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Statistical Replacement for Systems with Delta-Correlated Fluctuations

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Nonlinear systems with stochastic parameters are approximated by simpler systems using a method that we call "statistical replacement." This method is an extension of the previously developed AGREE which was restricted to systems with additive fluctuations. Statistical replacement incorporates the distinctions between globally stable thermodynamically closed systems and thermodynamically open systems that can be unstable.

KEY WORDS: Statistical replacement; statistical linearization; Gaussian representation; additive fluctuations; multiplicative fluctuations; stable systems; unstable systems.

1. INTRODUCTION

Nonlinear stochastic differential equations (SDE's) that arise in the modeling of physical and chemical phenomena are seldom amenable to exact analytic solution. Monte Carlo numerical techniques become exact as the number of realizations becomes infinite, but the computer expense diverges in the same limit. Thus it is highly desirable to develop approximation techniques suitable for studying the equilibrium and time-dependent properties of classes of such nonlinear stochastic equations. Some investigators have developed methods of obtaining approximate solutions to nonlinear SDE's.[1–5] Alternatively, several others have focused their attention on approximating the equations themselves and then finding exact solutions to the approximate equations.[6–13] In this paper we

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implement the latter philosophy. For example, since a linear SDE can always be solved exactly, we can seek the best linear equation that will reproduce the important features of the solution of the nonlinear SDE. The method to be used requires the replacement of the nonlinear equation with a linear equation in a prescribed optimal manner. The parameters in the linear equation are selected so that the mean squared error (suitably defined) made by this replacement is a minimum. Such a minimization procedure provides explicit expressions for the parameters of the linear equation in terms of moments of the dynamical variables.

The detailed implementation of the procedure to a particular nonlinear system depends on the properties that one wishes to represent most accurately. "Statistical linearization" has as its aim the accurate calculation of steady state moments, steady state correlation functions, and steady state spectra.[6–10] For this purpose, the moments that are needed to obtain the linearization parameters are evaluated using the steady state distribution for the process. The linearization parameters obtained from statistical linearization are consequently time independent. If the exact steady state distribution for the nonlinear process is used in the moment evaluation, then this procedure leads to a linear stochastic equation whose variables have exactly the same first and second steady state moments as those of the original nonlinear equation. We note that in some cases the full steady state distribution for the nonlinear problem is indeed available even if the time-dependent one (which is needed to calculate correlation functions and spectra) is not. If the exact steady state distribution is not available, then one must use that of the linearized problem. This leads to a self-consistent approximation for the moments and for the linearization parameters. The procedure is then equivalent to a Gaussian closure of the moment equations followed by the use of these moments to calculate the parameters of the linearized system.

Statistical linearization is a particularly useful technique for the calculation of steady state (time-independent) low-order moments. It has been shown that better accuracy in the calculation of time-dependent properties can be achieved by using the instantaneous *time-dependent* distribution to calculate the moments that must be obtained to obtain the linearization parameters.[11–13] In other words, the parameters of the linear equation are allowed to vary with time and are determined by the time-dependent moments. The linear equation is thus nonstationary. Since the exact time-dependent distribution is not known, one must use that of the linearized problem. The moment equations are therefore solved via time-dependent Gaussian closure. We named our method AGREE (*a*pproximate *G*aussian *r*epresentation of *e*volution *e*quations).[13]

SDE's can be classified according to the way in which the fluctuations

occur in them. The simplest kind of SDE is one in which the fluctuations are independent of the dynamical variables.[14] These are referred to as additive fluctuations. Statistical linearization and AGREE have so far been developed for and applied to SDE's with additive fluctuations.[15] The next class of SDE's in order of complexity contains parametric fluctuations, i.e., fluctuations that occur in the coefficients of functions of the dynamical variables. These are referred to as multiplicative fluctuations. Because of the multiplicative nature of the fluctuations, *all* such equations are nonlinear. The final class involves fluctuations that are not factorable from the dynamical variables. Almost nothing is known about the properties of the SDE's in the latter class, and we will not discuss them further. Herein we extend the technique AGREE to multivariable equations with δ-correlated multiplicative fluctuations.

Many physical phenomena are described by SDE's with multiplicative fluctuations. Examples include such phenomena as wave propagation through random media in which the index of refraction is a stochastic quantity,[16,17] chemical reactions with fluctuating rate coefficients,[18,19] laser emission with a fluctuating pump parameter,[20] diffusion of a passive scalar in a turbulent fluid,[21] and transport of excitons in molecular chains at finite temperatures.[22,23] One can distinguish two types of multiplicative fluctuations. There are those fluctuations occurring in thermodynamically open systems in which the environment does not respond to the dynamics of the system. Such systems need not be asymptotically stable, i.e., it is possible that they never achieve a steady state and may in fact become unstable.[18] It is also well known that some systems of this type can display very interesting fluctuation-induced organizational properties.[18] A thermodynamically closed system, on the other hand, necessarily achieves equilibrium asymptotically. This requires that the fluctuations be balanced by appropriate dissipative terms in the SDE.[24] When the fluctuations are additive, the dissipation is linear in the dynamical variables of the system. Multiplicative fluctuations require the dissipation to be nonlinear in the dynamical variables.[24,25] In either case there exists a fluctuation–dissipation relation (FDR) that guarantees the attainment of a steady state. In thermodynamically closed systems there is thus a constraint on the linearization technique whereby the resulting linear equation should itself obey some balancing condition that insures equilibration to the same temperature as the original nonlinear equation. This additional physical constraint on the linearization technique has not been previously addressed.

In Section 2 we review the methods of statistical linearization and AGREE as developed for nonlinear systems with additive fluctuations. In Section 3 we develop analogous techniques for approximating systems with multiplicative fluctuations in both thermodynamically open and closed

systems. In that section we also touch upon the difficulties associated with approximating systems with multiple stationary states. A number of conclusions about these techniques are summarized in Section 4.

2. ADDITIVE FLUCTUATIONS

Let us review the linearization techniques for a single-degree-of-freedom nonlinear system with additive fluctuations.[6-10] Consider a Langevin equation of the form

$$\dot{x} = F(x) + \xi(t) \tag{2.1}$$

where $F(x)$ is a nonlinear function of the dynamical variable and $\xi(t)$ is a stochastic function of time. The intent of linearization techniques is to replace this equation with a suitably chosen "best" linear equation.

2.1. Statistical Linearization

In statistical linearization the "best" linear equation is of the form

$$\dot{x} = \alpha + \beta x + \xi(t) \tag{2.2}$$

where the constant variational parameters α and β are determined by minimizing the mean square value of the error

$$\varepsilon \equiv F(x) - \alpha - \beta x \tag{2.3}$$

made in the steady state by the replacement. From the variational conditions $\partial\langle\varepsilon^2\rangle/\partial\alpha = \partial\langle\varepsilon^2\rangle/\partial\beta = 0$ one finds the relations

$$\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = M_2^{-1}\begin{pmatrix}\langle F(x)\rangle_s\\ \langle xF(x)\rangle_s\end{pmatrix} \tag{2.4}$$

where M_2 is the 2×2 moment matrix

$$M_2 = \begin{pmatrix}1 & \langle x\rangle_s\\ \langle x\rangle_s & \langle x^2\rangle_s\end{pmatrix} \tag{2.5}$$

Explicit inversion of (2.5) is trivial and yields

$$\alpha = \frac{\langle x^2\rangle_s\langle F(x)\rangle_s - \langle x\rangle_s\langle xF(x)\rangle_s}{\langle x^2\rangle_s - \langle x\rangle_s^2} \tag{2.6}$$

$$\beta = \frac{\langle xF(x)\rangle_s - \langle x\rangle_s\langle F(x)\rangle_s}{\langle x^2\rangle_s - \langle x\rangle_s^2} \tag{2.7}$$

The steady state average $\langle\ \rangle_s$ indicated in Eqs. (2.4)–(2.7) is taken over an ensemble of realizations of the stochastic function $\xi(t)$ at long times t. This average is equivalent to an average over an ensemble of the corresponding realizations of the dynamical variable. This latter ensemble is specified by a steady state phase space density $P_s(x)$, so that for any function $G(x)$ we have

$$\langle G(x)\rangle_s \equiv \int dx\, G(x)\, P_s(x) \tag{2.8}$$

With this prescription it can be seen by direct calculation that (2.2) with (2.6) and (2.7) gives exactly the same equations for the first two moments $\langle x\rangle_s$ and $\langle x^2\rangle_s$ as does the original nonlinear equation (2.1) at equilibrium.

