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Strategies for Fluctuation Renormalization in Nonlinear Transport Theory

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We are concerned here with the problems encountered in the derivation of nonlinear transport equations from a correspondingly nonlinear Langevin equation. A dynamical coupling between the time-dependent averages and the fluctuations must be accounted for by a procedure which leads to a renormalization of the nonlinear transport equation. Generalizing the familiar phenomenological approach to Brownian motion to nonlinear dynamics, we illustrate how the problem arises and show how the fluctuation renormalization can be obtained exactly by a formal procedure or approximately by more tractable methods.

KEY WORDS: Nonlinear transport equation; statistical fluctuations; fluctuation renormalization.

1. INTRODUCTION

Many problems in nonequilibrium statistical mechanics lead to a nonlinear transport theory. Nonlinearity adds a new complication to the derivation of the statistical transport theory due to the dynamical coupling between ensemble averaged properties and the fluctuations of these priorities in the ensemble. This problem will be analyzed here. We illustrate how the problem arises in a simple phenomenological theory and discuss a formal decoupling scheme together with several modifications which under appropriate conditions would allow the derivation of nonlinear fluctuation-renormalized transport equations.

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The approach to nonequilibrium statistical mechanics that we use here has evolved out of traditional Brownian motion theory,[1,2] which in recent years has been obtained on a microscopic first principle basis by Zwanzig[3] and Mori[4] using projection operator techniques and applied in the nonlinear regime by Kawasaki.[5] On the basis of Mori's microscopic derivation, which yielded a non-Markovian linear Langevin equation, Kubo[6] extended the phenomenological Brownian motion theory to the non-Markovian regime. Here we apply the phenomenological theory to a general class of nonlinear, essentially Markovian problems and focus on the role played by the fluctuations. The need for a fluctuation renormalization has been pointed out previously by way of a model calculation.[7] A more general analysis of the problem is presented here.

It will be evident that the problem of fluctuation effects in nonlinear statistical theories is a very general one appearing in many different forms depending on the specific problem. We shall not attempt to review here the many specific applications in which the same problem, in a broad sense, has been encountered and somehow overcome or neglected. Rather we shall save some comments about relevant previous work to the end of the paper, hoping by then to have given the reader a clear conception of the problem. This work has been motivated by the fact that while systematic and very general methods have now been developed which yield Langevin or Fokker–Planck equations for nonlinear processes,[3,5,8] a systematic treatment of the effects of fluctuations on nonlinear transport equations has been lacking.

The example of a nonlinear oscillator in a heat bath is studied briefly in Section 2 in order to expose the main content of the phenomenological transport theory used in the following. We generalize the theory and proceed to discuss in Section 3 the cumulant expansion for the fluctuations and a formal iteration procedure which when convergent leads to the desired fully fluctuation-renormalized transport equations. Approximate renormalization methods that may be practically useful are discussed in Section 4, and we conclude with a brief discussion of the need for nonlinear theories and fluctuation renormalization.

2. NONLINEAR BROWNIAN MOTION

In order to illustrate the content of the phenomenological transport theory to be used in the following and the problem posed by nonlinearity, we consider here the motion of a Duffing oscillator in a heat bath[3] which may be taken to be a dilute fluid. The motion of the oscillator in the absence of the heat bath is given by the equations

$$(\partial/\partial t)x(t) = v(t), \qquad (\partial/\partial t)v(t) = -kx(t) - x^3(t) \tag{1}$$

[3] A linearized transport equation for the Duffing oscillator in a heat bath has been studied in Ref. 9.

The point of the exercise is to understand the effect of the fluid on the motion of the oscillator. Clearly it contributes a force of interaction so that the acceleration becomes

$$(\partial/\partial t)v(t) = -kx(t) - x^3(t) + F_H(t) \tag{2}$$

Rigorous classical mechanics would direct us to obtain $F_H(t)$ from the equations of motion of the whole system but we shall be content with a completely phenomenological treatment. Rigorous derivations verifying the properties we shall rely upon below for a special class of systems have been discussed by Ford *et al.*[10] and by Zwanzig.[11] Here we merely assume that $F_H(t)$ consists of a frictional part proportional to the velocity of the oscillator and a remainder that fluctuates in a random manner. Thus the motion of the oscillator is given by

$$\frac{\partial}{\partial t}x(t) = v(t), \qquad \frac{\partial}{\partial t}v(t) = -kx(t) - x^3(t) - \xi v(t) + F(t) \tag{3}$$

These are the Langevin equations of our Brownian motion problem, and they will form the starting point for our discussion.

