PHYSICAL REVIEW A VOLUME 33, NUMBER 6 JUNE 1986

Relationship of fluctuations and transport for nonlinear Markov processes

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(Received 2 December 1985)

An exact relationship between the equations for the dynamics of average variables and those for their fluctuations is established for Markov processes. The result includes the general case of nonlinear and nonstationary dynamics and provides an extension of Onsager's regression hypothesis to a broad class of systems far from equilibrium.

I. INTRODUCTION

There is a growing literature on fluctuations in nonequilibrium systems that indicates a close relationship of the dynamics of fluctuations to the transport equations.[1] For states near equilibrium such a relationship is well established and is summarized by Onsager's regression hypothesis: spontaneous fluctuations in equilibrium decay according to the macroscopic transport equations linearized around the equilibrium state. This relationship not only simplifies calculations, but it also provides an important link between transport properties and experimental techniques that detect fluctuations. For states far from equilibrium Onsager's hypothesis does not apply as stated above, but it may be expected that a suitable generalization would maintain the close relationship of fluctuations and transport equations. Indeed, during the last several years many different problems have been described using a variety of models and techniques that lead to a common feature for the dynamics of fluctuations: time correlation functions obey bilinear equations equivalent in form to the transport equations linearized around the nonequilibrium state. Furthermore, the initial conditions for these equations (equal time correlation functions, or nonequilibrium susceptibilities) are related to the microscopic degrees of freedom by a linear dynamical "fluctuation-dissipation" equation. Once this coupling to the microscopic components is specified (e.g., a "noise" amplitude) a structurally simple closed set of equations for the macroscopic variables and their fluctuations is obtained, with the same appeal and utility as Onsager's hypothesis near equilibrium. Unfortunately, the generality of this result does not seem to be fully appreciated due to the disperse topics, methods, and approximations that have been used. The objective here is to provide an example which is both specific enough for the above structure to be derived as an exact consequence of the model, and general enough to encompass a broad class of nonequilibrium phenomena. The system considered is a set of stochastic variables governed by a Markov process.[2] The description is based on the introduction of a generating functional from which both average variables and their correlation functions can be obtained,[3] and the proof is simplified by a lemma due to Lax.[4]

Before discussing the details, the primary results can be stated easily. Let $\hat{\mathbf{a}}\equiv\{\hat{\mathbf{a}}_\alpha(t)\}$ denote a set of stochastic variables whose time dependence is governed by a Markov process. The mean values, $\mathbf{A}=\{A_\alpha(t)\}$, and the correlation functions $C_{\alpha\beta}(t,t')$ are defined by

$$A_\alpha(t)\equiv\langle\hat{\mathbf{a}}_\alpha(t)\rangle\ ,$$
$$C_{\alpha\beta}(t,t')\equiv\langle[\hat{\mathbf{a}}_\alpha(t)-A_\alpha(t)][\hat{\mathbf{a}}_\beta(t')-A_\beta(t')]\rangle\ , \tag{1.1}$$

where the brackets denote an average over the stochastic process and over a prescribed distribution of initial values, $\{\hat{\mathbf{a}}_\alpha(0)\}$. The times are assumed to be ordered according to $t>t'>0$. Then, it is shown below that these quantities obey the set of closed first-order equations,

$$\frac{\partial}{\partial t}A_\alpha(t)+N_\alpha[\mathbf{A};t]=0\ , \tag{1.2}$$

$$\frac{\partial}{\partial t}C_{\alpha\beta}(t,t')+L_{\alpha\sigma}[\mathbf{A};t]C_{\sigma\beta}(t,t')=0\ , \tag{1.3}$$

$$\frac{\partial}{\partial t}C_{\alpha\beta}(t,t)+L_{\alpha\sigma}[\mathbf{A};t]C_{\sigma\beta}(t,t)+L_{\beta\sigma}[\mathbf{A};t]C_{\sigma\alpha}(t,t)=I_{\alpha\beta}(t)\ . \tag{1.4}$$

Here $N_\alpha[\mathbf{A};t]$ is a function (or functional) of $\mathbf{A}$ that defines the average transport equations. The correlation functions obey bilinear equations parametrized by $\mathbf{A}(t)$, where the matrix, $L_{\alpha\beta}[\mathbf{A};t]$, is obtained from the transport equation according to

$$L_{\alpha\beta}[\mathbf{A},t]=\frac{\partial N_\alpha}{\partial A_\beta(t)}[\mathbf{A};t] \tag{1.5}$$

(or a suitable generalization to functional differentiation). The source term, $I_{\alpha\beta}(t)$, in the equation for the equal time correlation function is given by the second moment of the transition rate for the Markov process [Eq. (3.12), below].

