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On the Microscopic Derivation of Mode–Mode Coupling Equations

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Alternative results derived on a microscopic basis for the mode–mode coupling kinetic equations are shown to be identical. It is also emphasized that nonlinear kinetic equations for the gross variables describing the system are only suggested but not implied by the corresponding equations obeyed by their dynamical variables. Finally an equivalent closed form for the renormalized transport coefficients is shown to hold in mode–mode coupling theory.

KEY WORDS: Mode–mode coupling equations; dynamical and gross variables; stochastic Gaussian and Markovian processes; renormalized transport coefficients; nonlinear kinetic equations.

1. INTRODUCTION

The enormous success of mode–mode coupling theory[1] in giving an adequate picture of how transport coefficients behave in the vicinity of critical points has motivated some work on its microscopic foundations. In particular, Kawasaki has proposed a derivation of the kinetic equations for the set of phase space functions which are associated with the corresponding gross variables.[1,2] A similar approach has been followed by using a systematic set of approximations on the exact kinetic equation satisfied by such phase space functions.[3] However, the immediate step of going from this description to another one in terms of the gross or mesoscopic variables is not very clear, nor is it straightforward.[4] This paper has two objectives. One is to show trivially that the kinetic equations for the phase space functions are identical. This will avoid any source of confusion when looking at the two apparently different results. The second one is much deeper. We would like to emphasize

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that from a given kinetic equation in phase space, the corresponding equation in the gross variable space does not follow automatically. It also appears that the renormalization formula for the transport coefficients can be written according to the particular manner in which this latter equation is regarded. This will, we hope, cast some light on our present understanding of this theory at a more fundamental level.

2. DERIVATION OF MODE–MODE COUPLING EQUATIONS

We shall start by stressing the fact that the dynamical state of a many-body system will be described by a set of dynamical variables, e.g., phase space functions, a subset of which denoted by $\{A_i(\Gamma)\}$ constitutes the "slowly" varying variables. The gross, mesoscopic or coarse-grained variables $\{a_i\}$ are defined by the numerical values of these dynamical functions. The former set obeys exact equations of motion in Γ-space, whereas, as has been emphasized several times before,[4–6] the a's form a set of stochastic variables whose time evolution has to be dealt with correspondingly. Now, without burdening the reader with unnecessary tedious algebra, which can be found in the references, it is sufficient to point out that the equation of motion for the state vector $\mathbf{A} = (A_1, A_2, \ldots)$, which is clearly Liouville's equation, may be uniquely transformed into a different form which resembles that of, but is not quite, a Langevin equation. If the vector $\mathbf{A}$ corresponds to the slowly varying variables, then the idea of the decomposition is to obtain an equation with a "systematic" non-Markovian term linear in $\mathbf{A}$, plus a fluctuating "random" term which arises solely from the rapidly varying variables, this term acting, presumably, as a "random force." Furthermore, this force is related to the "memory" term which appears in the systematic motion through a generalization of the ordinary fluctuation-dissipation theorem as it appears in ordinary Brownian motion. It must be clear that, although appealing, this transformation is purely a mathematical one and cannot be identified from the physical point of view with a description of a real system by means of a stochastic process. Examples of these results, appropriate to our further discussion, are Eq. (5.6) of Ref. 1 and Eq. (32) of Ref. 3.

In particular, we now want to show that these two results lead to the same equation for the set $\{A_i\}$ upon which the mode–mode coupling theory in its usual context is based. In fact, if we take Eq. (5.6) of 1 and assume that the process is Markovian, namely that the memory kernel in the systematic term is instantaneous, we get that

$$\frac{dA_i(t)}{dt} = v_i(\{A\}) + g_{\text{eq}}^{-1}(\{A(t)\}) \sum_l \frac{\partial}{\partial A_l^*} \{g_{\text{eq}}(\{A(t)\}) \times \mathring{L}_{kl}(\{A(t)\})\} + f_i(t) \tag{1}$$

where, by definition, $g_{eq}(\{A(t)\})$ is the equilibrium distribution at time t

$$g_{eq}(\{A(t)\}) = \int d\Gamma\, \rho_{eq}(\Gamma)\, \delta[A(\Gamma, t) - \mathbf{a}] \tag{2}$$

and all the other quantities appearing in (1) are defined in Refs. 1 and 3. Equation (1) is also explicitly written in this way in earlier work.[2] However, the corresponding result given by Eq. (84) in Ref. 3 appears to be different from Eq. (1). To show that this is not the case we take Eq. (32) of Ref. 3, which is exact, and by identifying $[G(\mathbf{b}, 0)]$ with $g_{eq}(\{b\})$, which is its definition, using Eq. (46) of Ref. 3, which is the Markovian approximation on $L_{kl}(\mathbf{a}, s)$, and carrying out the elementary integrations involved, we arrive at Eq. (1) with $\mathring{K}_{ij} \equiv \mathring{L}_{ij}$.[3]