The following points concerning the content of the Langevin equations should be noted. The form of Eq. (3) represents a simplification in that the dissipative force of the heat bath is assumed instantaneous rather than delayed in time, as is generally the case. The many-body character of the dynamics is now hidden in the fluctuating force $F(t)$, which is dependent on the positions and velocities of the fluid particles. Since the initial conditions for the fluid can be experimentally controlled only in a very crude sense such as the specification of a temperature, we associate with the Langevin equation an ensemble of initial conditions for the whole system. This ensemble may be taken to represent a sequence of repeated experiments, and it is a requirement of the theory that the ensemble average of the fluctuating force vanish,

$$\langle F(t)\rangle = 0 \tag{4}$$

The Langevin equation describes the motion of the Duffing oscillator as it would appear in a single experiment. The trajectory depends through $F(t)$ on the initial state of both oscillator and fluid. We are, however, usually interested only in some systematic aspects of the motion. In particular, it is often sufficient to obtain the motion of the averaged properties as observed in the ensemble of experiments referred to above. Thus we take the ensemble average of the Langevin equations and get

$$\frac{\partial}{\partial t}\langle x\rangle_t = \langle v\rangle_t, \qquad \frac{\partial}{\partial t}\langle v\rangle_t = -k\langle x\rangle_t - \langle x^3\rangle_t - \xi\langle v\rangle_t \tag{5}$$

In the absence of the cubic term, that is, if our Langevin equations had been linear, the above equations would have been closed in the first moments $\langle x\rangle_t$

and $\langle v \rangle_t$. Such equations of motion, closed in the first moments of the properties studied, are called transport equations and their derivation is a significant part of nonequilibrium dynamics and our concern in this paper. Our problem is that in the presence of the cubic term and dispersion in the ensemble we have

$$\langle x^3 \rangle_t \neq \langle x \rangle_t^3 \tag{6}$$

and the equations of motion (5) are not closed in the first moments. Only if the fluctuations in the ensemble from one experiment to the next can be neglected so that (6) can be made an identity do we obtain a bare nonlinear transport equation

$$(\partial/\partial t)\langle v \rangle_t = -k\langle x \rangle_t - \langle x \rangle_t^3 - \xi \langle v \rangle_t \tag{7}$$

In the general case we must seek to correct the bare equation (7) for the effects of the fluctuations entering in the form of $\langle x^3 \rangle_t - \langle x \rangle_t^3$ to obtain a fluctuation-renormalized nonlinear transport equation. This will require that we learn something about the time development of the fluctuations in the ensemble. Thus we turn now to consider the probability density $f(t; x, v)$ describing the instantaneous distribution of oscillators in the ensemble over position and velocity. Note that this function contains the time development of the average of any function of the oscillator coordinates $A(x, v)$ through the relation

$$\langle A(x, v) \rangle_t = \int\int dx\, dv\, A(x, v) f(t; x, v) \tag{8}$$

It is clear then that obtaining an expression for $f(t; x, v)$ constitutes a complete solution for our problem and, in particular, $f(t; x, v)$ contains information about the fluctuations in the ensemble as required to obtain a correction to (7). Given that the fluctuating force $F(t)$ in addition to (4) satisfies the relation

$$\langle F(t)F(t') \rangle = 2\alpha\, \delta(t - t') \tag{9}$$

and is a Gaussian random process, the equation of motion satisfied by $f(t; x, v)$ can be found to be[1,2]

$$\frac{\partial}{\partial t} f(t; x, v) = \left[- v \frac{\partial}{\partial x} + (kx + x^3) \frac{\partial}{\partial v} + \xi \frac{\partial}{\partial v} v + \alpha \frac{\partial^2}{\partial v^2} \right] f(t; x, v) \tag{10}$$

This is the well-known Fokker–Planck for our Brownian motion problem.

Finally, we shall point out a useful connection between equilibrium and nonequilibrium theory. Let us, for example, assume that after the excess

velocity of the oscillator has been damped out it settles down into an equilibrium motion such that the oscillator density becomes

$$f_{\text{eq}}(x, v) = C \exp[-\tfrac{1}{2}\beta M(v^2 + kx^2 + \tfrac{1}{2}x^4)] \tag{11}$$

as determined by Gibbs' canonical ensemble. We must then demand that this equilibrium density be a stationary solution of the Fokker–Planck equation (10). Substituting (11) into (10), we then immediately obtain the well-known fluctuation-dissipation theorem relating the friction coefficient to the correlations in the fluctuating force,

$$\xi = \alpha M\beta = M(k_{\text{B}}T)^{-1} \int_0^\infty dt' \langle F(t)F(t + t')\rangle \tag{12}$$

Thus we have reduced to one the number of parameters occurring in the phenomenological Fokker–Planck equation.