In order to complete the above algorithm one must specify the probability density $P_s(x)$. This in turn requires knowledge of the statistical properties of $\xi(t)$. If the fluctuations are Gaussian, zero centered ($\langle\xi\rangle = 0$), and with correlation function

$$\langle\xi(t)\,\xi(\tau)\rangle = 2D\delta(t-\tau) \tag{2.9}$$

then $P_s(x) = \lim_{t\to\infty} P(x, t)$ is the steady state solution of the Fokker–Planck equation associated with (2.1):

$$\frac{\partial}{\partial t} P(x, t) = \left[-\frac{\partial}{\partial x} F(x) + D\frac{\partial^2}{\partial x^2}\right] P(x, t) \tag{2.10}$$

Direct integration of (2.10) with the left-hand side set to zero gives

$$P_s(x) = \frac{\exp\left[-D^{-1}\int_{-\infty}^{x} F(x')\,dx'\right]}{\int_{-\infty}^{\infty} dx \exp\left[-D^{-1}\int_{-\infty}^{x} F(x')\,dx'\right]} \tag{2.11}$$

Use of (2.11) in (2.6) and (2.7) then yields explicit values for α and β in the linear equation (2.2).

If the steady state solution $P_s(x)$ cannot be obtained (e.g., for most multivariable processes), then the averages in (2.6) and (2.7) must be calculated using the steady state distribution $W_s(x)$ for the linearized process, i.e., the $t\to\infty$ solution of the Fokker–Planck equation

$$\frac{\partial}{\partial t} W(x, t) = \left[-\frac{\partial}{\partial x}(\alpha+\beta x) + D\frac{\partial^2}{\partial x^2}\right] W(x, t) \tag{2.12}$$

This distribution is Gaussian and depends on the linearization parameters α and β:

$$W_s(x) = \frac{\exp[-D^{-1}(\alpha x + \beta x^2/2)]}{\int_{-\infty}^{\infty} dx \exp[-D^{-1}(\alpha x + \beta x^2/2)]} \tag{2.13}$$

Use of this distribution in (2.6) and (2.7) gives equations in which α and β appear on both sides. Their solution then gives self-consistent approximations to the more exact values obtained from the exact distribution. It can easily be checked that this procedure is equivalent to the determination of α and β via the closure of the first- and second-moment equations obtained from (2.1) as $t \to \infty$.

2.2. AGREE[13]

The method AGREE replaces (2.1) with a linear equation of the form

$$\dot{x} = \alpha(t) + \beta(t)x + \xi(t) \tag{2.14}$$

The deterministic functions $\alpha(t)$ and $\beta(t)$ are time dependent and are determined by minimizing at each time the mean-squared error resulting from the replacement of $F(x)$ by $[\alpha(t) + \beta(t)x]$. The mean square error is

$$\langle \varepsilon^2(t) \rangle = \langle [F(x) - \alpha(t) - \beta(t)x]^2 \rangle \tag{2.15}$$

The average $\langle\ \rangle$ is taken over an ensemble of realizations of the stochastic function $\xi(t)$ *at time* t or, alternately, over the corresponding realizations of $x(t)$ as specified by the time-dependent phase space density $P(x, t)$. Thus for any function $G(x)$ we have

$$\langle G(x) \rangle \equiv \int dx\, G(x)\, P(x, t) \tag{2.16}$$

The derivative conditions $\partial \langle \varepsilon^2 \rangle / \partial \alpha(t) = \partial \langle \varepsilon^2 \rangle / \partial \beta(t) = 0$ then lead to equations (2.4) and (2.5) and hence to (2.6) and (2.7) for $\alpha(t)$ and $\beta(t)$ but with the stationary averages $\langle\ \rangle_s$ replaced by the time-dependent averages $\langle\ \rangle$:

$$\alpha(t) = \frac{\langle x^2 \rangle \langle F(x) \rangle - \langle x \rangle \langle xF(x) \rangle}{\langle x^2 \rangle - \langle x \rangle^2} \tag{2.17}$$

$$\beta(t) = \frac{\langle xF(x) \rangle - \langle x \rangle \langle F(x) \rangle}{\langle x^2 \rangle - \langle x \rangle^2} \tag{2.18}$$

The transport equations for the first two moments $\langle x \rangle$ and $\langle x^2 \rangle$ obtained from (2.14) with (2.17) and (2.18) are identical to those obtained from the original nonlinear equation (2.1) at all times.

Since it is precisely the density $P(x, t)$ that is unknown, a further approximation must again be made: the averages in (2.17) and (2.18) must be evaluated using the probability density $W(x, t)$, i.e., the solution of the Fokker–Planck equation (2.12). Since the solution clearly depends on the functions $\alpha(t)$ and $\beta(t)$, (2.17) and (2.18) then become self-consistent (*integral*) equations for these functions. The resulting equations are most straightforwardly expressed as follows. The density function $W(x, t)$ is a Gaussian with time-dependent mean $s(t)$ and variance $v(t)$:

$$W(x, t) = [2\pi v(t)]^{-1/2} \exp\{-[x - s(t)]^2 / 2v(t)\} \tag{2.19}$$

The mean and variance are uniquely related to $\alpha(t)$ and $\beta(t)$ via the differential relations

$$\dot{s}(t) = \int x \frac{\partial}{\partial t} W(x, t)\, dx = \alpha(t) + \beta(t)\, s(t) \tag{2.20a}$$

$$\dot{v}(t) = \int x^2 \frac{\partial}{\partial t} W(x, t)\, dx - 2s(t)\, \dot{s}(t) = 2\beta(t)\, v(t) + 2D \tag{2.20b}$$

The use of Eqs. (2.20) together with (2.17) and (2.18) with the averages evaluated using (2.19) provides a self-consistent algorithm for the evaluation of $\alpha(t)$ and $\beta(t)$. Note that the procedure just outlined is equivalent to a time-dependent Gaussian closure of the moment equations.

We end this section by pointing out that the accuracy of the methods reviewed above has been tested by us and by others for a variety of examples including generalizations to many degrees of freedom. We refer the reader to some appropriate references.[11–13,26–29] Suffice it here to say that the accuracy is excellent for a variety of systems over wide ranges of parameter values in the original nonlinear equations.

3. MULTIPLICATIVE FLUCTUATIONS

3.1. Statistical Replacement

Let us now consider a more general process governed by the SDE

$$(\mathrm{S}) \quad \dot{\mathbf{x}} = \mathbf{F}(\mathbf{x}) + \mathbf{g}(\mathbf{x})\, \xi(t) \tag{3.1}$$

where $\xi(t)$ is a random vector with the following statistical properties:

$$\langle \xi(t) \rangle = \mathbf{0} \tag{3.2}$$

$$\langle \xi(t)\, \xi^T(\tau) \rangle = 2\mathbf{d}\, \delta(t-\tau) \tag{3.3}$$

with all higher cumulants being zero. Thus the components $\xi_i(t)$ of the random vector $\xi(t)$ are mutually dependent, each with Gaussian statistics of zero mean, δ correlated in time, and constant correlation elements d_{jk}. It is well known that the choice of white noise in (3.1) requires one to specify the calculus to be used in defining the SDE.[30] We have chosen to interpret (3.1) in the Stratonovich sense since we are concerned with physical systems for which the correlation time of the fluctuations is small but nonzero. The same equation when written as an Itô SDE takes the form

$$\text{(I)}\quad \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})\, \xi(t) \tag{3.4}$$

where the vector $\mathbf{f}(\mathbf{x})$ has components

$$f_i(\mathbf{x}) = F_i(\mathbf{x}) + \sum_{j,k,l} \left[\frac{\partial}{\partial x_k}\, g_{ij}(\mathbf{x}) \right] d_{jl}\, g_{kl}(\mathbf{x}) \tag{3.5}$$

A significant difference between the Itô and the Stratonovich specification of integration lies in the average time integral of the fluctuating term $\mathbf{g}(\mathbf{x})\, \xi(t)$. The average of the Itô integral is zero whereas the corresponding Stratonovich integral need not vanish on the average. It is precisely this correlation that is added to $\mathbf{F}(\mathbf{x})$ to get $\mathbf{f}(\mathbf{x})$.

The many-degree-of-freedom Fokker–Planck equation associated with (3.1) is

$$\frac{\partial}{\partial t} P(\mathbf{x}, t) = -\sum_i \frac{\partial}{\partial x_i} [F_i(\mathbf{x})\, P(\mathbf{x}, t)] + \sum_{j,k,l,m} d_{km} \frac{\partial}{\partial x_j} \left\{ g_{jk}(\mathbf{x}) \frac{\partial}{\partial x_l} [g_{lm}(\mathbf{x})\, P(\mathbf{x}, t)] \right\} \tag{3.6}$$

In terms of the drift vector $\mathbf{f}(\mathbf{x})$ and the diffusion tensor $\mathbf{D}(\mathbf{x})$ with components

$$D_{jk}(\mathbf{x}) = \sum_{l,m} g_{jl}(\mathbf{x})\, d_{lm}\, g_{km}(\mathbf{x}) \tag{3.7}$$

the Fokker–Planck equation (3.6) can also be written as

$$\frac{\partial}{\partial t} P(\mathbf{x}, t) = -\sum_i \frac{\partial}{\partial x_i} [f_i(\mathbf{x})\, P(\mathbf{x}, t)] + \sum_{j,k} \frac{\partial^2}{\partial x_j\, \partial x_k} [D_{jk}(\mathbf{x})\, P(\mathbf{x}, t)] \tag{3.8}$$

This second form could have been written down directly from (3.4).

