eta}\mathbf{x}^T \rangle \quad \langle \mathbf{x}\boldsymbol{\eta}^T \rangle \boldsymbol{\gamma}^T \tag{2.10}$$

Equations (2.7) and (2.8) are formally identical to (2.9) and (2.10) by virtue of Eqs. (2.4) and (2.5). In practice this identity can of course not be

implemented, because one does not know how to solve (2.1) and therefore one does not know the dependence of $\mathbf{x}$ on $\boldsymbol{\eta}(t)$ implicit in the nonlinear equation (2.1) (cf. Section 3).

We obtained three sets of algebraic equations for fixing three sets of parameters. We have shown that two moment equations are exactly reproduced. An interesting question is whether there is another feature of the original equation that is exactly reproduced by the approximating equations. This question can be answered by considering the evolution of the quantity $\langle \mathbf{x}\boldsymbol{\eta}^T \rangle$. From Eq. (2.1) we have

$$\frac{d}{dt}\langle \mathbf{x}\boldsymbol{\eta}^T \rangle = \langle \mathbf{x}\boldsymbol{\eta}^T \rangle + \langle \mathbf{F}\boldsymbol{\eta}^T \rangle + \langle \mathbf{g}\boldsymbol{\eta}\boldsymbol{\eta}^T \rangle \tag{2.11}$$

and from Eq. (2.2)

$$\frac{d}{dt}\langle \mathbf{x}\boldsymbol{\eta}^T \rangle = \langle \mathbf{x}\boldsymbol{\eta}^T \rangle + \boldsymbol{\alpha}\langle \boldsymbol{\eta}^T \rangle + \boldsymbol{\beta}\langle \mathbf{x}\boldsymbol{\eta}^T \rangle + \boldsymbol{\gamma}\langle \boldsymbol{\eta}\boldsymbol{\eta}^T \rangle \tag{2.12}$$

Equations (2.11) and (2.12) are identical by virtue of (2.6). Therefore, the present linearization scheme formally reproduces the evolution equations for the first- and second-order quantities $\langle \mathbf{x} \rangle$, $\langle \mathbf{x}\mathbf{x}^T \rangle$, and $\langle \boldsymbol{x}\boldsymbol{\eta}^T \rangle$.

3. WHITE NOISE LIMIT

To compare with previously established results, we now specialize the general scheme of the last section to the case where $\boldsymbol{\eta}(t)$ goes to the limit of a delta-correlated noise. Thus, we wish to take the limit $\boldsymbol{\eta}(t) \to \boldsymbol{\xi}(t)$, where

$$\langle \boldsymbol{\xi}(t) \rangle = 0 \tag{3.1}$$

$$\langle \boldsymbol{\xi}(t)\, \boldsymbol{\xi}^T(t+t') \rangle = 2\mathbf{D}\delta(t') \tag{3.2}$$

Then Eq. (2.1) is

$$(\mathrm{S}) \quad \dot{\mathbf{x}} = \mathbf{F}(\mathbf{x}) + \mathbf{g}(\mathbf{x})\, \boldsymbol{\xi}(t) \tag{3.3}$$

where (S) denote that the equation is written in Stratonovich calculus.

The linearization scheme of Eqs. (2.4)–(2.6) involves averages of the form $\langle \mathbf{u}(\mathbf{x})\, \boldsymbol{\xi}(t) \rangle$ for several forms of $\mathbf{u}(\mathbf{x})$. Hence, we first evaluate this average for an arbitrary vector function $\mathbf{u}(\mathbf{x})$. Since the white noise is defined only as a differential for mathematical manipulation, we interpret $\langle \mathbf{u}(\mathbf{x})\, \xi_i(t) \rangle$ as follows:

$$\langle \mathbf{u}(\mathbf{x})\, \xi_i(t) \rangle = \left\langle \lim_{\Delta t \to 0} \frac{1}{\Delta t} (S) \int_t^{t+\Delta t} \mathbf{u}(\mathbf{x})\, dw_i \right\rangle \tag{3.4}$$

where w_i is the Wiener process associated with $\xi_i(t)$. In writing Eq. (3.4), we first integrated $\mathbf{u}(\mathbf{x})\,\xi_i(t)$ with respect to time and then differentiated it again. Since Eq. (3.3) is a Stratonovich equation, all the integrals arising from it are Stratonovich integrals (unless deliberately transformed to another representation). Based on the definition of the Stratonovich integral,[8] Eq. (3.4) is written as

$$\langle \mathbf{u}(\mathbf{x})\,\xi_i(t)\rangle = \lim_{\Delta t\to 0}\left\langle \frac{1}{2\Delta t}\left[\mathbf{u}(t)+\mathbf{u}(t+\Delta t)\right]\Delta w_i\right\rangle \tag{3.5}$$

where

$$\Delta w_i = w_i(t+\Delta t) - w_i(t) \tag{3.6}$$

is the increment of the Wiener process. The statistical properties of the Wiener increment are

$$\langle \Delta w_i(t)\rangle = 0 \tag{3.7}$$

$$\langle \Delta w_i(t)\,\Delta w_j(t+\Delta t)\rangle = 2D_{ij}\,\Delta t + O(\Delta t^2) \tag{3.8}$$

Next we expand $\mathbf{u}(t+\Delta t)$ as a Taylor series around $\mathbf{u}(t)$:

$$\mathbf{u}(t+\Delta t) = \mathbf{u}(t) + \sum_j \frac{\partial \mathbf{u}}{\partial x_j}\,\Delta x_j\bigg|_t + O(\Delta t^2) \tag{3.9}$$

Using Eq. (3.9) in (3.5) and recognizing that $\Delta x_j = \dot{x}_j\,\Delta t$, we obtain

$$\langle \mathbf{u}(\mathbf{x})\,\xi_i(t)\rangle = \lim_{\Delta t\to 0}\left\langle \frac{1}{\Delta t}\left[\mathbf{u}(t) + \frac{1}{2}\sum_j \frac{\partial \boldsymbol{u}}{\partial x_j}F_j(\dot{\mathbf{x}})\,\Delta t + \sum_k g_{jk}(\mathbf{x})\,\Delta w_k\right]\Delta w_i\right\rangle \tag{3.10}$$

