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Regression Law and the Renormalization of the Transport Coefficients

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Using Mazur's lemma we show that the coarse-grained variables used in nonequilibrium statistical mechanics are the Onsager's regression variables. With this result we find a regression law for the fluctuations which is both non-Markovian and nonlinear. Considering the Markovian approximation and generalizing Onsager's ideas leading to the symmetry of the transport matrix, we formulate Mori and Fujisaka's method for the renormalization of transport coefficients due to nonlinear interactions.

KEY WORDS: Coarse-grained variables; Onsager's regression variables; Mazur's lemma; renormalization of the transport coefficients; Mori–Fujisaka method; projector operator.

1. INTRODUCTION

In 1972 Zwanzig[1] presented a model theory for the nonlinear interactions of collective modes in fluids, which is equivalent to Kawasaki's mode–mode coupling theory.[2] In Zwanzig's proposed model, the equations of motion of the phase functions are associated with the observables in a nonlinear Langevin equation of the form

$$\frac{d\mathbf{A}(\Gamma, t)}{dt} = \mathbf{v}(\mathbf{A}(\Gamma, t)) - \mathring{\gamma} \cdot \mathbf{A}(\Gamma, t) + \mathbf{R}(\Gamma, t) \tag{1}$$

where the streaming velocity $\mathbf{v}$ contains nonlinear contributions in the phase functions, $\mathring{\gamma}$ is the "bare" matrix for the transport coefficients, and $\mathbf{R}(\Gamma, t)$ is a fluctuating force which satisfies the fluctuation dissipation

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relation, namely,

$$\langle \mathbf{R}(\Gamma, t)\mathbf{R}(\Gamma, 0)\rangle = 2\mathring{\gamma}\delta(t) \tag{2}$$

Zwanzig obtained the Fokker–Planck equation associated with Eq. (1), rewrote this equation in terms of creation–destruction operators in such form that it is possible to use quantum field-theory methods, calculated the equilibrium time correlation function of dynamical variables, and finally comparing this result with the exact expression for the correlation function obtained from Mori's linear theory,[3] he showed that the linear transport matrix consists of two parts, one containing the bare matrix which relaxes rapidly compared with the hydrodynamic times and the second part which is the contribution of the nonlinear modes contained in the streaming velocity. Thus,

$$\phi(t) = 2\mathring{\gamma}\delta(t) + \psi(t) \tag{3}$$

where $\phi(t)$ is the time-dependent linear transport matrix, and $\psi(t)$ is the so-called renormalization matrix of the transport coefficients due to nonlinear interactions.

After this work Mori and Fujisaka's paper[4] appeared where using the projector operator method they justified from first principles the nonlinear Langevin equation proposed by Zwanzig and presented an alternative procedure for finding the renormalization of the transport coefficients. The physical ideas behind this calculation were greatly clarified in a paper by García–Colín and Velasco.[5]

The purpose of this paper is a twofold one: first, to show that the coarse-grained variables used in nonequilibrium statistical mechanics are the Onsager regression variables.[6] Second, to show that the Mori–Fujisaka method is a generalization of Onsager's ideas leading to the symmetry of the transport matrix, in the nonlinear case. These results allow one to see the similarity between Zwanzig's and Mori and Fujisaka's methods of renormalization.

The paper has the following structure: in Section 2 we give a brief review of the dynamics of coarse-grained variables,[7] and using Mazur's lemma[8] we show that these variables are Onsager's regression variables. With this result we find the non-Markovian and nonlinear fluctuation's regression law for systems which are initially prepared in a constrained equilibrium state. In Section 3 we present an alternative procedure for obtaining Zwanzig's model equation and we discuss the meaning of the renormalization of the transport coefficients in the context of Onsager's regression law. Furthermore, we generalize step by step Onsager's ideas to the Markovian nonlinear case and obtain Mori and Fujisaka's result. In Section 4 we calculate for a simple model the renormalization of the transport coefficients up to the second order in the nonlinear coupling constants.

2. LAW OF REGRESSION FOR THE FLUCTUATIONS

We begin our analysis with a brief review about the coarse grained variables which are used in several treatments of nonequilibrium statistical mechanics.[7]

We denote by $\mathbf{A}(\Gamma, 0)$ the complete set of phase functions associated with the macroscopic system's observables $\alpha(t)$, i.e.,

$$\boldsymbol{\alpha}(t) = \int d\Gamma\, \rho(\Gamma, 0)\mathbf{A}(\Gamma, t) \tag{4}$$

where $\rho(\Gamma, 0)$ is the initial nonequilibrium phase probability density and $\Gamma = (\mathbf{q}, \mathbf{p})$. Another quantity of interest is $g_k^{n\text{-}e}(\mathbf{a}_1, t_1; \ldots; \mathbf{a}_k, t_k)d\mathbf{a}_1 \ldots d\mathbf{a}_k$ which is the probability that $\mathbf{a}_i < \mathbf{A}(\Gamma, t_i) < \mathbf{a}_i + d\mathbf{a}_i$ for $i = 1, \ldots, k$. This quantity can be expressed as

$$\begin{aligned} &g_k^{n\text{-}e}(\mathbf{a}_1, t_1; \ldots; \mathbf{a}_k, t_k) \\ &\quad = \int d\Gamma\, \rho(\Gamma, 0)\delta(\mathbf{A}(\Gamma, t_1) - \mathbf{a}_1) \ldots \delta(\mathbf{A}(\Gamma, t_k) - \mathbf{a}_k) \end{aligned} \tag{5}$$