As has long been known, Brownian motion theory can be applied to a wide range of problems in which some relevant properties collectively denoted by the vector **a** couple to a heat bath of irrelevant properties of the system. Retaining the Markovian assumption, the generalized Langevin equation would then be

$$(\partial/\partial t)\mathbf{a}(t) = \mathbf{h}(\mathbf{a}(t)) + \boldsymbol{\eta}(\mathbf{a}(t)) + \mathbf{F}(t) \tag{13}$$

where the vector notation summarizes a system of equations. The first term on the right represents nondissipative streaming, while the second term contains the systematic, generally dissipative effects of the heat bath, and both terms may be nonlinear. The last term is the fluctuating force due to the nonsystematic effects of the heat bath, and it is assumed to satisfy

$$\langle \mathbf{F}(t)\tilde{\boldsymbol{F}}(t')\rangle = 2\alpha\, \delta(t - t') \tag{14}$$

Here $\mathbf{F}$ is a column matrix, $\tilde{\boldsymbol{F}}$ its transpose, and α is a constant square matrix.

The Fokker–Planck equation can be obtained by a standard method and we get

$$\frac{\partial}{\partial t} f(t; \mathbf{a}) = -\frac{\partial}{\partial \mathbf{a}} \cdot [\mathbf{h}(\mathbf{a}) + \boldsymbol{\eta}(\mathbf{a})] f(t; \mathbf{a}) + \frac{\partial}{\partial \mathbf{a}} \cdot \alpha \frac{\partial}{\partial \mathbf{a}} f(t; \mathbf{a}) \tag{15}$$

Self-consistency relations for the parameters of the theory can again be obtained by demanding that the equilibrium density $f_{\text{eq}}(\mathbf{a})$ be a stationary solution of (15). However, they will generally be more complicated than the fluctuation-dissipation theorem (12).

Taking the ensemble average of the Langevin equation (13), we obtain

$$(\partial/\partial t)\langle \mathbf{a}\rangle_t = \langle \mathbf{h}(\mathbf{a})\rangle_t + \langle \boldsymbol{\eta}(\mathbf{a})\rangle_t \tag{16}$$

which becomes a bare transport equation

$$(\partial/\partial t)\langle \mathbf{a}\rangle_t = \mathbf{h}(\langle \mathbf{a}\rangle_t) + \boldsymbol{\eta}(\langle \mathbf{a}\rangle_t) \tag{17}$$

only if the fluctuations contained in higher moments can be neglected. However, there are interesting problems such as critical dynamics where the fluctuations can be expected to have important effects, and we shall seek in the following the proper corrections to the bare transport equation.

3. FLUCTUATION RENORMALIZATION

The fluctuations that we must now consider are conveniently described by the cumulant averages well known in probability theory. Kubo[12] has pointed out their usefulness in statistical physics. Each higher-order moment can be expanded in terms of cumulant averages indicated here by the subindex c

$$\langle a_{l_1} \cdots a_{l_r} \rangle = \langle a_{l_1} \cdots a_{l_r} \rangle_c + \sum_{i=1}^{r} \langle a_{l_1} \cdots a_{l_{i-1}} a_{l_{i+1}} \cdots a_{l_r} \rangle_c \langle a_{l_i} \rangle_c + \cdots + \langle a_{l_1} \rangle_c \cdots \langle a_{l_r} \rangle_c \tag{18}$$

There is one term on the right of (18) for each partition of the natural numbers $1,\ldots, r$ into nonoverlapping sets. The first-order cumulant average $\langle a_{l_i} \rangle_c$ is identical to the first moment $\langle a_{l_i} \rangle$ but the higher-order cumulant average $\langle a_{l_1} \cdots a_{l_r} \rangle_c$ represents only the correlations among *all* the variables $a_{l_1},\ldots, a_{l_r}$. If these variables can be divided up into two independent subgroups, then the cumulant average will vanish.

A systematic definition of the cumulant average is given in terms of the characteristic function for the random vector $\mathbf{a}$ defined by

$$\phi_{\mathbf{a}}(\boldsymbol{\xi}) = \langle \exp(i\boldsymbol{\xi} \cdot \mathbf{a}) \rangle \tag{19}$$

The characteristic function generates the moments by the relation

$$\langle a_{l_1} \cdots a_{l_r} \rangle = [(-i)^r (\partial^r / \partial \xi_{l_1} \cdots \partial \xi_{l_r}) \phi_{\mathbf{a}}(\boldsymbol{\xi})_{\boldsymbol{\xi}=0}] \tag{20}$$

and the cumulant averages by

$$\langle a_{l_1} \cdots a_{l_r} \rangle_c = [(-i)^r (\partial^r / \partial \xi_{l_1} \cdots \partial \xi_{l_r}) \ln \phi_{\mathbf{a}}(\boldsymbol{\xi})]_{\boldsymbol{\xi}=0} \tag{21}$$

Expanding $\ln \phi_{\mathbf{a}}(\boldsymbol{\xi})$ in terms of moments using (19), one then finds from (21) an expansion of the cumulant average in terms of moments.

