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A Unified Approach for Deriving Kinetic Equations in Nonequilibrium Statistical Mechanics. II. Approximate Results

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The exact form for the kinetic equation derived by Mori, Fujisaka, and Shigematsu (MFS) is used to obtain several approximations better suited to be compared with macroscopic transport equations. Three approximations are discussed, namely, those known as the diagonal, the slow process, and the Markovian. The corresponding results are emphasized and their relationship is established. In particular, the Kramers–Moyal expansion for the Markovian kinetic equation is obtained from a microscopic basis.

KEY WORDS: Kinetic equation; diagonal, slow process, and Markovian approximations; slowness parameter; Kramers–Moyal expansion; mode–mode coupling; Fokker–Planck equation; derivative moments.

1. INTRODUCTION

In a previous paper[1] (hereafter referred to as I) we have discussed a unified method for deriving exact kinetic equations which govern the time evolution of the phase space functions describing the states of many-body systems. The relationship between the well-known methods of Zwanzig[2] and Mori *et al.*[3] was established as well as the equivalence among the many forms of the generalized projector operator which are of common use in the literature. In particular, the so-called Mori, Fujisaka, Shigematsu[3] (MFS) form is very useful because they have succeeded in expanding it in terms of a "slowness" parameter which leads to a Kramers–Moyal type of expansion for the exact kinetic equation.

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The purpose of this work is to use the ideas behind the MFS approach to present a systematic derivation of the approximate kinetic equations, which are known to allow a comparison with macroscopic transport equations in many situations of physical interest. It is hoped this will lead to a clear understanding of the nature of the approximations themselves and of the corresponding equations. In our belief that this is a rather obscure point in the present stage of our understanding of such complex phenomena.

In order to make this paper self-contained, a very brief resume of the main results obtained in I are given in Section 2. In Section 3 we derive Zwanzig's[2] approximate kinetic equation for slow processes. Also, another approximate result, which is referred to as the "diagonal" form, is obtained. This form has been widely used in the study of the dynamics of nonlinear fluctuations[4,5] and is often confused with the former one. In Section 4 we show that under a Markovian assumption the MFS equation reduces to the Kramers–Moyal (KM) expansion for the kinetic equation with explicit, microscopic, expressions for the derivative moments. Furthermore, if one introduces the diagonal approximation, then the KM expansion becomes a Fokker–Planck type of equation, which may be cast into the nonlinear form used in the study of the renormalization of transport coefficients[6] and to find the stationary states of a system not in equilibrium.[7] We also want to point out there how this equation is related to the nonlinear Langevin equation proposed by Kawasaki[8] for the mode–mode coupling theory. Finally, we show that if the "slow process" approximation is introduced in the KM expansion, one obtains the Fokker–Planck equation used by Green[9] in his pioneering work on this subject.

2. RESUME OF USEFUL RESULTS

As we showed in I, if $g(\mathbf{a}, t)\, d\mathbf{a}$ is the probability that at time t, $a_k \leqslant A_k(\Gamma) \leqslant a_k + da_k$ for all k, $A_k(\Gamma)$ being the kth phase space function selected using the criteria discussed by Green[9] and a_k its numerical value, and if we choose the initial probability density $\rho(\Gamma, 0)$ as

$$\rho(\Gamma, 0) = W(\Gamma)\nu\{A(\Gamma)\} \tag{1}$$

where $W(\Gamma)$ depends on the invariants of the system and $\nu\{A(\Gamma)\}$ is a function of the phase space functions, then

$$dg(\mathbf{a}, t)/dt = Z(\mathbf{a}, t)g(\mathbf{a}, t) \tag{2}$$

where $Z(\mathbf{a}, t)$ is Zwanzig's operator (ZO) given by

$$Z(\mathbf{a}, t)g(\mathbf{a}, t) = \int d\mathbf{b}\, i\Omega(\mathbf{a}, \mathbf{b})g(\mathbf{b}, t) - \int_0^t ds \int d\mathbf{b}\, K(\mathbf{a}, \mathbf{b}, s)g(\mathbf{b}, t - s) \tag{3}$$

If the inner product of two phase space functions A and B is defined through

$$(A, B) = \int d\Gamma\ W(\Gamma)A(\Gamma)B^*(\Gamma) \tag{4}$$

then

$$i\Omega(\mathbf{a}, \mathbf{b}) = [G(\mathbf{b}, 0)]^{-1}(i\Gamma G(\mathbf{a}, 0), G(\mathbf{b}, 0)) \tag{5}$$

$$K(\mathbf{a}, \mathbf{b}, s) = [G(\mathbf{b}, 0)]^{-1}(F(\mathbf{a}, s), F(\mathbf{b}, 0)) \tag{6}$$

$$[G(\mathbf{b}, 0)] = \int d\Gamma\ W(\Gamma)G(\mathbf{b}, 0) \tag{7}$$

L is Liouville's operator and $G(\mathbf{a}, t) = \prod_k \delta(A_k(\Gamma, t) - a_k) = \delta(A(\Gamma, t) - \mathbf{a})$, the hypercell in phase space at time t. Also,

$$F(\mathbf{a}, t) = e^{(1-P_G)iLt}(1 - P_G)iLG(\mathbf{a}, 0) \tag{8}$$

P_G being the projection operator defined as

$$P_G = \int d\mathbf{b}\, \frac{(\ldots, G(\mathbf{b}, 0))}{[G(\mathbf{b}, 0)]}\, G(\mathbf{b}, 0) \tag{9}$$

The exact kinetic equation (2) may be expressed in different equivalent ways. The generalized Fokker–Planck form (GFP) is shown to be

$$\frac{dg(\mathbf{a}, t)}{dt} = -\sum_k \frac{\partial}{\partial a_k}[v_k(\mathbf{a})g(\mathbf{a}, t)] + \int_0^t ds \int d\mathbf{b} \sum_k \sum_l \times \frac{\partial}{\partial a_k}[G(\mathbf{b}, 0)]K_{kl}(\mathbf{a}, \mathbf{b}, s)\frac{\partial}{\partial b_l^*}\frac{g(\mathbf{b}, t-s)}{[G(\mathbf{b}, 0)]} \tag{10}$$

where

$$v_k(\mathbf{a}) = \langle \dot{A}_k(\Gamma, 0); \mathbf{a}\rangle \tag{11}$$

$$K_{kl}(\mathbf{a}, \mathbf{b}, s) = \langle X_k(\mathbf{a}, s)R_l^*(0); \mathbf{b}\rangle \tag{12}$$

$\langle \ldots, \mathbf{a}\rangle$ being the microcanonical average taken over the hypercell specified by $A(\Gamma) = \mathbf{a}$, so that

$$\langle f(\Gamma), \mathbf{a}\rangle = [G(\mathbf{a}, 0)]^{-1} \int d\Gamma\ W(\Gamma)f(\Gamma)\ \delta(A(\Gamma) - \mathbf{a})$$

$$= [G(\mathbf{a}, 0)]^{-1}(f(\Gamma), G(\mathbf{a}, 0)) \tag{13}$$

The phase space functions $X_k(\mathbf{a}, t)$ and $R_k(t)$ are defined by,

$$X_k(\mathbf{a}, t) = e^{(1-P_G)iLt}\{R_k(0)G(\mathbf{a}, 0)\} \tag{14}$$

$$R_k(t) \quad = e^{(1-P_G)iLt}(1 - P_G)iLA_k(0) \tag{15}$$

with $R_k(t)$ playing the role of a fluctuating force, as has been emphasized in Eq. (57) of I.

