

Projector Formalism of Generalized Brownian Motion Theory Applied to Dissipative and Noisy Systems

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The projector formalism of Zwanzig–Mori type is extended to obtain generalized Fokker–Planck and generalized nonlinear Langevin equations for coarse-grained variables when the underlying microscopic dynamics is dissipative and noisy (stochastic).

KEY WORDS: Brownian motion theory; projector formalism; Fokker–Planck equation; nonlinear Langevin equation.

1. INTRODUCTION

Brownian motion theory⁽¹⁾ and its generalizations⁽²⁾ have successfully described the behavior of slow variables in complex many-body systems which have time scales well separated from those of other degrees of freedom of the system. The theory was provided with a new foundation in the sixties with the introduction of the projector formalisms^(3,4) which provided a direct though formal link between the existing phenomenological Brownian motion theories and the underlying microscopic dynamics. The projector formalism was originally developed for the case of classical non-dissipative dynamical systems.⁽³⁾ Extensions to other dynamical systems (quantum systems⁽⁴⁾ and also dissipative systems with noise⁽⁵⁾) have so far been limited to the case of linear Brownian dynamics. On the other hand, the limited usefulness of linear Brownian motion theories is now well recognized.^(6–8) A source of difficulty when the underlying dynamics is dissipative and noisy is the following. Consider a product of coarse-grained dynamical variables $A_1 A_2 \dots$. This product averaged over the noise is generally different from the product of the noise-averaged variables. Thus,

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straightforward extensions of the existing projector formalisms^(3,8) are not enough to obtain, for example, a closed generalized Fokker–Planck equation for the probability distribution function of the coarse-grained dynamical variables.

In recent years the statistical mechanics of mesoscopic objects has drawn a great deal of attention. Examples are polymers, colloids, emulsions, and membranes⁽⁹⁾ as well as varieties of topological defects associated with the spontaneous breakdown of symmetry.⁽¹⁰⁾ Mesoscopic equations of motion governing these objects are generally dissipative and noisy. In these areas one is often interested in understanding macroscopic behavior, such as rheological behavior, on the basis of mesoscopic (or “microscopic”) equations. This requires coarse-graining of the mesoscopic equations themselves. This circumstance motivated us to develop a projector formalism which is general enough to incorporate a wider class of underlying “microscopic” equations.

The paper is organized as follows. After some preliminary discussion in Section 2, the projector formalism is explained and the generalized Fokker–Planck equation is obtained in Section 3. Section 4 considers a corresponding generalized nonlinear Langevin equation and Section 5 concludes the paper. Some of the more involved algebras is deferred to an Appendix.

2. PRELIMINARIES

We consider a general system whose state can be described in some stage of coarse-graining by a set of “microscopic” variables which can be represented by a point x in the multidimensional space of the “microscopic” variables characterizing the system. We call this space the phase space and x the phase point. As long as we have no access to complete “microscopic” information about a state of the system, we can only deal with a phase space distribution function $D(x, t)$. The time evolution of the system is then described by the equation for D of the following general form:

$$\frac{\partial}{\partial t} D(x, t) = \Omega(x) D(x, t) \quad (2.1)$$

where $\Omega(x)$ is an operator acting in the phase space. We assume the existence of a unique stationary (or equilibrium) distribution $D_e(x)$ such that

$$\Omega(x) D_e(x) = 0 \quad (2.2)$$

The normalization of $D(x, t)$ requires that

$$\int dx \Omega(x) \cdots = 0 \quad (2.3)$$

where \cdots is any phase function and the integral is over the entire phase space.

We point out that the operator $\Omega(x)$ does not need to be a first-order differential operator as with the usual Liouville operator of classical mechanics, nor is $i\Omega(x)$ necessarily a self-adjoint operator. As a consequence, the time-displacement operator defined by $\exp[-t\Omega(x)]$ in general has the following property (here and henceforth the argument x is often suppressed for brevity unless confusion might arise):

$$e^{-t\Omega} \Gamma_1(\Gamma_2(x)) \neq \Gamma_1(e^{-t\Omega} \Gamma_2(x)) \quad (2.4)$$

where $\Gamma_2(x)$ is any phase function and $\Gamma_1(\Gamma_2)$ is any function of Γ_2 . Such a more general class of the operator Ω is required when (2.1) already contains some stochastic processes, as with the Fokker–Planck equation, or when (2.1) is a quantum mechanical Liouville equation expressed in terms of c -number quantities like a Wigner function,⁽¹¹⁾ although we shall not discuss the quantum case in any detail here.

