Macroscopic dynamics through coarse-graining: A solvable example

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The recently derived fluctuation-dissipation formula [A. N. Gorban *et al.*, Phys. Rev. E **63**, 066124 (2001)] is illustrated by the explicit computation for McKean's kinetic model [H. P. McKean, J. Math. Phys. **8**, 547 (1967)]. It is demonstrated that the result is identical, on the one hand, to the sum of the Chapman-Enskog expansion, and, on the other hand, to the exact solution of the invariance equation. The equality between all three results holds up to the crossover from the hydrodynamic to the kinetic domain.

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Derivation of macroscopic equations from microscopic dynamics is the outstanding problem of nonequilibrium statistical physics [1]. In particular, a simple method to derive dissipative macroscopic models in the short memory approximation from Ehrenfest's coarse-graining concept has been suggested [2–4]. Let us consider microscopic dynamics given by an equation for the distribution function $f(x,t)$ over a configuration space x

$$\partial_t f = J(f), \tag{1}$$

where operator $J(f)$ may be linear or nonlinear. Let $\mathbf{m}(f)$ be a set of linear functionals whose values $\mathbf{M}=\mathbf{m}(f)$ represent the macroscopic variables, and also let $f(\mathbf{M},x)$ be a set of distribution functions satisfying the consistency condition,

$$\mathbf{m}(f(\mathbf{M}))=\mathbf{M}. \tag{2}$$

The choice of the relevant distribution functions is the point of central importance which we discuss later on but for the time being we need only specification (2).

The starting point has been the following observation [2,3]: Given a finite time interval τ, it is possible to reconstruct uniquely the macroscopic dynamics from a single condition. For the sake of completeness, we shall formulate this condition here. Let us denote as $\mathbf{M}(t)$ the initial condition at the time t to the *yet unknown* equations of the macroscopic motion, and let us take $f(\mathbf{M}(t),x)$ for the initial condition of the microscopic Eq. (1) at the time t. Then the condition for the reconstruction of the macroscopic dynamics reads as follows: For every initial condition $\{\mathbf{M}(t),t\}$, solutions to the macroscopic dynamic equations at the time $t+\tau$ are equal to the values of the macroscopic variables on the solution to Eq. (1) with the initial condition $\{f(\mathbf{M}(t),x),t\}$:

$$\mathbf{M}(t+\tau)=\mathbf{m}(T_\tau f(\mathbf{M}(t))), \tag{3}$$

where T_τ is the formal solution operator of the microscopic Eq. (1). The right-hand side of Eq. (3) represents an operation on trajectories of the microscopic Eq. (1), introduced in a particular form by Ehrenfest [1] (the coarse-graining): The solution at the time $t+\tau$ is replaced by the state on the manifold $f(\mathbf{M},x)$. Notice that the coarse-graining time τ in Eq. (3) is finite, and we stress the importance of the required independence from the initial time t, and from the initial condition at t.

The essence of the reconstruction of the macroscopic equations from the condition just formulated is in the following [2,3]: Seeking the macroscopic equations in the form,

$$\partial_t \mathbf{M}=\mathbf{R}(\mathbf{M},\tau), \tag{4}$$

we proceed with Taylor expansion of the unknown functions $\mathbf{R}$ in terms of powers τ^n, where $n=0,1,...$, and require that each approximation $\mathbf{R}^{(n)}$ of the order n is such that resulting macroscopic solutions satisfy the condition (4) to the order τ^{n+1}. This process of successive approximation is solvable. Thus, the unknown macroscopic Eq. (4) can be reconstructed to any given accuracy.