We can rewrite (4) in terms of $g_1^{n\text{-}e}(a, t)$ through the identity

$$\mathbf{A}(\Gamma, t) = \int d\mathbf{a}\, \mathbf{a}\delta(\mathbf{A}(\Gamma, t) - \mathbf{a}) \tag{6}$$

and obtain that

$$\boldsymbol{\alpha}(t) = \int d\mathbf{a}\, \mathbf{a} g_1^{n\text{-}e}(\mathbf{a}, t) \tag{7}$$

Using the relationship

$$g_1^{n\text{-}e}(\mathbf{a}, t) = \int d\mathbf{b}\; g_1^{n\text{-}e}(\mathbf{b}, 0)P_{n\text{-}e}(\mathbf{a}, t \mid \mathbf{b}) \tag{8}$$

the macroscopic observables can be expressed as

$$\boldsymbol{\alpha}(t) = \int d\mathbf{b}\; g_1^{n\text{-}e}(\mathbf{b}, 0)\, \overline{\mathbf{a}(t)}^{\mathbf{b}} \tag{9}$$

where $\overline{\mathbf{a}(t)}^{\mathbf{b}}$ are the so-called coarse-grained variables, defined by

$$\overline{\mathbf{a}(t)}^{\mathbf{b}} = \int d\mathbf{a}\, \mathbf{a}P_{n\text{-}e}(\mathbf{a}, t \mid \mathbf{b}) \tag{10}$$

The time evolution equations for the $\overline{\mathbf{a}(t)}^{\mathbf{b}}$, can be found if we know the kinetic equation for $P_{n\text{-}e}(\mathbf{a}, t \mid \mathbf{b})$. This kinetic equation is obtained using the Liouville's equation of motion for the hypercell,[5] which is the way used by Mori and Fujisaka. In both cases Zwanzig's nonlinear projector operator is used. Furthermore, in both methods the nonequilibrium initial distribution function corresponds to a constrained equilibrium state. In other words,

$$\rho(\Gamma, 0) = \rho_{\text{eq}}(\Gamma)\Phi(\mathbf{A}(\Gamma, 0)) \tag{11}$$

Hence $\rho_{\text{eq}}(\Gamma)$ is the density distribution function in the final equilibrium state and $\Phi(\mathbf{A}(\Gamma,0))$ is any function of the phase functions with a convenient normalization. When we consider Zwanzig's method the kinetic equation for $P_{n\text{-}e}(\mathbf{a}, t\,|\,\mathbf{b})$ is given by[7]

$$\frac{\partial P_{n\text{-}e}(\mathbf{a}, t\,|\,\mathbf{b})}{\partial t} = Z(\mathbf{a}, t) P_{n\text{-}e}(\mathbf{a}, t\,|\,\mathbf{b}) \tag{12}$$

where $Z(\mathbf{a}, t)$ is Zwanzig's operator and (12) is a generalized Fokker–Planck equation. On the other hand when we consider the time evolution equation for the phase hypercell $\delta(\mathbf{A}(\Gamma, t) - \mathbf{a})$ and follow in a systematic way Mori's technique[3] with Zwanzig's nonlinear projector operator[9] the kinetic equation takes the form[10]

$$\frac{\partial P_{n\text{-}e}(\mathbf{a}, t\,|\,\mathbf{b})}{\partial t} = \Lambda(\mathbf{b}, t) P_{n\text{-}e}(\mathbf{a}, t\,|\,\mathbf{b}) \tag{13}$$

where $\Lambda(\mathbf{b}, t)$ is Mori's operator which is the transpose of $Z(\mathbf{a}, t)$. Equation (13) corresponds to the generalized Kolomogorov equation or the backward kinetic equation.[11]

Thus with the two equivalent kinetic equations (12) and (13) it is possible to find the equation of motion for the coarse-grained variables. When we insert Eq. (12) into Eq. (10) we have that

$$\frac{\partial \overline{\mathbf{a}(t)}^{\mathbf{b}}}{\partial t} = \int_0^t ds \int d\mathbf{a} \left[2\mathbf{v}(\mathbf{a})\delta(s) + \mathbf{c}(\mathbf{a}, s) \right] P_{n\text{-}e}(\mathbf{a}, t - s|\mathbf{b}) \tag{14}$$

where $\mathbf{v}(\mathbf{a})$ is the streaming velocity given by

$$\mathbf{v}(\mathbf{a}) = \langle iL\mathbf{A}(\Gamma, 0); \mathbf{a} \rangle \tag{15}$$

and $\mathbf{c}(\mathbf{a}, s)$ is defined by

$$\mathbf{c}(\mathbf{a}, s) = g_{\text{eq}}^{-1}(\mathbf{a}) \frac{\partial}{\partial \mathbf{a}} \cdot g_{\text{eq}}(\mathbf{a}) \langle \mathbf{R}(\Gamma, t)\mathbf{R}(\Gamma, 0); \mathbf{a} \rangle \tag{16}$$

where $\langle \ldots ; \mathbf{a} \rangle$ denotes the average over the hypercell characterized by the condition $\mathbf{A}(\Gamma, 0) = \mathbf{a}$, i.e.,

$$\langle \ldots ; \mathbf{a} \rangle = g_{\text{eq}}^{-1}(\mathbf{a}) \int d\Gamma\, \rho_{\text{eq}}(\Gamma) \cdots \delta(\mathbf{A}(\Gamma, 0) - \mathbf{a}) \tag{17}$$