It often happens in statistical physics that the level of description provided by (2.1) is too detailed for our need and further coarse-graining is desired, as was mentioned in the preceding section. In the new coarse-grained description the original set of variables x is replaced by a new set of a fewer number of phase functions collectively denoted as $A(x)$. A state in this newly coarse-grained description is specified by a set of numbers a taken by $A(x)$. Instead of the phase space distribution $D(x, t)$ we now have the reduced distribution $g(a, t)$ defined by

$$g(a, t) \equiv \int dx \delta(a - A(x)) D(x, t) \quad (2.5)$$

where the delta function is in fact the product of delta functions for every member of the set $a - A(x)$. We shall refer the multidimensional space in which a is defined as the state space.

Our goal here is to find a closed equation for $g(a, t)$ starting from (2.1). The fact that this is not an easy task can be seen by looking at

$$\frac{\partial}{\partial t} g(a, t) = \int dx \delta(a - A) \Omega D(x, t) \quad (2.6)$$

and the rhs is not readily expressible in $g(a, t)$. This is an inevitable consequence of coarse-graining associated with (2.5). That is, $g(a, t)$ cannot be uniquely determined by knowing $g(a, t')$ at some earlier time $t' < t$ only, but additional information at t' is also required, and in particular, $\partial g(a, t)/\partial t$ cannot be given solely in terms of $g(a, t)$ at the same time. The missing information can be supplied if we know $g(a, t')$ at *all* the earlier times $t' < t$. As a trivial example, consider two variables which decay exponentially in time, and then couple them linearly. Now, under suitable conditions each variable is a sum of two exponentially decaying functions with two arbitrary coefficients in front. Then the time rate of change of one of the variables cannot be determined by the value of that variable at the same time, since this is not enough to determine both coefficients in front, the missing information being supplied by knowledge of that variable at another time. The projector formalism is a succinct way to incorporate this missing information for a general case.

3. PROJECTOR FORMALISM

In order to prepare for the introduction of a projector, we start from the following formal solution of (2.1):

$$D(t) = e^{t\Omega} D(0) \quad (3.1)$$

Substituting this into (2.5) and using (2.3), we find

$$g(a, t) = \int \hat{g}(a, t) D(0) dx \quad (3.2)$$

where

$$\hat{g}(a, t) \equiv e^{-t\Omega} \delta(a - A) e^{t\Omega} = \delta(a - \hat{A}(t)) \quad (3.3)$$

and

$$\hat{A}(t) \equiv e^{-t\Omega} A e^{t\Omega} \quad (3.4)$$

Note that $\hat{A}(t)$ for $t > 0$ is in general still an operator in the phase space, since Ω in general contains higher-order differentiation operators. Hence $\hat{g}(a, t)$ is also a phase space operator. It is convenient to define the commutator operator O_c for an arbitrary phase space operator O by

$$O_c(\dots) \equiv [O, (\dots)] \equiv O(\dots) - (\dots)O \quad (3.5)$$

where (\dots) is anything that stands to the right of O_c . Here we note that the

relation $e^O f e^{-O} \equiv e^{O_c} f$ holds for arbitrary phase space operators f and O , which can easily be shown by expanding the operator e^O , etc., in Taylor series in O . Then (3.3) and (3.4) are rewritten as

$$\hat{g}(a, t) = e^{-t\Omega_c} \hat{g}(a, 0) \tag{3.6}$$

$$\hat{A}(t) = e^{-t\Omega_c} A \tag{3.7}$$

(3.2) thus becomes

$$g(a, t) = \int [e^{-t\Omega_c} \hat{g}(a, 0)]_c D(0) dx \tag{3.8}$$

where the subscript c attached to the bracket implies that the commutation operation of (3.5) is to be confined within the bracket, although, of course, the phase space operator inside the bracket acts to the right.

We now transform the operator $(d/dt)e^{-t\Omega_c}$ that governs the time evolution of the reduced distribution. A useful feature of Ω_c in contrast to Ω with the property (2.4) is that we now have

$$e^{-t\Omega_c} \Gamma_1(\Gamma_2) = \Gamma_1(e^{-t\Omega_c} \Gamma_2) \tag{3.9}$$

where Γ_2 can be a phase space operator. This turns out to be crucial in the projector formalism to be employed in this transformation. It is precisely this property of Ω_c in contrast to Ω which requires the phase space operator $\hat{g}(a, t)$ in order to achieve a consistent projector formalism in the following.

We now introduce a projector P acting on a phase space operator $O(x)$ as follows:

$$PO(x) = g_e^{-1}(A(x)) \int O(x') \delta(A(x) - A(x')) D_e(x') dx' \tag{3.10}$$

where g_e is the equilibrium reduced distribution defined by (2.5) in which D is replaced by D_e . Note that PO is no longer a phase space operator, but a phase space function, even though O is a phase space operator.