We now come to the core of this paper. The standard way of arriving at the nonlinear kinetic equation for the gross variables $\{a_i\}$ is by simply regarding the $\{A_i\}$ as the set of random variables $\{a_i\}$ and simply using (1) in a space by substituting the A's by the a's.[1,7] We wish to stress very clearly the fact that this is a nontrivial assumption whose consequences are not quite straightforward. This problem is extensively dealt with in Ref. 4, so that unnecessary repetitions of algebraic steps will be avoided. The crucial point is that the condition $\{A_i = a_i \text{ for all } i\}$ determines the hypersurface $\delta[A(\Gamma) - \mathbf{a}]$ in Γ space whose motion is determined uniquely by Liouville's equation through the motion of all the microscopic states contained therein and which are compatible with the coarse-grained state determined by the a's. Of course, this motion could also be determined by the exact equations of motion of the a's, which are clearly unknown because of their own nature, namely, they are regarded as stochastic variables. This implies that, if we intuitively or pragmatically propose some dynamical scheme in a space, the motion of this hypercell will be modeled by it in the sense that the values of the set $\{A_i\}$ will be determined by the values of the set $\{a_i\}$ at any time t. Furthermore, the a space as such has a status of its own so that any equation of motion that we propose has to be written in terms of operators, scalar products, etc. defined in that space, not in phase space.[5,6] This now brings us to the nature of Kawasaki's assumption[7] (see Ref. 1, p. 193). If we assume, it cannot be otherwise, that the a's are described by a stochastic Gaussian Markovian process such that Eq. (1) is obeyed, then the fluctuating term $f_j(t)$ has to be different from the one appearing in the equation for $A_i(t)$ in Γ space, because the projector P_a involved in it has to be defined in a space, not in Γ space. Now, going along with this assumption, it is also clear that the dynamics in

[3] Equation (1) is identical to Eq. (86) of Ref. 3.

Γ space is no longer determined by Eq. (1) itself. This arises from the fact that trivially

$$A_j(t) = \int a_j \, \delta[A(\Gamma, t) - \mathbf{a}] \, d\mathbf{a} \tag{3}$$

which when applied to Eq. (1) in a space [see Eq. (5.17) in Ref. 1] leads back formally to the same equation except that the fluctuating force is given by

$$f_j(t) = \int f_j^a(t) \, \delta[A(\Gamma, t) - \mathbf{a}] \, d\mathbf{a} \tag{4}$$

where f_j^a is the fluctuating term in a space. That $f_j(t) \neq f_j^a(t)$ has been clearly pointed out in the literature.[8] Of course, since in the practical applications of mode–mode coupling this force disappears when computing the correlation functions for the a's, which requires, by the way, that $\langle f_j^a(t) a_k(0) \rangle = 0$, its specific form has no importance whatsoever.

Moreover, Kawasaki's assumption could be interpreted in a different, but equally valid, manner. As it was shown in Ref. 3, Eq. (1) is completely equivalent to the Markovian form for the MFS (Mori–Fujisaka–Shigematsu)[8] dynamical operator which is explicitly written in Eq. (51) of Ref. 3. Now one can take up the same philosophy as in Ref. 4 and assume that the dynamics in a space will be determined by the corresponding operator Λ, and that it is linear in the a's

$$a_j(t) = e^{\Lambda t} a_j(0) \tag{5}$$

where Λ is given by (53) of Ref. 3. Then the whole machinery worked out in Section III of Ref. 4 can be applied step by step[8] to derive an equation of motion for the set $\{a_i\}$ which will formally look like Eq. (3.10) of Ref. 4. When this result is used together with Eq. (3) to obtain the corresponding dynamics in Γ space, then we find that, as a consequence of the nonlinear interactions among the gross variables, such dynamics simulates the exact one, provided that the corresponding transport coefficients are "renormalized," namely if L_{ij} is an element of the "exact" Onsager matrix, then

$$L_{ij}(i\omega) = 2\mathring{L}_{ij} + \psi_{ij}(i\omega) \tag{6}$$

where $\mathring{L}_{ij}$ is the bare transport coefficient, as it appears in Eq. (1), $\psi_{ij}(i\omega)$ is given by