As is well known, such general SDE's and/or their associated Fokker–Planck equations are usually intractable. This is precisely the set of equations for which we intend to generalize the linearization techniques discussed in the previous section. We thus intend to approximate (3.1) [i.e., (3.4)] with a more tractable SDE, again chosen so as to minimize the error made by this replacement.

General nonlinear SDE's such as (3.1) with multiplicative fluctuations arise from a variety of physical problems. From a practical viewpoint, it is desirable that the simpler equation used to approximate a general SDE be able to reproduce the salient features of the physical problem described by the original equation. In other words one should avoid simplifying the equation to the extent of losing important qualitative aspects of the physical system. The simpler equation used in the method of statistical linearization discussed in the previous section is a linear SDE with additive noise. At the outset we note that there are some definite qualitative properties associated with such a linear equation and therefore it should be used only to approximate a class of general equations which themselves exhibit these same qualitative properties. Thus it becomes necessary to associate a solvable simple equation to each class of SDE. The particular classification is motivated by the associated physical systems.

In the Introduction we classified SDE's according to the manner in which the fluctuations appear in the equation. Having specialized to a particular kind of equation (3.1) we then refined the classification according to whether or not the SDE describes a thermodynamically closed system. There exists a special class of closed systems which exhibit unique characteristics not associated with other closed systems. A typical member of this class is a Brownian particle moving in a bistable potential. We reserve this type of closed system as a separate class in itself.

Having recognized these three classes, we proceed to replace all the complicated SDE's in a class with a corresponding equation of the simplest form belonging to the *same* class. Since not all SDE's can be replaced with a linear equation, we propose the name "statistical replacement" for the procedure developed here.

3.2. Closed Systems with a Single Stationary State

3.2.1. Extension of AGREE. If a closed system has a single stationary state, the laws of thermodynamics dictate that the system approach this state asymptotically in time. If the dynamics of the system is described by a SDE, then the corresponding probability distribution describing the system asymptotically approaches a unimodal stationary distribution. Since this requirement applies to all equations in this class and

since this asymptotic stability is an immensely important physical property, we seek the simplest forms of SDE's consistent with this property as approximations to the more complicated equations in this class. From several candidate SDE's we select

$$\dot{\mathbf{x}} = \boldsymbol{\alpha} + \boldsymbol{\beta}\mathbf{x} + \boldsymbol{\gamma}\boldsymbol{\xi}(t) \tag{3.9a}$$

This equation is linear and can be formally solved. In order to keep the simplification to a minimum we selected the most general SDE that can be solved exactly and at the same time retains the required property of asymptotic stability.

Now the parameters $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ are to be chosen in such a way that the error made in approximating (3.1) with (3.9a) is a minimum. We first attempt an error minimization in the usual manner in order to emphasize that it is sometimes necessary to treat SDE's with white noise with some care. Following the procedure adopted in Section 2 we calculate the error by "subtracting" the right-hand side of Eqs. (3.4) and (3.9a):

$$\boldsymbol{\varepsilon} = \mathbf{f}(\mathbf{x}) - \boldsymbol{\alpha} - \boldsymbol{\beta}\mathbf{x} + [\mathbf{g}(\mathbf{x}) - \boldsymbol{\gamma}]\boldsymbol{\xi}(t) \tag{3.9b}$$

This expression contains the white noise $\boldsymbol{\xi}(t)$ explicitly. Clearly the single time correlation matrix $\langle \boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^T \rangle$ involves the mean square of white noise, $\langle \xi_i^2 \rangle$ which is an ill-defined quantity. Thus we are faced with the problem of finding a more appropriate quantity (or quantities!) to minimize in such replacement(s).

Now we argue that there are two linearly independent quantities to consider in the general SDE with multiplicative noise and we determine them. A SDE describes two kinds of motion, namely, drift and diffusion. When an ensemble of random paths described by the SDE is considered, the mean rate of change of the random variables is given by the ensemble average of the drift component given by Eq. (3.5), and the fluctuations around this mean path are contained in the coefficient of the noise term $[\mathbf{g}(\mathbf{x})$ in Eqs. (3.1) and (3.4)]. Thus the functions $\mathbf{f}(\mathbf{x})$ and $\mathbf{g}(\mathbf{x})$ play different roles. In other words, a stochastic process constructed by superimposing any diffusive motion (of the factorable white noise type) on any drift motion can be described by Eqs. (3.1)–(3.8). Moreover, the mapping (3.7) from $\mathbf{g}(\mathbf{x})$ to $\mathbf{D}(\mathbf{x})$ is many-to-one. Even though the diffusion tensor $\mathbf{D}(\mathbf{x})$ is defined from $\mathbf{g}(\mathbf{x})$ uniquely, $\mathbf{g}(\mathbf{x})$ cannot be determined from a given $\mathbf{D}(\mathbf{x})$. The solutions of all SDE's with different $\mathbf{g}(\mathbf{x})$ corresponding to the same $\mathbf{D}(\mathbf{x})$ are statistically equivalent. For example, the equation

$$\text{(I)}\quad \dot{x} = f(x) + [g_1(x)\ \ g_2(x)] \begin{pmatrix} \xi_1(t) \\ \xi_2(t) \end{pmatrix} \tag{3.10a}$$

as well as the equation

$$(\mathrm{I})\quad \dot{x} = f(x) + \left[g_1^2(x) + 2\frac{d_{12}}{d_{11}} g_1(x)\, g_2(x) + \frac{d_{22}}{d_{11}} g_2^2(x) \right]^{1/2} \xi_1(t) \qquad (3.10b)$$

give rise to the same diffusion coefficient, namely,

$$D_{11}(x) = d_{11}\, g_1^2(x) + 2d_{12}\, g_1(x)\, g_2(x) + d_{22}\, g_2^2(x) \qquad (3.10c)$$

and hence to the same Fokker–Planck equation. To illustrate further the fundamental roles played by the functions $\mathbf{f}(\mathbf{x})$ and $\mathbf{D}(\mathbf{x})$, let us consider the transition probability of the process $\mathbf{x}(t)$,

$$\Pi_{\mathbf{x}}(\Delta\mathbf{x}, \Delta t)\, d\Delta\mathbf{x} = P(\mathbf{x} + \Delta\mathbf{x}, t + \Delta t \,|\, \mathbf{x}, t)\, d\Delta\mathbf{x} \qquad (3.11)$$

Equation (3.11) gives the probability of an increment $\Delta\mathbf{x}$ within the interval Δt given that the process is $\mathbf{x}$ at time t. It is well known that the first and second moments of the increment $\Delta\mathbf{x}$ are given by

$$\langle \Delta\mathbf{x} \rangle_{\mathbf{x}} \equiv \int \Delta\mathbf{x} \Pi_{\mathbf{x}}(\Delta\mathbf{x}, t)\, d\Delta\mathbf{x} = \mathbf{f}(\mathbf{x})\, \Delta t + o(\Delta t) \qquad (3.12)$$

and

$$\langle \Delta\mathbf{x}\, \Delta\mathbf{x}^T \rangle_{\mathbf{x}} = \mathbf{D}(\mathbf{x})\, \Delta t + o(\Delta t) \qquad (3.13)$$

Therefore, for parameterizing a given SDE we choose the drift vector $\mathbf{f}(\mathbf{x})$ and the diffusion tensor $\mathbf{D}(\mathbf{x})$ rather than choosing $\mathbf{f}(\mathbf{x})$ and $\mathbf{g}(\mathbf{x})$. With this parametrization the set of all SDE's of the form (3.1) can be viewed as a linear space spanned by a "unit drift" and a "unit diffusion," $\mathbf{f}(\mathbf{x})$ and $\mathbf{D}(\mathbf{x})$ being the coefficients of drift and diffusion, respectively.[3]

Based on the *complete* representation of a SDE of the form (3.1) by the drift vector and the diffusion tensor, we propose the following procedure for constructing an approximate SDE of the form (3.9) from the original nonlinear SDE. We replace the drift vector $\mathbf{f}(\mathbf{x})$ by the approximate drift vector $\boldsymbol{\alpha}(t) + \boldsymbol{\beta}(t)\mathbf{x}$ in such a way that the error in this replacement, namely,

$$\boldsymbol{\varepsilon}_1 = \boldsymbol{\alpha} + \boldsymbol{\beta}\mathbf{x} - \mathbf{f}(\mathbf{x}) \qquad (3.14)$$