The next step is to use the following operator identity⁽¹²⁾:

$$\frac{d}{dt} e^{-t\Omega_c} = -e^{-t\Omega_c} P\Omega_c + \int_0^t ds e^{-(t-s)\Omega_c} P\Omega_c e^{-sQ\Omega_c} Q\Omega_c - e^{tQ\Omega_c} Q\Omega_c \tag{3.11}$$

where

$$Q \equiv 1 - P \tag{3.12}$$

This then leads to the following equation for $\hat{g}(a, t)$:

$$\begin{aligned} \frac{\partial}{\partial t} \hat{g}(a, t) = & -e^{-t\Omega_c} P\Omega_c \delta(a - A) + \int_0^t ds e^{-(t-s)\Omega_c} \\ & \times P\Omega_c e^{-sQ\Omega_c} Q\Omega_c \delta(a - A) - e^{-tQ\Omega_c} Q\Omega_c \delta(a - A) \end{aligned} \quad (3.13)$$

Each term on the rhs must now be transformed into a more transparent form that permits one to see its relationship with \hat{g} . Since this involves considerable algebra, details are deferred to the Appendix and only the final results are presented here. Namely, (3.13) is formally transformed into

$$\begin{aligned} \frac{\partial}{\partial t} \hat{g}(a, t) = & -\frac{\partial}{\partial a} \cdot V(a) \hat{g}(a, t) + \int_0^t ds \int da' \frac{\partial}{\partial a} \cdot g_e(a) K(aa', s) \cdot \frac{\partial}{\partial a'} \\ & \times g_e^{-1}(a') \hat{g}(a', t-s) - \frac{\partial}{\partial a} \cdot [e^{-tQ\Omega_c} \hat{f}(a, x) \delta(a - A)]_c \end{aligned} \quad (3.14)$$

where $V(a)$ is the state space operator defined by

$$V(a) \equiv \int dx \hat{V}(a, x) \delta(a - A(x)) \frac{D_e(x)}{g_e(a)} \quad (3.15)$$

$$\hat{V}(a, x) \equiv \int_0^1 ds :e^{-s(A-a) \cdot \partial/\partial a} : [-\Omega, A] \quad (3.16)$$

and

$$\hat{f}(a, x) \equiv \hat{V}(a, x) - V(a) \quad (3.17)$$

Here the symbol $::$ means that the differential operator $\partial/\partial a$ must always be placed at the extreme left. $K(aa', s)$ is the memory kernel, itself a tensor in the state space, given by

$$K(aa', t) \equiv g_e(a)^{-1} \int dx [e^{-tQ\Omega_c} \hat{f}(a, x) \delta(a - A)]_c \hat{f}(a', x) \delta(a' - A) D_e(x) \quad (3.18)$$

Now, both sides of (3.14) are still phase space operators. The equation for $g(a, t)$ is then obtained, using (3.2), as

$$\begin{aligned} \frac{\partial}{\partial t} g(a, t) = & -\frac{\partial}{\partial a} \cdot V(a) g(a, t) + \int_0^t ds \int da' \frac{\partial}{\partial a} \cdot g_e(a) K(aa', s) \cdot \frac{\partial}{\partial a'} \\ & \times g_e^{-1}(a') g(a', t-s) - \frac{\partial}{\partial a} \cdot y(a, t) \end{aligned} \quad (3.19)$$

where

$$y(a, t) \equiv \int dx [e^{-tQ\Omega_c} \hat{f}(a, x) \delta(a - A)]_c D(0) \tag{3.20}$$

It should be recalled that the projectors in (3.20) do not act on $D(0)$.

Now, if our coarse-grained description is a physically sensible one, the information about the system which cannot be described by the state variables should be irrelevant and no harm will be done by throwing them away at the outset. In other words, $D(0)$ may be chosen to be a constrained equilibrium phase space distribution $D_c(x; a_0)$ given by

$$D_c(x; a_0) = \delta(A(x) - a_0) D_e(x)/g_e(a_0) \tag{3.21}$$

(Care is needed for quantum mechanical cases.⁽⁸⁾) In this case the last term of (3.19) can be shown to vanish in view of the property $V(a) = P(x') \hat{V}(A(x'), x)$ with $A(x') = a$ and the following result is valid for an arbitrary phase space operator $O(x)$:

$$\begin{aligned} \int dx [PO] \delta(A - a_0) D_e &= \int dx \int dx' g_e^{-1}(A) O' \delta(A - A') D'_e \delta(A - a_0) D_e \\ &= \int dx \int dx' O' \delta(a_0 - A') D'_e \delta(A - a_0) D_e / g_e(a_0) \\ &= \int dx O \delta(a_0 - A) D_e \end{aligned} \tag{3.22}$$