$$\psi_{ij}(i\omega) = \int_0^\infty \langle f_i^{a*}(0) f_j^a(t) \rangle e^{-i\omega t} \, dt \tag{7}$$

and the "fluctuating force" f_i^a defined in a space contains only the nonlinear interactions among the a's. This brings us to a very interesting situation. On the one hand the a space version of Eq. (1) when subject to the standard perturbation method as described in Ref. 1 yields renormalized expressions for the transport coefficients in the critical region which are in astonishing

agreement with experiment. On the other hand one can interpret the same assumption in the sense that the dynamics of the a variables is determined by the same operator that describes the time evolution of the phase space functions, or equally well, the hypersurface $\delta[A(\Gamma) - \mathbf{a}]$ in Γ space. If this approach is taken we are led to a "renormalization" scheme which has a closed form in a space and from which, in principle, the behavior of the transport coefficients could be predicted. Unfortunately, very little work has been done along these lines. Since the operator Λ is completely equivalent to the operator that acts on the A's in Eq. (1), the two methods are strictly equivalent. However, in one case one proceeds to apply perturbative methods to the nonlinear kinetic equation for the a's to get the renormalization formula for the transport coefficients, whereas in the second method this renormalization appears when one studies the "modeled" dynamics in Γ space obtained through Eq. (5). Mori[9] has applied this method to study some systems close to critical points and finds results which agree with dynamic scaling, but it is clear at this point that much more work is needed to weigh the advantages of one method over the other one.

As a last remark, we would also like to point out that another way of approaching the mode–mode coupling theory is by casting the kinetic equation for the gross variables in terms of a stochastic equation for their probability distribution function $g(\mathbf{a}, t)$.[1,3,7]

It has been discussed previously[10] how exact equations of motion for this distribution function can be obtained from Liouville's equation, and have the following structure,

$$dg(\mathbf{a}, t)/dt = Z(\mathbf{a}, t)g(\mathbf{a}, t) \tag{8}$$

where the operator $Z(\mathbf{a}, t)$ may be written in several identical ways. In particular, the so called generalized Fokker–Planck form for $Z(\mathbf{a}, t)$ [see Eq. (10) in Ref. 1] is useful for our discussion. Indeed, if in this equation we introduce three approximations, namely (a) we assume that the process is diagonal, $K_{kl}(\mathbf{a}, \mathbf{b}; s) = L_{kl}(\mathbf{a}, s)\delta(\mathbf{a} - \mathbf{b})$, (b) we assume that it is Markovian, $L_{kl}(\mathbf{a}, t) = 2\mathring{L}_{kl}(\mathbf{a})\delta(t)$, and (c) we assume that $g_{eq}(\mathbf{b})$ is Gaussian, then, carrying through the elementary algebra involved, we come out with the result that

$$dg(\mathbf{a}, t)/dt = -\sum_i \left[v_i(\{a\}) + \sum_j \mathring{L}_{ij}F_j(\{a\})\right]g(\mathbf{a}, t) + \sum_{i,j} \frac{\partial}{\partial a_i}\left[\mathring{L}_{ij}\frac{\partial}{\partial a_j^*}g(\mathbf{a}, t)\right] \tag{9}$$

which is the form quoted in the literature[7] as the mode–mode coupling approximation for $g(\mathbf{a}, t)$. It is worthwhile to emphasize the difference in nature of Eqs. (1) and (9), since the latter follows from an exact result for the

distribution function of the numerical values of the slowly varying variables. The first moments of this distribution, say

$$\alpha_i = \int a_i(t) g(\mathbf{a}, t)\, d\mathbf{a} \tag{10}$$

would correspond to the macroscopic variables of the system and their corresponding equations ought to be equivalent to those that describe the behavior of hydrodynamic variables near critical points.[11] This connection remains, to the author's knowledge, rather unexplored.

3. CONCLUDING REMARKS

As was shown above, the nonlinear kinetic equations for the gross variables used in mode–mode coupling theory are indeed assumptions about the dynamics in a space which are at most suggested by the corresponding equations satisfied by their own phase space functions. The other result worth emphasizing is that if one models the dynamics in Γ space through a Markovian operator in a space, this induces a renormalization of the transport coefficients which can be expressed in a closed form in terms of the nonlinear interactions among the gross variables. Since this is equivalent to Kawasaki's conventional treatment of the renormalization scheme, it could be advantageous to explore its applicability, for instance, before doing perturbation expansions. Some applications along these lines have been suggested by Mori.[9]

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