With the purpose of displaying the meaning of Eq. (16) it is convenient to remember that when we rewrite the equation of motion of $A(\Gamma, t)$ following Mori's technique but using Zwanzig's projector (see Appendix), we obtain that

$$\frac{d\mathbf{A}(\Gamma,t)}{dt} = \int_0^t ds \int d\mathbf{a}\left[2\mathbf{v}(\mathbf{a})\delta(s) + \mathbf{c}(\mathbf{a},s)\right]\delta(\mathbf{A}(\Gamma,t-s)-\mathbf{a}) + \mathbf{R}(\Gamma,t) \tag{18}$$

where $\mathbf{R}(\Gamma,t)$ is an orthogonal function to any function of $\mathbf{A}(\Gamma,0)$, and therefore (16) is the fluctuation–dissipation relation in the nonlinear case.

Equation (18) is the basic equation used by Kawasaki in his mode–mode coupling theory,[2] and as was shown by Mori and Fujisaka, it leads, after some approximations to be discussed later to Zwanzig's model equation (1).

We can also obtain an alternative form of the equation of motion for the coarse-grained variables when we use the backward kinetic equation into Eq. (7)[7]

$$\frac{d\overline{\mathbf{a}(t)}^{\mathbf{b}}}{dt} = \Lambda(\mathbf{b},t)\,\overline{\mathbf{a}(t)}^{\mathbf{b}} \tag{19}$$

Equation (19) is very important in Mori and Fujisaka's renormalization method as we shall see in the following section. Now we are in a position to discuss the fluctuation's regression law using the lemma proved by Mazur,[8] namely, that if $\rho(\Gamma,0) = \rho_{\mathrm{eq}}(\Gamma)\Phi(\mathbf{A}(\Gamma,0))$ then the nonequilibrium conditional probability is identical with the equilibrium conditional probability, i.e.,

$$P_{n\text{-}e}(\mathbf{a},t\,|\,\mathbf{b},t=0) = P_{\mathrm{eq}}(\mathbf{a},t\,|\,\mathbf{b}) \tag{20}$$

a relation which holds true at $t = 0$ but not at all times (see Appendix).

Mazur's lemma allows a connection between two alternative points of view in nonequilibrium statistical mechanics, the study of fluctuations around the equilibrium states, which is the point of view of Onsager,[6] M. S. Green,[12] Kubo,[13] and the study of the relaxation to the equilibrium state of a system which is initially prepared in a constrained equilibrium state and some of its constrictions are suddenly removed. This is the point of view adopted by Zwanzig,[9] and Mori and co-workers.[4,14]

A trivial implication of Mazur's lemma is that the coarse-grained variables are identical with Onsager's regression variables.[6] In fact since these variables are defined as

$$\overline{\mathbf{a}_R(t)}^{\mathbf{b}} = \int d\mathbf{a}\,\mathbf{a}P_{\mathrm{eq}}(\mathbf{a},t\,|\,\mathbf{b}) \tag{21}$$

Mazur's lemma implies that

$$\overline{\mathbf{a}(t)}^{\mathbf{b}} = \overline{\mathbf{a}_R(t)}^{\mathbf{b}} \tag{22}$$

Thus, the transport equations and the regression law are now given by

$$\frac{d}{dt}\begin{bmatrix} \alpha(t) \\ \overline{\mathbf{a}_R(t)}^{\mathbf{b}} \end{bmatrix} = \int_0^t ds \int d\mathbf{a}\, \mathbf{K}(\mathbf{a}, s) \begin{bmatrix} g_1^{n\text{-}e}(\mathbf{a}, t-s) \\ P_{\text{eq}}(\mathbf{a}, t-s \mid \mathbf{b}) \end{bmatrix} \tag{23}$$

where $\mathbf{K}(\mathbf{a}, s)$ is defined as

$$\mathbf{K}(\mathbf{a}, s) = 2\mathbf{v}(\mathbf{a})\delta(s) + \mathbf{c}(\mathbf{a}, s) \tag{24}$$

The transport equation arises when we introduce Eq. (12) and Eq. (10) into Eq. (9) and use Eq. (8). Equation (23) shows that both equations are governed by the same function $\mathbf{K}(\mathbf{a}, s)$ in the general nonlinear case. Also it is easy to see that in the special case in which $\mathbf{K}(\mathbf{a}, s)$ is a function of the form

$$\mathbf{K}(\mathbf{a}, s) = -\mathsf{M}\cdot\mathbf{a}\delta(s) \tag{25}$$

where M is a constant matrix, Eq. (23) reduces to the familiar linear Onsager's regression law. Equation (23) may be regarded as a more general regression law whose structure depends on the explicit form of $\mathbf{K}(\mathbf{a}, s)$. The other form of the regression law is obtained when we use Eqs. (19) and (22),

$$\frac{\partial\, \overline{\mathbf{a}_R(t)}^{\mathbf{b}}}{\partial t} = \Lambda(b, t)\, \overline{\mathbf{a}_R(t)}^{\mathbf{b}} \tag{26}$$

Eq. (26) is used in Mori and Fujisaka's method of the renormalization of the transport coefficients.