Recall that we are dealing in this equation with delta-correlated noise and therefore quantities at different times in Eq. (3.10) can be averaged separately. Specifically,

$$\langle \mathbf{u}(t)\,\Delta w_i(t)\rangle = \langle \mathbf{u}(t)\rangle\langle \Delta w_i(t)\rangle$$

because $\Delta w_i(t)$ is the increment occurring *after* time t. Finally, using Eqs. (3.7) and (3.8), we have

$$\langle \mathbf{u}(\mathbf{x})\,\xi_i(t)\rangle = \sum_{jk} D_{ik}\left\langle g_{jk}\frac{\partial \mathbf{u}}{\partial x_j}\right\rangle \tag{3.11}$$

From this general result for an arbitrary $\mathbf{u}(\mathbf{x})$ we get the moments we need in the linearization scheme as follows:

$$\langle \mathbf{g}\xi(t)\rangle_i = \sum_{jkl} D_{jl} \left\langle g_{kl} \frac{\partial g_{ij}}{\partial x_k} \right\rangle \tag{3.12}$$

$$\langle \mathbf{g}\xi\mathbf{x}^T\rangle_{ij} = \sum_{klm} D_{km} \left\langle x_j g_{lm} \frac{\partial g_{ik}}{\partial x_l} \right\rangle + \sum_{km} D_{km} \langle g_{ik} g_{jm} \rangle \tag{3.13}$$

where the subscripts i and j on the left-hand side indicate the ith component of the (i, j)th element.

For Eq. (3.10) we tacitly used the nonlinear equation (3.3) for x_j. This is appropriate for evaluating moments of the type $\langle \mathbf{g}(\mathbf{x})\, \xi(t)\rangle$ arising from the nonlinear equation. Clearly the left-hand side of Eqs. (2.4)–(2.6) involve moments that arise from the linear portion of the error expression (2.3). In evaluating these quantities, therefore, we should use for x_j the linear equation

$$\dot{\mathbf{x}} = \boldsymbol{\alpha} + \boldsymbol{\beta}\mathbf{x} + \boldsymbol{\gamma}\xi(t) \tag{3.14}$$

When this linear equation is used, the result corresponding to Eq. (3.11) is

$$\langle \mathbf{u}(\mathbf{x})\, \xi_i(t)\rangle = \sum_{jk} D_{ik}\gamma_{jk} \left\langle \frac{\partial \mathbf{u}}{\partial x_j} \right\rangle \tag{3.15}$$

When all these results are used, in the case of white noise Eq. (2.4) becomes

$$\boldsymbol{\alpha} + \boldsymbol{\beta}(\mathbf{x}) = \langle \mathbf{f}\rangle \tag{3.16}$$

and (2.5) becomes

$$\boldsymbol{\alpha}\langle \mathbf{x}^T\rangle + \boldsymbol{\beta}\langle \mathbf{x}\mathbf{x}^T\rangle + \boldsymbol{\gamma}\mathbf{D}\boldsymbol{\gamma}^T = \langle \mathbf{f}\mathbf{x}^T\rangle + \langle \mathbf{g}\mathbf{D}\mathbf{g}^T\rangle \tag{3.17}$$

where $\mathbf{f}$ is a vector with components given by

$$f_i(\mathbf{x}) = F_i(\mathbf{x}) + \sum_{jkl} D_{jl}\, g_{kl} \left(\frac{\partial}{\partial x_k}\, g_{ij} \right) \tag{3.18}$$

To find the white noise limit of Eq. (2.6) let us write it as

$$[\beta\langle \mathbf{x}\xi^T\rangle + \gamma\langle \xi\xi^T\rangle][\langle \mathbf{F}\xi^T\rangle + \langle \mathbf{g}\xi\xi^T\rangle]^{-1} = 1 \tag{3.19}$$

As before, we replace $\langle \xi_i \xi_j \rangle$ with

$$\frac{\langle \Delta w_i\, \Delta w_j\rangle}{(\Delta t)^2} = \frac{1}{\Delta t}\,[2D_{ij} + O(\Delta t)] \tag{3.20}$$

and $\langle g_{ij}\xi_k\xi_l\rangle$ with

$$\frac{1}{2(\Delta t)^2}\langle[g_{ij}(t)+g_{ij}(t+\Delta t)]\,\Delta w_i\,\Delta w_j\rangle-\frac{1}{\Delta t}[\langle g_{ij}\rangle D_{ij}+O(\Delta t)] \tag{3.21}$$

After using (3.15), (3.20), and (3.21) in (3.19) and taking the limit $\Delta t\to 0$, we find

$$\boldsymbol{\gamma}=\langle\mathbf{g}\rangle \tag{3.22}$$

Summarizing, the present linearization scheme for equations with white noise is given by

$$\boldsymbol{\alpha}+\boldsymbol{\beta}\langle\mathbf{x}\rangle=\langle\mathbf{f}\rangle \tag{3.23}$$

$$\boldsymbol{\alpha}\langle\mathbf{x}^T\rangle+\boldsymbol{\beta}\langle\mathbf{x}\mathbf{x}^T\rangle+\boldsymbol{\gamma}\mathbf{D}\boldsymbol{\gamma}^T=\langle\mathbf{f}\mathbf{x}^T\rangle+\langle\mathbf{g}\mathbf{D}\mathbf{g}^T\rangle \tag{3.24}$$

$$\boldsymbol{\gamma}=\langle\mathbf{g}\rangle \tag{3.25}$$

This differs somewhat from the results reported earlier in Ref. 7 based on our work confined to white noise equations alone. The differences are discussed in the Appendix. Equations (3.23)–(3.25) yield for $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$

$$\begin{aligned}\boldsymbol{\beta}(t)=&[\langle\mathbf{f}\mathbf{x}^T\rangle-\langle\mathbf{f}\rangle\langle\mathbf{x}^T\rangle+\langle\mathbf{g}\mathbf{D}\mathbf{g}^T\rangle-\langle\mathbf{g}\rangle\,\mathbf{D}\langle\mathbf{g}^T\rangle]\\&\times[\langle\mathbf{x}\mathbf{x}^T\rangle-\langle\mathbf{x}\rangle\langle\mathbf{x}^T\rangle]^{-1}\end{aligned} \tag{3.26}$$

$$\boldsymbol{\alpha}(t)=\langle\mathbf{f}\rangle-\boldsymbol{\beta}(t)\langle\mathbf{x}\rangle \tag{3.27}$$