which takes the form

$$\int dx [QO] \delta(A - a_0) D_e = 0 \tag{3.23}$$

Here primed phase space functions and operators mean that their arguments are x' . In this case (3.19) reduces to

$$\begin{aligned} \frac{\partial}{\partial t} g(a, t) &= -\frac{\partial}{\partial a} \cdot V(a) g(a, t) \\ &+ \int_0^t ds \int da' \frac{\partial}{\partial a} \cdot g_e(a) K(aa', s) \cdot \frac{\partial}{\partial a'} \frac{g(a', t-s)}{g_e(a')} \end{aligned} \tag{3.24}$$

This completes the derivation of a closed-form equation for the state space distribution $g(a, t)$ for the constrained equilibrium initial phase distribu-

tion. As demonstrated in the Appendix, this equation has $g_e(a)$ as its stationary solution.

A familiar special case is when (2.1) is a classical Liouville equation with

$$\Omega(x) = -iL(x) \quad (3.25)$$

where $L(x)$ is the Liouville first-order differential operator. Here $[-\Omega, A] = [iL, A]$ is simply a phase space function which is also equal to $\hat{V}(a, x)$ when operated on $\delta(a - A)$ by (A.6), where in fact there is no dependence on a . Thus, by (A.8), $V(a)$ simply reduces to $v(a)$, which is the average of the rate of change $\dot{A} \equiv [iL, A]$ in the constrained equilibrium state and is no longer an operator:

$$V(a) = v(a) \equiv \int dx \dot{A}(x) \delta(a - A(x)) D_e(x) / g_e(a) \quad (3.26)$$

where we have also used (A.27). This is also equal to $P\dot{A}$, that is, $P\hat{V}(a', x)$ evaluated at $A(x) = a$ by (3.10). Therefore, by (3.17) we find

$$\hat{f}(a, x) = f(x) \equiv Q\hat{V}(a', x) = Q\dot{A} \quad (3.27)$$

which is valid at $a = A(x)$ but does not depend on a' . In this case (3.24) reduces to the generalized Fokker-Planck equation due originally to Zwanzig.⁽³⁾ In particular, the $\alpha\beta$ element of the tensor K becomes

$$K_{\alpha\beta}(aa', t) = g_e^{-1}(a) \int dx f_\beta(x) \delta(a' - A) [e^{iQL} f_\alpha(x) \delta(a - A)] D_e(x) \quad (3.28)$$

It is useful to note the following symmetry property reflecting the detailed balance:

$$g_e(a) K_{\alpha\beta}(aa', t) = g_e(a') K_{\beta\alpha}(a'a, -t) \quad (3.29)$$

For a proof, multiply the integrand of (3.28) by e^{-iQL} from the left, which does not change (3.28) in view of $\int dx QL \cdots = 0$. Then (3.28) becomes

$$K_{\alpha\beta}(aa', t) = g_e^{-1}(a) \int dx [e^{-iQL} f_\beta(x) \delta(a' - A)] f_\alpha(x) \delta(a - A) D_e(x)$$

Then (3.29) follows automatically.

The result (3.24) differs from the Zwanzig generalized Fokker-Planck equation⁽³⁾ in that $V(a)$ in general contains differential operators with

respect to the state space variables and also K does not necessarily satisfy (3.29).

As a second example we consider the case where (2.1) is a purely dissipative equation of the form

$$\Omega = k_B T \frac{\partial}{\partial A} \cdot \mu(A) \cdot D_e \frac{\partial}{\partial A} D_e^{-1} \tag{3.30}$$

where $\mu(a)$ is a mobility tensor in the a space. Then we find, as shown in the Appendix,

$$V(a) = -k_B T \mu(a) \cdot g_e(a) \frac{\partial}{\partial a} g_e^{-1}(a) \tag{3.31}$$

Thus, in this case the first term on the rhs of (3.24) already gives the usual Fokker–Planck equation in the state space and the second term in (3.24) gives a correction which is normally neglected.