For example, in a Fokker-Planck process $I_{\alpha\beta}(t)$ is equal to twice the average diffusion matrix. Several observations may be useful to put these results in context. (a) Equations (1.2)–(1.5) are exact. In particular, the bilinearity of the correlation function equation does not require that the fluctuations be small as in some previous discussions. (b) The correlation function equation, (1.3), is the same as that for the linear stability analysis of the transport equation, suggesting that the detection of correlation functions would provide a useful passive probe of systems near macroscopic instabilities. (c) The functional form of $N_\alpha[\mathbf{A};t]$, and hence $L_{\alpha\beta}[\mathbf{A},t]$, is that for the true macroscopic equations and not the deterministic limit of the Markov process; i.e., fluctuation-renormalization effects are already accounted for in these results. (d) For stationary states Eq. (1.4) is formally quite similar to an equilibrium fluctuation-dissipation relation (or Einstein relation). More generally, the equal time correlation functions are dynamical variables whose time evolution is governed by the same bilinear operator, $L_{\alpha\beta}[\mathbf{A}]$. Equation (1.5) therefore provides the key link of the correlation functions to the transport equations; the only additional information not contained in the latter is given by $I_{\alpha\beta}(t)$. Further comments on these results are given in the discussion section.

II. GENERATING FUNCTIONAL

A Markov process can be conveniently described by the conditional probability $P(\mathbf{a},t\mid\mathbf{a}',t')$ for finding the values $\mathbf{a}=\{a_\alpha\}$ of the stochastic variables at time t, given the values $\mathbf{a}'=\{a'_\alpha\}$ at time $t'\leq t$. It obeys the Chapman-Kolmogorov or Master equation

$$\left[\frac{\partial}{\partial t}-L\right]P(\mathbf{a},t\mid\mathbf{a}',t')=0\ , \tag{2.1}$$

where L is the linear operator

$$LP(\mathbf{a},t\mid\mathbf{a}',t')=\int d\mathbf{a}''[W(\mathbf{a}'',\mathbf{a})P(\mathbf{a}'',t\mid\mathbf{a}',t')-W(\mathbf{a},\mathbf{a}'')P(\mathbf{a},t\mid\mathbf{a}',t')]\ . \tag{2.2}$$

Here $W(\mathbf{a},\mathbf{a}')$ denotes the transition rate for changes from the state $\mathbf{a}$ to the state $\mathbf{a}'$. This transition rate completely specifies the Markov process. For a given initial condition, the knowledge of $P(\mathbf{a},t\mid\mathbf{a}',t')$ is enough to construct all the multitime probability distributions.

The averages at a single time can be represented in terms of the one-time distribution $P(\mathbf{a},t)$, defined by

$$P(\mathbf{a},t)=\langle\delta(\mathbf{a}-\hat{\mathbf{a}}(t))\rangle\ . \tag{2.3}$$

It is related to the conditional probability through

$$P(\mathbf{a},t)=\int d\mathbf{a}'P(\mathbf{a},t\mid\mathbf{a}',0)P(\mathbf{a}',0)\ , \tag{2.4}$$

where the initial value, $P(\mathbf{a}',0)$, is assumed to be given at some time (arbitrarily chosen to be $t=0$) and is normalized to 1. Then, for example, the average variables, $\mathbf{A}(t)$, are given by

$$\mathbf{A}(t)=\int d\mathbf{a}\,\mathbf{a}P(\mathbf{a},t)\ . \tag{2.5}$$

An nth-order correlation function is defined by

$$C_{\alpha_1,\ldots,\alpha_n}(t_1,\ldots,t_n)\equiv\langle[\hat{\mathbf{a}}_{\alpha_1}(t_1)-A_{\alpha_1}(t_1)]\cdots[\hat{\mathbf{a}}_{\alpha_n}(t_n)-A_{\alpha_n}(t_n)]\rangle\ . \tag{2.6}$$

These functions can be represented in a manner similar to (2.5) by the introduction of a joint probability function for values of the stochastic variables at n different times. However, from a formal point of view, it is more economical to obtain all of the correlation functions from generating functionals, $\mathbf{A}[t;\boldsymbol{\lambda}]$ that are closely related to the variables, $\mathbf{A}(t)$. They are defined in terms of some arbitrary test functions, $\boldsymbol{\lambda}=\{\lambda_\alpha\}$, by[5]

$$\mathbf{A}[t;\boldsymbol{\lambda}]\equiv\langle\hat{\mathbf{a}}(t)U[t;\boldsymbol{\lambda}]\rangle/\langle U[t;\boldsymbol{\lambda}]\rangle \tag{2.7}$$

with

$$U[t;\boldsymbol{\lambda}]\equiv\exp\left[\int_0^t d\tau\,\boldsymbol{\lambda}(\tau)\cdot\hat{\mathbf{a}}(\tau)\right]\ . \tag{2.8}$$

