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THE MATHEMATICAL PROCEDURE OF COARSE GRAINING: FROM GRAD'S TEN-MOMENT EQUATIONS TO HYDRODYNAMICS*

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Abstract. We employ systematic coarse graining techniques to derive hydrodynamic equations from Grad's ten-moment equations. The coarse graining procedure is designed such that it manifestly preserves the thermodynamic structure of the equations. The relevant thermodynamic structure and the coarse graining recipes suggested by statistical mechanics are described in detail and are illustrated by the example of hydrodynamics. A number of mathematical challenges associated with structure-preserving coarse graining of evolution equations for thermodynamic systems as a generalization of Hamiltonian dynamic systems are presented. Coarse graining is a key step that should always be considered before attempting to solve an equation.

Key words. coarse graining, dynamic systems, Poisson brackets, dissipative brackets, general equation for the nonequilibrium reversible-irreversible coupling structure, nonequilibrium thermodynamics, hydrodynamics, Grad's moment equations

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1. Introduction.

Physicists and engineers want to solve problems, and they hence try to solve equations. The purpose of this paper is to emphasize and to illustrate that an essential first step to solve a problem may be to coarse grain a given set of equations before studying the solutions. We here consider problems that can be investigated on different levels of description associated with different length and time scales, and we specify a set of rules for systematic coarse graining. From a mathematical perspective, it is important to specify the structure which should be left invariant in the coarse graining procedure. The relevant structure, which is known as GENERIC ("general equation for the nonequilibrium reversible-irreversible coupling") or "metriplectic," is a generalization of Hamiltonian structures to dissipative systems and is of thermodynamic origin. The design of structure-preserving coarse graining procedures and approximation schemes is presented as a general mathematical challenge. It is important to note that coarse graining is fundamentally different from reduction based on the idea of invariant manifolds because the transition from reversible to irreversible equations, or even increasing degrees of irreversibility, is allowed. The fundamental distinction between reduction (or solving) and coarse graining has been elaborated in detail in [27].

We first describe the GENERIC structure. The coarse graining recipes of statistical mechanics are then presented and explained in the context of rarefied gas flow. In particular, we shall illustrate the statistical mechanical coarse graining procedure by reducing Grad's ten-moment equations to hydrodynamics. It is well known that this can be done by various methods [16]. Our emphasis therefore lies on the method

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which was designed to preserve the GENERIC structure in the coarse graining procedure, and not on the relation between Grad's equations and hydrodynamics. Some specific mathematical challenges are further elaborated in section 5.

2. Thermodynamic structure. To employ a systematic coarse graining procedure for dynamic systems, it is necessary to write evolution equations in a properly structured form. For reversible systems, symplectic structures provide a natural setting to formulate time evolution generated by Hamiltonians, and Poisson and Dirac structures offer useful generalizations [5, 17]. For irreversible systems, thermodynamically consistent evolution equations consist of contributions constructed from two generators by means of Poisson and dissipative brackets [11, 14, 19]. We here summarize the GENERIC formulation of this idea for closed systems [12, 28]. In [20], an almost identical formulation of the original idea of [11, 14, 19] has been referred to as the metriplectic structure.

Once we have specified the list of independent variables x, for example the ten moments in Grad's approximate solution of Boltzmann's kinetic equation, thermodynamically admissible equations can be expressed in the form [12, 28]

$$\frac{dx}{dt} = L \cdot \frac{\delta E}{\delta x} + M \cdot \frac{\delta S}{\delta x}, \tag{2.1}$$

where the generators E and S are the total energy and entropy expressed in terms of the variables x, and L and M are certain linear operators, or matrices, which can also depend on x. We refer to L as a Poisson operator and to M as a friction operator. The two contributions to the time evolution of x generated by the total energy E and the entropy S in (2.1) are the reversible and irreversible contributions, respectively. Because x contains position-dependent fields, the state variables are labeled by a continuous position label in addition to the discrete one running from one to ten in the following. A matrix multiplication, which can alternatively be considered as the application of a linear operator, hence implies not only a summation over the discrete index but also integration over space, and $\delta/\delta x$ typically implies functional rather than partial derivatives (for a definition of functional derivatives, see, for example, Appendix C of [24]). Equation (2.1) is supplemented by the complementary degeneracy requirements

$$L \cdot \frac{\delta S}{\delta x} = 0 \tag{2.2}$$

and

$$M \cdot \frac{\delta E}{\delta x} = 0. \tag{2.3}$$

The requirement that the entropy gradient $\delta S/\delta x$ is in the null-space of L in (2.2) expresses the reversible nature of the L-contribution to the dynamics: the functional form of the entropy is such that it cannot be affected by the operator generating the reversible dynamics. The requirement that the energy gradient $\delta E/\delta x$ is in the null-space of M in (2.3) expresses the conservation of the total energy in a closed system by the M-contribution to the dynamics (for a discussion of open systems, see [26]). For Grad's ten-moment equations, for example, (2.2) determines the functional form of the entropy once the Poisson bracket is known (see Exercise 181 of [24]), and (2.3) allows an unrestricted relaxation of the traceless second-moment tensor (because the energy depends only on the trace of the second-moment tensor).