3. RENORMALIZATION OF THE TRANSPORT COEFFICIENTS

We begin discussing the way in which Zwanzig's model equation is obtained from the exact evolution equation of the phase functions.

In the Markovian approximation, namely,

$$\mathbf{c}(\mathbf{a}, s) = 2\mathbf{c}(\mathbf{a})\delta(s) = 2\left[\int_0^\infty \mathbf{c}(\mathbf{a}, t)\, dt\right]\delta(s) \tag{27}$$

Eq. (18) reduces to

$$\frac{d\mathbf{A}(\Gamma, t)}{dt} = \int d\mathbf{a}\,[\mathbf{v}(\mathbf{a}) + \mathbf{c}(\mathbf{a})]\,\delta(\mathbf{A}(\Gamma, t) - \mathbf{a}) + \mathbf{R}(\Gamma, t) \tag{28}$$

We now define a mesoscopic inner product as

$$\langle\langle f(\mathbf{a}), h(\mathbf{a})\rangle\rangle = \int d\mathbf{a}\; g_{\text{eq}}(\mathbf{a}) f(\mathbf{a}) h(\mathbf{a}) \tag{29}$$

and for simplicity we consider that $\langle\langle a_i, a_j\rangle\rangle = \delta_{ij}$. Introducing the mesoscopic linear projector operator

$$P_a \equiv \langle\langle\ , \mathbf{a}\rangle\rangle\cdot\mathbf{a} \tag{30}$$

we now state our second assumption, namely, that the nonlinear part of $\mathbf{c}(\mathbf{a})$ is an irrelevant one,

$$\mathbf{c}(\mathbf{a}) \simeq P_a \mathbf{c}(\mathbf{a}) = \langle\langle \mathbf{c}(\mathbf{a}), \mathbf{a} \rangle\rangle \cdot \mathbf{a} \tag{31}$$

Using now Eqs. (16), (17), and (29) we obtain that

$$\langle\langle \mathbf{c}(\mathbf{a}), \mathbf{a} \rangle\rangle = -\int_0^\infty \langle \mathbf{R}(\Gamma, t)\mathbf{R}(\Gamma, 0)\rangle \, dt = -\mathring{\gamma} \tag{32}$$

where $\langle\ \rangle$ denotes the average taken with $\rho_{\text{eq}}(\Gamma)$. If we insert Eqs. (31) and (32) into (28) the equation of motion for the phase functions reduces to Eq. (1). The procedure presented here to obtain Zwanzig's model is different to Mori and Fujisaka's procedure and has the advantage of simplicity.

Now we proceed with the problem of the renormalization of the transport coefficients and restrict ourselves to the Markovian case.

The regression law takes then the two following alternative forms:

$$\frac{\partial\, \overline{\mathbf{a}_R(t)}^{\mathbf{b}}}{\partial t} = \int d\mathbf{a} \left[\mathbf{v}(\mathbf{a}) + \mathbf{c}(\mathbf{a}) \right] P_{\text{eq}}(\mathbf{a}, t \mid \mathbf{b}) \tag{33}$$

$$\frac{\partial\, \overline{\mathbf{a}_R(t)}^{\mathbf{b}}}{\partial t} = \Lambda(\mathbf{b})\, \overline{\mathbf{a}_R(t)}^{\mathbf{b}} \tag{34}$$

The first one is obtained from Eqs. (14) and (27), and the second one from Eq. (26). Here $\Lambda(\mathbf{b})$ is the Markovian form for $\Lambda(\mathbf{b}, t)$.[7] The form of the regression law given by (33) is the most convenient one for understanding the meaning of the basic equation in Mori and Fujisaka's method. For clarity purposes we first discuss the renormalization in terms of Eq. (33). The point is that both terms $\mathbf{v}(\mathbf{a})$ and $\mathbf{c}(\mathbf{a})$ contain linear and nonlinear contributions in $\mathbf{a}$'s variables which may be separated with the projector defined in Eq. (30):

$$\mathbf{v}(\mathbf{a}) + \mathbf{c}(\mathbf{a}) = P_a \left[\mathbf{v}(\mathbf{a}) + \mathbf{c}(\mathbf{a}) \right] + \mathbf{K}'(\mathbf{a}) \tag{35}$$

where $\mathbf{K}'(\mathbf{a})$ denotes the nonlinear part.

Using Eqs. (15), (30), and (32) we obtain that

$$P_a \left[\mathbf{v}(\mathbf{a}) + \mathbf{c}(\mathbf{a}) \right] = \left[\dot{\mathsf{C}}(0) - \mathring{\gamma} \right] \cdot \mathbf{a} \tag{36}$$

where $\dot{\mathsf{C}}(t)$ is the time derivative of the correlation function. Thus Eq. (33) takes the form

$$\frac{d\, \overline{\mathbf{a}_R(t)}^{\mathbf{b}}}{dt} = \left[\dot{\mathsf{C}}(0) - \mathring{\gamma} \right] \cdot \overline{\mathbf{a}_R(t)}^{\mathbf{b}} + \int d\mathbf{a}\, \mathbf{K}'(\mathbf{a}) P_{\text{eq}}(\mathbf{a}, t \mid \mathbf{b}) \tag{37}$$

which is clearly a nonlinear regression law.