4. FLUCTUATION-DISSIPATION RELATION (FDR)

As we did earlier,[7] let us consider the set of equations

$$\dot{x}=p \tag{4.1}$$

$$\dot{p}=-V'(x)-B(x)\,p+A_1(x)\,\xi_1(t)+A_2(x)\,\xi_2(t) \tag{4.2}$$

This set describes the time evolution of the displacement x and momentum p of an anharmonic oscillator of unit mass moving in a potential $V(x)$.[9] The oscillator is also influenced by a heat bath consisting of a large number of harmonic oscillators with a broad frequency distribution. The fluctuating terms represent the energy input to the anharmonic oscillator from the heat bath due to nonlinear interactions. The term $-B(x)\,p$ describes the dissipation of energy as a frictional force exerted by the heat bath oscillators. These two transactions of energy are balanced and this is reflected by the relation

$$B(x)=\lambda_{11}A_1^2(x)+2\lambda_{12}A_1(x)\,A_2(x)+\lambda_{22}A_2^2(x) \tag{4.3}$$

where

$$\langle \xi_i(t)\, \xi_j(t') \rangle = 2k_B T \lambda_{ij}\, \delta(t-t') \tag{4.4}$$

and T is the temperature of the heat bath. Equation (4.3) is part of the formulation of the SDE describing the anharmonic oscillator and is the familiar FDR. This relation ensures eventual equilibration of the oscillator with the heat bath environment.

We replace Eqs. (4.1) and (4.2) with the linear set

$$\dot{x} = \alpha_1 + \beta_{11} x + \beta_{12} p + \gamma_{11} \xi_1(t) + \gamma_{12} \xi_2(t) \tag{4.5}$$

$$\dot{p} = \alpha_1 + \beta_{21} x + \beta_{22} p + \gamma_{21} \xi_1(t) + \gamma_{22} \xi_2(t) \tag{4.6}$$

We can now proceed to obtain expressions for α_i, β_{ij}, and γ_{ij} and we can then use these results to calculate first and second moment equations from the linearized equation as well as the average energy envelope

$$\langle E \rangle = \tfrac{1}{2} \langle p^2 \rangle + \langle V(x) \rangle \tag{4.7}$$

for certain $V(x)$ and $A_i(x)$. These steps yield the same results obtained earlier.

An important conclusion that was reached earlier and that we wish to reiterate within the present scheme is that the coefficients β_{ij} and γ_{ij} in the linear equation satisfy a FDR. Equations (3.16) and (3.17) yield

$$\alpha_1 = 0, \qquad \beta_{11} = 0, \qquad \beta_{12} = 1, \qquad \gamma_{11} = 0, \qquad \gamma_{12} = 0 \tag{4.8}$$

$$\begin{aligned} \alpha_2 = [&\langle Q \rangle (\langle x^2 \rangle \langle p^2 \rangle - \langle xp \rangle^2) - \langle xQ \rangle (\langle x \rangle \langle p^2 \rangle - \langle xp \rangle \langle p \rangle) \\ &+ (\langle pQ \rangle + R)(\langle x \rangle \langle xp \rangle - \langle x^2 \rangle \langle p \rangle)]/\mathrm{DET} \end{aligned} \tag{4.9}$$

$$\begin{aligned} \beta_{21} = [&-\langle Q \rangle (\langle x \rangle \langle p^2 \rangle - \langle p \rangle \langle xp \rangle) + \langle xQ \rangle (\langle p^2 \rangle - \langle p \rangle^2) \\ &- (\langle pQ \rangle + R)(\langle xp \rangle - \langle x \rangle \langle p \rangle)]/\mathrm{DET} \end{aligned} \tag{4.10}$$

$$\begin{aligned} \beta_{22} = [&\langle Q \rangle (\langle x \rangle \langle xp \rangle - \langle x^2 \rangle \langle p \rangle) - \langle xQ \rangle (\langle xp \rangle - \langle x \rangle \langle p \rangle) \\ &+ (\langle pQ \rangle + R)(\langle x^2 \rangle - \langle x \rangle^2)]/\mathrm{DET} \end{aligned} \tag{4.11}$$

where

$$Q = -V'(x) - B(x)\, p \tag{4.12}$$

$$\begin{aligned} R = 2k_B T [&A_{11}(\langle A_1^2 \rangle - \langle A_1 \rangle^2) + 2\lambda_{12}(\langle A_1 A_2 \rangle - \langle A_1 \rangle \langle A_2 \rangle) \\ &+ \lambda_{22}(\langle A_2^2 \rangle - \langle A_2 \rangle^2)] \end{aligned} \tag{4.13}$$

and

$$\begin{aligned} \mathrm{DET} = &\langle x^2 \rangle \langle p^2 \rangle - \langle xp \rangle^2 - \langle x \rangle^2 \langle p^2 \rangle \\ &+ 2\langle x \rangle \langle p \rangle \langle xp \rangle - \langle x^2 \rangle \langle p \rangle^2 \end{aligned} \tag{4.14}$$

(The expressions for α_2, β_{21}, and β_{22} differ from our previous expressions[7] by the presence of R.) Finally,

$$\gamma_{21} = \langle A_1 \rangle \tag{4.15}$$

$$\gamma_{22} = \langle A_2 \rangle \tag{4.16}$$

Therefore, the linearized equation is

$$\dot{x} = p \tag{4.17}$$

$$\dot{p} = \alpha_2 + \beta_{21} + \beta_{22} p + \langle A_1 \rangle \xi_1(t) + \langle A_2 \rangle \xi_2(t) \tag{4.18}$$

The coefficients α_2, β_{21}, and β_{22} involve higher order moments of x and p, which we do not know exactly. The power of the linearization method rests on the fact that these moments can be evaluated approximately using the linearized equation, because the distribution corresponding to the linear equation is Gaussian at all times.