(The dot between the two vectors, $\boldsymbol{\lambda}$ and $\hat{\mathbf{a}}$, implies a summation over indices.) The functional derivatives of $A_{\alpha_1}[t_1;\boldsymbol{\lambda}]$ with respect to $\lambda_{\alpha_2}(t_2),\ldots,\lambda_{\alpha_n}(t_n)$ are denoted by

$$C_{\alpha_1,\ldots,\alpha_n}[t_1,\ldots,t_n;\boldsymbol{\lambda}]\equiv\frac{\delta^{n-1}A_{\alpha_1}[t_1;\boldsymbol{\lambda}]}{\delta\lambda_{\alpha_2}(t_2)\cdots\delta\lambda_{\alpha_n}(t_n)}\ . \tag{2.9}$$

The right side vanishes if any of the times of the functional derivatives are greater than t_1, as follows from Eq. (2.8). It will be assumed from here on that the time, t_1, in (2.9) is greater than or equal to all other times, t_α. The quantities $A_\alpha[t;\boldsymbol{\lambda}]$ and $C_{\alpha_1,\ldots,\alpha_n}[t_1,\ldots,t_n;\boldsymbol{\lambda}]$ have the obvious limits,

$$A_\alpha[t;\boldsymbol{\lambda}=0]=A_\alpha(t)\ , \tag{2.10}$$

$$C_{\alpha_1,\ldots,\alpha_n}[t_1,\ldots,t_n;\boldsymbol{\lambda}=0]=C_{\alpha_1,\ldots,\alpha_n}(t_1,\ldots,t_n)\ . \tag{2.11}$$

Thus, the macroscopic variables and all of the correlation functions can be determined from the generators, $\mathbf{A}[t;\boldsymbol{\lambda}]$.

The averages appearing in Eq. (2.7) cannot be expressed in terms of the one-time distribution, as they are functionals of $\hat{\mathbf{a}}(\tau)$ for $t\geq\tau\geq0$. Nevertheless, $\mathbf{A}[t;\boldsymbol{\lambda}]$ can be calculated from a generalization of Eq. (2.5) as

$$\mathbf{A}[t;\boldsymbol{\lambda}]=\int d\mathbf{a}\,\mathbf{a}P[\mathbf{a},t;\boldsymbol{\lambda}] \tag{2.12}$$

with

$$P[\mathbf{a},t;\boldsymbol{\lambda}]=\langle\delta(\mathbf{a}-\hat{\mathbf{a}}(t))U[t;\boldsymbol{\lambda}]\rangle/\langle U[t;\boldsymbol{\lambda}]\rangle\ . \tag{2.13}$$

The interesting feature of this representation is that $P[\mathbf{a},t;\boldsymbol{\lambda}]$ obeys a linear equation that is closely related to that for the conditional probability, Eq. (2.1),

$$\left[\frac{\partial}{\partial t}-L-\boldsymbol{\lambda}(t)\cdot(\mathbf{a}-\mathbf{A}[t;\boldsymbol{\lambda}])\right]P[\mathbf{a},t;\boldsymbol{\lambda}]=0\ . \tag{2.14}$$

This result is due to Lax,[4] and an abbreviated proof is given in the Appendix. The operator L is the same as that of Eq. (2.2), so the transition rates, $W(\mathbf{a},\mathbf{a}')$, are unchanged by the additional fields, $\boldsymbol{\lambda}(t)$. The equations for $\mathbf{A}[t;\boldsymbol{\lambda}]$ follows immediately from (2.12) and (2.14),

$$\frac{\partial}{\partial t}\mathbf{A}[t;\boldsymbol{\lambda}]+\langle \mathbf{D}^{(1)}(\mathbf{a});t\rangle_{\boldsymbol{\lambda}}=\mathbf{C}[t,t;\boldsymbol{\lambda}]\cdot\boldsymbol{\lambda}(t)\ , \tag{2.15}$$

where

$$\mathbf{D}^{(1)}(\mathbf{a})=\int d\mathbf{a}'(\mathbf{a}-\mathbf{a}')W(\mathbf{a},\mathbf{a}') \tag{2.16}$$

and

$$\mathbf{C}[t,t;\boldsymbol{\lambda}]=\langle(\mathbf{a}-\mathbf{A}[t;\boldsymbol{\lambda}])(\mathbf{a}-\mathbf{A}[t;\boldsymbol{\lambda}]);t\rangle_{\boldsymbol{\lambda}}\ . \tag{2.17}$$