If one writes $K_{kl}(\mathbf{a}, \mathbf{b}, s)$ given by Eq. (12) so that the correlation of the fluctuating forces $R_k(t)$ and $R_l(0)$ over the hypercell appears in an explicit way, namely

$$K_{kl}(\mathbf{a}, \mathbf{b}, t) = L_{kl}(\mathbf{b}, t)\, \delta(\mathbf{a} - \mathbf{b}) + K'_{kl}(\mathbf{a}, \mathbf{b}, t) \tag{16}$$

where

$$L_{kl}(\mathbf{b}, t) = \langle R_k(t) R_l^*(0); \mathbf{b} \rangle \tag{17}$$

and

$$K'_{kl}(\mathbf{a}, \mathbf{b}, t) = \langle Y_k(\mathbf{a}, t) R_l^*(0); \mathbf{b} \rangle \tag{18}$$

and $Y_k(\mathbf{a}, t)$ is defined by

$$X_k(\mathbf{a}, t) = R_k(t) G(\mathbf{a}, 0) + Y_k(\mathbf{a}, t) \tag{19}$$

and now $K'_{kl}(\mathbf{a}, \mathbf{b}, t)$ is expressed in terms of the correlation force, Eq. (15), then the MFS form of Eq. (2) is obtained, namely

$$\begin{aligned} \frac{dg(\mathbf{a}, t)}{dt} = & -\sum_k \frac{\partial}{\partial a_k} [v_k(\mathbf{a}) g(\mathbf{a}, t)] + \sum_{n=0}^{\infty} (-1)^n \sum_{k_0} \cdots \sum_{k_n} \frac{\partial}{\partial a_{k_0}} \cdots \frac{\partial}{\partial a_{k_n}} \\ & \times \sum \int_0^t dt' \, [G(\mathbf{a}, 0)] \langle S(k_0, \ldots, k_n; t') R_l^*; \mathbf{a} \rangle \\ & \times \frac{\partial}{\partial a_l^*} \frac{g(\mathbf{a}, t - t')}{[G(\mathbf{a}, 0)]} \end{aligned} \tag{20}$$

where

$$\begin{aligned} S(k_0, \ldots, k_n; t') = & \int_0^{t'} dt_1 \cdots \int_0^{t_{n-1}} dt_n \, U(t' - t_1)(1 - P_G) \dot{A}_{k_1}(0) \\ & \times \cdots U(t_{n-1} - t_n)(1 - P_G) \dot{A}_{k_n}(0) R_{k_0}(t_n) \end{aligned} \tag{21}$$

with the U operator defined through

$$U(t) = e^{(1 - P_G) iLt} \tag{22}$$

Equation (20) may be alternatively written as

$$\begin{aligned} \frac{dg(\mathbf{a}, t)}{dt} = & \sum_{n=0}^{\infty} \sum_{k_0} \cdots \sum_{k_n} \left(-\frac{\partial}{\partial a_{k_0}} \right) \cdots \left(-\frac{\partial}{\partial a_{k_n}} \right) \\ & \times \int_0^t dt' \, K_{k_0 \cdots k_n}(\mathbf{a}, t') g(\mathbf{a}, t - t') \end{aligned} \tag{23}$$

where

$$K_{k_0}(\mathbf{a}, t') = v_{k_0}(\mathbf{a})\, \delta(t') + C_{k_0}(\mathbf{a}, t') \tag{24}$$

$$K_{k_0 \cdots k_n}(\mathbf{a}, t') = G_{k_0 \cdots k_n}(\mathbf{a}, t') + L_{k_0 \cdots k_{n-1}; -k_n}(\mathbf{a}, t') \tag{25}$$

and

$$L_{k_0\cdots k_n;l}(\mathbf{a}, t') = \langle S(k_0,\ldots, k_n, t')R_l^*(0); \mathbf{a}\rangle \tag{26}$$

$$G_{k_0\cdots k_n}(\mathbf{a}, t') = [G(\mathbf{a}, 0)]^{-1}\sum_l \frac{\partial}{\partial a_l^*}[G(\mathbf{a}, 0)]L_{k_0\cdots k_n;l}(\mathbf{a}, t') \tag{27}$$

Equation (23) resembles the KM expansion for the kinetic equation in the Markovian approximation. In Section 3 this will be shown to hold true for the MFS equation under such an assumption, which suggests that Eq. (23) could be considered as the KM expansion for a non-Markovian process.

3. DIAGONAL AND SLOW PROCESSES APPROXIMATIONS

The different forms for the kinetic equation (2) mentioned in the previous section are still exact. Also, they are too complicated in their structure to allow a comparison with macroscopic equations. In this section we shall discuss two approximate kinetic equations and their relationship as well.

The diagonal approximation assumes that the leading term of the memory kernel $K_{kl}(\mathbf{a}, \mathbf{b}, t)$ which appears in Eq. (10) and is defined in Eqs. (12) and (16) is given by $L_{kl}(\mathbf{a}, t)$, that is, by the correlation of the fluctuating force $R_k(t)$ over the hypercell $A(\Gamma) = \mathbf{a}$ in phase space. Thus,

$$K_{kl}(\mathbf{a}, \mathbf{b}, t) \simeq L_{kl}(\mathbf{a}, t)\,\delta(\mathbf{a} - \mathbf{b}) \tag{28}$$

implying that $K_{kl}(\mathbf{a}, \mathbf{b}, t)$ is diagonal in a space.

A justification for such an approximation may be found in the fact that the time evolution for the collective variables of the system is unaffected by Eq. (28), so that both the exact kinetic equation (2) and its diagonal approximation give rise to the same nonlinear and non-Markovian Langevin equation for the collective variables $\{A_k(\Gamma, t)\}$. In order to show this, we start from the exact time evolution equation for the hypercell $G(\mathbf{a}, t)$, which was shown in I to be

$$dG(\mathbf{a}, t)/dt = Z(\mathbf{a}, t)G(\mathbf{a}, t) + F(\mathbf{a}, t) \tag{29}$$

The time evolution equation for $\{A_k(\Gamma, t)\}$ is obtained from Eq. (29), integrating over $d\mathbf{a}$ and using the identity

$$A_k(\Gamma, t) = \int d\mathbf{a}\, a_k G(\mathbf{a}, t) \tag{30}$$

to yield

$$\frac{dA_k(\Gamma, t)}{dt} = \int a_k Z(\mathbf{a}, t)G(\mathbf{a}, t)\, d\mathbf{a} + R_k(t) \tag{31}$$

Using Eqs. (2) and (10) to evaluate the integral on the rhs of Eq. (31), one arrives at

$$\frac{dA_k(\Gamma, t)}{dt} = \int d\mathbf{a}\, v_k(\mathbf{a}) G(\mathbf{a}, t) + \int_0^t ds \int d\mathbf{b}\, \frac{G(\mathbf{b}, t-s)}{[G(\mathbf{b}, 0)]} \times \sum_l \frac{\partial}{\partial b_l^*} [G(\mathbf{b}, 0)] \int d\mathbf{a}\, K_{kl}(\mathbf{a}, \mathbf{b}, s) + R_k(t) \tag{32}$$