Coming back to the problem of chosing the distribution function $f(\mathbf{M},x)$, we recall that many physically relevant cases of the microscopic dynamics (1) are characterized by the existence of a concave functional $S(f)$ (the entropy functional) (discussions of S can be found in [5–7]). Traditionally, two cases are distinguished, the conservative [$dS/dt \equiv 0$ due to Eq. (1)], and the dissipative [$dS/dt \geqslant 0$ due to Eq. (1), where the equality sign corresponds to the stationary solution]. The approach (3) and (4) is applicable to both situations. In both of these cases, among the possible sets of distribution functions $f(\mathbf{M},x)$, the distinguished role is played by the well-known quasi-equilibrium approximations $f^*(\mathbf{M},x)$, which are maximizers of the functional $S(f)$ for fixed $\mathbf{M}$. We recall that, due to concavity of the functional S, if such a maximizer exists then it is unique. The special role of the quasi-equilibrium approximations is due to the well-known fact that they preserve the type of dynamics: If $dS/dt \geqslant 0$ due to Eq. (1), then $dS^*/dt \geqslant 0$ due to the quasi-equilibrium dynamics, where $S^*(\mathbf{M})=S(f^*(\mathbf{M}))$ is the quasi-equilibrium entropy, and where the quasi-equilibrium dynamics coincides with zeroth order in the above construction $\mathbf{R}^{(0)}=\mathbf{m}(J(f^*(\mathbf{M}))$. We notice it in passing that, since the well-known work of Jaynes [8], the usefulness of quasi-

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equilibrium approximations is well understood in various versions of projection operator formalism for the conservative case [9–12], as well as for the dissipative dynamics [7,13,14]. Relatively less studied remains the case of open or externally driven systems, where invariant quasi-equilibrium manifolds may become unstable [15]. The use of the quasi-equilibrium approximations for the above construction has been stressed in [2–4]. In particular, the strict increase in the quasi-equilibrium entropy has been demonstrated for first- and higher-order approximations [3]. Examples have been provided [3], focusing on the conservative case, and demonstrating that several well-known dissipative macroscopic equations, such as the Navier-Stokes equation and the diffusion equation for the one-body distribution function, are derived as the lowest-order approximations of this construction.

The advantage of the approach [2,3] is the locality of construction, because only Taylor series expansion of the microscopic solution is involved. This is also its natural limitation. From the physical standpoint, finite and fixed coarse-graining time τ remains a phenomeno-logical device which makes it possible to infer the form of the macroscopic equations by a noncomplicated computation rather than to derive a full form thereof. For instance, the form of the Navier-Stokes equations can be derived from the simplest model of free motion of particles, in which case the coarse-graining is a substitution for collisions. Going away from the limitations imposed by the finite coarse-graining time [2,3] can be recognized as the major problem of a consistent formulation of nonequilibrium statistical thermodynamics. Intuitively, this requires taking the limit $\tau\to\infty$, allowing for all the relevant correlations to be developed by the microscopic dynamics, rather than to be cut off at the finite τ. Indeed, in the case of the dissipative dynamics, in particular, for the linearized Boltzmann equation, one typically expects an initial layer [16] which is completely cut off in the short-memory approximation, whereas those effects can be made small by making τ large enough. A way of doing this in the general nonlinear setting for entropy-conserving systems still requires further work at the time of this writing.

However, there is one important exception when the "$\tau\to\infty$ problem" is readily solved [3,4]. This is the case where Eq. (1) is linear,

$$\partial_t f = Lf, \tag{5}$$

and where the quasi-equilibrium is a linear function of $\mathbf{M}$. This is, in particular, the classical case of linear irreversible thermodynamics where one considers the linear macroscopic dynamics near the equilibrium, f^{eq}, $Lf^{\mathrm{eq}}=0$. We assume, for simplicity of presentation, that the macroscopic variables $\mathbf{M}$ vanish at equilibrium, and are normalized in such a way that $\mathbf{m}(f^{\mathrm{eq}}\mathbf{m}^{\dagger})=\mathbf{1}$, where † denotes transposition, and one is an appropriate identity operator. In this case, the linear dynamics of the macroscopic variable $\mathbf{M}$ has the form

$$\partial_t \mathbf{M} = \mathbf{R}\mathbf{M}, \tag{6}$$

where the linear operator $\mathbf{R}$ is determined by the coarse-graining condition (3) in the limit $\tau\to\infty$:

$$\mathbf{R} = \lim_{\tau\to\infty} \frac{1}{\tau} \ln[\mathbf{m}(e^{\tau L} f^{\mathrm{eq}} \mathbf{m}^{\dagger})]. \tag{7}$$

Formula (7) has been already briefly mentioned in [3], and its relation to the Green-Kubo formula has been demonstrated in [4]. In our case, the Green-Kubo formula reads

$$\mathbf{R}_{\mathrm{GK}} = \int_0^\infty \langle \dot{\mathbf{m}}(0)\dot{\mathbf{m}}(t)\rangle, \tag{8}$$

where angular brackets denote equilibrium averaging, and where $\dot{\mathbf{m}}=L^{\dagger}\mathbf{m}$. The difference between formulas (7) and (8) stems from the fact that condition (3) does not use an *a priori* hypothesis of the separation of the macroscopic and microscopic time scales. For the classical N-particle dynamics, Eq. (7) is a complicated expression, involving a logarithm of noncommuting operators. It is therefore very desirable to gain understanding in simple model situations.