The brackets, $\langle ;t\rangle_{\boldsymbol{\lambda}}$, are defined for an arbitrary function, $X(\mathbf{a})$, by

$$\langle X(\mathbf{a});t\rangle_{\boldsymbol{\lambda}}=\int d\mathbf{a}X(\mathbf{a})P[\mathbf{a},t;\boldsymbol{\lambda}]\ . \tag{2.18}$$

If $\mathbf{D}^{(1)}(\mathbf{a})$ is not a linear function of $\mathbf{a}$, then its average will be different from $\mathbf{D}^{(1)}(\mathbf{A}[t;\boldsymbol{\lambda}])$ due to fluctuations. This is the fluctuation-renormalization problem that is at the heart of most difficulties in a given application. Schematically, the renormalization can be implemented using the auxiliary variables, $\boldsymbol{\lambda}(t)$. The average of $\mathbf{D}^{(1)}$ is some specific functional of these variables,

$$\langle \mathbf{D}^{(1)}(\mathbf{a});t\rangle_{\boldsymbol{\lambda}}\equiv\mathbf{F}[\boldsymbol{\lambda};t]\ . \tag{2.19}$$

In addition, $\mathbf{A}[t;\boldsymbol{\lambda}]$ is also a functional of $\boldsymbol{\lambda}$, defined by Eq. (2.12). Assuming this latter relationship is invertible, Eq. (2.19) can be expressed in terms of the $\mathbf{A}[t;\boldsymbol{\lambda}]$,

$$\langle \mathbf{D}^{(1)}(\mathbf{a});t\rangle_{\boldsymbol{\lambda}}=\mathbf{F}[\boldsymbol{\lambda}[t;\mathbf{A}];t]\equiv\mathbf{N}[\mathbf{A}[t;\boldsymbol{\lambda}];t]\ . \tag{2.20}$$

In this form the functional dependence on $\boldsymbol{\lambda}$ occurs only through $\mathbf{A}[t;\boldsymbol{\lambda}]$. This has the important consequence that the average of $\mathbf{D}^{(1)}$ for $\boldsymbol{\lambda}=0$ is the same function of $\mathbf{A}(t)$. More specifically, Eq. (2.15) is written

$$\frac{\partial}{\partial t}\mathbf{A}[t;\boldsymbol{\lambda}]+\mathbf{N}[\mathbf{A}[t;\boldsymbol{\lambda}];t]=\mathbf{C}[t,t;\boldsymbol{\lambda}]\cdot\boldsymbol{\lambda}(t) \tag{2.21}$$

and the macroscopic transport equations are obtained simply by setting $\boldsymbol{\lambda}=0$,

$$\frac{\partial}{\partial t}\mathbf{A}(t)+\mathbf{N}[\mathbf{A};t]=0\ . \tag{2.22}$$

This structural similarity of the equations for the generating functional and the macroscopic variables can be exploited now to relate the equations for the correlation functions to the transport equations, (2.22).

III. DYNAMICS OF CORRELATIONS

To simplify the discussion, attention will be limited here to correlations of only two variables. Using Eq. (2.9), the $\boldsymbol{\lambda}$-dependent correlation function is obtained from the generating functional by

$$C_{\alpha\beta}[t,t';\boldsymbol{\lambda}]\equiv\frac{\delta A_\alpha[t;\boldsymbol{\lambda}]}{\delta\lambda_\beta(t')},\quad t>t'\geq 0\ . \tag{3.1}$$

Also for $t\neq t'$ the functional differentiation at t' and time differentiation at t commute,

$$\frac{\partial}{\partial t}\frac{\delta A_\alpha[t;\boldsymbol{\lambda}]}{\delta\lambda_\beta(t')}=\frac{\delta}{\delta\lambda_\beta(t')}\frac{\partial}{\partial t}A_\alpha[t;\boldsymbol{\lambda}]\ . \tag{3.2}$$

Application of (2.21) on the right side and (3.1) on the left gives the equations for the correlation functions at two different times, $t>t'\geq 0$,

$$\frac{\partial}{\partial t}C_{\alpha\beta}[t,t';\boldsymbol{\lambda}]+\frac{\delta N_\alpha[\mathbf{A}[t;\boldsymbol{\lambda}];t]}{\delta\lambda_\beta(t')}=C_{\alpha\sigma\beta}[t,t,t';\boldsymbol{\lambda}]\lambda_\sigma(t)\ . \tag{3.3}$$