Now we wish to show that β_{22} is related to the coefficients of the noise $\langle A_1 \rangle$ and $\langle A_2 \rangle$ at equilibrium in a manner analogous to the original FDR. Since the coefficients α_2, β_{21}, etc., are time-dependent, the Fokker–Planck equation is of the form

$$\frac{\partial}{\partial t} P(x, p, t) = L(t) P(x, p, t) \tag{4.19}$$

where $L(t)$ is a time-dependent differential operator. Therefore, the stationary distribution satisfies

$$L(\infty) P(x, p, \infty) = 0 \tag{4.20}$$

The importance of the FDR is reflected in the fact that it ensures a solution to Eq. (4.20). It is sufficient for solving (4.21) to evaluate the $t \to \infty$ limit of $\beta_{22}(t)$, $\langle A_1 \rangle$, and $\langle A_2 \rangle$. Equation (4.11) gives $\beta_{22}(t)$ in terms of moments of x and p. These moments can be factored into the first and second moments alone, because of the Gaussian nature of the solution to the linearized equation. By directly solving the moment equations for the stationary values, we get

$$\langle p \rangle_s = \langle xp \rangle_s = 0 \tag{4.21}$$

Using this and the factorizability of Gaussian moments, we also get

$$\langle p^2 \rangle_s = 2k_B T \tag{4.22}$$

Finally, from Eq. (4.11) through similar arguments we have

$$\lim_{t\to\infty} \beta_{22}(t) = -[\lambda_{11}\langle A_{11}\rangle^2 - 2\lambda_{12}\langle A_1\rangle\langle A_2\rangle + \lambda_{22}\langle A_2\rangle^2] \quad (4.23)$$

which is the required FDR.

5. BISTABLE SYSTEMS AND SYMMETRY

The method of linearization can be used only in studying closed systems that attain a unique stationary state. For example, it cannot be used for thermodynamically open systems, which can exhibit multiple stationary states.[5] The statistical distribution corresponding to such a situation consists of multiple peaks. Since the distribution obtained from a linear SDE is always Gaussian and hence has a single peak, in these situations the replacement equation necessarily has to be nonlinear.

Let us consider, for example, the equation

$$(\mathrm{S}) \quad \dot{x} = F(x) + g(x)\,\xi(t) \quad (5.1)$$

or equivalently,

$$(\mathrm{I}) \quad \dot{x} = f(x) + g(x)\,\xi(t) \quad (5.2)$$

where

$$f(x) = F(x) + Dgg' \quad (5.3)$$

and the (I) on (5.2) indicates that it is written as an Itô equation. Let us suppose that (5.1) has no low-order moment instabilities and that $f(x) = 0$ has three roots. The simplest equation in this class is

$$\dot{x} = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \alpha_3 x^3 + \beta\xi(t) \quad (5.4)$$

which arises from a two-well potential. Though Eq. (5.4) cannot be solved exactly for the time-dependent solution, much insight has been obtained by approximation methods. We propose to replace the general equation (5.1) with Eq. (5.4) and select α_i and β so that the mean square difference between the equations is minimized.

The scheme of Section 3 is applicable only when the replacement equation is linear. To use the nonlinear equation (5.4), we again perform the error minimization. The error is

$$\varepsilon = \sum_{k=0}^{3} \alpha_k x^k - F(x) + (\beta - g)\,\xi(t) \quad (5.5)$$

Minimizing $\langle \varepsilon^2 \rangle$ with respect to α_k, we have

$$-\begin{pmatrix} 1 & \langle x \rangle & \langle x^2 \rangle & \langle x^3 \rangle \\ \langle x \rangle & \langle x^2 \rangle & \langle x^3 \rangle & \langle x^4 \rangle \\ \langle x^2 \rangle & \langle x^3 \rangle & \langle x^4 \rangle & \langle x^5 \rangle \\ \langle x^3 \rangle & \langle x^4 \rangle & \langle x^5 \rangle & \langle x^6 \rangle \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} + \beta \begin{pmatrix} 0 \\ \langle x\xi \rangle \\ \langle x^2\xi \rangle \\ \langle x^2\xi \rangle \\ \langle x^3\xi \rangle \end{pmatrix} = \begin{pmatrix} \langle F \rangle + \langle g\xi \rangle \\ \langle xF \rangle + \langle xg\xi \rangle \\ \langle x^2F \rangle + \langle x^2g\xi \rangle \\ \langle x^3F \rangle + \langle x^3g\xi \rangle \end{pmatrix} \tag{5.6}$$