The question that arises concerns now the contribution to the transport coefficients due to the nonlinear terms. This question can be formulated in a more transparent form in terms of the time correlation function. From first principles we know that the exact equation of motion for the correlation function[3] is given by

$$\frac{d\mathbf{C}(t)}{dt} = i\omega \cdot \mathbf{C}(t) - \int_0^t ds\, \boldsymbol{\phi}(s) \cdot \mathbf{C}(t-s) \tag{38}$$

where $i\omega = \dot{\mathbf{C}}(0)$ and $\boldsymbol{\phi}(s)$ is the generalized matrix of the transport coefficients.

On the other hand we can obtain the time evolution of the correlation function from (37), using the fact that

$$\mathbf{C}(t) = \left\langle \left\langle \overline{\mathbf{a}_R(t), }^{\mathbf{b}}\mathbf{b} \right\rangle \right\rangle \tag{39}$$

this leads to using Eqs. (39) and (37); we then get that

$$\frac{d\mathbf{C}(t)}{dt} = \left[i\omega - \mathring{\gamma} \right] \cdot \mathbf{C}(t) + \int d\mathbf{b} \int d\mathbf{a}\, \mathbf{K}'(\mathbf{a})\mathbf{b} g_2^{\text{eq}}(\mathbf{a}, t; \mathbf{b}, 0) \tag{40}$$

The problem now is to find the contribution of the second term in Eq. (40) to the matrix $\boldsymbol{\phi}(s)$. To solve this problem we proceed using Mori and Fujisaka's method to understand the physical content behind this process, and generalize step by step Onsager's ideas leading to the symmetry of the matrix of transport coefficients, using Eq. (34), the nonlinear regression law.

Onsager's first step was to introduce the linear regression law, namely, that the macroscopic variables satisfy the equation

$$\frac{d\boldsymbol{\alpha}(t)}{dt} = -\mathsf{M} \cdot \boldsymbol{\alpha}(t) \tag{41}$$

then the regression law is given by

$$\frac{d\overline{\mathbf{a}_R(t)}^{\mathbf{b}}}{dt} = -\mathsf{M} \cdot \overline{\mathbf{a}_R(t)}^{\mathbf{b}} \tag{42}$$

We now generalize this step using Eq. (34), rewriting this equation using Mori's identity,

$$e^{\hat{Q}t} = e^{\hat{Q}t}P + e^{(1-P)\hat{Q}t}(1-P) + \int_0^t ds\, e^{\hat{Q}(t-s)} P \hat{Q} e^{(1-P)\hat{Q}s}(1-P) \tag{43}$$

where $\hat{Q}$ is a time-independent operator and P is a projector operator, making $\hat{Q} = \Lambda(b)$ and $P = P_b$ leads to

$$\frac{d\overline{\mathbf{a}_R(t)}^{\mathbf{b}}}{dt} = i\boldsymbol{\Omega} \cdot \overline{\mathbf{a}_R(t)}^{\mathbf{b}} - \int_0^t ds\, \boldsymbol{\psi}(s) \cdot \overline{\mathbf{a}_R(t-s)}^{\mathbf{b}} + \mathbf{q}(t) \tag{44}$$

where

$$i\Omega = \langle\langle \Lambda(\mathbf{b})\mathbf{b}, \mathbf{b} \rangle\rangle \tag{45a}$$

$$\psi(t) = -\langle\langle \Lambda(\mathbf{b})\mathbf{q}(t), \mathbf{b} \rangle\rangle \tag{45b}$$

$$\mathbf{q}(t) = e^{(1-P_b)\Lambda(\mathbf{b})t}(1 - P_b)\Lambda(\mathbf{b})\mathbf{b} \tag{45c}$$

and $\mathbf{q}(t)$ is orthogonal to $\mathbf{b}$, $\langle\langle \mathbf{q}(t), \mathbf{b} \rangle\rangle = 0$. The following step in Onsager's derivation is to find the time evolution equation for the correlation function, taking the inner product of Eq. (42) with $\mathbf{b}$ and using Eq. (39), then,

$$\frac{d\mathbf{C}(t)}{dt} = -\mathsf{M} \cdot \mathbf{C}(t) \tag{46}$$

whose solution is given by

$$\mathbf{C}(t) = k_B e^{-\mathsf{M}t} \cdot \mathsf{g}^{-1} \tag{47}$$

Here we used that $\mathrm{C}(0) = k_B \mathsf{g}^{-1}$, k_B being Boltzmann's constant and $\mathsf{g} = |\partial^2 s / \partial \mathbf{a}\, \partial \mathbf{a}|$ is a symmetric matrix.