Since $\mathbf{N}[\mathbf{A}[t;\boldsymbol{\lambda}];t]$ depends on $\boldsymbol{\lambda}$ only through $\mathbf{A}[t;\boldsymbol{\lambda}]$ the functional derivative in (3.3) may be evaluated as[7]

$$\frac{\delta N_\alpha[\mathbf{A}[t;\boldsymbol{\lambda}]]}{\delta\lambda_\beta(t')}=\frac{\partial N_\alpha[\mathbf{A}[t;\boldsymbol{\lambda}];t]}{\partial A_\sigma[t;\boldsymbol{\lambda}]}\frac{\delta A_\sigma[t;\boldsymbol{\lambda}]}{\delta\lambda_\beta(t')}=\frac{\partial N_\alpha[\mathbf{A}[t;\boldsymbol{\lambda}];t]}{\partial A_\sigma[t;\boldsymbol{\lambda}]}C_{\sigma\beta}[t,t';\boldsymbol{\lambda}]$$

and Eq. (3.3) becomes

$$\frac{\partial}{\partial t}C_{\alpha\beta}[t,t';\boldsymbol{\lambda}]+L_{\alpha\sigma}[\mathbf{A}[t;\boldsymbol{\lambda}];t]C_{\sigma\beta}[t,t';\boldsymbol{\lambda}]=C_{\alpha\sigma\beta}[t,t,t';\boldsymbol{\lambda}]\lambda_\sigma(t) \tag{3.4}$$

with

$$L_{\alpha\beta}[\mathbf{A}[t;\boldsymbol{\lambda}];t]\equiv\frac{\partial N_\alpha[\mathbf{A}[t;\boldsymbol{\lambda}];t]}{\partial A_\beta[t;\boldsymbol{\lambda}]}\ . \tag{3.5}$$

Setting $\boldsymbol{\lambda}=0$ in these last two equations gives the desired results for the correlation functions at two different times,[8] Eqs. (1.3) and (1.5).

To obtain the equation for correlations at the same time, i.e., $C_{\alpha\beta}(t,t)$, a somewhat different method is required since the commutation relation (3.2) does not hold for $t'=t$. Instead, a direct calculation from (2.14) is possible,

$$\begin{aligned}\frac{\partial}{\partial t}C_{\alpha\beta}[t,t;\boldsymbol{\lambda}]&=\frac{\partial}{\partial t}\langle(a_\alpha-A_\alpha[t;\boldsymbol{\lambda}])(a_\beta-A_\beta[t;\boldsymbol{\lambda}]);t\rangle_{\boldsymbol{\lambda}}\\&=\langle L^\dagger\{(a_\alpha-A_\alpha[t;\boldsymbol{\lambda}])(a_\beta-A_\beta[t;\boldsymbol{\lambda}])\};t\rangle_{\boldsymbol{\lambda}}\\&\quad+C_{\alpha\beta\gamma}[t,t,t;\boldsymbol{\lambda}]\lambda_\gamma(t)\ ,\end{aligned} \tag{3.6}$$

where $L^\dagger$ is the adjoint of L,

$$L^\dagger F(\mathbf{a})\equiv\int d\mathbf{a}'W(\mathbf{a},\mathbf{a}')[F(\mathbf{a}')-F(\mathbf{a})]\ . \tag{3.7}$$

Carrying out the operation of $L^\dagger$ in (3.6) leads to

$$\begin{aligned}\frac{\partial}{\partial t}C_{\alpha\beta}[t,t;\boldsymbol{\lambda}]=&-\langle D_\alpha^{(1)}(\mathbf{a})(a_\beta-A_\beta[t;\boldsymbol{\lambda}]);t\rangle_{\boldsymbol{\lambda}}\\&-\langle(a_\alpha-A_\alpha[t;\boldsymbol{\lambda}])D_\beta^{(1)}(\mathbf{a});t\rangle_{\boldsymbol{\lambda}}\\&+2\langle D_{\alpha\beta}^{(2)}(\mathbf{a});t\rangle_{\boldsymbol{\lambda}}+C_{\alpha\beta\gamma}[t,t,t;\boldsymbol{\lambda}]\lambda_\gamma(t)\ .\end{aligned} \tag{3.8}$$

Here $\mathbf{D}^{(2)}(\mathbf{a})$ is defined in terms of the transition rate by

$$\mathbf{D}^{(2)}(\mathbf{a})\equiv\frac{1}{2}\int d\mathbf{a}'(\mathbf{a}-\mathbf{a}')(\mathbf{a}-\mathbf{a}')W(\mathbf{a},\mathbf{a}') . \qquad (3.9)$$