Let us now return to the ensemble average of the Langevin equation (16). Assuming that the components of $\mathbf{h}(\mathbf{a})$ and $\boldsymbol{\eta}(\mathbf{a})$ are well-behaved functions which can be expanded in multidimensional Taylor series, we use these expansions together with the cumulant expansion (18) for the moments to rewrite (16) in the form

$$(\partial / \partial t) \langle \mathbf{a} \rangle_t = \mathbf{h}(\langle \mathbf{a} \rangle_t) + \boldsymbol{\eta}(\langle \mathbf{a} \rangle_t) + \mathcal{N}(\langle \mathbf{a} \rangle_t, \langle \mathbf{aa} \rangle_{c,t}, \langle \mathbf{aaa} \rangle_{c,t} \cdots) \tag{22}$$

The last term summarizes the corrections to the bare transport equation, and we note that it vanishes when the fluctuations represented by all cumulant averages of order two and higher vanish. We shall not be concerned with the exact form of the functions summarized in $\mathcal{N}$. The whole term is a sum of products of cumulant averages, and the important point is that it exposes the dependence on the instantaneous first moments and upon the fluctuations.

Our task then is to replace the dependence on unknown instantaneous fluctuations by further dependence on first moments or on other quantities that can be considered known. To do so, we must produce solutions of proper form for the higher-order cumulants. Since the cumulant average $\langle a_{l_1} \cdots a_{l_r} \rangle_{c,t}$ can be expanded as a sum of products of moments of the same or lower order, its equation of motion can be obtained from those of the moments. Note now that an equation of motion for the average of the function $B(\mathbf{a})$ can be obtained from the Fokker–Planck equation in the following manner:

$$(\partial/\partial t)\langle B(\mathbf{a})\rangle_t = \int d\mathbf{a}\, B(\mathbf{a})(\partial/\partial t) f(t; \mathbf{a})$$

$$= \int d\mathbf{a}\, B(\mathbf{a}) \mathscr{D} f(t; \mathbf{a}) = \int d\mathbf{a}\, [\mathscr{D}^+ B(\mathbf{a})] f(t; \mathbf{a}) \tag{23}$$

Here $\mathscr{D}$ is the Fokker–Planck operator defined by (15) as

$$\mathscr{D} = -\frac{\partial}{\partial \mathbf{a}} \cdot [\mathbf{h}(\mathbf{a}) + \boldsymbol{\eta}(\mathbf{a})] + \frac{\partial}{\partial \mathbf{a}} \cdot \alpha \frac{\partial}{\partial \mathbf{a}} \tag{24a}$$

and $\mathscr{D}^+$ is its adjoint, which can be obtained by partial integration if $f(t; \mathbf{a})$ vanishes at the boundaries

$$\mathscr{D}^+ = [\mathbf{h}(\mathbf{a}) + \boldsymbol{\eta}(\mathbf{a})] \cdot \frac{\partial}{\partial \mathbf{a}} + \frac{\partial}{\partial \mathbf{a}} \cdot \alpha \frac{\partial}{\partial \mathbf{a}} \tag{24b}$$

Replacing $B(\mathbf{a})$ by the product $a_{l_1} \cdots a_{l_r}$, we obtain from (23) the equation of motion for $\langle a_{l_1} \cdots a_{l_r} \rangle_t$, and the equations of motion for the cumulant averages follow in a straightforward manner. We shall adopt a notation which suppresses all of the details and focuses on the basic principle of the formal manipulations we now proceed to discuss. Let $\mathscr{A}(t)$ be an infinite-dimensional vector which has as components all of the time-dependent cumulant averages,

$$\mathscr{A}_{l_1 \ldots l_r}(t) = \langle a_{l_1} \cdots a_{l_r} \rangle_{c,t} \tag{25}$$

We can summarize all of the equations of motion of the cumulants in the vector notation

$$(\partial/\partial t)\mathscr{A}(t) = \mathbf{M}(\mathscr{A}(t)) \tag{26}$$

Corresponding to our separation of all information in our ensemble into first moments and fluctuations, we separate $\mathscr{A}(t)$ into

$$\mathscr{A}(t) = \mathscr{A}_1(t) + \mathscr{A}_2(t)$$

where $\mathscr{A}_1(t)$ lies in the subspace corresponding to first moments and $\mathscr{A}_2(t)$ in the subspace of higher-order cumulants or fluctuations. That is,

$$\mathscr{A}_{1,l_1,\ldots,l_n}(t) = 0 \qquad \text{for} \quad n > 1; \qquad \mathscr{A}_{2,l_1}(t) = 0$$