Using Eq. (18), one can show (see Appendix A) that

$$\int d\mathbf{a}\, K'_{kl}(\mathbf{a}, \mathbf{b}, s) = 0 \tag{33}$$

so that Eq. (32) is transformed into

$$\frac{dA_k(\Gamma, t)}{dt} = \int d\mathbf{a}\, v_k(\mathbf{a}) G(\mathbf{a}, t) + \int_0^t ds \int d\mathbf{b} \left\{ [G(\mathbf{b}, 0)]^{-1} \times \sum_l \frac{\partial}{\partial b_l^*} [G(\mathbf{b}, 0)] L_{kl}(\mathbf{b}, s) \right\} G(\mathbf{b}, t-s) + R_k(t) \tag{34}$$

which is an alternative form of Eq. (59) of I. It is now clear from Eq. (33) that the nonlinear, non-Markovian Langevin equation for the collective variables $\{A_k(\Gamma)\}$ corresponding to the exact kinetic equation (2) is invariant under the diagonal approximation, where $K'_{kl}(\mathbf{a}, \mathbf{b}, t) = 0$. Thus, the assumption expressed by Eq. (28) may be justified by the fact that it leads to an equation for the $\{A_k(\Gamma)\}$ that is identical to Eq. (34). However, it is important to underline the fact that the diagonal approximation differs from the exact kinetic equation, since it predicts different time evolution equations for the higher moments of the A_ks.

The diagonal approximation was introduced by Mori and Fujisaka[4] and by García-Colín and Velasco[5] in a way that is different from the one presented above. This equation will be referred to as the Mori-García-Colín equation (MGC) and is readily found if Eq. (28) is used in Eq. (10), namely,

$$\frac{dg(\mathbf{a}, t)}{dt} = -\sum_k \frac{\partial}{\partial a_k} [v_k(\mathbf{a}) g(\mathbf{a}, t)] + \sum_k \sum_l \frac{\partial}{\partial a_k} \int_0^t ds\, [G(\mathbf{a}, 0)] \times L_{kl}(\mathbf{a}, s) \frac{\partial}{\partial a_l^*} \frac{g(\mathbf{a}, t-s)}{[G(\mathbf{a}, 0)]} \tag{35}$$

It may be obtained in an alternative fashion from the MFS equation (20), neglecting all the terms in the series for $n \geqslant 1$. This is equivalent to ignoring the nondiagonal contributions of $K_{kl}(\mathbf{a}, \mathbf{b}, s)$.

Another approximate kinetic equation is found in those cases where the time rate of change of the phase space functions is controlled by a "slowness" parameter δ,[3] which implies that $\dot{A}_k \sim \delta$. When $\delta \ll 1$ the relevant or

dominant terms in the resulting equation are those that are of order δ and δ^2 and characterize the slow behavior. This is, however, possible, provided that the A_k and the slowness parameter have been chosen in an appropriate manner so that the power series expansion in the latter is valid. Equation (20) is very well suited for deriving the kinetic equation for slow processes, since it contains the different terms to all orders in δ. Let us now study this equation in terms of δ, by noticing that since $\dot{A}_k(\Gamma, 0) \sim \delta$, Eqs. (11) and (15) imply that

$$v_k(a) \sim \delta, \qquad R_k(0) \sim \delta \tag{36}$$

When $(iLP_G)^n$ is applied to a phase function $I(\Gamma)$ that changes as δ^r, then (see Appendix A)

$$[iLP_G]^n I(\Gamma) \sim \delta^{n+r} \tag{37}$$

Using Eq. (37), it follows easily that $U(t)(1 - P_G)I(\Gamma)$ has at least terms of order δ^r,

$$U(t)(1 - P_G)I(\Gamma) = (1 - P_G)e^{iL(1-P_G)t}I(\Gamma) \sim \delta^r \tag{38}$$

and also, by Eq. (15),

$$R_k(t) \sim \delta \tag{39}$$

Use of Eq. (39) in Eq. (21) leads also to the result that

$$S(k_0,..., k_n, t') \sim \delta^{n+1} \tag{40}$$

whence

$$\langle S(k_0,..., k_n, t')R_l^*(0); \mathbf{a}\rangle \sim \delta^{n+2} \tag{41}$$

From Eqs. (36) and (41) it follows readily that the first term in Eq. (20) is linear in δ, whereas the nth term has terms of order δ^{n+2} and higher powers in δ. This implies that the MFS equation is *not* a systematic power series expansion in terms of the slowness parameter δ. However, if $\delta < 1$, we can obtain the kinetic equation for slow processes by neglecting all terms of order δ^3 and higher, recovering Zwanzig's approximate equation.[2] Indeed, we may proceed in two steps, setting first $n = 0$. This leads to the MGC equation (35). In this equation the term $L_{kl}(\mathbf{a}, s)$ defined by Eq. (17) still has contributions of order higher than δ^2. To extract from it the linear and quadratic contributions in this parameter, we use Eq. (36) and notice also from Eq. (15) that any term in the expansion of the exponential operator containing at least one fact iLP_G is, according to (37), of order δ^2; hence

$$R_k(s) = (1 - P_G)\dot{A}_k(\Gamma, s) + O(\delta^2) \tag{42}$$

using the fact that $\dot{A}_k(\Gamma, s) = e^{iLs}\dot{A}_k(\Gamma, 0)$. Letting P_G act on the phase function, one obtains that

$$R_k(s) = \dot{A}_k(\Gamma, s) - \int d\mathbf{b}\, \langle \dot{A}_k(\Gamma, s); \mathbf{b}\rangle G(\mathbf{b}, 0) + O(\delta^2) \tag{43}$$

Thus, the δ^2 effect in $L_{kl}(\mathbf{a}, s)$ is obtained through the identity (A9), to yield

$$\langle R_k(s)R_l^*(0); \mathbf{a}\rangle = \langle [\dot{A}_k(\Gamma, s) - v_k(\mathbf{a})][\dot{A}_l(\Gamma, 0) - v_l(\mathbf{a})]^*; \mathbf{a}\rangle + O(\delta^3) \tag{44}$$

where use has been made of the fact that $\langle G(\mathbf{b}, 0)\dot{A}_l^*(0); \mathbf{a}\rangle = v_l^*(\mathbf{a})\,\delta(\mathbf{a} - \mathbf{b})$, so that to order δ^2 the correlation of the fluctuating forces is equal to the correlation of the velocities in the hypercell. If this term is denoted by $L_{kl}^{(2)}(\mathbf{a}, t)$, we can finally write, substituting Eq. (44) back into Eq. (35), that

$$\frac{dg(\mathbf{a}, t)}{dt} = -\sum_k \frac{\partial}{\partial a_k} v_k(\mathbf{a})g(\mathbf{a}, t) + \sum_k \sum_l \int_0^t ds\, [G(\mathbf{a}, 0)]L_{kl}^{(2)}(\mathbf{a}, s) \times \frac{\partial}{\partial a_l^*} \frac{g(\mathbf{a}, t - s)}{[G(\mathbf{a}, 0)]} \tag{45}$$

which is just Eq. (33) in Ref. 2.