In this paper we want to give an explicit example of formula (7). In order to make our point, we consider here dissipative rather than conservative dynamics in the framework of the well-known toy kinetic model introduced by McKean [17] for the purpose of testing various ideas in kinetic theory. In the dissipative case with a clear separation of time scales, existence of formula (7) is underpinned by the entropy growth in both the rapid and the slow parts of the dynamics. This physical idea underlies generically the extraction of the slow (hydrodynamic) component of motion through the concept of normal solutions to kinetic equations, as pioneered by Hilbert [18], and has been discussed by many authors, e.g., [16,19,20]. Case studies for linear kinetic equations help clarify the concept of this extraction [17,21,22].

Therefore, for the dissipative case there exist well-established approaches to the problem of reducing the description, and which are exact in the present setting. It is very instructive to see their relation to formula (7). Specifically, we compare the result with the exact sum of the Chapman-Enskog expansion [23], and with the exact solution in the framework of the method of invariant manifold [13,14]. We demonstrate that all three approaches, different in their nature, give the same result as long as the hydrodynamic and the kinetic regimes are separated.

The McKean model is the kinetic equation for the two-component vector function $\mathbf{f}(r,t)=(f_+(r,t),f_-(r,t))^{\dagger}$:

$$\partial_t f_+ = -\partial_r f_+ + \epsilon^{-1}\left(\frac{f_+ + f_-}{2} - f_+\right), \tag{9}$$

$$\partial_t f_- = \partial_r f_- + \epsilon^{-1}\left(\frac{f_+ + f_-}{2} - f_-\right).$$

Equation (9) describes the one-dimensional kinetics of particles with velocities $+1$ and -1 as a combination of free flight and a relaxation with the rate ϵ^{-1} to the local equilibrium. Using the notation, $(\mathbf{x},\mathbf{y})$, for the standard scalar product of the two-dimensional vectors, we introduce the fields, $n(r,t)=(\mathbf{n},\mathbf{f})$ [the local particle density, where $\mathbf{n}=(1,1)$],

and $j(r,t)=(\mathbf{j},\mathbf{f})$ [the local momentum density, where $\mathbf{j}=(1,-1)$]. Equation (9) can be equivalently written in terms of the moments,

$$\partial_t n = -\partial_r j, \tag{10}$$

$$\partial_t j = -\partial_r n - \epsilon^{-1} j.$$

The local equilibrium

$$\mathbf{f}^*(n) = \frac{n}{2}\mathbf{n} \tag{11}$$

is the conditional maximum of the entropy,

$$S = -\int (f_+ \ln f_+ + f_- \ln f_-)\, dr,$$

under the constraint which fixes the density, $(\mathbf{n},\mathbf{f}^*)=n$. The quasi-equilibrium manifold (11) is linear in our example, as well as is the kinetic equation.

The problem of reducing the description for the model (9) amounts to finding the closed equation for the density field $n(r,t)$. When the relaxation parameter ϵ^{-1} is small enough (the relaxation dominance), then the first Champan-Enskog approximation to the momentum variable $j(r,t) \approx -\epsilon \partial_r n(r,t)$ amounts to the standard diffusion approximation. Let us consider now how the formula (7), and other methods, extend this result.