We emphasize that no fundamental importance is attached to the introduction of this vector space of cumulants. It merely allows us to write the equations which follow in a compact form. In the same way the equation of motion (26) splits into

$$(\partial/\partial t)\mathscr{A}_1(t) = \mathbf{M}_1(\mathscr{A}_1(t) + \mathscr{A}_2(t)) \tag{27a}$$

$$(\partial/\partial t)\mathscr{A}_2(t) = \mathbf{M}_2(\mathscr{A}_1(t) + \mathscr{A}_2(t)) \tag{27b}$$

Note now that if the right-hand side of (27a) did not contain any dependence on $\mathscr{A}_2(t)$, as in the linear theory, then this relation summarizes the transport equations we are seeking. In the nonlinear theory there is such a dependence on $\mathscr{A}_2(t)$. The bare transport equations follow by setting $\mathscr{A}_2(t)$ equal to zero,

$$(\partial/\partial t)\mathscr{A}_1(t) \cong \mathbf{M}_1(\mathscr{A}_1(t)) \tag{28}$$

When the fluctuations cannot be neglected we must solve (27b) to obtain a relation for $\mathscr{A}_2(t)$ in terms of first moments and initial values. Substituting this relation for $\mathscr{A}_2(t)$ into (27a), we would then obtain our fluctuation-renormalized transport equation. How to obtain such a solution for $\mathscr{A}_2(t)$ is the problem.

Let us first integrate (27b) over time to obtain

$$\mathscr{A}_2(t) = \mathscr{A}_2(0) + \int_0^t ds\, \mathbf{M}_2(\mathscr{A}_1(s) + \mathscr{A}_2(s)) \tag{29}$$

We note now that for a physically well-behaved Hamiltonian the dynamics of variables such as the cumulants above will be analytic in time (as they must for their equations of motion to make sense). Thus we can find an exact solution for $\mathscr{A}_2(t)$ in the form of a Taylor series expansion in time. The coefficients in that expansion will be time derivatives of the respective components of $\mathscr{A}_2(t)$ and they can be obtained as functions of the initial conditions $\mathscr{A}(0)$ by repeated differentiation of (29) with the use of (27a) and (27b) to reduce the dependence on derivatives. We would obtain

$$\mathscr{A}_2(t) = \sum_{n=0}^{\infty} \mathbf{C}_{2,n}(\mathscr{A}(0))(1/n!)t^n \tag{30}$$

where, for example,

$$\mathbf{C}_{2,0} = \mathscr{A}_2(0), \qquad \mathbf{C}_{2,1} = \mathbf{M}_2(\mathscr{A}_1(0) + \mathscr{A}_2(0)) \tag{31}$$

and so on.

However, the solution (30) does not have the desired form. It would merely introduce further dependence on initial conditions in the renormalized transport equations while we are seeking a solution which would introduce further dependence on the time-dependent first moments themselves and thus renormalize the transport coefficients. Such a solution can be obtained by a successive approximation procedure in which the self-consistency relation (29) is used recursively to generate higher-order approximations to $\mathscr{A}_2(t)$. The zeroth-order approximation is taken to be the initial value

$$\mathscr{A}_2^{(0)}(t) = \mathscr{A}_2(0) \tag{32}$$

and the higher-order approximations are obtained from the recursion relation

$$\mathscr{A}_2^{(n)}(t) = \mathscr{A}_2(0) + \int_0^t ds\, \mathbf{M}_2(\mathscr{A}_1(s) + \mathscr{A}_2^{(n-1)}(s)) \tag{33}$$

It should be noted that this method is a straightforward generalization of Picard's method of successive approximations[13] as applied to nonlinear integral equations. Given that the functional in the integrand of (33) satisfies some physically reasonable conditions (see, for example, Ref. 13, p. 415), we can expect the successive approximations to converge to the unique solution

$$\lim_{n \to \infty} \mathscr{A}_2^{(n)}(t) = \mathscr{A}_2^{(\infty)}(t) = \mathscr{A}_2(t) \tag{34}$$

Clearly the convergence properties will be most favorable in the limit of short time but we can reasonably expect the convergence to be faster than that characterizing the n first terms of the Taylor series expansion (30) as n goes to infinity. More importantly, the successive approximation method does retain the explicit dependence of $\mathscr{A}_2(t)$ on first moments at earlier times. That is, upon substitution of $\mathscr{A}_2^{(n)}(t)$ into (27a), we would find the fluctuation-renormalized transport equation to contain memory effects.