In spite of the formal similarity between Eqs. (35) and (45), which has occasionally led to an identification of the slow process and the diagonal approximations, they are different kinetic equations. As indicated above, Eq. (45) has an additional restriction over Eq. (35), namely that the correlation of the fluctuating forces is replaced by the correlation of the velocities on the hypercell, which is a δ^2 effect.

4. MARKOVIAN KINETIC EQUATIONS

The main purpose of this section is to show how the MFS result, Eq. (20), behaves under a Markovian assumption. The KM expansion for the kinetic equation is obtained, which under further approximations, namely the diagonal one, leads to the nonlinear Fokker–Planck equation used by Zwanzig and Kawasaki in their study of the renormalization of transport coefficients and in the mode–mode coupling theory. Also, the KM expansion together with the slow process approximation reduces to the Fokker–Planck equation used by Green in his general theory of irreversible processes.

The usual way of introducing the Markovian approximation within a microscopic context is to assume that the times over which the phase space functions $A_k(\Gamma)$ change appreciably are much longer than the correlation time of the kernel $K(\mathbf{a}, \mathbf{b}, t)$. Thus one writes that

$$K(\mathbf{a}, \mathbf{b}, t) = 2K(\mathbf{a}, \mathbf{b})\,\delta(t) \tag{46}$$

where

$$K(\mathbf{a}, \mathbf{b}) = \int_0^\infty K(\mathbf{a}, \mathbf{b}, t)\, dt \tag{47}$$

Introducing Eq. (46) into Eq. (2) and using the convention that $\int_0^\infty dt\ \delta(t) = \frac{1}{2}$ yields

$$dg(\mathbf{a}, t)/dt = M(\mathbf{a})g(\mathbf{a}, t) \tag{48}$$

where the time-independent operator $M(\mathbf{a})$ is given by

$$M(\mathbf{a})g(\mathbf{a}, t) = \int d\mathbf{b}\ [i\Omega(\mathbf{a}, \mathbf{b}) - K(\mathbf{a}, \mathbf{b})]g(\mathbf{b}, t) \tag{49}$$

Introduce now $\Lambda(\mathbf{a})$, the adjoint operator of $M(\mathbf{a})$, through the following equality:

$$\int f(\mathbf{a})M(\mathbf{a})h(\mathbf{a})\, d\mathbf{a} = \int h(\mathbf{a})\Lambda(\mathbf{a})f(\mathbf{a})\, d\mathbf{a} \tag{50}$$

where $f(\mathbf{a})$ and $h(\mathbf{a})$ are arbitrary functions of the variables $\{a_k\}$.

Upon substitution of $K(\mathbf{a}, \mathbf{b}, t)$ in Eq. (20) by its approximate value given by Eqs. (46) and (47) and using Eqs. (76), (92), and (68) of I, one can show that the kinetic equation is transformed into

$$\frac{dg(\mathbf{a}, t)}{dt} = -\sum_k \frac{\partial}{\partial a_k}[v_k(\mathbf{a})g(\mathbf{a}, t)] + \sum_{n=0}^{\infty}(-1)^n \sum_{k_0} \cdots \sum_{k_n} \times \frac{\partial}{\partial a_{k_0}} \cdots \frac{\partial}{\partial a_{k_n}} \sum_l [G(\mathbf{a}, 0)]L_{k_0 \cdots k_n;l}(\mathbf{a}) \frac{\partial}{\partial a_l^*} \frac{g(\mathbf{a}, t)}{[G(\mathbf{a}, 0)]} \tag{51}$$

where

$$L_{k_0 \cdots k_n;l}(\mathbf{a}) = \int_0^\infty \langle R_l^*(0)S(k_0 \cdots k_n, t); \mathbf{a}\rangle\, dt \tag{52}$$

Notice should be made of the fact that Eq. (51) also can be obtained from Eq. (20) if the Markovian approximation is used in the form $L_{k_0 \cdots k_n;l}(\mathbf{a}, t) = 2L_{k_0 \cdots k_n;l}(\mathbf{a})\ \delta(t)$.

Also, it is easy to show that $\Lambda(\mathbf{a})$ is obtained via Eqs. (51) and (50) with the following result:

$$\Lambda(\mathbf{a})f(\mathbf{a}) = \sum_{n=0}^{\infty} \sum_{k_0} \cdots \sum_{k_n} K_{k_0 \cdots k_n}(\mathbf{a}) \frac{\partial}{\partial a_{k_0}} \cdots \frac{\partial}{\partial a_{k_n}} f(\mathbf{a}) \tag{53}$$

where

$$K_{k_0}(\mathbf{a}) = v_{k_0}(\mathbf{a}) + C_{k_0}(\mathbf{a}) \tag{54}$$

$$K_{k_0 \cdots k_n}(\mathbf{a}) = L_{k_0 \cdots k_{n-1};-k_n}(\mathbf{a}) + C_{k_0 \cdots k_n}(\mathbf{a}) \tag{55}$$

and

$$C_{k_0 \cdots k_n}(\mathbf{a}) = [G(\mathbf{a}, 0)]^{-1} \sum_l \frac{\partial}{\partial a_l^*}[G(\mathbf{a}, 0)]L_{k_0 \cdots k_n;l}(\mathbf{a}) \tag{56}$$

Using Eqs. (48), (50), and (53), one can show after some elementary straightforward algebra that the kinetic equation (51) may be rewritten in the following way:

$$\frac{dg(\mathbf{a}, t)}{dt} = \sum_{n=0}^{\infty} \sum_{k_0} \cdots \sum_{k_n} \left(-\frac{\partial}{\partial a_{k_0}}\right) \cdots \left(-\frac{\partial}{\partial a_{k_n}}\right) K_{k_0 \cdots k_n}(\mathbf{a}) g(\mathbf{a}, t) \tag{57}$$

Equation (57) plays an essential role in our analysis in view of its similarity with the KM expansion of the master equation. In the theory of stochastic processes it is shown that, starting from the master equation defining a Markov process, the time evolution for the probability density $g(\mathbf{a}, t)$ may be expressed in its KM form,[10,11] namely

$$\frac{dg(\mathbf{a}, t)}{dt} = \sum_{n=0}^{\infty} \frac{1}{(n+1)!} \sum_{k_0} \cdots \sum_{k_n} \left(-\frac{\partial}{\partial a_{k_0}}\right) \cdots \left(-\frac{\partial}{\partial a_{k_n}}\right) \mathbb{K}_{k_0 \cdots k_n}(\mathbf{a}) g(\mathbf{a}, t) \tag{58}$$

where $\mathbb{K}_{k_0 \cdots k_n}(\mathbf{a})$ is the $n+1$ moment of the transition probability per unit time or derivative moment, defined by

$$\mathbb{K}_{k_0 \cdots k_n}(\mathbf{a}) = \lim_{\tau \to 0} \frac{1}{\tau} \int (b_{k_0} - a_{k_0}) \cdots (b_{k_n} - a_{k_n}) P(\mathbf{b}, \tau | \mathbf{a})\, d\mathbf{a} \tag{59}$$

$P(\mathbf{b}, \tau|\mathbf{a})$ being the conditional probability that at time τ the stochastic variable takes the value $\mathbf{b}$, given its value $\mathbf{a}$ at time $t = 0$.