Further general properties of L and M are discussed most conveniently in terms of the Poisson and dissipative brackets

$$\{A,B\} = \frac{\delta A}{\delta x} \cdot L \cdot \frac{\delta B}{\delta x}, \tag{2.4}$$

$$[A,B] = \frac{\delta A}{\delta x} \cdot M \cdot \frac{\delta B}{\delta x}, \tag{2.5}$$

where A, B are sufficiently regular real-valued functions on the space of independent variables. In terms of these brackets, (2.1) and the chain rule lead to the following time-evolution equation of an arbitrary function A in terms of the two separate generators E and S:

$$\frac{dA}{dt} = \{A,E\} + [A,S]. \tag{2.6}$$

The further conditions for L can now be stated as the antisymmetry property

$$\{A,B\} = -\{B,A\} \tag{2.7}$$

and the Jacobi identity

$$\{A,\{B,C\}\} + \{B,\{C,A\}\} + \{C,\{A,B\}\} = 0, \tag{2.8}$$

where C is another arbitrary sufficiently regular real-valued function on the state space. These properties are well known from the Poisson brackets of classical mechanics. In an abstract approach to Poisson brackets, one may use the product or Leibniz rule

$$\{AB,C\} = A\{B,C\} + B\{A,C\}, \tag{2.9}$$

instead of the explicit representation in (2.4), to capture the essence of reversible dynamics.

Further properties of M can be formulated in terms of the symmetry condition

$$[A,B] = [B,A] \tag{2.10}$$

and the nonnegativeness condition

$$[A,A] \geq 0. \tag{2.11}$$

This nonnegativeness condition, together with the degeneracy requirement (2.2), guarantees that the entropy is a nondecreasing function of time,

$$\frac{dS}{dt} = \frac{\delta S}{\delta x} \cdot M \cdot \frac{\delta S}{\delta x} = [S,S] \geq 0. \tag{2.12}$$

The existence of a Lyapunov function S provides a powerful tool for stability analysis and, in particular, implies the consistency of the time-evolution equations (2.1) with equilibrium thermodynamics. The properties (2.10) and (2.11) imply the symmetry and the positive-semidefiniteness of M (for a more sophisticated discussion of the Onsager–Casimir symmetry properties of M, see sections 3.2.1 and 7.2.4 of [24]). The Jacobi identity (2.8), which is a highly restrictive condition for formulating proper reversible dynamics, expresses the invariance of Poisson brackets in the course of time (time-structure invariance).

In thermodynamic modeling, we focus on the thermodynamic building blocks E, S, L, and M rather than on the time-evolution equations. One of the advantages of this approach is that we can coarse grain the basic building blocks by systematic procedures so that the coarse grained equations are guaranteed to be thermodynamically admissible.

3. Grad's ten-moment equations. As a first step, we need to define a thermodynamic system by specifying the list of independent variables. In addition to the usual five hydrodynamic fields, the mass density ρ, the velocity $\boldsymbol{v}$, and the temperature T, we use a traceless second-moment tensor $\boldsymbol{\sigma}$ in velocity space. Note that we consider a traceless tensor because the trace of the second-moment tensor is represented by the temperature T. Further note that the tensor $\boldsymbol{\sigma}$ is symmetric so that it has five independent components in addition to the five hydrodynamic fields and we arrive at a total of ten moment variables. If we add the trace part,

$$\boldsymbol{\pi} = p\mathbf{1} + \boldsymbol{\sigma}, \tag{3.1}$$

the tensor $\boldsymbol{\pi}$ is positive definite, where p is the local thermodynamic pressure and $\mathbf{1}$ is the unit tensor. Equation (3.1) also implies the normalization of the independent variable $\boldsymbol{\sigma}$.

The ten-moment equations for the independent variables $x = (\rho, \boldsymbol{v}, T, \boldsymbol{\sigma})$ are derived from Boltzmann's kinetic equation, and we hence expect them to be restricted to rarefied gases. The detailed derivation of the functional form of the building blocks E, S, L, and M of the thermodynamic structure can be found in section 7.4.3 of [24]. The energy is given in terms of the five hydrodynamic variables alone,

$$E = \int \left(\frac{1}{2}\rho \boldsymbol{v}^2 + \frac{3}{2}\frac{\rho}{m} k_{\mathrm{B}} T \right) d^3r, \tag{3.2}$$

in which the kinetic energy and the internal energy of a monatomic ideal gas of particles with mass m can be recognized. The entropy, which can be obtained by evaluating Boltzmann's entropy with a Gaussian velocity distribution, is composed of the local equilibrium contribution for an ideal gas determined by ρ and T, and a configurational contribution depending on $\boldsymbol{\sigma}$,

$$S = \frac{k_{\mathrm{B}}}{2} \int \frac{\rho}{m} \left[\ln\left(c\frac{T^3}{\rho^2} \right) + \ln\det\left(\mathbf{1} + \frac{\boldsymbol{\sigma}}{p} \right) \right] d^3r, \tag{3.3}$$

where $p = p(\rho, T) = \rho k_{\mathrm{B}} T/m$ is the ideal gas pressure and c is a constant. The occurrence of the logarithm and determinant in the configurational entropy reflects the Gaussian nature of the velocity distribution [16]. For the gradients of the energy and entropy functionals, we then find

$$\frac{\delta E}{\delta x} = \begin{pmatrix} \frac{1}{2}\boldsymbol{v}^2 + \frac{3}{2}\frac{k_{\mathrm{B}}T}{m} \\ \rho\boldsymbol{v} \\ \frac{3}{2}\frac{\rho}{m}k_{\mathrm{B}} \\ 0 \end{pmatrix} \tag{3.4}$$

and

$$\frac{\delta S}{\delta x} = \frac{k_{\mathrm{B}}}{2m} \begin{pmatrix} \ln(\rho^{-5}\det\boldsymbol{\pi}) + p\,\mathrm{tr}(\boldsymbol{\pi}^{-1}) \\ 0 \\ \rho^2 \frac{k_{\mathrm{B}}}{m}\mathrm{tr}(\boldsymbol{\pi}^{-1}) \\ \rho\boldsymbol{\pi}^{-1} \end{pmatrix}. \tag{3.5}$$

In calculating the functional derivatives in (3.4) and (3.5), we have neglected contributions resulting from constraints, such as the conserved total mass or the traceless nature of $\boldsymbol{\sigma}$, because they lead to constant contributions that are irrelevant in the subsequent calculations.