4. LOW-ORDER RENORMALIZATION METHODS

The successive approximation method described above seems well suited to the basic theoretical task of proving the existence of an exact fluctuation renormalization of the proper form for the bare nonlinear transport equations. However, it may not, in its present form, be very well suited to generate practically useful approximate fluctuation renormalization. It should be noted that the series $\{\mathscr{A}_2^{(n)}(t)\}_{n=0}^{\infty}$ will share many of the problems of a

straightforward Taylor series expansion in time. That is, the rate of convergence can be expected to decrease rapidly with time and, moreover, for finite n the approximation $\mathscr{A}_2^{(n)}(t)$ will show nonphysical divergencies for long times.

From a practical point of view it is immediately clear that exact fluctuation renormalization will be beyond reach in nontrivial cases, and we must find ways of accounting approximately for the effects of the fluctuations by methods that are tractable either analytically or numerically. Since we are normally particularly interested in the long-time limit in which we expect to find decay to stationary equilibrium values of the moments and cumulants, the long-time inadequacies of $\mathscr{A}_2^{(n)}(t)$ as given above are particularly unfortunate. Thus we shall now discuss some approximations that may eliminate the long-time difficulties and prove practically useful.

Approximation 1. Our concern with the long-time limit of the time dependence suggests that we should consider replacing the fluctuations as they enter (27a) by their long-time limit which we presume to be the equilibrium values, i.e.,

$$\mathscr{A}_2(t) \cong \mathscr{A}_{2,\mathrm{eq}} \tag{35}$$

$$(\partial/\partial t)\mathscr{A}_1(t) = \mathbf{M}_1(\mathscr{A}_1(t) + \mathscr{A}_{2,\mathrm{eq}}) \tag{36}$$

This approximation would be reasonable in cases when the initial conditions represent a small deviation from equilibrium conditions. Moreover, it would imply that as first moments and cumulants decay toward their equilibrium values only the coupling of the first moments to the static part of the fluctuations need be considered. Nevertheless, the bare transport equation may be significantly renormalized in this way. In the case of the Duffing oscillator discussed in Section 2, we would get

$$\langle x^3\rangle_t = \langle x^3\rangle_{c,t} + 3\langle x^2\rangle_{c,t}\langle x\rangle_t + \langle x\rangle_t^3 \cong 3\langle x^2\rangle_{c,\mathrm{eq}}\langle x\rangle_t + \langle x\rangle_t^3$$

since $\langle x^3\rangle_{c,\mathrm{eq}}$ vanishes and inserting into (5)

$$\frac{\partial}{\partial t}\langle x\rangle_t = \langle v\rangle_t, \qquad \frac{\partial}{\partial t}\langle v\rangle_t = -(k + 3\langle x^2\rangle_{c,\mathrm{eq}})\langle x\rangle_t - \xi\langle v\rangle_t - \langle x\rangle_t^3 \tag{37}$$

where we see that one of the linear transport coefficients has been renormalized by the fluctuations.

Approximation 2. In the case that the equilibrium approximation for the fluctuations is too crude, one may try a local equilibrium approximation. That is, the time dependence of the fluctuations is assumed to be rapid compared to that of the first moments so that the statistical ensemble is always close to local equilibrium as given by

$$f_{l,\mathrm{eq}}(\Gamma; \mathscr{A}_1(t)) = C\exp[-\beta H(\Gamma) + \mathbf{A}(\Gamma)\cdot\boldsymbol{\gamma}(t)] \tag{38}$$

where $\gamma(t)$ is determined so that the first moments become just $\mathscr{A}_1(t)$. Here β is $(k_B T)^{-1}$ and Γ is the coordinate of the underlying phase space in which the properties we are studying take the form of phase space functions, $\{\mathscr{A}_i(\Gamma)\}$, in classical theory. The local equilibrium approximation for the fluctuations $\mathscr{A}_{2,l.\mathrm{eq}}(\mathscr{A}_1(t))$ would then be calculated directly from the density $f_{l.\mathrm{eq}}$ in (38). Although less convenient mathematically, this approximation has many advantages over the equilibrium approximation. We note that in nonequilibrium statistical mechanics it is customary to choose the initial conditions to be obtained from just such a local equilibrium ensemble. If this is done, then $\mathscr{A}_{2,l.\mathrm{eq}}(t)$ will be exact both in the long- and in the short-time limits. Moreover, the local equilibrium approximation need not necessarily be limited to describing the time development of the first moments from initial conditions that correspond to a small deviation from equilibrium. We note also that the local equilibrium approximation makes contact with thermodynamic reasoning in that it assigns the fluctuations a value that would maximize the entropy for given values of the first moments.