Averages involving $\xi(t)$ are calculated using

$$\langle u(x)\, \xi(t) \rangle = D \langle u'(x)\, g(x) \rangle \tag{5.7}$$

on the right-hand side and

$$\langle u(x)\, \xi(t) \rangle = D\beta(t) \langle u'(x) \rangle \tag{5.8}$$

on the left-hand side, as before. Minimizing $\langle \varepsilon^2 \rangle$ with respect to β gives

$$\beta = \langle g \rangle \tag{5.9}$$

Using Eq. (5.7)–(5.9) in Eq. (5.6), we find for the latter

$$\begin{pmatrix} 1 & \langle x \rangle & \langle x^2 \rangle & \langle x^3 \rangle \\ \langle x \rangle & \langle x^2 \rangle & \langle x^3 \rangle & \langle x^4 \rangle \\ \langle x^2 \rangle & \langle x^3 \rangle & \langle x^4 \rangle & \langle x^5 \rangle \\ \langle x^3 \rangle & \langle x^4 \rangle & \langle x^5 \rangle & \langle x^6 \rangle \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} + \begin{pmatrix} \langle f \rangle \\ \langle xf \rangle \\ \langle x^2 f \rangle \\ \langle x^3 f \rangle \end{pmatrix} + D \begin{pmatrix} 0 \\ \langle g^2 \rangle - \langle g \rangle^2 \\ 2(\langle xg^2 \rangle - \langle x \rangle \langle g \rangle^2) \\ 3(\langle x^2 g^2 \rangle - \langle x^2 \rangle \langle g \rangle^2) \end{pmatrix} = 0 \tag{5.10}$$

If the original equation (5.1) involves a symmetric potential [$V(x)$ such that $V'(x) = -f(x)$] and the initial distribution is symmetric about $x = 0$, then the replacement equation (5.4) should also involve a symmetric potential, i.e., $\alpha_0 = \alpha_2 = 0$.[7] Suppose $f(x)$ is an odd function of x and all odd moments of the initial distribution $P(x, 0)$ vanish. Our argument is based on the fact that the matrix in Eq. (5.10) contains the odd and even moments regularly arranged in the lattice and that the vector involving f also alternates between odd and even symmetry. The terms involving g in Eq. (5.10) have exactly the same parity as the corresponding moments involving f. These facts lead to the conclusion that if α_0 and α_2 are zero initially, then they remain zero always, and the symmetry present in the original problem is thus preserved.

6. GAUSSIAN CLOSURE FOR CLOSED SYSTEMS DRIVEN BY COLORED NOISE

Now we return to the general treatment in Section 2, i.e., we remove the restriction to white noise. The general replacement scheme given by Eqs. (2.4)–(2.6) is written in terms of moments involving the noise $\eta(t)$. For practical use of these equations these moments should be expressed in terms of the moments in x_i alone. In Section 3 we evaluated these moments in the case of white noise. Here we wish to evaluate them for a more general stationary Gaussian noise. Therefore let us assign the following statistical properties to $\eta(t)$:

$$\langle \eta_i(t) \rangle = 0 \tag{6.1}$$

$$\langle \eta_i(t)\, \eta_j(t') \rangle = 2D_{ij}\phi_{ij}(t-t') \tag{6.2}$$

and all higher cumulants are zero. The correlation times are defined as

$$\tau_{ij} = \int_0^\infty \tau \phi_{ij}(\tau)\, d\tau \tag{6.3}$$

The white noise is a special case with a delta function for $\phi_{ij}(t-t')$, i.e., $\tau_{ij}=0$. Subsequently we specialize to the Ornstein–Uhlenbeck stationary process, where $\phi_{ij}(t-t')$ is an exponential function. Even though Gaussian noise with short correlation time seems to be only a small class of random functions, it covers many situations encountered in physical and chemical studies.

When $\eta(t)$ is Gaussian with short correlation times, one can derive an approximate equation of evolution for the probability density in phase space valid to lowest order in the D_{ij} analogous to the Fokker–Planck equation. For the system (2.1) this approximate equation is

$$\frac{\partial}{\partial t} P(\mathbf{x}, t) = \left[-\sum_i \frac{\partial}{\partial x_i} f_i(\mathbf{x}) + \sum_{ij} \frac{\partial^2}{\partial x_i\, \partial x_j} D_{ij}(\mathbf{x}) \right] P(\mathbf{x}, t) \tag{6.4}$$

where $f_i(\mathbf{x})$ and $D_{ij}(\mathbf{x})$ are given

$$f_i(\mathbf{x}) = F_i(\mathbf{x}) + \sum_{jkl} \sum_{n=0}^{\infty} \frac{1}{n!} \tau_{jk}^{(n)} D_{jk} \left(\frac{\partial}{\partial x_l} g_{ij}(\mathbf{x}) \right) Q_{lk}^{(n)}(\mathbf{x}) \tag{6.5a}$$

$$D_{il}(\mathbf{x}) = \sum_{jk} \sum_{n=0}^{\infty} \frac{1}{n!} \tau_{jk}^{(n)} D_{jk}\, g_{ij}(\mathbf{x})\, Q_{lk}^{(n)}(\mathbf{x}) \tag{6.5b}$$

Here the $\tau_{jk}^{(n)}$ are moments of the correlation function defined by

$$\tau_{jk}^{(n)} = \int_0^\infty \tau^n \phi_{jk}(\tau)\, d\tau \tag{6.6}$$

and the $Q_{ij}^{(n)}$ are generated by the recursion relation

$$Q_{ij}^{(1)}(\mathbf{x}) = g_{ij}(\mathbf{x}) \tag{6.7}$$

$$Q_{ij}^{(n+1)} = \sum_k \left[\left(\frac{\partial}{\partial x_j} F_i \right) Q_{jk}^{(n)} - \left(\frac{\partial}{\partial x_j} Q_{ik}^{(n)} \right) F_j \right] \tag{6.8}$$

From the Fokker–Planck equation (6.3) we can derive the following moment equations:

$$\frac{d}{dt} \langle \mathbf{x} \rangle = \langle \mathbf{f} \rangle \tag{6.9}$$

$$\frac{d}{dt} \langle \mathbf{x}\mathbf{x}^T \rangle = \langle \mathbf{f}\mathbf{x}^T \rangle + \langle \mathbf{x}\mathbf{f}^T \rangle + \langle \mathbf{D}(\mathbf{x}) \rangle + \langle \mathbf{D}^T(\mathbf{x}) \rangle \tag{6.10}$$