4. GENERALIZED LANGEVIN EQUATION

Instead of the state space distribution $g(a, t)$, one can also consider the state variables themselves as dynamical variables, and thus obtain a generalized Langevin equation. The first step is to multiply (3.14) by a and integrate over a . With the use of (3.3), (3.4), and (3.7) we then find

$$\frac{d}{dt} \hat{A}(t) = v(\hat{A}(t)) + \int_0^t ds \Psi(s, \hat{A}(t-s)) + \hat{F}(t) \tag{4.1}$$

where $v(a)$ is a function of a redefined as

$$v(a) \equiv V(a) \cdot 1 \tag{4.2}$$

$$\hat{F}(t) \equiv e^{-tQ\Omega} \hat{f}(\hat{A}(x), x) e^{tQ\Omega} \tag{4.3}$$

and

$$\Psi_x(t, a) \equiv g_e^{-1}(a) \sum_{\beta} \frac{\partial}{\partial a_{\beta}} \bar{K}_{\alpha\beta}(t, a) g_e(a) \tag{4.4}$$

with

$$\begin{aligned} \bar{K}_{\alpha\beta}(t, a) &\equiv g_e^{-1}(a) \int da' g_e(a') K_{\alpha\beta}(t, a'a) \\ &= \int dx \hat{F}_x(t) \hat{f}_{\beta}(a, x) \delta(a - A(x)) D_e(x) g_e(a)^{-1} \end{aligned} \tag{4.5}$$

In general, (4.1) is still an operator equation, which reflects the fact that (1.1) does not describe a deterministic trajectory in phase space, in contrast to the classical Liouville equation. That is, the corresponding phase space equation of motion is written as

$$\dot{\mathbf{x}}(t) \equiv \frac{d}{dt} \mathbf{x}(t) = \boldsymbol{\omega}(\mathbf{x}(t), t) \quad (4.6)$$

where $\boldsymbol{\omega}(x, t)$ contains random elements and $\mathbf{x}(t)$ represents the set of phase space variables. The stochastic phase space equation of motion for

$$\mathbf{D}(x, t) = \delta(x - \mathbf{x}(t)) \quad (4.7)$$

is

$$\frac{\partial}{\partial t} \mathbf{D}(x, t) = \boldsymbol{\Omega}(t) \mathbf{D}(x, t) \quad (4.8)$$

where

$$\boldsymbol{\Omega}(t) \equiv \frac{\partial}{\partial x} \boldsymbol{\omega}(x, t) \quad (4.9)$$

is a stochastic Liouville operator. That is, choosing $\mathbf{D}(x, 0) = D(x, 0)$, we have

$$\mathbf{D}(x, t) = \exp_+ \left[\int_0^t ds \boldsymbol{\Omega}(s) \right] D(x, 0) \quad (4.10)$$

where \exp_+ is the time-ordered exponential. The phase space distribution $D(x, t)$ is obtained by averaging (4.10) over random elements contained in $\boldsymbol{\omega}$.⁽¹³⁾ That is,

$$D(x, t) = \langle \mathbf{D}(x, t) \rangle_{\boldsymbol{\omega}} = \left\langle \exp_+ \left[\int_0^t ds \boldsymbol{\Omega}(s) \right] \right\rangle_{\boldsymbol{\omega}} D(x, 0) \quad (4.11)$$

Then Ω is related to $\boldsymbol{\Omega}(t)$ through⁽¹⁴⁾

$$\Omega = \frac{1}{t} \left\langle \exp_+ \left[\int_0^t dx \boldsymbol{\Omega}(s) \right] - 1 \right\rangle_{\text{cm}} \quad (4.12)$$

where $\langle \dots \rangle_{\text{cm}}$ is the cumulant average over $\boldsymbol{\omega}$. That (4.12) is independent of t is the restriction imposed on the nature of random elements in $\boldsymbol{\omega}$ which

must be delta-correlated in time. The phase function $\mathbf{A}(t) \equiv A(\mathbf{x}, t)$ corresponding to the state space variable a is

$$\mathbf{A}(t) = \exp_- \left[\int_0^t ds \mathbf{\Omega}^\dagger(\mathbf{x}(s), s) \right] A(\mathbf{x}(0)) \tag{4.13}$$

where $\mathbf{\Omega}^\dagger$ is the adjoint operator of $\mathbf{\Omega}$:

$$\mathbf{\Omega}^\dagger(x, t) \equiv \boldsymbol{\omega}(x, t) \partial / \partial x \tag{4.14}$$

and \exp_- is the same as \exp_+ except that time-ordering is now reversed. $\hat{A}(t)^\dagger \cdot 1$ is obtained by averaging (4.13) over $\boldsymbol{\omega}$:

$$\hat{A}(t)^\dagger \cdot 1 = e^{i\Omega^\dagger(x)} A(0) \cdot 1 \tag{4.15}$$

with

$$\Omega^\dagger(x) = t^{-1} \left\langle \exp_- \left[\int_0^t ds \mathbf{\Omega}^\dagger(x, s) \right] - 1 \right\rangle_{\text{cm}} \tag{4.16}$$

which is the adjoint operator of $\Omega(x)$, (4.12). Since Ω^\dagger operating on a constant vanishes, we have

$$\hat{A}(t)^\dagger = e^{i\Omega^\dagger} A(0) e^{-i\Omega^\dagger} \tag{4.17}$$