Because of the linearity of Eq. (9), and of the local equilibrium, it is natural to use the Fourier transform $h_k = \int \exp(ikr) h(r)\, dr$. Equation (9) is then written,

$$\partial_t \mathbf{f}_k = \mathbf{L}_k \mathbf{f}_k, \tag{12}$$

where

$$\mathbf{L}_k = \begin{pmatrix} -ik - \dfrac{1}{2\epsilon} & \dfrac{1}{2\epsilon} \\ \dfrac{1}{2\epsilon} & ik - \dfrac{1}{2\epsilon} \end{pmatrix}. \tag{13}$$

Derivation of formula (7) in our example goes as follows: We seek the macroscopic dynamics of the form

$$\partial_t n_k = R_k n_k, \tag{14}$$

where the function R_k is yet unknown. In the left-hand side of Eq. (3) we have

$$n_k(t+\tau) = e^{\tau R_k} n_k(t). \tag{15}$$

In the right-hand side of Eq. (3) we have

$$(\mathbf{n}, e^{\tau \mathbf{L}_k} \mathbf{f}^*[n_k(t)]) = \tfrac{1}{2}(\mathbf{n}, e^{\tau \mathbf{L}_k}\mathbf{n}) n_k(t). \tag{16}$$

After equating the expressions (15) and (16), we require that the resulting equality holds in the limit $\tau \to \infty$ independently of the initial data $n_k(t)$. Thus, we arrive at formula (7):

$$R_k = \lim_{\tau\to\infty} \frac{1}{\tau} \ln[(\mathbf{n}, e^{\tau \mathbf{L}_k}\mathbf{n})]. \tag{17}$$

Equation (17) defines the macroscopic dynamics (14) within the present approach. Explicit evaluation of expression (17) is straightforward in the present model. Indeed, operator $\mathbf{L}_k$ has two eigenvalues, $\Lambda_k^{\pm}$, where

$$\Lambda_k^{\pm} = -\frac{1}{2\epsilon} \pm \sqrt{\frac{1}{4\epsilon^2} - k^2}. \tag{18}$$

Let us denote as $\mathbf{e}_k^{\pm}$ the two (arbitrary) eigenvectors of the matrix $\mathbf{L}_k$, corresponding to the eigenvalues $\Lambda_k^{\pm}$. Vector $\mathbf{n}$ has a representation $\mathbf{n} = \alpha_k^+ \mathbf{e}_k^+ + \alpha_k^- \mathbf{e}_k^-$, where $\alpha_k^{\pm}$ are complex valued coefficients. With this, we obtain in Eq. (17),

$$R_k = \lim_{\tau\to\infty} \frac{1}{\tau} \ln[\alpha_k^+ (\mathbf{n},\mathbf{e}_k^+) e^{\tau\Lambda_k^+} + \alpha_k^- (\mathbf{n},\mathbf{e}_k^-) e^{\tau\Lambda_k^-}]. \tag{19}$$

For $k \leqslant k_c$, where $k_c^2 = 4\epsilon$, we have $\Lambda_k^+ > \Lambda_k^-$. Therefore,

$$R_k = \Lambda_k^+, \quad \text{for} \quad k < k_c. \tag{20}$$

As was expected, formula (7) in our case results in the exact hydrodynamic branch of the spectrum of the kinetic Eq. (9). The standard diffusion approximation is recovered from Eq. (20) as the first nonvanishing approximation in terms of the $(k/k_c)^2$.

At $k = k_c$, the crossover from the extended hydrodynamic to the kinetic regime takes place, and $\mathrm{Re}\,\Lambda_k^+ = \mathrm{Re}\,\Lambda_k^-$. However, we may still extend the function R_k for $k \geqslant k_c$ on the basis of formula (17)

$$R_k = \mathrm{Re}\,\Lambda_k^+ \quad \text{for} \quad k \geqslant k_c. \tag{21}$$

Notice that the function R_k as given by Eqs. (20) and (21) is continuous but nonanalytic at the crossover.