The first two terms on the right side of Eq. (3.8) can be put in a more useful form as

$$\begin{aligned}\langle D_\alpha^{(1)}(\mathbf{a})(a_\beta-A_\beta[t;\boldsymbol{\lambda}]);t\rangle_\lambda &= \lim_{\tau\to 0^+}\frac{\delta}{\delta\lambda_\beta(t-\tau)}\langle D_\alpha^{(1)}(\mathbf{a});t\rangle_\lambda \\ &= \frac{\delta N_\alpha[\mathbf{A}[t;\boldsymbol{\lambda}];t]}{\delta\lambda_\beta(t)} \\ &= L_{\alpha\sigma}[\mathbf{A}[t;\boldsymbol{\lambda}];t]C_{\sigma\beta}[t,t;\boldsymbol{\lambda}] , \qquad (3.10)\end{aligned}$$

where the definition (3.5) has been used. Equation (3.8) can then be written

$$\begin{aligned}\frac{\partial}{\partial t}C_{\alpha\beta}[t,t,;\boldsymbol{\lambda}]+L_{\alpha\sigma}[\mathbf{A}[t;\boldsymbol{\lambda}];t]C_{\sigma\beta}[t,t;\boldsymbol{\lambda}] \\ +L_{\beta\sigma}[\mathbf{A}[t;\boldsymbol{\lambda}];t]C_{\sigma\alpha}[t,t;\boldsymbol{\lambda}] \\ =I_{\alpha\beta}[t;\boldsymbol{\lambda}]+C_{\alpha\beta\gamma}[t,t,t;\boldsymbol{\lambda}]\lambda_\gamma(t) \qquad (3.11)\end{aligned}$$

with

$$I_{\alpha\beta}[t;\boldsymbol{\lambda}]\equiv 2\langle D_{\alpha\beta}^{(2)}(\mathbf{a});t\rangle_\lambda . \qquad (3.12)$$

Now, setting $\boldsymbol{\lambda}=0$, Eqs. (1.4) and (1.5) for the equal time correlation functions are obtained. This completes the verification of Eqs. (1.2)—(1.5).

IV. DISCUSSION

For states near equilibrium the results (1.2) and (1.3) confirm Onsager's regression hypothesis since in that case the nonlinear transport equations can be linearized and the resulting equations for fluctuations and transport are the same. More generally, these two sets of equations differ but the dynamics of fluctuations can always be obtained from the general form of the transport equations through Eq. (1.5). This latter observation and its generality is the primary result of this paper. It extends to a wide class of nonequilibrium states the intuitive notion that the dynamics of low-order correlation functions is essentially macroscopic. The statistical features appear in Eq. (1.4), which expresses the relationship of the macroscopic transport matrix, $L_{\alpha\beta}$, to the "noise amplitude," $I_{\alpha\beta}$. This interpretation of $I_{\alpha\beta}$ follows from its definition, (3.12), and also from the fact that $I_{\alpha\beta}$ is the average covariance of the noise in an equivalent Langevin formulation.[4] Some further comments regarding these results may be useful to clarify their general context.

(1) Although the stochastic process considered here is Markovian, the contracted description for the average value $\mathbf{A}(t)$ will generally be nonlocal in time ("memory effects"). The differential operator in Eq. (1.5) relating $L_{\alpha\beta}$ and N_α then must be replaced by a functional derivative, so that Eq. (1.3) becomes

$$\frac{\partial}{\partial t}C_{\alpha\beta}(t,t')+\int_{t'}^{t}ds\, L_{\alpha\sigma}[\mathbf{A};t,s]C_{\sigma\beta}(s,t')=0 ,$$

$$L_{\alpha\beta}[\mathbf{A};t,s]\equiv\frac{\delta N_\alpha[\mathbf{A};t]}{\delta A_\beta(s)}$$

with similar changes in Eq. (1.4) for the equal time correlation functions. Also, it is possible to generalize the equations to the case of variables $\{A_\alpha\}$ with α being a continuous rather than a discrete label.