These moment equations, unlike Eqs. (2.7) and (2.8), involve the moments of $\mathbf{x}$ only. Since both this set and the set of moment equations in Section 2 are exact (to order D_{ij}), we can conclude by comparison that

$$\sum_j \langle g_{ij}\eta_j \rangle = \sum_{jkl} D_{jk} \sum_{n=1}^{\infty} \frac{1}{n!} \tau_{jk}^{(n)} \left\langle \left(\frac{\partial}{\partial x_l} g_{ij} \right) Q_{kl}^{(n)} \right\rangle \tag{6.11}$$

and that

$$\sum_j \langle g_{ij}\eta_j x_s \rangle = \sum_{jkl} D_{ji} \sum_{n=1}^{\infty} \frac{1}{n!} \tau_{jk}^{(n)} \left\langle \left(\frac{\partial}{\partial x_l} g_{ij} \right) Q_{lk}^{(n)} x_s \right\rangle + \langle D_{is}(\mathbf{x}) \rangle \tag{6.12}$$

In the case of white noise, the moments of the correlation function vanish except for the zeroth one, i.e., when $\phi(\tau) = \delta(\tau)$,

$$\tau_{ij}^{(0)} = 1 \tag{6.13}$$

$$\tau_{ij}^{(n)} = 0, \qquad n \geqslant 1 \tag{6.14}$$

In this case Eqs. (6.11) and (6.12) properly reduce to Eqs. (3.12) and (3.13). Equations (6.11) and (6.12) also simplify when $\boldsymbol{\eta}(t)$ is an exponentially correlated Gaussian noise, i.e., an Ornstein–Uhlenbeck (OU) process. The OU correlation function is

$$\phi_{ij}(t - t') = (1/\tau_{ij}) \exp(-|t - t'|/\tau_{ij}) \tag{6.15}$$

In this case, the moments of ϕ_{ij} are given in terms of the nth power of the correlation time τ_{ij} by

$$\tau_{ij}^{(n)} = n!\, \tau_{ij}^n \tag{6.16}$$

For a single-variable process, Eq. (6.5) can then be expressed in the more compact form

$$D(x) = D\frac{F(x)}{g(x)}\left[1 + \tau F(x)\frac{d}{dx}\right]^{-1}\frac{g(x)}{F(x)} \tag{6.17}$$

In principle, Eqs. (6.11) and (6.12) can be substituted into Eqs. (2.4)–(2.6), thereby obtaining equations for $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, and $\boldsymbol{\gamma}$ in terms of the moments of $\mathbf{x}$ alone. However, if we are only interested in the first and second moment equations, a shortcut can be used. We have already seen that the lowest moment equations are retained by the linearization procedure. This means that when the final expressions for $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, and $\boldsymbol{\gamma}$ are substituted in the moment equations [Eqs. (2.9) and (2.10)] obtained from the linearized equation, we should get exactly Eqs. (6.9) and (6.10), which we obtained straight from the Fokker–Planck equation (6.3) corresponding to the nonlinear SDE. Treating Eqs. (6.9) and (6.10) as having arisen from the linearized equation, we can factorize the higher moments on the right-hand side by invoking the Gaussian nature of the solution. Therefore, $\langle \mathbf{f} \rangle$, $\langle \mathbf{f}\mathbf{x}^T \rangle$, and $\langle \mathbf{D}(\mathbf{x}) \rangle$ can be expressed in terms of $\langle \mathbf{x} \rangle$ and $\langle \mathbf{x}\mathbf{x}^T \rangle$ alone.

7. AN EXAMPLE

We apply the replacement procedure developed here to a simple nonlinear SDE and illustrate the method of Gaussian closure. Let us consider the SDE

$$\dot{x} = -ax - bx^3 + \eta(t) \tag{7.1}$$

where $\eta(t)$ is an Ornstein–Uhlenbeck process and $a, b > 0$. The correlation function for this process is

$$\phi(t) = (D/\tau)\, e^{-t/\tau} \tag{7.2}$$

where τ is the correlation time. The distribution corresponding to (7.1) is expected to be singly peaked. Therefore we apply the linearization procedure to this example. Linearization amounts to approximating the singly peaked distribution with a Gaussian distribution.

The approximate Fokker–Planck equation corresponding to Eq. (7.1) is

$$\frac{\partial}{\partial t}P(x, t) = \left[\frac{\partial}{\partial x}(bx^3 + ax) + \frac{\partial^2}{\partial x^2}D(x)\right]P(x, t) \tag{7.3}$$

where

$$D(x) = D\{1 - (a + 3bx^2)\,\tau + O(\tau^2)\} \tag{7.4}$$

Equation (7.3) can be solved exactly for the stationary distribution to give

$$\begin{aligned} P_s(x) &= \frac{1}{D(x)} \exp \int^x \frac{-ay - by^3}{D[1 + (a - 3by^2)\,\tau]}\, dy \\ &= \exp\left\{ -\frac{ax^2}{2D} - \frac{bx^4}{4D} + \left[\left(3b - \frac{a^2}{2D} \right) x^2 \right.\right. \\ &\quad \left.\left. - \frac{ab}{D} x^4 - \frac{b^2 x^6}{2D} \right] \tau + O(\tau^2) \right\} \end{aligned} \tag{7.5}$$

up to a normalization constant. We apply the linearization and compute the stationary distribution to compare with the solution (7.5). We also compare the steady-state moments $\langle x \rangle_s$ and $\langle x^2 \rangle_s$ for several sets of parameter values. Since $P_s(x)$ is an even function of x,

$$\langle x \rangle_s = 0 \tag{7.6}$$

The second moment $\langle x^2 \rangle_s$ can be calculated by two simple numerical integrations.