The generalization of this step is to find the equation of motion of the correlation function when we use the nonlinear regression law. Using Eqs. (39) and (44) we correspondingly find that

$$\frac{d\mathbf{C}(t)}{dt} = i\Omega \cdot \mathbf{C}(t) - \int_0^t ds\, \psi(s) \cdot \mathbf{C}(t-s) \tag{48}$$

which is the counterpart of Eq. (46). At this point it is convenient to say that when we introduce the explicit form of $\Lambda(b)$ given in Ref. 14 and calculate $i\Omega$ using (45a), we get that

$$i\Omega = i\omega - \mathring{\gamma} \tag{49}$$

Comparing Eqs. (48) and (49) with Eq. (40) we see that the second term in the right-hand side of Eq. (48) contains the nonlinear contributions to the transport coefficients.

The third step in Onsager's derivation is to make use of the microscopic definition for the correlation function

$$\mathbf{C}(t) = \int d\Gamma\, \rho_{\mathrm{eq}}(\Gamma)\mathbf{A}(\Gamma, t)\mathbf{A}(\Gamma, 0) \tag{50}$$

and show that due to the time reversal invariance of the mechanical equations of motion, it has the property that

$$\mathbf{C}(t) = \mathbf{C}^T(t) \tag{51}$$

when the phase functions are even in the velocities.

The generalization of this step is given by Eq. (38) where we identified the matrix of transport coefficients with $\phi(t)$.

The last step in Onsager's method is to demand that the phenomenological expression for $C(t)$ given by Eq. (47) satisfies the symmetry property (51) which is a microscopic result; the result of this requirement is that M satisfies the relation

$$e^{-\mathsf{M}t}\cdot\mathsf{g}^{-1}=\mathsf{g}^{-1}\cdot e^{-\mathsf{M}^T t} \tag{52}$$

which implies that $L = L^T$ where

$$\mathsf{L}=\mathsf{M}\cdot\mathsf{g}^{-1} \tag{53}$$

The generalization of this step is to demand that the exact time evolution equation of $\mathbf{C}(t)$, Eq. (38) is identical with Eq. (48). This requirement implies that

$$\phi(t)=2[i\omega-i\Omega]\delta(t)+\psi(t) \tag{54}$$

and if we introduce Eq. (49), then

$$\phi(t)=2\mathring{\gamma}\delta(t)+\psi(t) \tag{55}$$

Therefore $\psi(t)$ defined by Eq. (45b) is the renormalization of the transport coefficients due to the nonlinear interactions. The form of $\psi(t)$ can be calculated introducing the explicit form of $\Lambda(\mathbf{b})$,[14] but for our purpose this is irrelevant.

It is now clear that Mori and Fujisaka's method may be understood as a generalization of Onsager's ideas to the nonlinear case. Also this point of view allows one to establish a connection with Zwanzig's method, and the details of this will be given in a future communication.

4. RENORMALIZATION IN A SIMPLE MODEL

To illustrate the ideas presented in the previous sections, we now calculate the renormalization of the transport coefficients due to the nonlinear modes using a perturbation theory in the simple case in which (a) the equilibrium distribution $g_{\text{eq}}(a)$ is Gaussian, i.e.,

$$g_{\text{eq}}(a)=C\exp\left(-\tfrac{1}{2}\sum_k a_k a_k\right) \tag{56}$$

(b) $\mathbf{R}(\Gamma,t)$ is a Gaussian fluctuating force, and satisfies the fluctuation–dissipation theorem given by Eq. (2); (c) the streaming velocity $\mathbf{v}(a)$ is given by

$$v_k(a)=\sum_l i\omega_{kl}a_l+\sum_l\sum_m V_{klm}(a_l a_m-\langle a_l a_m\rangle_{\text{eq}}) \tag{57}$$

where the coupling constants V_{klm} obey the symmetry relationships

$$V_{klm}=V_{kml}, \qquad V_{klm}+V_{mkl}+V_{lmk}=0 \tag{58}$$

which are a consequence of the fact that $\mathbf{v}(a)$ satisfies the conditions

$$\langle v_k(a)\rangle_{\text{eq}} = 0 \tag{59}$$

$$\sum_k \frac{\partial}{\partial a_k} v_k(a) g_{\text{eq}}(a) = 0 \tag{60}$$

implied by the definition of the streaming velocity.(1,15) This model has been used by R. Zwanzig in several treatments of the renormalization of transport coefficients.(1,16,17) When the conditions (a) and (b) are satisfied, the explicit form of the Λ operator is given by(4,5)

$$\Lambda(b) = \left[\mathbf{v}(b) - \mathring{\gamma} \cdot \mathbf{b}\right] \cdot \frac{\partial}{\partial \mathbf{b}} + \mathring{\gamma} : \frac{\partial^2}{\partial \mathbf{b}\, \partial \mathbf{b}} \tag{61}$$

and (45b) takes the simple form(4,5)

$$\psi(t) = \langle\langle\left[\exp(1 - P_b)\Lambda(b)t\right]\mathbf{v}^1(b), \mathbf{v}^1(b)\rangle\rangle \tag{62}$$