When transformed into the current set of variables x, the Poisson operator for the ten-moment equations derived in [24] becomes

$$L = \begin{pmatrix} 0 & -\frac{\partial}{\partial \boldsymbol{r}} & 0 & 0 \\ -\frac{\partial}{\partial \boldsymbol{r}} & \frac{1}{\rho}\boldsymbol{\omega} & \frac{1}{\rho}\frac{\partial T}{\partial \boldsymbol{r}} - \frac{1}{\rho}\frac{\partial}{\partial \boldsymbol{r}} \cdot \boldsymbol{\pi}\frac{2m}{3\rho k_{\mathrm{B}}} & L_{24} \\ 0 & -\frac{1}{\rho}\frac{\partial T}{\partial \boldsymbol{r}} - \frac{2m}{3\rho k_{\mathrm{B}}}\boldsymbol{\pi} \cdot \frac{\partial}{\partial \boldsymbol{r}}\frac{1}{\rho} & 0 & L_{34} \\ 0 & L_{42} & L_{43} & L_{44} \end{pmatrix}, \tag{3.6}$$

where $\boldsymbol{\omega}$ is the vorticity tensor

$$\boldsymbol{\omega} = \boldsymbol{\kappa}^T - \boldsymbol{\kappa}, \tag{3.7}$$

expressed in terms of the transposed velocity gradient tensor $\boldsymbol{\kappa}$ with components

$$\kappa_{jk} = \frac{\partial v_j}{\partial r_k}, \tag{3.8}$$

and the beyond-hydrodynamic entries in this Poisson operator are

$$(L_{24})_{ikl} = -\frac{1}{\rho}\sigma_{kl}\frac{\partial}{\partial r_i} - \frac{1}{\rho}\left[\frac{\partial}{\partial r_k}\pi_{il} + \frac{\partial}{\partial r_l}\pi_{ki} - \frac{2}{3}\delta_{kl}\left(\frac{\partial}{\partial \boldsymbol{r}} \cdot \boldsymbol{\pi}\right)_i\right], \tag{3.9}$$

$$(L_{42})_{ijk} = -\frac{\partial}{\partial r_k}\frac{1}{\rho}\sigma_{ij} - \left[\pi_{kj}\frac{\partial}{\partial r_i} + \pi_{ik}\frac{\partial}{\partial r_j} - \frac{2}{3}\delta_{ij}\left(\boldsymbol{\pi} \cdot \frac{\partial}{\partial \boldsymbol{r}}\right)_k\right]\frac{1}{\rho}, \tag{3.10}$$

$$L_{34} = -L_{43} = \frac{2m}{3\rho k_{\mathrm{B}}}(\boldsymbol{\sigma} \cdot \boldsymbol{\omega} - \boldsymbol{\omega} \cdot \boldsymbol{\sigma}), \tag{3.11}$$

and

$$\begin{aligned}(L_{44})_{ijkl} = \frac{2}{3}(\boldsymbol{\sigma} \cdot \boldsymbol{\omega} - \boldsymbol{\omega} \cdot \boldsymbol{\sigma})_{ij}\delta_{kl} - \frac{2}{3}\delta_{ij}(\boldsymbol{\sigma} \cdot \boldsymbol{\omega} - \boldsymbol{\omega} \cdot \boldsymbol{\sigma})_{kl} \\ +\pi_{ik}\omega_{jl} + \omega_{ik}\pi_{jl} + \pi_{il}\omega_{jk} + \omega_{il}\pi_{jk}.\end{aligned} \tag{3.12}$$

The Jacobi identity for this Poisson operator follows from the fact that it can be obtained by a rigorous reduction procedure from the Poisson bracket for Boltzmann's kinetic equation [24]. In principle, the Poisson and friction matrices should depend on two position arguments $\boldsymbol{r}$ and $\boldsymbol{r}'$, and a matrix multiplication should involve an integration over space. For local field theories, however, L and M contain Dirac δ-functions of $\boldsymbol{r} - \boldsymbol{r}'$ (and their derivatives) so that we can, as in (3.6), use an operator notation without integrations over space (for more details, see sections 2.2.2 and 2.2.3 of [24]). One should note the following careful distinction made in our notation. When we write $\frac{\partial f}{\partial \boldsymbol{r}}$ for any function f, the derivative applies to f only, whereas writing $\frac{\partial}{\partial \boldsymbol{r}} f$ would imply the derivation of all functions to the right of $\frac{\partial}{\partial \boldsymbol{r}}$, including the functions resulting from a vector multiplied from the right.