Next we consider the product

$$\begin{aligned} \mathbf{A}_\alpha(t) \mathbf{A}_\beta(t) &= \left\{ \exp_- \left[\int_0^t ds \mathbf{\Omega}^\dagger(s) \right] A_\alpha \right\} \left\{ \exp_- \left[\int_0^t ds \mathbf{\Omega}^\dagger(s) \right] A_\beta \right\} \\ &= \exp_- \left[\int_0^t ds \mathbf{\Omega}^\dagger(s) \right] A_\alpha A_\beta \end{aligned} \tag{4.18}$$

The second step is justified since $\mathbf{\Omega}^\dagger$ is the first-order differential operator. Averaging over $\boldsymbol{\omega}$, we now find

$$\langle \mathbf{A}_\alpha(t) \mathbf{A}_\beta(t) \rangle_\omega = e^{i\Omega^\dagger} A_\alpha A_\beta = \hat{A}_\alpha^\dagger(t) \hat{A}_\beta^\dagger(t) \cdot 1 \tag{4.19}$$

This applies to any function $X(A(t))$ of $A_\alpha(t)$, so that

$$\langle X(\mathbf{A}(t)) \rangle_\omega = e^{i\Omega^\dagger} X(A) = X(\hat{A}(t)^\dagger) \cdot 1 \tag{4.20}$$

The results obtained in this section up to now permit us to interpret the adjoint of the operator equation (4.1) operating onto unity to the right as the $\boldsymbol{\omega}$ -averaged equation for $\mathbf{A}(t)$ of the same form as (4.1) where $\hat{A}(t)^\dagger$

everywhere is replaced by $\mathbf{A}(t)$ except for the last term, which is replaced by the phase function $\mathbf{F}(x, t)$ defined by

$$\mathbf{F}(x, t) \equiv \hat{F}(t)^+ \cdot 1 \quad (4.21)$$

The desired generalized Langevin equation is then the equation for $\mathbf{A}(t)$ before taking ω -averaging. Thus, we split $\omega(\mathbf{x}(t), t)$ as

$$\omega(\mathbf{x}(t), t) = \bar{\omega}(\mathbf{x}(t), t) + \mathbf{f}_\omega(\mathbf{x}(t), t) \quad (4.22)$$

where $\bar{\omega}$ is the ω -averaged part and \mathbf{f}_ω is the remainder that vanishes after ω -averaging. In this way the generalized Langevin equation for the random variable $\mathbf{A}(t)$ is obtained as

$$\frac{d}{dt} \mathbf{A}(t) = v(\mathbf{A}(t)) + \int_0^t ds \Psi(s, \mathbf{A}(t-s)) + \mathbf{F}(t) + \mathbf{f}_A(t) \quad (4.23)$$

where

$$\mathbf{f}_A(t) \equiv \mathbf{f}_\omega(t) \cdot \frac{\partial}{\partial \mathbf{x}(t)} A(\mathbf{x}(t)) \quad (4.24)$$

and $\bar{\omega}$ is assimilated into the first two terms on the rhs of (4.23).

The generalized Langevin equation now has two kinds of random forces. $\mathbf{f}_A(t)$ originates from the random force inherent in the starting equation (1.1). This term is connected to the dissipative part of $v(\mathbf{A}(t))$ through a ‘‘microscopic’’ fluctuation-dissipation relation. We shall not elaborate on this any further, since this is more or less known. Another random force $\mathbf{F}(t)$ arises from the coarse-graining process of reducing the phase space into the state space. The corresponding fluctuation-dissipation relation is already given through (4.4) and (4.5). Equation (4.5) can be put in a slightly different form as

$$\bar{K}_{\alpha\beta}(t, a) = g_e^{-1}(a) \int dx D_e(x) \delta(a - A(x)) \hat{f}_\beta^+(a, x) \langle \mathbf{F}_\alpha(x, t) \rangle_\omega \quad (4.25)$$

When (1.1) is the classical Liouville equation with (3.25), Eq. (4.23) reduces to the known result.⁽¹²⁾

Finally we note that the generalized Langevin equation derived here does not give complete information on the stochastic processes under consideration, since this is the first moment equation of the generalized Fokker–Planck equation and must be supplemented by equations for higher moments. Nevertheless, this type of generalized Langevin equation

has been useful to generate various approximation schemes, such as the mode coupling approximation,^(7,10) where random forces are assumed to be Gaussian.