Let us now compare this result with the Chapman-Enskog method. Since the exact Chapman-Enskog solution for the systems like Eq. (10) has been recently discussed in detail elsewhere [24–26], we shall be brief here. Following the Chapman-Enskog method, we seek the momentum variable j in terms of an expansion,

$$j^{\mathrm{CE}} = \sum_{n=0}^{\infty} \epsilon^{n+1} j^{(n)}. \tag{22}$$

The Chapman-Enskog coefficients $j^{(n)}$, are found from the recurrence equations,

$$j^{(n)} = -\sum_{m=0}^{n-1} \partial_t^{(m)} j^{(n-1-m)}, \tag{23}$$

where the Chapman-Enskog operators $\partial_t^{(m)}$ are defined by their action on the density n

$$\partial_t^{(m)} n = -\partial_r j^{(m)}. \tag{24}$$

The recurrence Eqs. (22), (23), and (24), become well-defined as soon as the aforementioned zeroth-order approximation $j^{(0)}$ is specified,

$$j^{(0)} = -\partial_r n. \tag{25}$$

From Eqs. (23), (24), and (25), it follows that the Chapman-Enskog coefficients $j^{(n)}$ have the following structure:

$$j^{(n)} = b_n \partial_r^{2n+1} n, \tag{26}$$

where coefficients b_n are found from the recurrence equation,

$$b_n = \sum_{m=0}^{n-1} b_{n-1-m} b_m, \quad b_0 = -1. \tag{27}$$

Notice that coefficients (27) are real-valued, by the sense of the Chapman-Enskog procedure. The Fourier image of the Chapman-Enskog solution for the momentum variable has the form,

$$j_k^{\mathrm{CE}} = ikB_k^{\mathrm{CE}} n_k, \tag{28}$$

where

$$B_k^{\mathrm{CE}} = \sum_{n=0}^{\infty} b_n (-\epsilon k^2)^n. \tag{29}$$

Equation for the function B (29) is easily found upon multiplying Eq. (27) by $(-k^2)^n$, and summing in n from zero to infinity,

$$\epsilon k^2 B_k^2 + B_k + 1 = 0. \tag{30}$$

Solution to the latter equation which respects condition (25), and which constitutes the exact Chapman-Enskog solution (29) is

$$B_k^{\mathrm{CE}} = \begin{cases} k^{-2}\Lambda_k^+, & k < k_c \\ \text{none}, & k \geqslant k_c. \end{cases} \tag{31}$$

Thus, the exact Chapman-Enskog solution derives the macroscopic equation for the density as follows:

$$\partial_t n_k = -ikj_k^{\mathrm{CE}} = R_k^{\mathrm{CE}} n_k, \tag{32}$$

where

$$R_k^{\mathrm{CE}} = \begin{cases} \Lambda_k^+, & k < k_c \\ \text{none}, & k \geqslant k_c. \end{cases} \tag{33}$$

The Chapman-Enskog solution does not extend beyond the crossover at k_c. This happens because the full Chapman-Enskog solution appears as a continuation of the diffusion approximation, whereas formula (17) is not based on such an extension *a priori*.

Finally, let us discuss briefly the comparison with the solution within the method of invariant manifold [13,14]. Specifically, the momentum variable $j_k^{\mathrm{inv}} = ikB_k^{\mathrm{inv}} n_k$ is required to be invariant of both the microscopic and the macroscopic dynamics, that is, the time derivative of j_k^{inv} due to the macroscopic subsystem,

$$\frac{\partial j_k^{\mathrm{inv}}}{\partial n_k} \partial_t n_k = ikB_k^{\mathrm{inv}}(-ik)[ikB_k^{\mathrm{inv}}], \tag{34}$$

should be equal to the derivative of j_k^{inv} due to the microscopic subsystem,

$$\partial_t j_k^{\mathrm{inv}} = -ikn_k - \epsilon^{-1} ikB_k^{\mathrm{inv}} n_k, \tag{35}$$

and that the equality between Eqs. (34) and (35) should hold independently of the specific value of the macroscopic variable n_k. This amounts to a condition for the unknown function B_k^{inv}, which is essentially the same as Eq. (30), and it is straightforward to show that the same selection procedure of the hydrodynamic root as above in the Chapman-Enskog case results in Eq. (33).

In conclusion, in this paper we have given the explicit illustration for formula (7). The example considered above demonstrates that formula (7) gives the exact macroscopic evolution equation, which is identical to the sum of the Chapman-Enskog expansion, as well as to the invariance principle. This identity holds up to the point where the hydrodynamics and the kinetics cease to be separated. Whereas the Chapman-Enskog solution does not extend beyond the crossover point, formula (7) demonstrates a nonanalytic extension. The example considered adds to the confidence of the correctness of the approach suggested in [2–4].

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