We assume that the friction operator is composed of two contributions describing momentum relaxation and spatial diffusion, respectively:

$$M = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \boldsymbol{M}^{\text{relax}} \end{pmatrix} + C_M^{\text{diff}} \frac{Dm}{\rho k_{\text{B}}} (C_M^{\text{diff}})^T. \tag{3.13}$$

The first contribution has been derived from Boltzmann's kinetic equation [24]. It reflects the idea that only the nonconserved second moments are affected by dissipative relaxation processes. To obtain a convenient expression for the components of the fourth-rank tensor $\boldsymbol{M}^{\text{relax}}$, we evaluate the integral expression (7.175) of [24] for the special interaction potential of Maxwell molecules,

$$\begin{aligned} M_{ijkl}^{\text{relax}} = \frac{m}{\rho k_{\text{B}}} \frac{1}{\tau} \Bigg[& \frac{p}{2}(\pi_{ik}\delta_{jl} + \delta_{ik}\pi_{jl} + \pi_{il}\delta_{jk} + \delta_{il}\pi_{jk}) - \frac{2}{3}\pi_{ij}\pi_{kl} \\ & + \frac{1}{3}(\sigma_{ik}^2\delta_{jl} - 2\sigma_{ik}\sigma_{jl} + \delta_{ik}\sigma_{jl}^2 + \sigma_{il}^2\delta_{jk} - 2\sigma_{il}\sigma_{jk} + \delta_{il}\sigma_{jk}^2) \Bigg]. \end{aligned} \tag{3.14}$$

Note that the terms with the prefactor 1/3 in the second line of this equation do not contribute to the double contraction $\sum_{kl} M_{ijkl}^{\text{relax}} A_{kl}$, where the tensor $\boldsymbol{A}$ can be an arbitrary function of $\boldsymbol{\sigma}$ or $\boldsymbol{\pi}$. The tensor $\boldsymbol{M}^{\text{relax}}$ describes the standard dissipative mechanism of Grad's ten-moment equations. The inclusion of an additional diffusion mechanism with diffusion coefficient D into hydrodynamics, which is achieved through the second contribution to the friction operator in (3.13), has been forcefully postulated and convincingly substantiated by Brenner in recent years [1, 2, 3]. The corresponding friction operator for Grad's moment expansion with an arbitrary set of moments was derived by coarse graining Boltzmann's kinetic equation [25]. When transformed into the present set of moment variables, the results for the related vectors C_M^{diff} and $(C_M^{\text{diff}})^T$ are

$$C_M^{\text{diff}} = \begin{pmatrix} -\frac{\partial}{\partial \boldsymbol{r}}\rho \\ -\frac{\partial \boldsymbol{v}}{\partial \boldsymbol{r}} \\ -\frac{\partial T}{\partial \boldsymbol{r}} \\ -\frac{\partial}{\partial \boldsymbol{r}}\boldsymbol{\sigma} \end{pmatrix}, \qquad (C_M^{\text{diff}})^T = \begin{pmatrix} \rho\frac{\partial}{\partial \boldsymbol{r}} & -\frac{\partial \boldsymbol{v}}{\partial \boldsymbol{r}} & -\frac{\partial T}{\partial \boldsymbol{r}} & \boldsymbol{\sigma}\frac{\partial}{\partial \boldsymbol{r}} \end{pmatrix}. \tag{3.15}$$

The spatial derivative operators in the two factors C_M^{diff} and $(C_M^{\text{diff}})^T$ in (3.13) are to be contracted with each other. For this choice of $(C_M^{\text{diff}})^T$, we have the identities

$$(C_M^{\text{diff}})^T \cdot \frac{\delta E}{\delta x} = 0 \tag{3.16}$$

and

$$(C_M^{\text{diff}})^T \cdot \frac{\delta S}{\delta x} = -\frac{\partial}{\partial \boldsymbol{r}} \frac{p}{T}. \tag{3.17}$$

By inserting the above building blocks E, S, L, and M into the fundamental equation (2.1), we obtain the following set of time-evolution equations:

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial \boldsymbol{r}} \cdot [(\boldsymbol{v} + \boldsymbol{v}^{\text{diff}})\rho], \tag{3.18}$$

$$\frac{\partial \boldsymbol{v}}{\partial t} = -(\boldsymbol{v} + \boldsymbol{v}^{\text{diff}}) \cdot \frac{\partial}{\partial \boldsymbol{r}} \boldsymbol{v} - \frac{1}{\rho} \frac{\partial}{\partial \boldsymbol{r}} \cdot \boldsymbol{\pi}, \tag{3.19}$$

$$\frac{\partial T}{\partial t} = -(\boldsymbol{v} + \boldsymbol{v}^{\text{diff}}) \cdot \frac{\partial T}{\partial \boldsymbol{r}} - \frac{2m}{3\rho k_{\text{B}}} \boldsymbol{\pi} : \boldsymbol{\kappa}, \tag{3.20}$$

$$\frac{\partial \boldsymbol{\sigma}}{\partial t} = -\frac{\partial}{\partial \boldsymbol{r}} \cdot [(\boldsymbol{v} + \boldsymbol{v}^{\text{diff}})\boldsymbol{\sigma}] - \boldsymbol{\kappa} \cdot \boldsymbol{\pi} - \boldsymbol{\pi} \cdot \boldsymbol{\kappa}^T + \frac{2}{3}\boldsymbol{1}(\boldsymbol{\pi} : \boldsymbol{\kappa}) - \frac{1}{\tau}\boldsymbol{\sigma}, \tag{3.21}$$

where the diffusive contribution to the convection velocity is given by

$$\boldsymbol{v}^{\text{diff}} = -\frac{Dm}{\rho k_{\text{B}}} \frac{\partial}{\partial \boldsymbol{r}} \frac{p}{T} = -\frac{D}{\rho} \frac{\partial \rho}{\partial \boldsymbol{r}}. \tag{3.22}$$

For $D = 0$, we have $\boldsymbol{v}^{\text{diff}} = 0$ and we recover the standard set of Grad's ten-moment equations [10, 30].