5. DISCUSSION

Equation (4.1) and similar equations for higher moments obtained from (3.1) by multiplying it by products of the a 's and integrating over a suggest an alternative way to derive the results of this work, which is closer to the procedure followed by Nordholm and Zwanzig.⁽⁸⁾ From Sections 2 and 4 we see that the time development of a physical quantity corresponding to the phase function $X(x)$ can be obtained by the operator

$$\hat{X}^\dagger(t) \equiv e^{t\Omega^\dagger} X e^{-t\Omega^\dagger} \tag{5.1}$$

We can then write down, using the standard projector formalism,⁽⁴⁾ the generalized linear Langevin equation in the operator form for a column vector of dynamical variables consisting of products of $\hat{A}^\dagger(t)$. Putting all these equations together, one should be able to derive an operator equation which is Hermitian conjugate to (3.14), although we have not yet verified this.

In the present paper we were able to extend the powerful projector formalism beyond what is currently available (Section 1). This will help us to examine the basis of some existing applications of the projector formalism to dissipative and noisy systems such as polymer systems. We hope to report on such studies in the future.

APPENDIX

First we consider the operator

$$O_1(x) \equiv [\Omega_c \delta(a - A(x))]_c \tag{A.1}$$

In order to transform this expression, we note the following expansion for small $t > 0$:

$$\begin{aligned} O_1(x) &\cong -\frac{1}{t} [\delta(a - \hat{A}(t)) - \delta(a - A)] \\ &= -\frac{1}{t} \int_k (\exp\{ik \cdot [a - A - t\hat{A}_t(0)]\} - \exp[ik \cdot (a - A)]) \\ &= \int_k \int_0^1 ds \exp[ik \cdot a - (1-s)ik \cdot A] ik \cdot \hat{A}_t(0) \exp(-isk \cdot A) \end{aligned} \tag{A.2}$$

Here k is a wave vector in the state space of a and \int_k is the integral over the k space divided by $(2\pi)^{-d_s}$, d_s being the dimensionality of the state space; the subscript t on \hat{A} stands for time derivative. The dot denotes the scalar product of vectors in the state space. Since $\hat{A}_t(0) = -[\Omega, A]$, we can also write

$$\begin{aligned} O_1(x) &= -\frac{\partial}{\partial a} \cdot \int_k \int_0^1 ds e^{i(1-s)k \cdot (a-A)} [\Omega, A] e^{isk \cdot (a-A)} \\ &= -\frac{\partial}{\partial a} \cdot \int_0^1 ds \int da' \delta(a' - A) [\Omega, A] \delta(a - A - s(a' - A)) \end{aligned} \quad (\text{A.3})$$

where s and $1-s$ were interchanged in the last step. We then use

$$\begin{aligned} \delta(a - A - s(a' - A)) &= \exp \left[-s(a' - A) \cdot \frac{\partial}{\partial a} \right] \delta(a - A) \\ &= : \exp \left[-s(a' - a) \cdot \frac{\partial}{\partial a} \right] : \delta(a - A) \end{aligned} \quad (\text{A.4})$$

where the symbol $::$ means that differential operators $\partial/\partial a$ must always be placed at the extreme left upon expanding the exponential differential operator. Hence (A.3) becomes

$$[\Omega_c \delta(a - A(x))]_c = \frac{\partial}{\partial a} \cdot \hat{V}(a, x) \delta(a - A(x)) \quad (\text{A.5})$$

where

$$\hat{V}(a, x) \equiv \int_0^1 ds : \exp \left[-s(A - a) \cdot \frac{\partial}{\partial a} \right] : [-\Omega, A] \quad (\text{A.6})$$

In obtaining (A.6), integration over a' was trivially carried out. Operating by P on (A.5), we then find after some straightforward algebra

$$P[\Omega_c \delta(a - A(x))]_c = \frac{\partial}{\partial a} \cdot V(a) \delta(a - A(x)) \quad (\text{A.7})$$

where

$$V(a) \equiv \int dx \hat{V}(a, x) \delta(a - A(x)) \frac{D_e}{g_e(a)} \quad (\text{A.8})$$

is the operator acting in the state space. Now the time displacement

operator $e^{-t\Omega_c}$ operating on (A.7) acts only on $A(x)$. Therefore we find the following for the second term of (3.13):

$$- [e^{-t\Omega_c} P\Omega_c \delta(a - A)]_c = - \frac{\partial}{\partial a} \cdot V(a) \hat{g}(a, t) \tag{A.9}$$