The first and second moment equations from Eq. (7.1) are

$$\frac{d}{dt} \langle x \rangle = -a\langle x \rangle - b\langle x^3 \rangle \tag{7.7}$$

$$\frac{d}{dt} \langle x^2 \rangle = -2a\langle x^2 \rangle - 2b\langle x^4 \rangle + 2\langle D(x) \rangle \tag{7.8}$$

The linearized equation is

$$\dot{x} = \alpha + \beta x + \eta(t) \tag{7.9}$$

where

$$\alpha = -b \frac{\langle x^2 \rangle \langle x^3 \rangle - \langle x^4 \rangle \langle x \rangle}{\langle x^2 \rangle - \langle x \rangle^2} \tag{7.10}$$

$$\beta = -a + b \frac{\langle x^3 \rangle \langle x \rangle - \langle x^4 \rangle}{\langle x^2 \rangle - \langle x \rangle^2} \tag{7.11}$$

The first and second moment equations obtained from the linear equation are

$$\frac{d}{dt}\langle x\rangle = \alpha + \beta\langle x\rangle \tag{7.12}$$

$$\frac{d}{dt}\langle x^2\rangle = 2\alpha\langle x\rangle + 2\beta\langle x^2\rangle + 2\langle D(x)\rangle \tag{7.13}$$

After substituting for α and β in (7.12) and (7.13) we get exactly (7.7) and (7.8). Since the linearized equation has a Gaussian solution, α and β can be evaluated using Gaussian factorization for the higher moments.

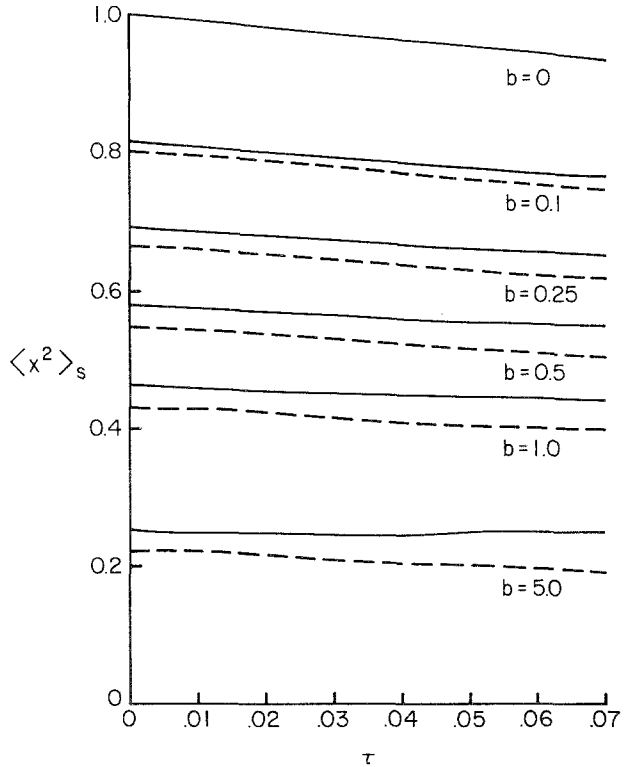

Fig. 1. Comparison of $\langle x^2\rangle_s$ from (—) the "exact" [Eq. (7.5)] and (- -) approximate [Eq. (7.17)] expressions for various values of b, with $D = 1$. The two results of course coincide when $b = 0$.

After this factorization the moment equations yield for the stationary moments

$$a\langle x\rangle_s - b\langle x\rangle_s(3\langle x^2\rangle_s - 2\langle x\rangle_s^2) = 0 \quad (7.14)$$

$$a\langle x^2\rangle_s - b(3\langle x^2\rangle_s^2 - 2\langle x\rangle_s^4) + D(1 - a\tau - 3\tau b\langle x^2\rangle_s) = 0 \quad (7.15)$$

The solution of (7.14) and (7.15) is

$$\langle x\rangle_s = 0 \quad (7.16)$$

$$\langle x^2\rangle_s = \frac{-2a - 6bD\tau[(2a + 6bD\tau)^2 + 48bD(1 - a\tau)]^{1/2}}{12b} \quad (7.17)$$

Both the exact (to order τ) solution and the linearized solution give $\langle x\rangle_s = 0$. The second moments $\langle x^2\rangle_s$ are compared in Fig. 1. We also compare the stationary distributions in Figs. 2 and 3. When $b = 0$, the

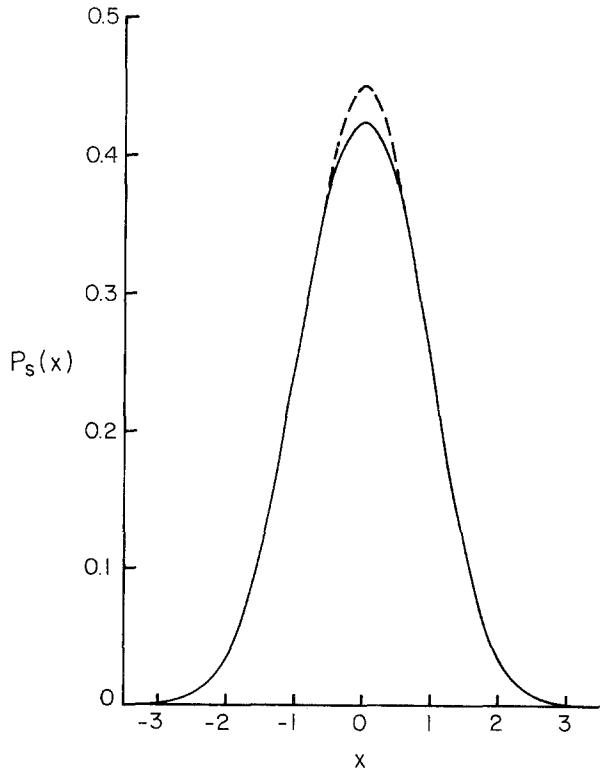

Fig. 2. Comparison of (- -) the stationary distribution given by the linearized equation with (—) the "exact" distribution. $\tau = 0.02$, $b = 0.1$, and $D = 1$.