[3] It should be noted that for a Markov process any multiple-time distribution function can be written as a product of two-time distribution functions each of which is a solution to the Fokker–Planck equation. Hence specification of the drift vector $\mathbf{f}(\mathbf{x})$ and diffusion tensor $\mathbf{D}(\mathbf{x})$ are sufficient to also uniquely determine higher-order moment properties of the process.

is minimized in the mean square sense. We also replace the diffusion tensor $\mathbf{D}(\mathbf{x})$ by the approximate diffusion tensor $\gamma(t)\,d\gamma^T(t)$ and again minimize the error

$$\varepsilon_2 = \gamma\, d\gamma^T - \mathbf{D}(\mathbf{x}) \tag{3.15}$$

in this replacement. Minimizing $\langle \varepsilon_1 \varepsilon_1{}^T \rangle$ with respect to $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ we obtain the set of equations

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

and

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

$\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are uniquely determined by solving this set of algebraic equations. Similarly, minimization of $\langle \varepsilon_2 \varepsilon_2^T \rangle$ yields the equation

$$\gamma\, d\gamma^T = \langle \mathbf{D}(\mathbf{x}) \rangle \tag{3.18}$$

Since the moments $\langle \mathbf{x} \rangle$, $\langle \mathbf{x}\mathbf{x}^T \rangle$, etc. are in general time dependent, we take the parameters $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ and γ as functions of time so that $\boldsymbol{\alpha}(t)$, $\boldsymbol{\beta}(t)$ and $\gamma(t)$ are given by the values of the moments at time t. Thus we have replaced the original nonlinear equation (3.1) by the linear additive equation

$$\dot{\mathbf{x}} = \boldsymbol{\alpha}(t) + \boldsymbol{\beta}(t)\mathbf{x} + \mathbf{h}(t) \tag{3.19}$$

where $\mathbf{h}(t)$ is a zero-centered, Gaussian, nonstationary random process with correlation function

$$\langle \mathbf{h}(t)\, \mathbf{h}^T(\tau) \rangle = 2\boldsymbol{\mu}(t)\, \delta(t-\tau) \tag{3.20}$$

and where $\boldsymbol{\mu}(t)$ is given by the error minimization as

$$\boldsymbol{\mu}(t) = \langle \mathbf{D}(\mathbf{x}) \rangle \tag{3.21}$$

Even though $\mathbf{h}(t)$ is nonstationary, the form of the correlation function (3.20) as a product involving a δ function implies that $\mathbf{h}(t)$ can be factored into a stationary white noise and a function of time. The distribution for the linearized problem is a multivariate Gaussian with time-dependent parameters.

Strictly speaking the averages indicated on the right-hand side of Eqs. (3.16)–(3.18) are to be performed using the distribution obtained by solv-

ing the exact Fokker–Planck equation (3.8), whereas those on the left-hand side are over the Gaussian distribution for the linearized problem. From the Fokker–Planck equation (3.6) one can derive the following equations for the time evolution of the first and the second moments:

$$\frac{d}{dt}\langle \mathbf{x} \rangle = \langle \mathbf{f} \rangle \tag{3.22}$$

$$\frac{d}{dt}\langle \mathbf{x}\mathbf{x}^T \rangle = \langle \mathbf{f}\mathbf{x}^T \rangle + \langle \mathbf{x}\mathbf{f}^T \rangle + 2\langle \mathbf{D} \rangle \tag{3.23}$$

These are the exact moment equations obtained from the original SDE. The linearized equation (3.19) yields for the moment equations

$$\frac{d}{dt}\langle \mathbf{x} \rangle = \boldsymbol{\alpha}(t) + \boldsymbol{\beta}(t)\langle \mathbf{x} \rangle \tag{3.24}$$

and

$$\frac{d}{dt}\langle \mathbf{x}\mathbf{x}^T \rangle = \boldsymbol{\alpha}(t)\langle \mathbf{x}^T \rangle + \langle \mathbf{x} \rangle \boldsymbol{\alpha}^T(t) + \boldsymbol{\beta}(t)\langle \mathbf{x}\mathbf{x}^T \rangle + \langle \mathbf{x}\mathbf{x}^T \rangle \boldsymbol{\beta}^T(t) + 2\boldsymbol{\mu}(t) \tag{3.25}$$

By virtue of Eqs. (3.16)–(3.18) these moment equations derived from the linear equation are identical to the exact ones (3.22) and (3.23). Thus the approximation involving separate error minimizations for the drift and the diffusion coefficients reproduces the first two moment equations exactly.

The explicit expressions for $\boldsymbol{\alpha}(t)$ and $\boldsymbol{\beta}(t)$ obtained by solving Eqs. (3.16) and (3.17) are the multidimensional generalization of Eqs. (2.17) and (2.18):

$$\boldsymbol{\beta}(t) = [\langle \mathbf{f}\mathbf{x}^T \rangle - \langle \mathbf{f} \rangle \langle \mathbf{x}^T \rangle][\langle \mathbf{x}\mathbf{x}^T \rangle - \langle \mathbf{x} \rangle \langle \mathbf{x}^T \rangle]^{-1} \tag{3.26}$$

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

The final step in the implementation of this prescription is the calculation of the averages in (3.26) and (3.27). Again one uses the distribution for the linearized problem, not only for $\langle \mathbf{x} \rangle$ and $\langle \mathbf{x}\mathbf{x}^T \rangle$ but also for $\langle \mathbf{f} \rangle$ and $\langle \mathbf{f}\mathbf{x}^T \rangle$. As before we obtain a set of ordinary differential equations from which the parameters are determined self-consistently.

The predictions of our results in a few special cases should be noted. If $\mathbf{g}(\mathbf{x})$ is a matrix with constant elements (additive noise), then (3.23) leaves the fluctuations unchanged. The present scheme then reduces to the old AGREE. If the drift vector $\mathbf{f}(\mathbf{x})$ is linear in $\mathbf{x}$ and the fluctuations are mul-

tiplicative, then the present scheme leaves the drift term unchanged and replaces the multiplicative fluctuations by additive ones.

3.2.2. Anharmonic Oscillator as Example. Just as the harmonic oscillator is the workhorse for the description of linear phenomena, so too is the anharmonic oscillator for modeling nonlinear phenomena. We too shall test our ideas on this generic system. The multiplicative fluctuations arise as rapid variations in the frequency of such an oscillator.

Let us consider the displacement x and momentum p of an oscillator of unit mass moving in a potential $V(x)$. We have shown elsewhere[25] that such an oscillator interacting in a particular nonlinear fashion with an initially equilibrated bath of oscillators can be described by the stochastic evolution equations

$$\dot{x} = p \tag{3.28a}$$

$$\dot{p} = -V'(x) - B(x)\, p + A_1(x)\, \xi_1(t) + A_2(x)\, \xi_2(t) \tag{3.28b}$$

where $B(x)$, $A_1(x)$, and $A_2(x)$ depend on the assumed system–bath interactions. The fluctuations $\xi_i(t)$ are Gaussian and δ correlated, with

$$\langle \xi_i(t)\, \xi_j(\tau) \rangle = 2kT\lambda_{ij}\, \delta(t-\tau) \tag{3.29}$$

and

$$B(x) = \lambda_{11} A_1^2(x) + 2\lambda_{12} A_1(x)\, A_2(x) + \lambda_{22} A_2^2(x) \tag{3.30}$$

In (3.29) T is the initial temperature of the bath, and (3.29) and (3.30) constitute the fluctuation–dissipation relation that ensures eventual equilibration of the oscillator with the environment at temperature T. We will return to a detailed discussion of this relation in Section 3.2.3.