Due to the structure of the kinetic equation (57), Mori *et al.*[3] identify it with the KM expansion by simply setting

$$\mathbb{K}_{k_0 \cdots k_n}(\mathbf{a}) = (n+1)!\, K_{k_0 \cdots k_n}(\mathbf{a}) \tag{60}$$

However, this is not quite convincing, because ultimately this relationship ought to be derived from Eq. (59). Indeed, one can establish this relationship starting directly from the kinetic equation that is satisfied by the conditional probability $P(\mathbf{b}, \tau|\mathbf{a})$. Recalling that this quantity $P(\mathbf{b}, \tau|\mathbf{a})$ satisfies Eq. (2) [see (37) of I]

$$dP(\mathbf{b}, t|\mathbf{a})/dt = Z(\mathbf{b}, t) P(\mathbf{b}, t|\mathbf{a}) \tag{61}$$

which, after introduction of Eq. (46), is transformed into

$$dP(\mathbf{b}, t|\mathbf{a})/dt = M(\mathbf{b}) P(\mathbf{b}, t|\mathbf{a}) \tag{62}$$

whose formal solution is

$$P(\mathbf{b}, t|\mathbf{a}) = \{\exp[M(\mathbf{b})t]\} P(\mathbf{b}, 0|\mathbf{a}) = \{\exp[M(\mathbf{b})t]\}\, \delta(\mathbf{a} - \mathbf{b}) \tag{63}$$

Substitution of Eq. (63) into Eq. (59) and use of Eq. (50) leads to the result

$$\mathbb{K}_{k_0 \cdots k_n}(\mathbf{a}) = \lim_{\tau \to 0} \frac{1}{\tau} \int d\mathbf{b}\, \delta(\mathbf{b} - \mathbf{a}) \exp[\Lambda(\mathbf{b})\tau] \prod_{r=0}^{n} (b_{k_r} - a_{k_r}) \tag{64}$$

which after expansion of the exponential reads

$$\mathbb{K}_{k_0\cdots k_n}(\mathbf{a}) = \lim_{\tau\to 0}\frac{1}{\tau}\left\{\int d\mathbf{b}\,\delta(\mathbf{b}-\mathbf{a})\prod_{r=0}^{n}(b_{k_r}-a_{k_r}) + \tau\int d\mathbf{b}\,\delta(\mathbf{b}-\mathbf{a})\Lambda(\mathbf{b})\prod_{r=0}^{n}(b_{k_r}-a_{k_r}) + O(\tau^2)\right\} \tag{65}$$

Since the first term is zero upon integration and all except the second one are zero when the time limit is taken, we are left with

$$\mathbb{K}_{k_0\cdots k_n}(\mathbf{a}) = \int d\mathbf{b}\,\delta(\mathbf{b}-\mathbf{a})\Lambda(\mathbf{b})\prod_{r=0}^{n}(b_{k_r}-a_{k_r}) \tag{66}$$

Using Eq. (53) for $\Lambda(\mathbf{b})$ and carrying out the integrations [see Eq. (B14)], one arrives at the following result:

$$\mathbb{K}_{k_0\cdots k_n}(\mathbf{a}) = \sum_{n+1P_{n+1}} K_{k_{\alpha 0}\cdots k_{\alpha n}}(\mathbf{a}) \tag{67}$$

where the notation beneath the sum indicates a summation over the permutations of the $n+1$ elements $k_0,\ldots,k_n$ taken $n+1$ times. Equation (67) differs from Mori's proposal in the fact that the moment derivatives are in this case conveniently symmetrized. For example, the third derivative moment is

$$\mathbb{K}_{k_0k_1k_2}(\mathbf{a}) = K_{k_0k_1k_2}(\mathbf{a}) + K_{k_0k_2k_1}(\mathbf{a}) + K_{k_1k_0k_2}(\mathbf{a}) + K_{k_1k_2k_0}(\mathbf{a}) + K_{k_2k_1k_0}(\mathbf{a}) + K_{k_2k_0k_1}(\mathbf{a}) \tag{68}$$

and not just $6K_{k_0k_1k_2}(\mathbf{a})$. Our result is in agreement with Green's in the case of a slow Markovian process, as we shall see later.

Regardless of this fine point, Eq. (57) may in fact be interpreted as the KM expansion of a Markovian process.[3] Indeed, noticing that $k_0,\ldots,k_n$ are dummy variables, the derivatives with respect to the a_k commute and the following identity holds true:

$$\sum_{k_0}\cdots\sum_{k_n}\left(-\frac{\partial}{\partial a_{k_0}}\right)\cdots\left(-\frac{\partial}{\partial a_{k_n}}\right)\left\{\sum_{n+1P_{n+1}} K_{k_{\alpha 0}\cdots k_{\alpha n}}(\mathbf{a})g(\mathbf{a},t)\right\} = (n+1)!\sum_{k_0}\cdots\sum_{k_n}\left(-\frac{\partial}{\partial a_{k_0}}\right)\cdots\left(-\frac{\partial}{\partial a_{k_n}}\right)K_{k_0\cdots k_n}(\mathbf{a})g(\mathbf{a},t) \tag{69}$$

When Eq. (69) is substituted back into Eq. (58), we recover precisely Eq. (57).

If we further regard the Markovian process as a continuous one,[11] then by definition

$$\mathbb{K}_{k_0\cdots k_n}(\mathbf{a}) = 0, \qquad n \geqslant 2 \tag{70}$$

Under this condition the KM expansion of the kinetic equation reduces to its first two terms. Using Eq. (57), one can easily see that for this case

$$\frac{dg(\mathbf{a}, t)}{dt} = -\sum_k \frac{\partial}{\partial a_k} K_k(\mathbf{a}) g(\mathbf{a}, t) + \sum_{k_0} \sum_{k_1} \frac{\partial}{\partial a_{k_0}} \frac{\partial}{\partial a_{k_1}} K_{k_0 k_1}(\mathbf{a}) g(\mathbf{a}, t) \tag{71}$$

which is the well-known Fokker–Planck equation. Notice should be made, however, that in this equation the quantities K_k and K_{k_0,k_1} may be in principle calculated from microscopic quantities through Eqs. (56), (55), (52), and (21).

As we mentioned in the previous section, the diagonal approximation consists in neglecting all terms for $n \geqslant 1$ in the MFS equation. If we introduce this approximation in Eq. (51), we get that

$$\frac{dg(\mathbf{a}, t)}{dt} = -\sum_k \frac{\partial}{\partial a_k} [v_k(\mathbf{a}) g(\mathbf{a}, t)] + \sum_{k_0} \frac{\partial}{\partial a_{k_0}} \sum_l [G(\mathbf{a}, 0)] \times L_{k_0;l}(\mathbf{a}) \frac{\partial}{\partial a_l^*} \frac{g(\mathbf{a}, t)}{[G(\mathbf{a}, 0)]} \tag{72}$$

which is the kinetic equation for diagonal Markovian processes. Making use of Eqs. (54) and (56), it may be rewritten as follows:

$$\frac{dg(\mathbf{a}, t)}{dt} = -\sum_k \frac{\partial}{\partial a_k} K_k(\mathbf{a}) g(\mathbf{a}, t) + \sum_{k_0} \sum_{k_1} \frac{\partial}{\partial a_{k_0}} \frac{\partial}{\partial a_{k_1}} L_{k_0;-k_1}(\mathbf{a}) g(\mathbf{a}, t) \tag{73}$$

Comparison of Eqs. (71) and (73) shows that a diagonal Markovian process is a particular case of a continuous process where the additional assumption is made that

$$K_{k_0 k_1}(\mathbf{a}) = L_{k_0;-k_1}(\mathbf{a}) \tag{74}$$

Also, as is shown in Appendix B, the stationary solution $g^{(s)}(\mathbf{a})$ for both cases, namely, Eqs. (57) and (73), is given by

$$g^{(s)}(\mathbf{a}) = [G(\mathbf{a}, 0)] \tag{75}$$

Equation (73) may be now used to derive the Zwanzig–Kawasaki equation under the following three assumptions: (i) $W(\Gamma)$ in Eq. (1) is substituted by an equilibrium distribution function $W(\Gamma) = \rho_{eq}(\Gamma)$. (ii) The distribution function of the coarse-grained variables $\{a\}$ is a Gaussian. (iii) $L_{k_0;-k_1}(\mathbf{a})$ may be replaced by its average value.