If we consider that the nonlinear coupling constants V_{klm} are small, we can obtain a second-order perturbation expression for $\psi(t)$. This is accomplished by separating the $\Lambda(b)$ operator in the following form, namely,

$$\Lambda(b) = \Lambda_0(b) + \Lambda_1(b) \tag{63}$$

where $\Lambda_1(b)$ contains the nonlinear contributions of the streaming velocity. Thus,

$$\Lambda_0(b) = \left[(i\omega - \mathring{\gamma}) \cdot \mathbf{b}\right] \cdot \frac{\partial}{\partial \mathbf{b}} + \mathring{\gamma} : \frac{\partial^2}{\partial \mathbf{b}\, \partial \mathbf{b}} \tag{64}$$

$$\Lambda_1(b) = \mathbf{v}^1(b) \cdot \frac{\partial}{\partial \mathbf{b}} \tag{65}$$

where $\mathbf{v}^1(b) = (1 - P_b)\mathbf{v}(b)$. Next the operator $\exp[(1 - P_b)\Lambda(b)t]$ is expanded in powers of $\Lambda_1(b)$

$$\begin{aligned} &\exp\{(1 - P_b)\Lambda(b)t\} \\ &\quad = \exp(1 - P_b)\Lambda_0(b)t - \int_0^t ds \exp\left[(1 - P_b)\Lambda_0(b)(t - s)\right] \\ &\quad\quad \times (1 - P_b)\Lambda_1(b)\exp\left[(1 - P_b)\Lambda_0(b)s\right] + \phi(\Lambda^2) \end{aligned} \tag{66}$$

After some algebraic manipulations one obtains that

$$\begin{aligned} (1 - P_b)\Lambda_0(\mathbf{bb} - 1) &= \Theta \cdot (\mathbf{bb} - 1) + (\mathbf{bb} - 1) \cdot \Theta^T \\ &\equiv \{\Theta, (\mathbf{bb} - 1)\} \end{aligned} \tag{67}$$

where use has been made of Eqs. (64), (30), and the symmetry property $i\omega = -i\omega^T$, and the definition

$$\boldsymbol{\Theta} = i\omega - \mathring{\gamma} \tag{68}$$

Now we define the tensor $\mathsf{A}(t)$ in the form

$$\mathsf{A}(t) = \exp\left[(1 - P_b)\Lambda_0(b)t\right](\mathbf{bb} - 1) \tag{69}$$

and compute its time derivative with the use of Eq. (67). The result is that

$$\frac{d\mathsf{A}(t)}{dt} = \{\Theta, \mathsf{A}(t)\} \tag{70}$$

whose solution is given by

$$\mathsf{A}(t) = (\exp \Theta t) \cdot \mathsf{A}(0) \cdot (\exp \Theta^T t) \tag{71}$$

as it can be easily verified.

Introducing Eq. (66) into (62), and using the fact that

$$v_k^1(a) = \sum_{lm} V_{klm}(b_l b_m - \delta_{lm}) \tag{72}$$

as it is implied by Eqs. (56) and (57), we find the second-order expression for the renormalization matrix is

$$\psi_{ij}^{(2)}(t) = \sum_{lm} \sum_{\alpha\beta} V_{ilm} V_{j\alpha\beta} \langle\langle \left[\exp(1 - P_b)\Lambda_0(b)t\right] \times (b_l b_m - \delta_{lm}), (b_\alpha b_\beta - \delta_{\alpha\beta}) \rangle\rangle \tag{73}$$

Using Eq. (71) this expression conveniently reduces to

$$\psi_{ij}^{(2)}(t) = \sum_{lm} \sum_{\alpha\beta} \sum_{pq} V_{ilm} V_{j\alpha\beta} (\exp \Theta t)_{lp} (\exp \Theta^T t)_{qm} \times \langle (b_p b_q - \delta_{pq})(b_\alpha b_\beta - \delta_{\alpha\beta}) \rangle_{eq} \tag{74}$$

where use was made of Eq. (29). Finally using Eqs. (58) and the fact $g_{\text{eq}}(b)$ is Gaussian, we obtain

$$\psi_{ij}^{(2)}(t) = 2 \sum_{lm} \sum_{\alpha\beta} V_{ilm} V_{j\alpha\beta} (\exp \Theta t)_{l\alpha} (\exp \Theta t)_{m\beta} \tag{75}$$

A similar expression for the renormalization of the transport coefficients was obtained by R. Zwanzig,[17] using the Fokker–Planck equation, from which he obtained a hierarchy of equations coupling successive cumulants which is solved using a perturbation scheme, based in the fact that the nonlinear coupling constants are small. Also it is important to note that in the case in which the phase functions are even in the momenta $\dot{C}(0) = i\omega = 0$ and if we assume that $\mathring{\gamma}$ is diagonal, i.e.,

$$\mathring{\gamma}_{kl} = \mathring{\gamma}_k \delta_{kl} \tag{76}$$

then Eq. (75) takes the form

$$\psi_{ij}^{(2)}(t) = 2 \sum_{lm} V_{ilm} V_{jlm} \left[\exp - (\mathring{\gamma}_l + \mathring{\gamma}_m)t\right] \tag{77}$$

which is the result found in Ref. 16. Clearly, the diagonal term is given by

$$\psi_{ii}^{(2)}(t) = 2\sum_{lm} |V_{ilm}|^2 \left[\exp - (\mathring{\gamma}_l + \mathring{\gamma}_m)t\right] \tag{78}$$

which is Zwanzig's result obtained via theoretical quantum-field methods.