Now we wish to apply the scheme developed in Section 3.2.1 to Eq. (3.28). Our aim is to replace the set of equations (3.28) with the set of linear equations

$$\dot{x} = \alpha_1 + \beta_{11} x + \beta_{12} p + h_1(t) \tag{3.31a}$$

$$\dot{p} = \alpha_2 + \beta_{21} x + \beta_{22} p + h_2(t) \tag{3.31b}$$

Equations (3.26) and (3.27) for the variational parameters yield

$$\alpha_1 = 0, \qquad \beta_{11} = 0, \qquad \beta_{12} = 1 \tag{3.32}$$

$$\begin{aligned} \alpha_2 = [&\langle Q \rangle (\langle x^2 \rangle \langle p^2 \rangle - \langle xp \rangle^2) - \langle xQ \rangle (\langle x \rangle \langle p^2 \rangle - \langle xp \rangle \langle p \rangle) \\ &+ \langle pQ \rangle (\langle x \rangle \langle xp \rangle - \langle x^2 \rangle \langle p \rangle)]/\mathrm{DET} \end{aligned} \tag{3.33}$$

$$\beta_{21} = [-\langle Q\rangle(\langle x\rangle\langle p^2\rangle - \langle p\rangle\langle xp\rangle) + \langle xQ\rangle(\langle p^2\rangle - \langle p\rangle^2) - \langle pQ\rangle(\langle xp\rangle - \langle x\rangle\langle p\rangle)]/\mathrm{DET} \tag{3.34}$$

$$\beta_{22} = [\langle Q\rangle(\langle x\rangle\langle xp\rangle - \langle x^2\rangle\langle p\rangle) - \langle xQ\rangle(\langle xp\rangle - \langle x\rangle\langle p\rangle) + \langle pQ\rangle(\langle x^2\rangle - \langle x\rangle^2)]/\mathrm{DET} \tag{3.35}$$

where

$$Q = -V'(x) - B(x)\,p \tag{3.36}$$

and

$$\mathrm{DET} = \langle x^2\rangle\langle p^2\rangle - \langle xp\rangle^2 - \langle x\rangle^2\langle p^2\rangle + 2\langle x\rangle\langle p\rangle\langle xp\rangle - \langle x^2\rangle\langle p\rangle^2 \tag{3.37}$$

Applying Eq. (3.20) yields

$$h_1(t) = 0 \tag{3.38a}$$

$$h_2(t) = (\langle B(x)\rangle/\lambda_{11})^{1/2}\,\xi_1(t) \tag{3.38b}$$

Therefore, the linearized equation is

$$\dot{x} = p \tag{3.39a}$$

$$\dot{p} = \alpha_2 + \beta_{21}x + \beta_{22}\,p + (\langle B(x)\rangle/\lambda_{11})^{1/2}\,\xi_1(t) \tag{3.39b}$$

We have written the expressions (3.33)–(3.35) for a general potential $V(x)$ and general interaction function $B(x)$. For a numerical test of the results obtained from the linearized equation it is necessary to specialize to particular functions for $V(x)$ and $B(x)$. The simplest multiplicative fluctuations are obtained if in Eq. (3.28)

$$A_1(x) = 1, \qquad A_2(x) = x \tag{3.40}$$

For the potential $V(x)$ in (3.28) we select

$$V(x) = \tfrac{1}{2}\omega_0^2 x^2 + \tfrac{1}{4}bx^4 \tag{3.41}$$

In previous applications we have analyzed in detail the effect of the quartic term in $V(x)$ when $A_2(x) = 0$, i.e., with additive fluctuations.[13] Here we study the cases of multiplicative fluctuations with both harmonic ($b = 0$) and anharmonic ($b \neq 0$) potentials.

Consider, then, the SDE

$$\dot{x} = p \tag{3.42a}$$

$$\dot{p} = -\omega_0^2 x - bx^3 - (\lambda_{11} + 2\lambda_{12}x + \lambda_{22}x^2)\,p + \xi_1(t) + x\xi_2(t) \tag{3.42b}$$

together with (3.29). The properties of (3.42) are to be reproduced by those of the linear Eq. (3.39). Of course a direct comparison of the moment

properties of the two would in general require the numerical solution of (3.42). We have elsewhere[25] been able to obtain an exact analytic expression for the average energy envelope

$$\langle E\rangle = \tfrac{1}{2}\langle p^2\rangle + \langle V(x)\rangle \tag{3.43}$$

of Eq. (3.42) in the limit of weak damping, thus providing us with an alternative test of the utility of the above method. The average energy envelope is given in terms of the initial energy $E_0 \equiv E(0)$ by

$$\langle E\rangle = \frac{kT(E_0 + ckT) - ckT(kT - E_0)\, e^{-(1+c^{-1})\lambda_{11} t}}{(E_0 + ckT) - (kT - E_0)\, e^{-(1+c^{-1})\lambda_{11} t}} \tag{3.44}$$

with the weak damping condition

$$\lambda_{11} + \frac{kT\lambda_{22}}{\omega_0^2} \ll b \tag{3.45}$$

and where

$$c = \lambda_{11}\omega_0^2/\lambda_{22}\, kT \tag{3.46}$$

The average energy envelope of the linearized system in terms of the first and second moments is

$$\langle E\rangle_{\text{lin}} = \tfrac{1}{2}\langle p^2\rangle + \tfrac{1}{2}\omega_0^2\langle x^2\rangle + \tfrac{1}{4}b[3\langle x^2\rangle^2 - 2\langle x\rangle^4] \tag{3.47}$$

The evolution equations for the moments are obtained by combining equations (3.24) and (3.25) with the expressions (3.32)–(3.35) for the parameters $\boldsymbol{\alpha}(t)$ and $\boldsymbol{\beta}(t)$. The resulting equations are

$$\frac{d}{dt}\langle x\rangle = \langle p\rangle \tag{3.48}$$

$$\frac{d}{dt}\langle p\rangle = -\omega_0^2\langle x\rangle - b\langle x^3\rangle - \lambda_{11}\langle p\rangle - 2\lambda_{12}\langle xp\rangle - \lambda_{22}\langle x^2 p\rangle \tag{3.49}$$

$$\frac{d}{dt}\langle x^2\rangle = 2\langle xp\rangle \tag{3.50}$$

$$\frac{d}{dt}\langle xp\rangle = \langle p^2\rangle - \omega_0^2\langle x^2\rangle - b\langle x^4\rangle - \lambda_{11}\langle xp\rangle - 2\lambda_{12}\langle x^2 p\rangle - \lambda_{22}\langle x^3 p\rangle \tag{3.51}$$

$$\frac{d}{dt}\langle p^2\rangle = -2\omega_0^2\langle xp\rangle - 2b\langle x^3 p\rangle - 2\lambda_{11}\langle p^2\rangle - 4\lambda_{12}\langle xp^2\rangle - 2\lambda_{22}\langle x^2 p^2\rangle + 2kT(\lambda_{11} + 2\lambda_{12}\langle x\rangle + \lambda_{22}\langle x^2\rangle) \tag{3.52}$$

Table I. Comparison of Energy Envelope from the Linearized Equation with the Exact Limiting Expression. The Parameter Values Are $\lambda_{11}=\lambda_{12}=\lambda_{22}=kT=1$; $\omega_0=50$ and $b=1$

Time	Linear	Exact
0.0	3.125	3.125
0.5	2.283	2.286
1.0	1.775	1.780
1.5	1.469	1.473
2.0	1.284	1.287
2.5	1.172	1.174
3.0	1.105	1.105
3.5	1.064	1.064
4.0	1.039	1.039
4.5	1.024	1.023
5.0	1.014	1.014

The time-dependent moments are obtained by solving these differential equations with given initial conditions compatible with the values of E_0, the initial energy of the oscillator. Finally, the energy envelope is obtained from these moments through Eq. (3.47). In Tables I, II, and III we compare the exact energy envelope (3.43) with the approximate result (3.47) for various values of the parameters ω_0, b, and λ_{ij}. The two results are found to be in excellent agreement at all the times considered.

Table II. Comparison of Energy Envelope from the Linearization Equation with the Exact Limiting Expression. The Parameter Values Are $\lambda_{11}=\lambda_{12}=\lambda_{22}=kT=1$; $\omega_0=20$ and $b=1$

Time	Linear	Exact
0.0	0.0201	0.0201
0.2	0.1973	0.1985
0.4	0.3429	0.3444
0.6	0.4615	0.4637
0.8	0.5598	0.5612
1.0	0.6395	0.6410
1.2	0.7043	0.7063
1.4	0.7584	0.7597
1.6	0.8023	0.8034
1.8	0.8379	0.8391

Table III. Comparison of Energy Envelope from the Linearization Equation with the Exact Limiting Expression. The Parameter Values Are $\lambda_{11}=\lambda_{12}=\lambda_{22}=kT=1$; $\omega_0=50$ and $b=0$

Time	Linear	Exact
0.0	12.500	12.500
0.5	7.948	7.917
1.0	5.201	5.199
1.5	3.542	3.548
2.0	2.540	2.546
2.5	1.934	1.938
3.0	1.567	1.569
3.5	1.345	1.345
4.0	1.210	1.209
4.5	1.128	1.127
5.0	1.078	1.077

3.2.3. Fluctuation–Dissipation Relation (FDR). We mentioned in the Introduction the importance of having an FDR between the fluctuation and dissipation terms of the SDE describing a closed system. For the anharmonic oscillator in contact with a heat bath such a relation naturally emerges in the derivation of the SDE (3.28). This relation is given by the FDR contained in Eqs. (3.29) and (3.30) and ensures the proper thermal equilibration of the system. It also implies that if the drift term in Eq. (3.28) is linear, then the noise is additive. Obviously, if the noise is multiplicative, then the equation is necessarily nonlinear. Because the nonlinear SDE (3.28) describes a thermodynamically closed system, any approximation to it should also reflect this property. In particular, the fluctuations and dissipation in the approximate description should also balance at the *same* temperature as that of the nonlinear system. Thus if we want to approximate the nonlinear oscillator equation with a linear oscillator equation, we should make the noise additive. Otherwise, the fluctuation–dissipation relation present in the original equation would definitely be lost by the approximation scheme. This supports the choice of the constant diffusion tensor in the general linearized equation (3.9). It will be shown now that this linearization schemes indeed preserves a relation required for the thermal *equilibration* of the system, even though it may not be called an FDR in the anticipated sense.