The first assumption implies that, by Eq. (7),

$$[G(\mathbf{a}, 0)] = \int d\Gamma\, \rho_{\text{eq}}(\Gamma) G(\mathbf{a}, 0) \tag{76}$$

or that the stationary solution to Eq. (73) is the equilibrium distribution function for the coarse-grained variables. Hence the equilibrium average of any function $f(a)$ is given by

$$\langle\langle f(\mathbf{a})\rangle\rangle = \int d\mathbf{a}\, f(\mathbf{a}) g_{\text{eq}}(\mathbf{a}) \tag{77}$$

and furthermore, if $f(\mathbf{a}) = \langle f(\Gamma); \mathbf{a}\rangle$, its average over the hypercell, then

$$\langle\langle f(\mathbf{a})\rangle\rangle = \int d\mathbf{a}\, g_{\text{eq}}(\mathbf{a}) \langle f(\Gamma); \mathbf{a}\rangle = \int d\Gamma\, \rho_{\text{eq}}(\Gamma) f(\Gamma) = \langle f(\Gamma)\rangle_{\text{eq}} \tag{78}$$

where use has been made of Eq. (13).

The equilibrium averages of $v_k(\mathbf{a})$ and $L_{k_0;-k_1}(\mathbf{a})$ may be readily found using Eqs. (11), (52), and (78). In fact,

$$\langle\langle v_k(\mathbf{a})\rangle\rangle = \langle \dot{A}_k(\Gamma, 0)\rangle_{\text{eq}} = 0 \tag{79}$$

$$\langle\langle L_{k_0;-k_1}(\mathbf{a})\rangle\rangle = \int_0^\infty \langle R_{k_0}(t) R_{k_1}(0)\rangle_{\text{eq}}\, dt \tag{80}$$

The second assumption simply states that

$$g_{\text{eq}}(\mathbf{a}) = C \exp\Big\{-\sum_k a_k a_k^*\Big\} \tag{81}$$

which may be achieved by an adequate selection of the variables A_k.[6] The third assumption (iii) postulates that if

$$L_{k_0;-k_1}(\mathbf{a}) \simeq \langle\langle L_{k_0;-k_1}(\mathbf{a})\rangle\rangle = \mathring{L}_{k_0;-k_1} \tag{82}$$

then by Eqs. (56) and (81)

$$C_k(\mathbf{a}) = -\sum_l \mathring{L}_{kl} a_l \tag{83}$$

Substitution of Eqs. (54), (82), and (83) into Eq. (73) leads to the result that

$$\frac{dg(\mathbf{a}, t)}{dt} = -\sum_k \frac{\partial}{\partial a_k}\Big[v_k(\mathbf{a}) - \sum_l \mathring{L}_{k;l} a_l \Big] g(\mathbf{a}, t) + \sum_{k_0, k_1} \mathring{L}_{k_0;-k_1} \frac{\partial}{\partial a_{k_0}} \frac{\partial}{\partial a_{k_1}} g(\mathbf{a}, t) \tag{84}$$

which is the Fokker–Planck equation used by Zwanzig[16] and Kawasaki.[7] The nonlinearity in this equation arises from the term $v_k(\mathbf{a})$.[8]

It is at this stage interesting to point out that the time evolution equation for the collective variables in the Markovian approximation is found to be (see Appendix B)

$$dA_k(\Gamma, t)/dt = \int d\mathbf{a}\, K_k(\mathbf{a}) G(\mathbf{a}, t) + R_k(t) \tag{85}$$

where $K_k(\mathbf{a})$ and $R_k(t)$ are given in Eqs. (54) and (15), respectively. As pointed out before, this result is invariant under the diagonal approximation and it may be further simplified if Eqs. (82), (80), and (83) are used, leading to

$$dA_k(\Gamma, t)/dt = v_k(\{\mathbf{a}(t)\}) + [G\{\mathbf{a}(t)\}]_{\text{eq}}^{-1} \sum_l \frac{\partial}{\partial a_l^*} [G(\{\mathbf{a}(t)\}]_{\text{eq}} \mathring{L}_{kl} + R_k(t) \tag{86}$$

In this equation, the fluctuating force $R_k(t)$ and the bare transport coefficients are related through Eq. (17). In fact, if the correlation time for the hypercell average of $R_k(t)$ is much smaller than the time interval in which an appreciable change in $A_k(\Gamma, t)$ takes place, then it is valid to introduce the approximation that $\langle R_k(t) R_l^*(0); \mathbf{a}\rangle \simeq 2L_{k;l}(\mathbf{a})\, \delta(t)$. Hence the bare transport coefficients and the fluctuating force are related through the fluctuation-dissipation theorem, namely

$$\langle R_k(t) R_l^*(0)\rangle_{\text{eq}} = 2\mathring{L}_{k;l}\, \delta(t) \tag{87}$$

as follows from Eq. (78). Also, $\langle R_k(t)\rangle_{\text{eq}} = 0$, which follows from the fact that $\langle R_k(t); \mathbf{a}\rangle = 0$. Equation (86) was first proposed by Kawasaki[8] in his mode–mode coupling theory and derived from first principles by Mori and Fujisaka[4] and García-Colín and Velasco.[5]

The kinetic equation for a slow Markovian process is easily obtained from Eq. (73) ignoring all terms of order δ^3 and higher. Thus,

$$\frac{dg(\mathbf{a}, t)}{dt} = -\sum_k \frac{\partial}{\partial a_k} [v_k(\mathbf{a}) g(\mathbf{a}, t)] + \sum_{k_0} \frac{\partial}{\partial a_{k_0}} \sum_l L_{k_0;l}^{(2)}(\mathbf{a}) \frac{\partial}{\partial a_l^*} \frac{g(\mathbf{a}, t)}{[G(\mathbf{a}, 0)]} \tag{88}$$

where

$$K_k^{(2)}(\mathbf{a}) = v_k(\mathbf{a}) + [G(\mathbf{a}, 0)]^{-1} \sum_l \frac{\partial}{\partial a_l^*} [G(\mathbf{a}, 0)] L_{kl}^{(2)}(\mathbf{a}) \tag{89}$$

$$K_{k_0, k_1}^{(2)}(\mathbf{a}) = L_{k_0; -k_1}^{(2)}(\mathbf{a}) \tag{90}$$

Comparing Eqs. (88) and (71) and using Eq. (67), we obtain the derivative moments for a slow process, namely

$$\mathbb{K}_{k_0}(\mathbf{a}) = K_{k_0}^{(2)}(\mathbf{a}) \tag{91}$$

$$\mathbb{K}_{k_0, k_1}(\mathbf{a}) = L_{k_0; -k_1}^{(2)}(\mathbf{a}) + L_{k_1; -k_0}^{(2)}(\mathbf{a}) \tag{92}$$

Equation (89) with the explicit forms given by Eqs. (91) and (92) for the first derivative moments was first derived by Green[9] in 1952.