4. Coarse graining to hydrodynamics. As a next step, we want to reduce the list of variables from the ten-moment variables $x = (\rho, \boldsymbol{v}, T, \boldsymbol{\sigma})$ to the five hydrodynamic fields $y = (\rho, \boldsymbol{v}, T)$. The usual assumption is that the relaxation time τ is small so that $\boldsymbol{\sigma}$ relaxes rapidly to a value of order τ. If $\boldsymbol{\sigma}$ in (3.21) is expanded in terms of τ, the lowest-order term is given by the explicit expression

$$\boldsymbol{\sigma} = -\eta \left(\boldsymbol{\kappa} + \boldsymbol{\kappa}^T - \frac{2}{3}\boldsymbol{1}\text{tr}\boldsymbol{\kappa} \right) \tag{4.1}$$

with the viscosity $\eta = \tau p$. The actual dimensionless expansion parameter is τ divided by the characteristic time scale of the flow, which is the inverse flow rate. In the context of kinetic theory, this small expansion parameter can be interpreted as a local Knudsen number. The Newtonian expression (4.1) for the pressure tensor is to be used together with (3.1) in the hydrodynamic equations (3.18)–(3.20). As a result of this singular perturbation procedure, the differential equation for $\boldsymbol{\sigma}$ is changed into an explicit constitutive expression.

Whereas the singular perturbation approach is very simple, it has the severe drawback that it is not intrinsically clear whether or not the resulting equations for the hydrodynamic variables y possess the GENERIC structure expressing thermodynamic admissibility. Not only is the nature of the equation for $\boldsymbol{\sigma}$ changed but also the role of $\boldsymbol{\sigma}$ or $\boldsymbol{\pi}$ in the hydrodynamic equations. Whereas in the ten-moment equations the occurrence of $\boldsymbol{\pi}$ in the equations for ρ, $\boldsymbol{v}$, and T results from the reversible contribution, the occurrence of η in (4.1) signals that reversible contributions are turned into irreversible terms. Such a conversion from reversible to irreversible is a characteristic of coarse graining.

Although the above procedure does not tell us anything about the GENERIC structure of the equations for the variables y, hydrodynamics is well known to be thermodynamically consistent. It would hence be desirable to have an equivalent coarse graining procedure that guarantees the GENERIC structure on the coarse grained level automatically.

Coarse graining of time-evolution equations can be regarded as the topic of nonequilibrium statistical mechanics. A general and systematic procedure is based on the idea that there exists a separation of time scales and that the fast variables can be eliminated from the equations for the slow variables by means of a projection-operator technique. The thermodynamic structure can be preserved in coarse graining by focusing on the building blocks E, S, L, and M. The two key ingredients required for the general procedure are (i) a mapping of the variables, $\Pi : x \mapsto y$, and (ii) a probability measure $\rho_y(x)$ on the space of independent variables x so that averages can be performed (for given y). The generalized microcanonical and canonical ensembles of statistical mechanics, or combinations of those, provide natural choices for such probability measures [24].

4.1. Ensemble. For our example of coarse graining from Grad's equations to hydrodynamics, the mapping Π merely selects five of the ten moment variables. We choose the probability measure $\rho_y(x)$ to be of the generalized microcanonical type,

$$\rho_y(x) = \frac{1}{\mathcal{N}(y)} \exp\left\{\frac{S(x)}{k_\mathrm{B}}\right\} \delta(\Pi(x) - y). \tag{4.2}$$

This measure is based on the idea that all microstates have equal weight. To count the microstates consistent with y, we make use of the fact that the microstates associated with x have already been counted to obtain $S(x)$. For a given y, this measure is concentrated on the manifold that is obtained as the inverse image of y. The weight of the states within the inverse image of y is governed by the entropy $S(x)$. For the normalization factor $\mathcal{N}(y)$ we have

$$\mathcal{N}(y) = \int \exp\left\{\frac{S(x)}{k_\mathrm{B}}\right\} \delta(\Pi(x) - y)\mathcal{D}x, \tag{4.3}$$

where we have used the symbol $\mathcal{D}$ to emphasize the occurrence of functional integrations. For our example with entropy (3.3), the normalization factor is given by the following functional:

$$\mathcal{N}(\rho, T) = \int \exp\left\{\frac{S(\rho, T, \boldsymbol{\sigma})}{k_\mathrm{B}}\right\} \mathcal{D}\boldsymbol{\sigma} = \exp\left\{\int \frac{\rho}{2m} \ln\left(c\frac{T^3}{\rho^2}\right) d^3r\right\} \Omega(\rho, T), \tag{4.4}$$

with

$$\Omega(\rho, T) = \int \exp\left\{\int \frac{\rho}{2m} \ln\det\left(\mathbf{1} + \frac{\boldsymbol{\sigma}}{p}\right) d^3r\right\} \mathcal{D}\boldsymbol{\sigma}. \tag{4.5}$$

Note that the proper definition of functional integrals requires great care, in particular, with normalization factors (see, for example, Chapter 9 of [13]). While ratios of functional integrals can be defined unambiguously, in the following, we use physical arguments for handling the normalization factors properly.