The two approximations discussed above either neglect or make a strong simplifying assumption about the time development of the fluctuations. When these assumptions fail the problem becomes, of course, much more difficult since we would then have to obtain and, in some adequate approximation, solve the equations of motion of the cumulants (27b). It may be possible to truncate the infinite set of coupled nonlinear equations by neglecting the time development of cumulants of order higher than some small integer N. However, there appears to be little a priori support for such a procedure so the effect of the truncation would have to be considered in each individual case.

Approximation 3. The full dynamical coupling between first moments and fluctuations which is introduced recursively in the successive approximation procedure above may perhaps be introduced in a more practical manner by a modification of this procedure. Note that the zeroth-order approximation $\mathscr{A}_2^{(0)}(t)$ can be generalized in the hope of obtaining more rapid convergence and eliminating the difficulties at long times. Clearly the rate of convergence is directly dependent on the extent to which the zeroth-order approximation differs from the correct functional form $\mathscr{A}_2(t)$. One may, for example, obtain corrections to the local equilibrium approximation discussed above by substituting

$$\mathscr{A}_2^{(0)}(t) = \mathscr{A}_{2,l.\mathrm{eq}}(t) \tag{39}$$

in the successive approximation method and generating the low-order approximations according to (33).

Approximation 4. Another possibility is the application of partial resummation techniques. One model calculation employing this technique as justified by the assumption of weakly nonlinear dynamics has been previously presented.[7] It can be summarized as follows. The equation of motion for the cumulants (27b) is rewritten by collecting the linear effects in a separate term to obtain (K is a square matrix)

$$(\partial/\partial t)\mathscr{A}_2(t) = K\mathscr{A}_2(t) + \lambda \mathbf{M}_2'(\mathscr{A}_1(t) + \mathscr{A}_2(t)) \tag{40}$$

where the nonlinear coupling parameter λ has been inserted to keep track of the order to which the nonlinear effects will appear. The equation can be partially solved to yield

$$\mathscr{A}_2(t) = e^{Kt}\mathscr{A}_2(0) + \lambda \int_0^t ds\, e^{(t-s)K}\mathbf{M}_2'(\mathscr{A}_1(s) + \mathscr{A}_2(s)) \tag{41}$$

We can now apply the method of successive approximation to Eq. (41), which is a partially resummed modification of the Eq. (29), using

$$\mathscr{A}_2^{(0)}(t) = e^{Kt}\mathscr{A}_2(0) \tag{42}$$

and higher-order approximations as given by Eq. (33). The advantage gained by the resummation lies in the fact that $\mathscr{A}_2^{(n)}(t)$ can now be seen to be correct to order λ^n if the λ expansion exists as assumed. The hope is, of course, that the convergence will now be rapid since all of the linear dynamical effects are already included in $\mathscr{A}_2^{(0)}(t)$ and the nonlinear effects are assumed to be small. Another important point is that the linear propagator exp Kt may now contain dissipative effects that would lead to exponential decay for the linear problem and which can eliminate the long-time problems that arise in the same method as applied to the original equation.

Since the nonlinearities are responsible for the coupling between the first moments and the fluctuations, the above method would only yield renormalization effects that were themselves small. However, the same general method may be based instead on the assumption of small deviations from equilibrium. If we assume that Eq. (27b) has been rewritten so that it gives the time development of the deviations of the cumulants from their equilibrium values, then the partial resummation can be carried out as follows. First, we separate out the linear dynamical effects to get

$$(\partial/\partial t)\mathscr{A}_2(t) = K\mathscr{A}_2(t) + L\mathscr{A}_1(t) + \mathbf{M}_2''(\mathscr{A}_1(t), \mathscr{A}_2(t)) \tag{43}$$

Here L will be not a square but a rectangular matrix since the vector space of

the first moments will be of lower dimensionality. This equation can again be integrated to yield

$$\mathscr{A}_2(t) = e^{Kt}\mathscr{A}_2(0) + \int_0^t ds\, e^{(t-s)K}L\mathscr{A}_1(s) + \int_0^t ds\, e^{K(t-s)}\mathbf{M}_2''(\mathscr{A}_1(s), \mathscr{A}_2(s)) \tag{44}$$

We can now apply the successive approximation method to Eq. (44) using

$$\mathscr{A}_2^{(0)}(t) = e^{Kt}\mathscr{A}_2(0) + \int_0^t ds\, e^{K(t-s)}L\mathscr{A}_1(s) \tag{45}$$

This time the approximations $\mathscr{A}_2^{(n)}(t)$ would contain effects of increasing order in the deviations from equilibrium as n increases. Moreover, strong renormalization effects can now appear through the coupling of first moments to the equilibrium part of the fluctuations.