Thus we seek a relation between $\beta_{22}(t)$ and the coefficient of the white noise in Eq. (3.39). For this purpose we consider a general potential $V(x)$ and a general interaction coefficient $B(x)$. Equation (3.35) gives $\beta_{22}(t)$ in

terms of some moments, which in turn can be expressed in terms of the first and second moments alone, because the distribution obtained by solving Eq. (3.39) is always Gaussian. The equilibrium values of the first two moments are easily obtained from the differential equations for the moments written down directly from Eq. (3.39). One finds that

$$\langle p \rangle_s = \langle xp \rangle_s = 0 \tag{3.53}$$

Using these and the factorizability of the moments of Gaussian variables, it can be shown that

$$\beta_{22,s} \equiv \lim_{t \to \infty} \beta_{22}(t) = -\langle B(x) \rangle_s \tag{3.54}$$

This relation can be called an asymptotic FDR and we argue that this relation plays the same role here as does the exact FDR contained in Eqs. (3.29) and (3.30). This exact relation is a *sufficient* condition for the existence of a stationary solution of the Fokker–Planck equation corresponding to the SDE (3.28). The Fokker–Planck equation for the nonstationary SDE (3.39) is of the form

$$\frac{\partial}{\partial t} P(x, p, t) = \mathscr{L}(t)\, P(x, p, t) \tag{3.55}$$

where $\mathscr{L}(t)$ is a time-dependent differential operator. Therefore, the stationary distribution $P(x, p, \infty)$ satisfies

$$\mathscr{L}(\infty)\, P(x, p, \infty) = 0 \tag{3.56}$$

The importance of the FDR is manifest in the existence of a solution to Eq. (3.56). Obviously Eq. (3.54) serves the purpose for the nonstationary equation. Of course in the case of a stationary SDE the operator $\mathscr{L}$ is time independent and hence asymptotic relations of the form (3.54) imply time-independent relations similar to Eqs. (3.29) and (3.30).

In summary we can state that the linearization procedure developed in Section 3.2.1 preserves the FDR present in the original oscillator equation.

3.3. Open System

3.3.1. Oscillator with an Instability. In contrast to closed systems, open systems need not reach a canonical stationary state as $t \to \infty$. Some open systems do not achieve *any* stationary state.[30] The fluctuations and dissipation in open systems need not be balanced since they result from distinct physical processes. As a result, when the dissipation is

unable to extract energy from the system at a sufficiently high rate the fluctuations can drive the system unstable. Classes of nonlinear oscillators have been studied as prototypes for such unstable systems. Herein we illustrate the method of *statistical replacement* applied to unstable systems using the nonlinear oscillator equations as examples.

A class of unstable oscillators is described by the SDE[31]

$$\begin{aligned} \dot{x} &= p \\ \dot{p} &= -\omega x^r - 2\lambda p + x^q \xi_1(t) + \xi_2(t) \end{aligned} \tag{3.57}$$

Because of the multiplicative fluctuation term $x^q \xi_1(t)$, Eq. (3.57) cannot satisfy a fluctuation–dissipation relation since the dissipation ($\lambda > 0$) is linear. In previous studies we have obtained equations for the energy distribution of such oscillators in the limit of weak damping, i.e., $\lambda \ll \omega$. Detailed analysis has shown that the stability properties of the oscillators depends on the discriminant

$$s = 2q - r - 1 \tag{3.58}$$

which measures the strength of the multiplicative fluctuations in relation to the steepness of the potential. A stationary distribution for the energy exists only if $s \leqslant 0$. When $s < 0$ all moments of the stationary energy distribution are finite and the ocillator is globally stable. However, the energy distribution is not of the Boltzmann form, but rather is

$$P(E) = c_1 E^{-c_2} \exp(-c_3 E^{c_4}) \tag{3.59}$$

where the c_i's are derived constants depending on the oscillator parameters. When $s = 0$, a normalizable stationary distribution is obtained only for a limited range of values of λ. Moreover, for each value of λ there is a critical value of m beyond which all moments $\langle E^n \rangle$ with $n \geqslant m$ diverge. Thus the parameter space of Eq. (3.57) is divided into stable and unstable regions for the oscillator.

As another example for this class of systems consider the Lorenz description of Bénard convection obtained by truncating the geophysical field equations to three degrees of freedom[32]:

$$\dot{x} = \sigma(y - x) \tag{3.60a}$$

$$\dot{y} = vx - y - xz \tag{3.60b}$$

$$\dot{z} = -vz + xy \tag{3.60c}$$

Knobloch[33] has shown that a further reduction of this set under appropriate conditions leads to a description of the form

$$\dot{x} = \sigma p \tag{3.61a}$$

$$\dot{p} = ax - bp - x\omega(t) \tag{3.61b}$$

where $p = y - x$, a and b are parameters, and $\omega(t) \equiv \sigma(z - \langle z \rangle)$ is assumed to be a zero-centered, Gaussian coefficient. By assuming $\omega(t)$ to be a stochastic process and neglecting its own dynamic origin, one loses the response of the surroundings (z) to the presence of the system (x and y). Therefore (3.61) is a SDE with "external" fluctuations which remain unbalanced by any associated dissipation.

Even though the stability properties of (3.57) were obtained from the energy distribution in a limiting case, a general study of systems described by Eq. (3.57) is very difficult. We explore the possibility of applying the method of statistical replacement to this class of systems.

An approximation method is usually suggested by the recognition of a physical property that simplifies the description. For the thermodynamically closed systems treated in the last section, the simplifying property is the existence of a stationary distribution guaranteed by the FDR. This suggested the use of Eq. (3.9). The class of open systems is lacking such a definite property to guide in the selection of the approximate equation to be used. However, in cases where an instability is indicated, we can formulate an approximate description using the simplest equation exhibiting the same instability. For example, the simplest case of Eq. (3.57) corresponds to the choices $r = q = 1$. In this special case the equation is formally linear (or quasilinear) even though the solution is not a Gaussian random variable. This case is much easier to study than the general case. The differential equations for the moments $\langle x^m p^n \rangle$ form a closed set and we can analyze the stability properties of these moments in addition to those of the energy moments.

Based on these considerations we propose to approximate (3.57) with the equation

$$\dot{x} = p \tag{3.62a}$$

$$\dot{p} = \alpha + \beta x + \gamma p + x h_1(t) + h_2(t) \tag{3.62b}$$

where $h_1(t)$ and $h_2(t)$ are mutually correlated white noise processes, i.e.,

$$\langle h_i(t)\, h_j(\tau) \rangle = 2\mu_{ij}\, \delta(t - \tau) \tag{3.63}$$

Equation (3.62) differs from all the approximate equations used so far in that it contains multiplicative fluctuations. Both in statistical linearization

and in AGREE a general SDE was replaced by one with additive noise. Here we show how a nonlinear multiplicative noise can be easily replaced with a linear multiplicative noise by following essentially the same procedure as in the case of closed systems.