Because ensemble averaging is the key step in coarse graining, we discuss the functional integration over $\boldsymbol{\sigma}$ in some detail. To discretize the integral, we assume that the volume occupied by the gas can be partitioned into cells of volume V_i on which the variables x may be considered to be independent of position. We then have

$$\Omega(\rho, T) = \prod_i \int \exp\left\{N_i \,\mathrm{tr} \ln\left(\mathbf{1} + \frac{\boldsymbol{\sigma}_i}{p_i}\right)\right\} d\boldsymbol{\sigma}_i, \tag{4.6}$$

where $2N_i = V_i\rho/m$ is the number of particles in the volume V_i. If we expand the logarithm, the linear contribution vanishes because $\boldsymbol{\sigma}_i$ is traceless and we find the Gaussian integrals

$$\Omega(\rho, T) = \prod_i \int \exp\left\{-\frac{1}{2}\frac{N_i}{p_i^2} \boldsymbol{\sigma}_i : \boldsymbol{\sigma}_i\right\} d\boldsymbol{\sigma}_i. \tag{4.7}$$

Because N_i is a large number, the Gaussian factors are sharply peaked and higher-order terms in the expansion of the logarithm can be neglected safely. We have thus reduced the problem to independent Gaussian integrations. In view of the symmetry of $\boldsymbol{\sigma}_i$, (4.7) describes a Gaussian distribution in the six components $(\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{12}, \sigma_{13}, \sigma_{23})$ of $\boldsymbol{\sigma}_i$ with inverse covariance matrix

$$C_\sigma^{-1} = \frac{N_i}{p_i^2} \begin{pmatrix} 1+\alpha & \alpha & \alpha & 0 & 0 & 0 \\ \alpha & 1+\alpha & \alpha & 0 & 0 & 0 \\ \alpha & \alpha & 1+\alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}. \tag{4.8}$$

The parameter α has been included to incorporate the constraint that $\boldsymbol{\sigma}_i$ should be traceless; in the limit $\alpha \to \infty$, we have introduced a Gaussian that converges to a Dirac δ-function of $\mathrm{tr}\boldsymbol{\sigma}_i$. The determinant of C_σ^{-1} is given by

$$\det C_\sigma^{-1} = 8(3\alpha + 1) \left(\frac{N_i}{p_i^2} \right)^6 . \tag{4.9}$$

By inverting C_σ^{-1} and performing the limit $\alpha \to \infty$, we obtain the covariance matrix for the Gaussian components $(\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{12}, \sigma_{13}, \sigma_{23})$ of $\boldsymbol{\sigma}_i$:

$$C_\sigma = \frac{p_i^2}{6N_i} \begin{pmatrix} 4 & -2 & -2 & 0 & 0 & 0 \\ -2 & 4 & -2 & 0 & 0 & 0 \\ -2 & -2 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{pmatrix}. \tag{4.10}$$

Our final result for the normalization factor then becomes

$$\Omega(\rho, T) = \prod_i \left[2 \left(\frac{\pi p_i^2}{N_i} \right)^{5/2} \right], \tag{4.11}$$

where we have left out the factor associated with the regularization needed to fulfill the trace condition. As mentioned before, such factors are somewhat ambiguous, but this ambiguity does not affect the physical results (as discussed below).

4.2. Energy. The energy on the coarse grained level is obtained by averaging the energy of the more detailed level,

$$E'(y) = \int E(x) \rho_y(x) \mathcal{D}x. \tag{4.12}$$

In view of the occurrence of the normalization factor (4.3) in $\rho_y(x)$, all averages performed with $\rho_y(x)$ are ratios of functional integrals so that any ambiguous normalization factors are cancelled. For our example, the energy does not depend on the fast variables $\boldsymbol{\sigma}$, so that we have a trivial representation of the type $E(x) = E'(\Pi(x))$. Note that Π merely picks out the hydrodynamic fields, so that we get the same energy expression as in (3.2),

$$E'(\rho, \boldsymbol{v}, T) = \int \left(\frac{1}{2} \rho \boldsymbol{v}^2 + \frac{3}{2} \frac{\rho}{m} k_{\mathrm{B}} T \right) d^3 r. \tag{4.13}$$

4.3. Entropy. The formula for the normalization factor in (4.3) expresses an iterated counting of microstates. The factor $\exp\{S(x)/k_{\mathrm{B}}\}$ represents the number of microstates compatible with the intermediate state x, and the integral sums up all the numbers of microstates for all the states x consistent with the more coarse grained state y. This interpretation suggests the definition of the entropy $S'(y)$ by

$$\mathcal{N}(y) = \exp\left\{\frac{S'(y)}{k_{\mathrm{B}}}\right\}. \tag{4.14}$$

In general, there might be a problem with this definition of entropy because it is not invariant under nonlinear one-to-one transformations of the coarse grained variables y. This and related problems with the definition of entropy have been discussed and resolved in the context of the theory of fluctuations on p. 228 of [24].