5. CONCLUDING COMMENTS

We have shown above how the phenomenological Brownian motion theory can be extended in a straightforward manner to nonlinear processes given that the coupling between first moments and fluctuations can be satisfactorily accounted for. The existence of renormalized nonlinear transport equations of the proper form has been argued on the basis of a method of successive approximations, and a number of methods have been suggested that may under favorable conditions considerably simplify the inherent practical difficulties so that reasonably accurate fluctuation renormalization could be obtained.

It should be emphasized that microscopic projection operator methods can be used to derive nonlinear Langevin equations and corresponding Fokker–Planck equations. In general, these equations will be non-Markovian, leading to non-Markovian character of the equations of motion for the cumulants (27a) and (27b). However, apart from a formal complication of the notation our analysis still applies, as is easily verified.

In view of the well-known complications of nonlinear dynamics the very real need for nonlinear theories must be emphasized. As illustrated here by the Brownian motion of a Duffing oscillator in a fluid and by the Boltzmann equation of kinetic theory, certain problems naturally lead to nonlinear dynamics. Provided that only small deviations from equilibrium are considered, it may still be possible to reformulate such a problem by methods of Zwanzig[9] and Mori[4] so that it becomes linear. But the nonlinear effects will then appear in the form of memory effects of significant magnitude and

duration hidden in the form of a propagator in the space of orthogonal variables. It seems unlikely that the nonlinear effects will be any easier to understand or to account for if they appear in this form. In fact, we believe the opposite will more often be the case.

The nonlinear theory will, of course, be particularly manageable when the effects of the fluctuations can be neglected and the bare transport equations used. However, many areas of current research seem certain to require the fluctuations to be accounted for. One such area is critical dynamics, where there is now widespread agreement that nonlinear mode–mode coupling theories are useful. The fact that the system studied is close to a phase transition means that the fluctuations may be large in magnitude and consequently they may contribute significantly to the dynamics.

The mode–mode coupling theory as formulated by Kawasaki is based on a generalized Brownian motion theory such as discussed here. Although at one point[14] in his derivations Kawasaki suggests a procedure which would be the equivalent of the local equilibrium approximation described under approximation 2 above, the present theory[5] does not attempt to account for the effects of fluctuations by a systematic renormalization scheme. It is our view that this aspect of the mode–mode coupling theories requires further investigation and we believe the methods outlined above will be helpful in this regard.

Finally, in order to place the fluctuation-renormalization schemes described above in a broader perspective it should be noted that the effects of fluctuations on nonlinear processes can, of course, be studied by obtaining the dynamics of a probability density rather than that of the first moments alone as given by the transport equation. Much work has been done along the former approach to the problem and we refer in particular to Van Kampen[15] and Lax,[16] who have applied master equation and Fokker–Planck equation methods to the study of nonlinear processes. It should be clear that while the formal problem of fluctuation renormalization can be avoided in this way, one can do so only by drastically expanding the scope of the problem. Note that the probability density contains all of the information which is contained in the moments or cumulants to all orders. This is reflected in the fact that for a discrete set of variables the transport equations for a Markovian process are a set of ordinary differential equations while, for example, the corresponding Fokker–Planck equation is a partial differential equation in a space of as many dimensions as there are variables.

Although the problem of dynamical coupling between first moments and fluctuations occurs in a number of applications of nonlinear statistical theories in the literature, it is rarely discussed in the terms we have used here. Typically the coupling is entirely neglected, which amounts to an assumption that the time-dependent cumulants of order two and higher are small enough

so that they will not significantly influence the dynamics of the first moments. This is the strongest form of what has been called the cumulant neglect hypothesis in statistical continuum theories.[17] The assumption can be made progressively weaker by neglecting only cumulants of order n and higher where n is 3, 4, 5,.... In this case one then ends up with coupled nonlinear equations for the cumulants of order one through $n - 1$ and in order to obtain the transport equations for the first moments one must solve for the cumulants of order 2 through $n - 1$ in terms of the first moments and substitute into the equations for the first moments. Further discussion of this technique as applied to turbulence theory and a stochastic harmonic oscillator problem can be found in the work of Kraichnan[18] and Richardson,[19] respectively. The same basic idea of imposing a cutoff on the cumulant expansion of higher moments has been drawn upon in applications of statistical methods to other physical problems (see Ref. 20 for a recent example). It should be noted that such a cutoff hypothesis can easily be imposed upon our coupled equations of motion (27b) for the infinite set of higher-order cumulants. The approximation procedures we have discussed here would then generally be simplified. However, the neglect of cumulants beyond a given order is difficult to justify a priori.

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