(2) The method used here to obtain Eqs. (1.2)—(1.5) makes explicit use of the renormalization of the deterministic equations. This renormalization has two different origins. The first one is associated with the fact that the dynamics of the set of variables $\{A_\alpha\}$ is not self-deterministic, and reflects the fundamental statistics of the stochastic process considered. The second origin is a quite different statistics associated with specification of the initial probability distribution, $P(\mathbf{a};0)$. If the latter is a stationary state these two sources of statistics are closely related. In general, however, $P(\mathbf{a};0)$ can be specified independently of the master equation. Consequently, one could take the point of view that the "true" transport equations should have a form that is independent of initial data and that only the first source of renormalization should be considered here. The results (1.2)—(1.5) are still obtained in this case, with only a change in the definition of the averages, (2.12), to conditional averages. Of course, ultimately an average over the initial distribution must be performed in a given application.

(3) The linear form of the correlation function equation is the same as that for the linear stability analysis of the transport equations, (1.2). In stability analysis these equations are obtained by a linearization of the transport equations, neglecting quadratic and higher-order nonlinearities. Here, however, these linear equations for the correlation functions are exact and do not imply an approximate linearization. It is expected, therefore, that they would apply even near an instability. Asymptotically close to an instability the decay of fluctuations slows to zero. At this point, the inversion of Eq. (2.12) to obtain (2.20) is presumably singular. For example, at a simple bifurcation, a specific one of the multiple solutions above the instability would have to be chosen to implement the renormalization. In this way, the dynamics of correlation functions would be well-defined on both sides of the instability, and would be characteristic of the particular solutions to the transport equations on each side.

(4) The general structure of the relationship between transport equations and the dynamics of correlation functions discussed here is also expected to apply approximately for non-Markovian processes with two well-separated time scales. Generally, Eqs. (1.2) and (1.3) would have sources representing initial short-time transients. The decay time for such transients sets the time scale on which the macroscopic transport equations apply (for example, the Boltzmann equation applies for times long compared to a collision time, hydrodynamics applies for times long compared to a mean free time). On the long time scale for which the transport equations (1.2) are a good approximation, it is possible to show that Eqs. (1.3)—(1.5) for the correlation functions apply to the same degree of approximation.[3] In practice, the determination of $I_{\alpha\beta}(t)$ can be quite difficult in this more general context.

ACKNOWLEDGMENTS

The authors thank Dr. M. Lax for helpful comments. The research of J.W.D. and J.J.B. is supported in part by National Science Foundation Grant No. CHE-84-11932, the U.S.-Spain Joint Committee for Scientific and Technological Cooperation (CCB-84-02062), and by the Alianza Espana-Florida. M.C.M. is supported in part by the U.S. Army Research Office.

APPENDIX: PROOF OF EQUATION (2.14)

The function $P[\mathbf{a};t;\boldsymbol{\lambda}]$ is defined by Eq. (2.13):

$$P[\mathbf{a},t;\boldsymbol{\lambda}]\equiv f[\mathbf{a},t;\boldsymbol{\lambda}]\Big/\int d\mathbf{a} f[\mathbf{a},t;\boldsymbol{\lambda}]\;, \tag{A1}$$

$$f[\mathbf{a},t;\boldsymbol{\lambda}]\equiv\left\langle \delta(\mathbf{a}-\hat{\mathbf{a}}(t))\exp\int_0^t d\tau\,\boldsymbol{\lambda}(\tau)\cdot\hat{\mathbf{a}}(\tau)\right\rangle\;. \tag{A2}$$

The time integral in (A2) may be represented as a series by dividing the interval 0 to t into N equal parts:

$$f[\mathbf{a},t;\boldsymbol{\lambda}]=\left\langle \delta(\mathbf{a}-\hat{\mathbf{a}}(t))\prod_{i=1}^{N} e^{\Delta t\boldsymbol{\lambda}(t_i)\cdot\hat{\mathbf{a}}(t_i)}\right\rangle \tag{A3}$$

with $\Delta t\equiv t/N$ and $t_i=i\Delta t$. This expression can be evaluated in terms of the N-time joint probability function $P(\mathbf{a},t;\mathbf{a}^{(N-1)},\,t_{N-1};\ldots;\mathbf{a}^{(1)},\,t_1)$,

$$\begin{aligned}f[\mathbf{a},t;\boldsymbol{\lambda}]&=\int d\mathbf{a}^{(1)}\cdots d\mathbf{a}^{(N-1)}P(\mathbf{a},t;\ldots;\mathbf{a}^{(1)},t_1)\prod_{i=1}^{N} e^{\Delta t\boldsymbol{\lambda}(t_i)\cdot\mathbf{a}^{(i)}}\\&=\int d\mathbf{a}^{(1)}\cdots d\mathbf{a}^{(N-1)}P(\mathbf{a},t\,|\,\mathbf{a}^{(N-1)},t_{N-1})\cdots P(\mathbf{a}^{(2)},t_2\,|\,\mathbf{a}^{(1)},t_1)\;\;P(\mathbf{a}^{(1)},t_1)\prod_{i=1}^{N} e^{\Delta t\boldsymbol{\lambda}(t_i)\cdot\mathbf{a}^{(i)}}\;.\end{aligned} \tag{A4}$$