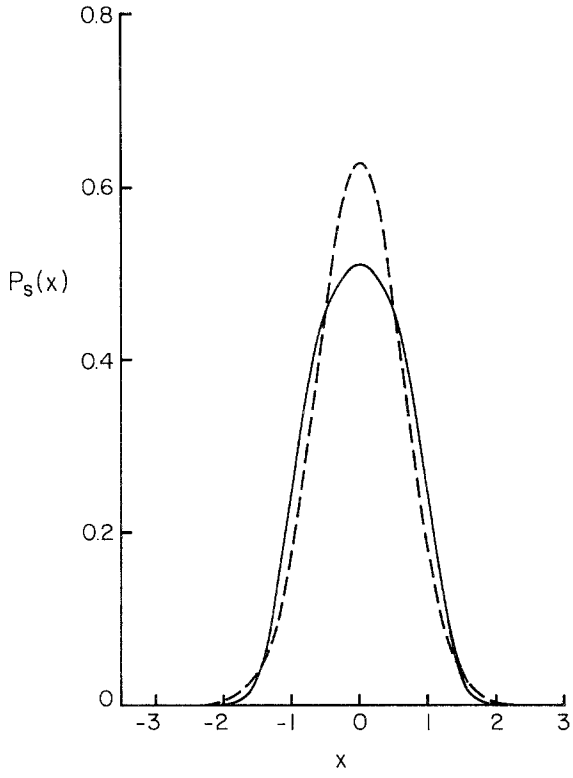

Fig. 3. Comparison of (- -) the stationary distribution given by the linearized equation with (—) the "exact" distribution. $\tau = 0.05$, $b = 1$, and $D = 1$.

original equation is linear and therefore the linearized solution must agree with the exact solution. The figure clearly shows that the deviations become larger as b increases. Moreover, for a given b, better approximation is achieved for smaller τ.

CONCLUSION

The method of statistical replacement reported here is applicable to equations in which the noise term can have general statistical properties. We have derived practical application methods for the cases of white noise, for an Ornstein–Uhlenbeck process, and for a multidimensional Gaussian process with finite correlation times. We found that the white noise limit of the present scheme is different from our earlier scheme, which was developed exclusively for equations with white noise. Nevertheless, *all* the

final conclusions we deduced earlier remain valid in the light of the new scheme.

The most powerful replacement is linearization, i.e., replacement with a linear equation. This is because the Gaussian nature of the solution permits a practical procedure for obtaining closed expressions for the first and second moments.

The drawback in this method is the lack of an *a priori* measure of the accuracy of the approximation. Minimizing $\langle \boldsymbol{\varepsilon}^2 \rangle$ implies that $\langle \boldsymbol{\varepsilon} \rangle = 0$, i.e., the difference between the replaced and replacement equations vanishes on the average. However, it is not clear how the error made in higher moments of $\boldsymbol{\varepsilon}$ translates into the errors made on the moments of $\mathbf{x}$. To apply the linearization method, for example, one should know beforehand that the true solution does not deviate significantly from a Gaussian shape. This is the basis for our criterion that linearization can be applied safely only to thermodynamically closed systems. It is not easy to extend similar criteria to nonlinear replacements.

APPENDIX

In place of Eqs. (3.23)–(3.25), in Ref. 7 we obtained the expressions

$$\boldsymbol{\alpha} + \boldsymbol{\beta}\langle \mathbf{x} \rangle = \langle \mathbf{f} \rangle \tag{A1}$$

$$\mathbf{a}\langle \mathbf{x}^T \rangle + \boldsymbol{\beta}\langle \mathbf{x}\mathbf{x}^T \rangle + \boldsymbol{\gamma}\boldsymbol{D}\boldsymbol{\gamma}^T = \langle \mathbf{f}\mathbf{x}^T \rangle + \langle \mathbf{g}\mathbf{D}\mathbf{g}^T \rangle \tag{A2}$$

$$\boldsymbol{\gamma}\mathbf{D}\boldsymbol{\gamma}^T = \langle \mathbf{g}\boldsymbol{D}\boldsymbol{g}^T \rangle \tag{A3}$$

and the expression for $\boldsymbol{\beta}$ in Ref. 7 did not contain the last two terms in the numerator of (3.26). However, both schemes reproduce the first and second moment equations exactly. This is because the change due to $\boldsymbol{\beta}$ cancels the change due to $\boldsymbol{\alpha}$ in both moment equations.

Equations (A1)–(A3) were based on separate consideration of the drift and diffusion contributions. If we had Eq. (A3) in place of Eq. (3.22), then the two schemes would be identical. This may lead to the thought that if we had minimized the error in $\mathbf{g}$ (i.e., minimized $\mathbf{g} - \boldsymbol{\gamma}$) rather than in the diffusion function $\mathbf{g}\mathbf{D}\mathbf{g}^T$, we would have obtained the present results earlier, but this is easily shown not to be the case. Thus minimizing the combined error in both terms of the equation and minimizing drift and diffusion contributions separately produces different expressions for $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, and $\boldsymbol{\gamma}$ even though the moment equations are the same.

To say this in different terms, let us decompose $\boldsymbol{\varepsilon}$ in Eq. (2.3) as

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_1 + \boldsymbol{\varepsilon}_2 \tag{A4}$$

where

$$\boldsymbol{\varepsilon}_1 = \boldsymbol{\alpha} + \boldsymbol{\beta}\mathbf{x} - \mathbf{F}(\mathbf{x}) \tag{A5}$$

Here we have minimized $\boldsymbol{\varepsilon}_1\boldsymbol{\varepsilon}_1^T + \boldsymbol{\varepsilon}_2\boldsymbol{\varepsilon}_2^T + \boldsymbol{\varepsilon}_1\boldsymbol{\varepsilon}_2^T + \boldsymbol{\varepsilon}_2\boldsymbol{\varepsilon}_1^T$. In Ref. 7 we minimized $\boldsymbol{\varepsilon}_1\boldsymbol{\varepsilon}_1^T + \boldsymbol{\varepsilon}_2\boldsymbol{\varepsilon}_2^T$ only. This was deliberately done because we did not understand then how to treat the cross terms involving white noise explicitly.

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