5. CONCLUDING REMARKS

Using the MFS form for the exact kinetic equation of a many-body system, one is able to find in a systematic way the several approximate equations that, in many instances, have been used in the literature. Although the nature of the approximations themselves have been stressed throughout the paper, it is important to mention that applications to concrete problems are small in number. In particular, explicit calculations of transport coefficients using these types of techniques have only been suggested, but numerical results are scarce, being difficult to accomplish.[12] We hope to deal explicitly with this question in a future publication.

It is also pertinent to comment here about the slowness parameter δ, which was introduced in Section 3 to derive one class of approximate kinetic equations. This parameter is, for instance, equal to $q_0\xi$, where q_0 is the maximum wave number and ξ the correlation length of density fluctuations in dense fluids when the set $\{A\}$ are the hydrodynamic variables. For the case of a Brownian particle of mass M suspended in a fluid where particles have a mass m, then δ is $(m/M)^{1/2}$ and so on. The nature of this parameter is thus inherent to the choice of the phase space function and under these circumstances will yield meaningful equations for slow processes. Once a kinetic equation is obtained and explicit expressions for the transport coefficients are given, say

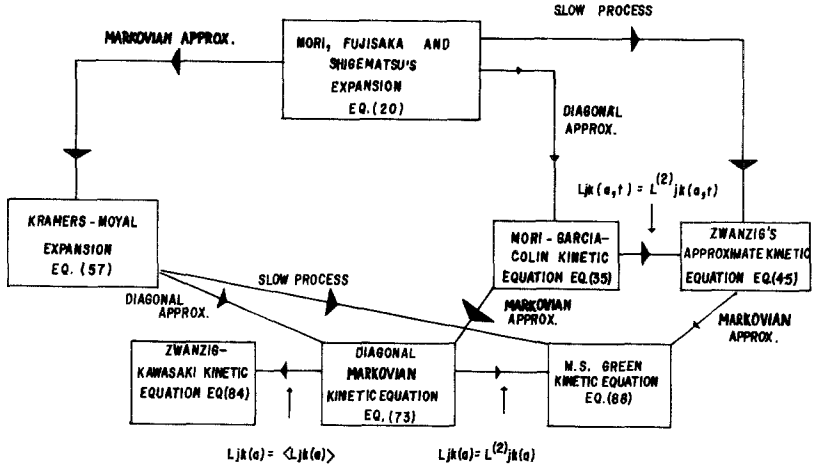

Fig. 1. Diagram illustrating the several results obtained from the MFS form of the kinetic equation. The relationship among these results is also exhibited.

as time correlation functions of the appropriate currents, their evaluation as power series in the density n is well known to present difficulties because of the so-called long-time tails, which give rise to terms like $n^2 \log n$, and in two dimensions these results even bring into question the validity of hydrodynamics. This is not the place to enter into a detailed discussion of such problems, but a word of caution must be advanced in connection with the use of these expansions, as well as with regard to the differences among them.

Finally, we condense all the different schemes used in this work, as well as the relationship among them, and the various results that they lead to in the diagram shown in Fig. 1.

APPENDIX A. PROOF OF EQS. (33) AND (37)

Equation (33) is obtained as follows. Using Eq. (18), defining $K'_{kl}(\mathbf{a}, \mathbf{b}, t)$, we see that

$$\int d\mathbf{a}\, K'_{kl}(\mathbf{a}, \mathbf{b}, t) = \left\langle \left\{ \int d\mathbf{a}\, Y_k(\mathbf{a}, t) \right\} R_l^*(0); \mathbf{b} \right\rangle \tag{A1}$$

From Eq. (19), one has that

$$\int d\mathbf{a}\, Y_k(\mathbf{a}, t) = \int d\mathbf{a}\, X_k(\mathbf{a}, t) - \int d\mathbf{a}\, G(\mathbf{a}, 0) R_k(t) \tag{A2}$$

But the first term is, according to Eq. (14), equal to $R_k(t)$ and $G(\mathbf{a}, 0)$ is normalized to unity in a space so that

$$\int d\mathbf{a}\, Y_k(\mathbf{a}, t) = 0 \tag{A3}$$

When Eq. (A3) is substituted back into Eq. (A1), it yields Eq. (33) of the text.

The proof of Eq. (37) starts by looking at the effect of applying the operator $[iLP_G]^n$ to an arbitrary phase space function $I(\Gamma)$. From Eqs. (9) and (13),

$$\begin{aligned}[iLP_G]^n I(\Gamma) &= [iLP_G]^n \int d\mathbf{b}_1 \langle I(\Gamma), \mathbf{b}_1 \rangle iLG(\mathbf{b}_1, 0) \\ &= \int d\mathbf{b}_1 \cdots \int d\mathbf{b}_n \langle I(\Gamma); \mathbf{b}_1 \rangle i\Omega(\mathbf{b}_1, \mathbf{b}_2) \cdots i\Omega(\mathbf{b}_{n-1}, \mathbf{b}_n) iLG(\mathbf{b}_n, 0)\end{aligned} \tag{A4}$$

by successive applications of iLP_G, $n - 1$ times to $iLG(\mathbf{b}_1, 0)$. The order in δ of the different terms appearing in Eq. (A4) is now easy to find. From the identity

$$iLG(\mathbf{b}, 0) = -\sum_k \frac{\partial G(\mathbf{b}, 0)}{\partial b_k} \dot{A}_k(0) \tag{A5}$$

$iLG(\mathbf{b}, 0) \sim \delta$, so that from Eq. (5) we see that $i\Omega(\mathbf{b}_i, \mathbf{b}_j) \sim \delta$, which in turn implies that if $I(\Gamma) \sim \delta^r$, its average value over the hypercell $A(\Gamma) = \mathbf{b}$ will be $\sim \delta^r$. These results used in Eq. (A4) show that

$$[iLP_G]^n I(\Gamma) \sim \delta^{n+r} \tag{A6}$$

which is Eq. (37) of the text.

Finally, to show the result used in the derivation of Eq. (44), we start with

$$\langle R_k(t')R_l^*(0); \mathbf{a}\rangle = \frac{(R_k(t')R_l^*(0); G(\mathbf{a}, 0))}{[G(\mathbf{a}, 0)]} = \frac{(R_k(t'), R_l(0)G(\mathbf{a}, 0))}{[G(\mathbf{a}, 0)]} \tag{A7}$$

where the second equality follows from the definition of inner product. Using the definition of $R_l(0)$ given in Eq. (15) and the identity $P_G\{f(\Gamma)G(\mathbf{a}, 0)\} = \{P_G f(\Gamma)\}G(\mathbf{a}, 0)$, one readily finds that

$$R_l(0)G(\mathbf{a}, 0) = (1 - P_G)[\dot{A}_l(0)G(\mathbf{a}, 0)] \tag{A8}$$

When Eq. (A8) is substituted back into Eq. (A7), it gives that

$$\langle R_k(t')R_l^*(0); \mathbf{a}\rangle = \langle R_k(t')\dot{A}_l^*(0); \mathbf{a}\rangle \tag{A9}$$

where use has been made of the fact that $(1 - P_G)$ is Hermitian and that acting on $R_k(t')$ leaves it unchanged.