The second equality holds only for a Markov process. The conditional probabilities obey Eq. (2.1), that is to be solved with a δ-function initial condition, i.e.,

$$P(\mathbf{a}^{(2)},t_2\,|\,\mathbf{a}^{(1)},t_1)=e^{(t_2-t_1)L}\delta(\mathbf{a}^{(1)}-\mathbf{a}^{(2)})\;. \tag{A5}$$

Substitution of (A5) into (A4) and integration over the $\mathbf{a}$ yields

$$\begin{aligned}f[\mathbf{a},t;\boldsymbol{\lambda}]&=e^{\Delta t\,\boldsymbol{\lambda}(t)\cdot\mathbf{a}}e^{(t-t_{N-1})L}e^{\Delta t\,\boldsymbol{\lambda}(t_{N-1})\cdot\mathbf{a}}e^{(t_{N-1}-t_{N-2})L}e^{\Delta t\,\boldsymbol{\lambda}(t_{N-1})\cdot\mathbf{a}}\cdots e^{t_1L}P(\mathbf{a},0)\\&=e^{tL}T\prod_{i=1}^{N}\exp[\Delta t\,\boldsymbol{\lambda}(t_i)\cdot\tilde{\mathbf{a}}(t_i)]P(\mathbf{a},0)\;.\end{aligned} \tag{A6}$$

Here $\tilde{\mathbf{a}}(t)$ is an operator

$$\tilde{\mathbf{a}}(t)\equiv e^{-tL}\mathbf{a}e^{tL}\;, \tag{A7}$$

and T is the time-ordering operator with latest times to the left. Taking the limit $N\to\infty$ ($\Delta t\to 0$), Eq. (A6) goes to

$$f[\mathbf{a},t;\boldsymbol{\lambda}]=e^{tL}T\exp\left[\int_0^t d\tau\,\boldsymbol{\lambda}(\tau)\cdot\tilde{\mathbf{a}}(\tau)\right]P(\mathbf{a},0)\;. \tag{A8}$$

Differentiation of this result with respect to time gives

$$\left[\frac{\partial}{\partial t}-L\right]f=\boldsymbol{\lambda}(t)\cdot\mathbf{a}f\;. \tag{A9}$$

Finally, the desired result is obtained by combining (A9) and (A1),

$$\left[\frac{\partial}{\partial t}-L-\boldsymbol{\lambda}(t)\cdot(\mathbf{a}-\mathbf{A}[t;\boldsymbol{\lambda}])\right]P[\mathbf{a},t;\boldsymbol{\lambda}]=0\;. \tag{A10}$$

[1]A recent review with extensive references is given by A. M. Tremblay in *Recent Developments in Nonequilibrium Thermodynamics,* Proceedings of the Meeting held at Bellaterra School of Thermodynamics, Autonomous University of Barcelona, Bellaterra (Barcelona), Spain, 1983, edited by J. Casas-Vazquez, D. Jou, and G. Lebon (Lecture Notes in Physics, Vol. 199) (Springer, Berlin, 1984). An early reference for the case of Markov processes is M. Lax, Phys. Rev. **172**, 350 (1968), Sec. 4.

[2]N. Van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).

[3]This method has been used in the same context by M. C. Marchetti and J. Dufty, Physica **118A**, **205** (1983); M. C. Marchetti, Ph.D. thesis, University of Florida, 1982.

[4]M. Lax, Rev. Mod. Phys. **38**, 359 (1966).

[5]It is more usual to define the single generating functional $G[\boldsymbol{\lambda}]=\ln\langle U[t=\infty;\boldsymbol{\lambda}]\rangle$, from which both the macroscopic variables and their correlations can be obtained. The choice (2.7) made here, however, allows more direct application of Lax's result (2.11).

[6]The definition of $U[t;\boldsymbol{\lambda}]$ here restricts the correlation functions to positive arguments, $t\geq 0$. The choice of $t=0$ for specification of initial conditions is easily changed in an obvious way.

[7]For simplicity of notation it has been assumed that $N_\alpha[\mathbf{A}[t;\boldsymbol{\lambda}]]$ is a function (rather than a functional) of $A[t;\boldsymbol{\lambda}]$. The more general case is described in the last section.

[8]For nonstationary states these functions actually depend on all three times t, t', and 0.