In our example, indeed, the situation is unproblematic. According to (4.11), the contribution of each cell to $\ln\Omega$ is of the order of $\ln N_i$ and hence negligible compared to the extensive entropy contribution of the other factor in (4.4), which is proportional to N_i. For the same reason, also constant factors associated with each cell are physically irrelevant. We hence find

$$S'(\rho, T) = \frac{k_{\mathrm{B}}}{2}\int \frac{\rho}{m}\ln\left(c\frac{T^3}{\rho^2}\right) d^3r. \tag{4.15}$$

The factor c is the same as in (3.3), so that the entropy S' is actually obtained by setting $\boldsymbol{\sigma} = 0$ in the entropy S. This observation justifies or explains the occurrence of the equilibrium entropy in (3.3), which is reduced by deviations of $\boldsymbol{\sigma}$ from its equilibrium value.

4.4. Poisson operator. The general expression for the coarse grained Poisson operator is given by the average of the Poisson bracket formed for all pairs of coarse grained variables,

$$L'(y) = \int \{\Pi, \Pi\}\rho_y(x)\mathcal{D}x. \tag{4.16}$$

The coarse graining procedure for the Poisson bracket can also be expressed in a different way. For any two functionals $A'(y)$ and $B'(y)$, one defines $A(x) = A'(\Pi(x))$, $B(x) = B'(\Pi(x))$ and evaluates the Poisson bracket $\{A, B\}$, which is a function of x. By averaging $\{A, B\}$ with $\rho_y(x)$, one obtains $\{A', B'\}'$ as a function of y.

For our example of coarse graining the ten-moment equations to hydrodynamic equations, we need only average the 3×3 block in (3.6) associated with the hydrodynamic fields. The average of $\boldsymbol{\sigma}$ vanishes, so that (3.1) implies

$$L'(\rho, \boldsymbol{v}, T) = \begin{pmatrix} 0 & -\frac{\partial}{\partial \boldsymbol{r}} & 0 \\ -\frac{\partial}{\partial \boldsymbol{r}} & \frac{1}{\rho}\boldsymbol{\omega} & \frac{1}{\rho}\frac{\partial T}{\partial \boldsymbol{r}} - \frac{1}{\rho}\frac{\partial}{\partial \boldsymbol{r}}\frac{2}{3}T \\ 0 & -\frac{1}{\rho}\frac{\partial T}{\partial \boldsymbol{r}} - \frac{2}{3}T\frac{\partial}{\partial \boldsymbol{r}}\frac{1}{\rho} & 0 \end{pmatrix}. \tag{4.17}$$

4.5. Friction operator. So far, no dynamic material properties are involved in the coarse graining procedure or in the building blocks E', S', and L'. Dynamic properties occur exclusively in the friction operator M'.

There are two contributions to the coarse grained friction operator, $M' = \bar{M}' + \bar{\bar{M}}'$. A direct contribution is obtained by averaging the dissipative bracket for all pairs of coarse grained variables in exactly the same way as for the Poisson operator in (4.16),

$$\bar{M}'(y) = \int [\Pi, \Pi] \rho_y(x) \mathcal{D}x. \tag{4.18}$$

A second contribution results from the fast variables in the list x that are considered as fluctuations on the coarser level of y, and they hence cause a new contribution to the friction operator,

$$\bar{\bar{M}}'(y) = \frac{1}{k_{\mathrm{B}}} \int_0^{\tau_{\mathrm{s}}} \left[\int \mathcal{K}^{\mathrm{f}} \Pi(x(t)) \, \mathcal{K}^{\mathrm{f}} \Pi(x) \, \rho_y(x) \mathcal{D}x \right] dt, \tag{4.19}$$

where τ_{s} separates the fast and slow variables. On the time scale τ_{s}, the slow variables do not change appreciably, whereas the fast variables relax completely so that the integral converges. In practice, there are no general rules for separating fast and slow variables; identifying the relevant slow variables is an art that is closely related to understanding the essential physics of a problem. The operator $\mathcal{K}^{\mathrm{f}}$ describing the rapid contribution to the time derivative of an observable is defined by the following equations:

$$\mathcal{K}^{\mathrm{f}} \Pi(x) = \mathcal{K}_0 \Pi(x) - \int \mathcal{K}_0 \Pi(x') \, \rho_y(x') \mathcal{D}x', \tag{4.20}$$

with

$$\mathcal{K}_0 = \mathcal{K}^+ = \left(L \cdot \frac{\delta E}{\delta x} + M \cdot \frac{\delta S}{\delta x} \right) \cdot \frac{\delta}{\delta x} + k_{\mathrm{B}} \frac{\delta}{\delta x} \cdot M \cdot \frac{\delta}{\delta x}. \tag{4.21}$$

The symbol $\mathcal{K}^+$ is used because this operator occurs in Kolmogorov's backward equation in the theory of Markovian solutions of stochastic differential equations; it is the adjoint of the Fokker–Planck operator occurring in the equation for the transition probabilities. Finally, $x(t)$ in (4.19) is obtained from $x(0) = x$ by solving the fast part of the time-evolution equations. Expressions for dissipative material properties in terms of time correlations of fluctuations as in (4.19) are known as Green–Kubo formulas (see, for example, [9, 15, 24]).