Then we immediately find

$$Q[\Omega_c \delta(a - A(x))]_c = \frac{\partial}{\partial a} \cdot \hat{f}(a, x) \delta(a - A(x)) \tag{A.10}$$

where

$$\hat{f}(a, x) \equiv \hat{V}(a, x) - V(a) \tag{A.11}$$

Next we take up

$$O_2(s, a, x) = P[\Omega_c e^{-sQ\Omega_c} Q\Omega_c \delta(a - A(x))]_c \tag{A.12}$$

By the definition of the projector (3.10) and noting (2.3), we find after some algebra

$$O_2(t, a, x) = - \int dx' Y'(a, t) Y'(A, 0) D'_e/g_e(A) \tag{A.13}$$

where

$$Y(a, t, x) \equiv - [e^{-tQ\Omega_c} Q\Omega_c \delta(a - A)]_c \tag{A.14}$$

and primes imply that x is to be replaced by x' in the arguments. To avoid confusion, we note that $Y'(A, 0)$ is explicitly written as

$$Y'(A, 0) = Y(A(x), 0, x') = -Q(x')[\Omega_c(x') \delta(A(x) - A(x'))]_c \tag{A.15}$$

Here we have used (2.2) and the following identity:

$$\int dx X_1(PX_2)D_e = \int dx (PX_1) X_2D_e \tag{A.16}$$

for a pair of arbitrary phase space operators X_1 and X_2 . Equation (A.15) can be directly verified using the definition (3.10). Let us rewrite (A.13) as

$$O_2(t, a, x) = - \int da' K^*(t, aa') \delta(A(x) - a') g_e^{-1}(a') \tag{A.17}$$

where

$$K^*(t, aa') \equiv \int dx Y(a, t, x) Y(a', 0, x) D_e(x) \quad (\text{A.18})$$

is no longer an operator. Now, using (A.10), we have for $Y(a, t, x)$ of (A.14)

$$Y(a, t, x) = -\frac{\partial}{\partial a} [e^{-tQ\Omega_c} \hat{f}(a, x) \delta(a-A)]_c \quad (\text{A.19})$$

and thus

$$K^*(t, aa') = \frac{\partial}{\partial a} \frac{\partial}{\partial a'} : g_e(a) K(aa', t) \quad (\text{A.20})$$

where K is the tensor function in the state space given by

$$K(aa', t) \equiv g_e(a)^{-1} \int dx [e^{-tQ\Omega_c} \hat{f}(a, x) \delta(a-A)]_c \\ \times \hat{f}(a', x) \delta(a'-A) D_e(x) \quad (\text{A.21})$$

and the symbol $:$ means a scalar product of two tensors. Here we recall that the notation $[\cdot]_c$ implies that the commutation with Ω extends only to the expression within $[\cdot]_c$ and that the phase operator with $[\cdot]_c$ extends all the way to its right.

Substituting (A.9), (A.17) with (A.20) and (A.10) into (3.13), we finally obtain

$$\frac{\partial}{\partial t} \hat{g}(a, t) = -\frac{\partial}{\partial a} \cdot V(a) \hat{g}(a, t) + \int_0^t ds \int da' \frac{\partial}{\partial a} \cdot g_e(a) K(aa'; s) \cdot \frac{\partial}{\partial a'} \\ \times g_e^{-1}(a') \hat{g}(a', t-s) - \frac{\partial}{\partial a} \cdot [e^{-tQ\Omega_c} \hat{f}(a, x) \delta(a-A)]_c \quad (\text{A.22})$$

which is reproduced as (3.14). One can readily verify that the second and third terms on the rhs vanish if \hat{g} is replaced by g_e . To see this for the second term, we use (A.5) and

$$\int dx [\Omega, \delta(a-A)] D_e = 0 \quad (\text{A.23})$$

on the rhs of

$$\frac{\partial}{\partial a} \cdot V(a) g_e(a) = \frac{\partial}{\partial a} \cdot \int dx \hat{V}(a, x) \delta(a-A) D_e \quad (\text{A.24})$$

For a purely dissipative case given by (3.30) we have

$$[\Omega, A] D_e = k_B T \left[2\mu \cdot D_e \frac{\partial}{\partial A} + \left(\frac{\partial}{\partial A} \cdot \mu D_e \right) \right] \quad (\text{A.25})$$

Using

$$:e^{-s(\partial/\partial a) \cdot (A-a)}: \frac{\partial \delta(A-a)}{\partial A} = \frac{\partial}{\partial a} (s-1) \delta(A-a) \quad (\text{A.26})$$

$$:e^{-s(\partial/\partial a) \cdot (A-a)}: \delta(a-A) = \delta(a-A) \quad (\text{A.27})$$

as well as (A.25), we can readily find (3.31).

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