The variational parameters α and β are again given by minimizing the mean square error in approximating the drift term. We find as before that

$$\alpha = -\omega[\langle x^r\rangle(\langle x^2\rangle\langle p^2\rangle - \langle xp\rangle^2) - \langle x^{r+1}\rangle(\langle x\rangle\langle p^2\rangle - \langle xp\rangle\langle p\rangle) + \langle x^r p\rangle(\langle x\rangle\langle xp\rangle - \langle x^2\rangle\langle p\rangle)]/\mathrm{DET} \tag{3.64a}$$

$$\beta = \omega[\langle x^r\rangle(\langle x\rangle\langle p^2\rangle - \langle p\rangle\langle xp\rangle) - \langle x^{r+1}\rangle(\langle p^2\rangle - \langle p\rangle^2) + \langle x^r p\rangle[\langle xp\rangle - \langle x\rangle\langle p\rangle)]/\mathrm{DET} \tag{3.64b}$$

and

$$\gamma = -2\lambda - \omega[\langle x^r\rangle(\langle x\rangle\langle xp\rangle - \langle x^2\rangle\langle p\rangle) - \langle x^{r+1}\rangle(\langle xp\rangle - \langle x\rangle\langle p\rangle) + \langle x^r p\rangle\langle x^2\rangle - \langle x\rangle^2)]/\mathrm{DET} \tag{3.64c}$$

where DET is given by Eq. (3.37). The error for the diffusion coefficient is

$$\varepsilon_2 = D(x) - \mu_{11}x^2 - 2\mu_{12}x - \mu_{22} \tag{3.65}$$

where

$$D(x) = d_{11}x^{2q} + 2d_{12}x^q + d_{22} \tag{3.66}$$

Minimizing $\langle \varepsilon_2^2\rangle$, we obtain the following set of equations, from which the $\mu_{ij}(t)$ can be determined:

$$\mu_{11}\langle x^2\rangle + 2\mu_{12}\langle x\rangle + \mu_{22} = \langle D(x)\rangle \tag{3.67}$$

$$\mu_{11}\langle x^3\rangle + 2\mu_{12}\langle x^2\rangle + \mu_{22}\langle x\rangle = \langle xD(x)\rangle \tag{3.68}$$

$$\mu_{11}\langle x^4\rangle + 2\mu_{12}\langle x^3\rangle + \mu_{22}\langle x^2\rangle = \langle x^2D(x)\rangle \tag{3.69}$$

As before we evaluate *all* averages appearing in Eqs. (3.67)–(3.69) using the distribution corresponding to the simplified equation (3.62). Again we note that the first two moment equations are exactly reproduced by this replacement. For example, the exact equation for $\langle p^2\rangle$ obtained from Eq. (3.57) is

$$\frac{d}{dt}\langle p^2\rangle = -2\omega\langle x^r p\rangle - 4\lambda\langle p^2\rangle + 2\langle D(x)\rangle \tag{3.70}$$

whereas the simplified equation (3.62) yields

$$\frac{d}{dt}\langle p^2\rangle = 2\alpha\langle p\rangle + 2\beta\langle xp\rangle - 4\lambda\langle p^2\rangle + 2\mu_{11}\langle x^2\rangle + 4\mu_{12}\langle x\rangle + 2\mu_{22} \tag{3.71}$$

It is easily seen that Eq. (3.71) is identical to Eq. (3.70) when the parameters α, β, and γ are substituted from (3.64a) to (3.64c) and Eqs. (3.67)–(3.69) are used.

3.3.2. Significance of the Number of Variational Parameters. The method of AGREE discussed in Section 2.2 involved two parameters α and β which we uniquely determined by minimizing $\langle \varepsilon^2 \rangle$ with respect to α and β. As a result we found that the first and second moment equations are exactly reproduced. If instead of minimizing the mean square error we require that the lowest two moment equations derived from Eq. (2.2) agree with the exact ones from Eq. (2.1), then we would obtain the same expressions for α and β as Eqs. (2.5) and (2.6). Thus in this case the method of error minimization and that of fitting the lowest two moment equations are equivalent. However, Eq. (3.9), used for replacing a SDE with multiplicative fluctuations, contains three variational parameters and yet only two moment equations are exactly reproduced. One can easily verify that the third moment equations derived from the approximate equation (3.9) with the parameters given by (3.16)–(3.18) cannot be identical to the third moment equations derived from the exact SDE (3.1). Similarly in Section 3.3.1, Eq. (3.62) contains six variational parameters, namely, α, β, γ, μ_{11}, μ_{12}, and μ_{22}. Even with these six parameters we are able to reproduce only the first and second moment equations. If we had only attempted to fit two moment equations, we would evidently not have had enough equations to determine all the parameters without additional constraints. We explain below the nature of these additional constraints and how the error minimization performs better than directly fitting moment equations. The discussion below also shows that the error minimization procedure can be extended to any desired degree.

For simplicity suppose we have a SDE in one variable with drift and diffusion coefficiens $f(x)$ and $D(x)$. Let us consider the replacement of the SDE with another one whose drift and diffusion coefficients are of the following form:

$$\bar{f}(x) = \sum_{i=0}^{n} \alpha_i x^i \tag{3.72}$$

i.e., a polynomial in x of degree n, and

$$\tilde{D}(x) = \sum_{i=0}^{m} \beta_i x^i \tag{3.73}$$

another polynomial in x of degree m. We stress that these polynomials are the most general ones of the given degree. None of the coefficients (not even α_0 or β_0) is taken as zero *a priori*. Then the error involved in the drift replacement is

$$\varepsilon_1 = \sum_{i=0}^{n} \alpha_i x^i - f(x) \tag{3.74}$$

Minimizing $\langle \varepsilon_1^2 \rangle$ we get the equations

$$\sum_{k=0}^{n} \alpha_k \langle x^{i+k} \rangle = \langle x^i f(x) \rangle, \qquad i = 0, 1, 2, \ldots n \tag{3.75}$$

Similarly, minimizing the mean square error in $D(x)$ we get

$$\sum_{k=0}^{n} \beta_k \langle x^{j+k} \rangle = \langle x^j D(x) \rangle, \qquad j = 0, 1, 2, \ldots, m \tag{3.76}$$

α_i and β_i are to be found by solving Eqs. (3.75) and (3.76). From the original SDE with the functions $f(x)$ and $D(x)$ we get the moment equations

$$\frac{d}{dt} \langle x^l \rangle = l \langle x^{l-1} f(x) \rangle + l(l-1) \langle x^{l-2} D(x) \rangle \tag{3.77}$$

The moment equations from the approximate SDE with parameters $\tilde{f}(x)$ and $\tilde{D}(x)$ are given by

$$\frac{d}{dt} \langle x^l \rangle = l \sum_{k=0}^{n} \alpha_k \langle x^{l+k-1} \rangle + l(l-1) \sum_{k=0}^{m} \beta_k \langle x^{l+k-2} \rangle \tag{3.78}$$

Now we wish to compare (3.77) and (3.78). The right-hand sides of these two equations can be equated using the relations (3.75) and (3.76) whenever possible. Since we have Eqs. (3.75) and (3.76) only for $i \leqslant n$ and $j \leqslant m$, Eqs. (3.77) and (3.78) are identical only for those l which satisfy $l-1 \leqslant n$ and $l-2 \leqslant m$. Thus the number of moment equations exactly reproduced by the minimization procedure is $\min(n+1, m+2)$.

As discussed in Section 3.2.1, the drift and the diffusion coefficients act as linearly independent contributions to the SDE (3.1). This is also obvious

from the moment equations (3.77). Each moment equation has two distinct parts, one arising from the drift coefficient and the other from diffusion. Therefore when we equate the right-hand sides of Eqs. (3.77) and (3.78), it is necessary to equate the two parts independently of each other. The two sides of Eq. (3.75) represent the drift parts of the ith moment equation from the exact and approximate SDE's. Similarly Eq. (3.76) involves the corresponding diffusion parts. The first moment equation consists of a drift part only. Thus the above minimization with nth and mth degree polynomials involves $n+m+2$ variational parameters. It reproduces the drift parts of the first $n+1$ moment equations and the diffusion parts of the second,..., $(m+2)$nd moment equations. As a result the lowest $\min(n+1, m+2)$ moment equations are completely reproduced. Thus the sum of the drift and diffusion parts reproduced in the moment equation is equal to the number of parameters.

3.4. Bistable Systems

An important class of systems is exemplified by a fictitious particle whose position x is described by the SDE

$$\dot{x} = -V'(x) + \beta\xi(t) \tag{3.79}$$

where the "potential" $V(x)$ is of the form

$$V(x) = \alpha_0 x + \tfrac{1}{2}\alpha_1 x^2 + \tfrac{1}{3}\alpha_2 x^3 + \tfrac{1}{4}\alpha_3 x^4 \tag{3.80}$$

and the parameters α_i are such that $V(x)$ has two minima and a maximum. Interesting physical phenomena are associated with the transfer of probability density between the two wells of such a potential.[15,18] Physical and chemical systems kept far from thermodynamic equilibrium can exhibit such multiple stable steady states. One would like to investigate the relative stability of these two states, predictability of the relative occurrence of these two states, the transfer rate of particles in one state to the other, etc.

In meteorology the persistence of certain weather conditions for unusually long periods is termed blocking.[34-39] To study this phenomenon several authors have proposed truncated hydrodynamic models. These models consist of equations of motion for three of the most important hydrodynamic modes in atmospheric circulation. These modes exhibit two stable regions in the state space corresponding to steady flow. The transition between these states needs to be studied by including the effects of fluctuations derived from the neglected hydrodynamic modes. As this problem involves three state variables, it is more complicated than Eq. (3.79). The Lorenz model of Bénard convection mentioned in

Section 3.3.1 has a strange attractor solution which has a number of qualitative features in common with bistable systems. In particular, the ergodic distribution of the deterministic trajectory is bimodal. In chemical kinetics the rate of reaction is related to the rate of transfer of molecules from the potential minimum corresponding to the reactant state to the minimum of the product state.