These results show the Mori-Fujisaka method and the variety of methods developed by Zwanzig and co-workers give the same results for the renormalization of the transport coefficients due to nonlinear interactions.

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APPENDIX

In this Appendix we outline the steps leading to Eq. (18) and to Mazur's lemma.

We write the equation of motion for the phase functions $\mathbf{A}(\Gamma, t)$ in a form which resembles a nonlinear Langevin-type equation. Thus, we begin with equation

$$\frac{d\mathbf{A}(\Gamma, t)}{dt} = iL\mathbf{A}(\Gamma, t) = e^{iLt} iL\mathbf{A}(\Gamma, 0) \tag{A.1}$$

where L is Liouville's operator. Now we use Zwanzig's projector operator defined by

$$P_z = \int d\mathbf{b} \langle\ ;\mathbf{b}\rangle \delta(\mathbf{A}(\Gamma, 0) - \mathbf{b}) \tag{A.2}$$

Using Mori's identity, Eq. (43), with $\hat{Q} = iL$ and $P = P_z$, into Eq. (A.1) we obtain

$$\begin{aligned} \frac{d\mathbf{A}(\Gamma, t)}{dt} &= \int d\mathbf{b}\, \mathbf{v}(\mathbf{b}) \delta(\mathbf{A}(\Gamma, t) - \mathbf{b}) \\ &\quad + \int_0^t ds \int d\mathbf{b} \langle iL\mathbf{R}(\Gamma, s); \mathbf{b}\rangle \delta(\mathbf{A}(\Gamma, t - s) - \mathbf{b}) + \mathbf{R}(\Gamma, t) \end{aligned} \tag{A.3}$$

where we used Eq. (A.2), which implies that

$$e^{iLt} P_z iL\mathbf{A}(\Gamma, 0) = \int d\mathbf{b}\, \mathbf{v}(\mathbf{b}) \delta(\mathbf{A}(\Gamma, t) - \mathbf{b}) \tag{A.4}$$

and we defined

$$\mathbf{R}(\Gamma, t) = e^{(1 - P_z) iLt} (1 - P_z) iL\mathbf{A}(\Gamma, 0) \tag{A.5}$$

Using the explicit form of the average over the hypercell given by Eq. (17), and the Hermitian property of the P_z and L operators, it is possible to show that

$$\langle iL\mathbf{R}(\Gamma, s); \mathbf{b}\rangle = g_{\text{eq}}(\mathbf{b})^{-1} \frac{\partial}{\partial \mathbf{b}} \cdot \langle \mathbf{R}(\Gamma, s)\mathbf{R}(\Gamma, 0); \mathbf{b}\rangle g_{\text{eq}}(\mathbf{b}) = \mathbf{c}(\mathbf{b}, s) \quad (A.6)$$

Finally introducing this result into Eq. (A.3), we obtain immediately Eq. (18).

To show Mazur's lemma, we use the definition of the nonequilibrium conditional probability

$$P_{n\text{-}e}(\mathbf{a}, t \mid \mathbf{b}) = \left[g_1^{n\text{-}e}(\mathbf{b}, 0) \right]^{-1} g_2^{n\text{-}e}(\mathbf{a}, t; \mathbf{b}, 0) \quad (A.7)$$

Using Eq. (5) and the fact that the initial phase distribution function has the form

$$\rho(\Gamma, 0) = \rho_{\text{eq}}(\Gamma)\Phi(\mathbf{A}(\Gamma, 0)) \quad (A.8)$$

we have that

$$g_2^{n\text{-}e}(\mathbf{a}, t; \mathbf{b}, 0) = \Phi(\mathbf{b}) g_2^{\text{eq}}(\mathbf{a}, t; \mathbf{b}, 0) \quad (A.9)$$

$$g_1^{n\text{-}e}(\mathbf{b}, 0) = \Phi(\mathbf{b}) g_{\text{eq}}(\mathbf{b}) \quad (A.10)$$

Putting Eqs. (A.9) and (A.10) into Eq. (A.7) we obtain

$$P_{n\text{-}e}(\mathbf{a}, t \mid \mathbf{b}) = \left[g_{\text{eq}}(\mathbf{b}) \right]^{-1} g_2^{\text{eq}}(\mathbf{a}, t; \mathbf{b}, 0) = P_{\text{eq}}(\mathbf{a}, t \mid \mathbf{b}) \quad (A.11)$$

which is Mazur's lemma.

Due to the fact that the nonequilibrium conditional probability is not stationary, it is clear that $P_{n\text{-}e}(\mathbf{a}, t_2 \mid \mathbf{b}, t_1) \neq P_{\text{eq}}(\mathbf{a}, t_2 - t_1 \mid \mathbf{b}, 0)$. On the other hand $P_{\text{eq}}(\mathbf{a}, t_2 \mid \mathbf{b}, t_1)$ is stationary, because this is weighted with $\rho_{\text{eq}}(\Gamma)$. Therefore $P_{n\text{-}e}(\mathbf{a}, t_2 \mid \mathbf{b}, t_1) \neq P_{\text{eq}}(\mathbf{a}, t_2 \mid \mathbf{b}, t_1)$, implying that the equality between the nonequilibrium and equilibrium conditional probability is only valid when $t_1 = 0$, but not for arbitrary values of time.

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