APPENDIX B

To obtain Eq. (67), one starts with Eq. (53) applied to a convenient function, namely

$$\Lambda(\mathbf{b})\prod_{r=0}^{n}(b_{k_r} - a_{k_r}) = \sum_{q=0}^{n}\sum_{l_0}\cdots\sum_{l_q} K_{l_0\cdots l_q}(\mathbf{b})\frac{\partial}{\partial b_{l_0}}\cdots\frac{\partial}{\partial b_{l_q}}\prod_{r=0}^{n}(b_{k_r} - a_{k_r}) \tag{B1}$$

Since

$$\frac{\partial}{\partial b_{l_0}}\prod_{r=0}^{n}(b_{k_r} - a_{k_r}) = \sum_{\alpha_0=0}^{n}\delta_{l_0,k_{\alpha_0}}\prod_{r\neq\alpha_0}(b_{k_r} - a_{k_r})$$

one sees immediately that

$$\frac{\partial}{\partial b_{l_q}}\cdots\frac{\partial}{\partial b_{l_0}}\prod_{r=0}^{n}(b_{k_r} - a_{k_r})$$

$$= \sum_{\alpha_0=0}^{n}\sum_{\alpha_1\neq\alpha_0}\cdots\sum_{\alpha_q\neq\alpha_0,\ldots,\alpha_{q-1}}\delta_{k_{\alpha_0}l_0}\delta_{l_1k_{\alpha_1}}\cdots\delta_{l_q,k_{\alpha_q}}\prod_{r\neq\alpha_0\cdots\alpha_q}(b_{k_r} - a_{k_r}) \tag{B2}$$

when $q \leqslant n$ and the lhs is equal to zero if $q > n$. Since all the summations

over $\alpha_0, \alpha_1, \ldots, \alpha_q$ are equal to the sum over all permutations of the $n+1$ elements $k_0 \cdots k_n$ taken in groups of $q+1$, we have that

$$\frac{\partial}{\partial b_{l_q}} \cdots \frac{\partial}{\partial b_{l_0}} \prod_{r=0}^{n} (b_{k_r} - a_{k_r}) = \sum_{n+1P_{q+1}} \delta_{l_0 k_{\alpha_0}} \cdots \delta_{l_q k_{\alpha_q}} \prod_{r \neq \alpha_0 \cdots \alpha_q} (b_{k_r} - a_{k_r}) \tag{B3}$$

Substituting Eq. (B3) into Eq. (B1) and carrying over the $l_0, \ldots, l_q$ summation gives that

$$\Lambda(\mathbf{b}) \prod_{r=0}^{n} (b_{k_r} - a_{k_r}) = \sum_{q=0}^{n} \sum_{n+1P_{q+1}} K_{\alpha_0 \cdots \alpha_q}(\mathbf{b}) \prod_{r \neq \alpha_0 \cdots \alpha_q} (b_{k_r} - a_{k_r}) \tag{B4}$$

When Eq. (B4) is put back into Eq. (66), then due to the $\delta(\mathbf{a} - \mathbf{b})$ in the integral, only the term $q = n$ survives and Eq. (67) is immediately obtained.

Let us show next that the stationary solution to Eqs. (57) and (73) is just $[G(\mathbf{a}, 0)]$. Introducing Eqs. (54) and (55) into Eq. (57) yields

$$\frac{dg(\mathbf{a}, t)}{dt} = -\sum_{k_0} \frac{\partial g(\mathbf{a}, t)}{\partial a_{k_0}} \{v_{k_0}(\mathbf{a}) + C_{k_0}(\mathbf{a})\} + \sum_{n=1}^{\infty} \sum_{k_0} \cdots \sum_{k_n}$$

$$\times \left(-\frac{\partial}{\partial a_{k_0}}\right) \cdots \left(-\frac{\partial}{\partial a_{k_n}}\right) [L_{k_0 \cdots k_{n-1}; -k_n}(\mathbf{a}) + C_{k_0 \cdots k_n}(\mathbf{a})] g(\mathbf{a}, t) \tag{B5}$$

From Eq. (56), on the other hand, it is readily seen that

$$\sum_{k_0} \cdots \sum_{k_n} \left(-\frac{\partial}{\partial a_{k_0}}\right) \cdots \left(-\frac{\partial}{\partial a_{k_n}}\right) C_{k_0 \cdots k_n}(\mathbf{a})[G(\mathbf{a}, 0)]$$

$$= -\sum_{k_0} \cdots \sum_{k_{n+1}} \left(-\frac{\partial}{\partial a_{k_0}}\right) \cdots \left(-\frac{\partial}{\partial a_{k_{n+1}}}\right) L_{k_0 \cdots k_n; -k_{n+1}}(\mathbf{a})[G(\mathbf{a}, 0)] \tag{B6}$$

so that for $g(\mathbf{a}, t) = [G(\mathbf{a}, 0)]$ the term containing $C_{k_0}(\mathbf{a})$ in the first summation and all the series of the second term cancel out among themselves. Also, the first term is zero because, according to Eq. (11),

$$-\sum_{k} \frac{\partial}{\partial a_k} v_k(\mathbf{a})[G(\mathbf{a}, 0)] = -\sum_{k} \frac{\partial}{\partial a_k} \int d\Gamma \, W(\Gamma) \dot{A}_k(0) G(\mathbf{a}, 0)$$

$$= \int d\Gamma \, [iLW(\Gamma)] G(\mathbf{a}, 0) = 0 \tag{B7}$$

after the identity given by Eq. (A5) and the fact that L is Hermitian are used. The equality follows because the metric $W(\Gamma)$ is stationary. Equations (B6) and (B7) lead directly to the result that $[G(\mathbf{a}, 0)]$ is the stationary solution to Eq. (57).

Noticing that if one cuts the KM expansion for $n = m$ and introduces the approximation

$$K_{k_0 \cdots k_m}(\mathbf{a}) = L_{k_0 \cdots k_{m-1}; -k_m}(\mathbf{a}) \tag{B8}$$

Equation (B6) keeps holding true; thus $[G(\mathbf{a}, 0)]$ is the stationary solution to the truncated equation (75).

Finally, to find the time evolution equation for the collective variables in the Markovian approximation, one substitutes the definition of $C_k(\mathbf{a}, s)$ given by Eq. (27) into Eq. (34) to obtain that

$$dA_k(\Gamma, t)/dt = \int d\mathbf{a}\, v_k(\mathbf{a}) G(\mathbf{a}, t) + \int_0^t ds \int d\mathbf{a}\, C_k(\mathbf{a}, s) G(\mathbf{a}, t - s) + R_k(t) \tag{B9}$$

From Eq. (27) and the Markovian approximation one gets that

$$C_k(\mathbf{a}, s) = 2C_k(\mathbf{a})\, \delta(s) \tag{B10}$$

Substituting Eq. (B10) back into Eq. (B9), carrying over the time integral and introducing Eq. (54) leads us directly to Eq. (85).

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