Suppose a physical process is described by an SDE of the form (3.1) where

$$\mathbf{f}(\mathbf{x}) = 0 \tag{3.81}$$

has three real solutions. These solutions correspond to the steady states of the physical system. If we replace this SDE with a linear SDE as in Section 3.2.1, then we would lose the property of multiple steady states. The simplest equation in this class is Eq. (3.79). Therefore we propose to replace more complicated equations with Eq. (3.79) following the method of statistical replacement. There are three kinds of simplification involved in such a replacement. First we attempt to get a single-variable equation from the multivariable Eq. (3.1). Secondly, if the drift $f(x)$ has a more complicated form than the derivative of (3.80), then we replace $f(x)$ by $-V'(x)$. Finally, in many problems the white noise fluctuations appear multiplicatively in the SDE. We replace this noise term with an additive one, since the multi-steady-state property stems from the drift and is not destroyed by the diffusion coefficient.

In systems of several variables, one is often able to find a variable that varies more slowly than the others. One can then reduce the dynamics of the system essentially to that of this degree of freedom by eliminating the fast variables. If we cannot perform such an elimination, we have to replace the original SDE with the simplest SDE in the same number of variables. Hereafter we assume that a reduction has been made and we have the single-variable equation

$$\text{(I)}\quad \dot{x} = f(x) + g(x)\,\xi(t) \tag{3.82}$$

When we minimize the mean square differences between the drift and the diffusion coefficients, we get the set of equations

$$\begin{pmatrix} 1 & \langle x\rangle & \langle x^2\rangle & \langle x^3\rangle \\ \langle x\rangle & \langle x^2\rangle & \langle x^3\rangle & \langle x^4\rangle \\ \langle x^2\rangle & \langle x^3\rangle & \langle x^4\rangle & \langle x^5\rangle \\ \langle x^3\rangle & \langle x^4\rangle & \langle x^5\rangle & \langle x^6\rangle \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} + \begin{pmatrix} \langle f\rangle \\ \langle xf\rangle \\ \langle x^2 f\rangle \\ \langle x^3 f\rangle \end{pmatrix} = 0 \tag{3.83}$$

and

$$\beta = \langle g^2\rangle^{1/2} \tag{3.84}$$

The parameters α_i and β can be expressed in terms of the time-dependent moments of x by solving Eq. (3.83).

The practical use of Eq. (3.83) would involve the derivation of a closed set of moment equations. The moment equations corresponding to the simplified SDE (3.79) do not form a closed set. The differential equation for a particular moment involves higher moments and therefore the hierarchy of moment equations cannot be truncated. This was also the case for statistical linearization. There the problem was overcome by invoking the Gaussian property of the linear SDE, thereby expressing all higher moments in terms of the first two. In the case of Eq. (3.79) no general characteristic of the solution is known. Thus the procedure in general would involve a numerical calculation of the time-dependent distribution. However, we may seek to further approximate this distribution. Valsakumar *et al.*[12] have successfully used a double Gaussian for this purpose in a special case. They studied the dynamics described by a SDE with additive noise [of the form (3.79)] and a symmetric potential. When the initial condition is also symmetric, the time-dependent distribution was taken to be of the form

$$P(x, t) = c\left\{H(-x)\exp\left[-\frac{(x+\bar{x})^2}{2\sigma_1^2}\right] + H(x)\exp\left[-\frac{(x-\bar{x})^2}{2\sigma_1^2}\right]\right\} \tag{3.85}$$

where c is the normalization constant and $H(x)$ is the Heaviside step function.

We have statistically replaced Eq. (3.82) with Eq. (3.79) with a *time-dependent* potential. The parameters in the potential function (3.80) are given by the time-dependent moments of x through (3.83). In the general problem of multistable systems, additional phenomena are involved if the potential in Eq. (3.82) [$V(x)$ such that $V'(x) = -f(x)$] is symmetric. These phenomena include equistability and coexistence of two phases. We now address the question of whether the statistical replacement preserves this symmetry. Suppose the drift $f(x)$ is an odd function of x. This in itself does not imply that α_0 and α_2 are zero. Equation (3.83) implies that the parameters $\alpha_i(t)$ are different for different initial values of the moments. Thus $\alpha_i(t)$ adjust themselves to describe the particular dynamics starting from the given initial distribution. The system dynamics is symmetric only if the initial condition is also symmetric in addition to the symmetry of the potential. Let us consider an initial distribution for which all the odd moments are zero. The matrix in Eq. (3.83) contains the odd and even moments regularly arranged in a lattice. Therefore its inverse also must have the same structure. In other words, wherever there is an odd moment in the matrix, the corresponding element in the inverse is a sum of terms

each of which has an odd number of odd moments as factors. Combining this with the fact that $f(x)$ is odd, we conclude that the expressions for $\alpha_0(t)$ and $\alpha_2(t)$ in terms of the moments are of odd symmetry, and $\alpha_1(t)$ and $\alpha_3(t)$ are of even symmetry. The equations for the moments obtained from the SDE (3.79) are given by

$$\frac{d}{dt}\langle x^n\rangle = n\alpha_0\langle x^{n-1}\rangle + n\alpha_1\langle x^n\rangle + n\alpha_2\langle x^{n+1}\rangle$$
$$+ n\alpha_3\langle x^{n+2}\rangle + n(n-1)\,\beta\langle x^{n-2}\rangle \tag{3.86}$$

It is verified that if all the odd moments are initially zero, they remain zero for all times. This means that $\alpha_0(t) = \alpha_2(t) = 0$ and the time-dependent distribution is always symmetric.

4. CONCLUSION

We have reviewed methods of approximating SDE's via methods that are generalizations of statistical linearization. To our knowledge all previous work has been restricted to SDE's with additive fluctuations. We have presented ways of extending these methods to include SDE's with multiplicative fluctuations. We found it necessary and convenient to treat the drift and diffusion coefficients as independent parameters of a SDE. We showed that such a description of the SDE is complete. This recognition led to an error minimization procedure whereby the drift and diffusion coefficients of the given SDE could be replaced by simpler drift and diffusion coefficients giving rise to a simpler SDE.

The optimization procedure developed here can be applied between any given pair of original SDE and simpler SDE provided the drift and diffusion coefficients of the simpler SDE are polynomials in the state variables. This leaves a freedom in the choice of the simple SDE. This choice was made based on two criteria. The more important criterion is that the simple SDE should reflect the important qualitative properties of the underlying physical system. The second criterion is that the approximate SDE should be as simple as possible without violating the first criterion. In order to implement the first criterion we classified physical systems into three classes according to whether the system is thermodynamically closed or open and according to the number of steady states.

For closed systems with a single equilibrium we used a linear SDE with additive fluctuations as an approximation. Using the Gaussian nature of the solution of the linear equation we were able to calculate the parameters in the linear equation in a self-consistent manner. This replacement process left the first two moment equations from the original

SDE unaltered, even though the equations for high moments were changed. We studied an anharmonic oscillator as an example using the linearized equation and compared the resulting energy envelope with the exact energy envelope. The agreement is excellent. We also showed that the balance between fluctuations and dissipation present in the original SDE is preserved by the replacement.

We treated mechanical oscillator systems with biased fluctuations and dissipation as examples for open systems. Unlike closed systems, this class of systems lacks a well-posed constraint. However, when an instability is indicated, we proposed to replace the SDE with a linear one but with multiplicative fluctuations. Again the first two moment equations were reproduced. In Section 3.3.2 we showed a relationship between the number of variational parameters used in the approximating equation and the number of moment equations reproduced.

The final class treated here consists of systems with two stable steady states. Even the simplest equation describing such systems cannot be solved exactly. However, Eq. (3.79) has been extensively studied in the literature and several approximation methods have been developed. Therefore we have taken Eq. (3.79) as essentially solvable. The corresponding multivariable SDE has not been studied to the same extent. Thus we have shown how to replace a one-variable general SDE with the SDE (3.79) with additive fluctuations. When the original problem (i.e., the SDE and its initial conditions) is symmetric, the approximating problem also involves a symmetric potential.

The spirit of this presentation has been to indicate how the method of statistical replacement is potentially useful in a variety of circumstances. We anticipate that this method would be most useful in the case of closed systems with a single equilibrium. This is due to the Gaussian nature of the approximating solution. In other cases the method of statistical replacement is equally well applicable; however, the resulting equations cannot be so readily solved.

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