The choice of $\mathcal{K}_0 = \mathcal{K}^+$ in the definition (4.20) of $\mathcal{K}^{\mathrm{f}}$ is controversial. In [6, 23], operators $\mathcal{K}^-$ occurred, and a simple coarse graining procedure summarized in the appendix suggests still another choice. All suggestions consist of

$$\mathcal{K}_0 = \left(L \cdot \frac{\delta E}{\delta x} + M \cdot \frac{\delta S}{\delta x} \right) \cdot \frac{\delta}{\delta x}, \tag{4.22}$$

plus fluctuation-related terms proportional to k_{B}. We here recommend that the simpler first-order differential operator (4.22) should be chosen in the definition of $\mathcal{K}^{\mathrm{f}}$ because the fluctuation terms are expected to be small, and these subtle terms actually depend on the particular coarse graining procedure. The friction operator has contributions from fluctuations on all time scales shorter than that of the fastest relevant variable, but interactions between fluctuations on different time scales are not taken into account. This is a standard assumption in calculating dynamic fluctuations. With (4.19), (4.20), and (4.22), the contribution $\bar{\bar{M}}'$ is defined and the coarse graining procedure is complete.

Because we often deal with position-dependent fields as variables, the meaning of differential operators such as the one in (4.21) is rather symbolic. Following the theory of stochastic partial differential equations [4], we define

$$\mathcal{K}^{+}\Pi = \left\langle \left(L \cdot \frac{\delta E}{\delta x} + M \cdot \frac{\delta S}{\delta x} \right), \frac{\delta \Pi}{\delta x} \right\rangle + \frac{1}{k_{\rm B}} \sum_{j=1}^{\infty} \left\langle e_j, \frac{\delta}{\delta x} \left\langle e_j, M \cdot \frac{\delta \Pi}{\delta x} \right\rangle \right\rangle, \tag{4.23}$$

where $\{e_j\}$ is a complete orthonormal system in the Hilbert space of independent variables x, $\langle \cdot, \cdot \rangle$ is the scalar product in that space, and $\delta/\delta x$ denotes the functional derivative associated with the scalar product of the Hilbert space. Kolmogorov's backward equation in section 9.3 of [4] is developed for infinite-dimensional Itô equations; the rigor and usefulness of infinite-dimensional stochastic equations in which M occurs between the derivatives remains to be explored.

If the rapid decay of $\mathcal{K}^{\rm f}\Pi(x(t))$ can be modeled by

$$\mathcal{K}^{\rm f}\Pi(x(t)) = e^{-t/\tau}\mathcal{K}^{\rm f}\Pi(x), \tag{4.24}$$

where $\tau \ll \tau_{\rm s}$ is an intrinsic time scale for the rapid motion, then we obtain the approximate formula

$$\bar{\bar{M}}'_{\rm app}(y) = \frac{\tau}{k_{\rm B}} \int \mathcal{K}^{\rm f}\Pi(x)\, \mathcal{K}^{\rm f}\Pi(x)\, \rho_y(x) \mathcal{D}x. \tag{4.25}$$

This expression in terms of static correlations is strongly reminiscent of the results of an alternative coarse graining procedure inspired by the work of Ehrenfest (see the appendix).

For our example, the first contribution is obtained by averaging the relevant 3×3 subblock of (3.13), which is actually independent of the eliminated rapid variable $\boldsymbol{\sigma}$. In the operator notation without integration over positions, we have

$$\bar{M}'(\rho, \boldsymbol{v}, T) = \begin{pmatrix} -\frac{\partial}{\partial \boldsymbol{r}}\rho \\ -\frac{\partial \boldsymbol{v}}{\partial \boldsymbol{r}} \\ -\frac{\partial T}{\partial \boldsymbol{r}} \end{pmatrix} \frac{Dm}{\rho k_{\rm B}} \begin{pmatrix} \rho \frac{\partial}{\partial \boldsymbol{r}} & -\frac{\partial \boldsymbol{v}}{\partial \boldsymbol{r}} & -\frac{\partial T}{\partial \boldsymbol{r}} \end{pmatrix}. \tag{4.26}$$

Note that, on the one hand, the nonconventional diffusive contribution to the hydrodynamic equations is already present on the level of the ten-moment equations. The viscous stress, on the other hand, results from the coarse graining procedure. To evaluate the coarse graining contribution to the friction matrix, we note that $\mathcal{K}_0\rho$, $\mathcal{K}_0\boldsymbol{v}$, and $\mathcal{K}_0 T$ are given by the right-hand sides of the hydrodynamic equations (3.18)–(3.20). We then find

$$\mathcal{K}^{\rm f}\rho = 0, \tag{4.27}$$

$$\mathcal{K}^{\rm f}\boldsymbol{v} = -\frac{1}{\rho}\frac{\partial}{\partial \boldsymbol{r}} \cdot \boldsymbol{\sigma}, \tag{4.28}$$

and

$$\mathcal{K}^{\rm f}T = -\frac{2m}{3\rho k_{\rm B}} \boldsymbol{\sigma} : \boldsymbol{\kappa}. \tag{4.29}$$

If all convection and codeformational effects are negligible on the rapid time scale, (3.21) suggests the simple exponential decay

$$\boldsymbol{\sigma}(t) = e^{-t/\tau}\boldsymbol{\sigma}, \tag{4.30}$$

so that the evaluation of (4.19), or of the equivalent Ehrenfest expression (4.25), requires only the static correlation function

$$\boldsymbol{C}(\boldsymbol{r},\boldsymbol{r}') = \frac{1}{\mathcal{N}(\rho,T)} \int \boldsymbol{\sigma}(\boldsymbol{r})\boldsymbol{\sigma}(\boldsymbol{r}') \exp\left\{\frac{S(\rho,T,\boldsymbol{\sigma})}{k_{\mathrm{B}}}\right\} \mathcal{D}\boldsymbol{\sigma}. \tag{4.31}$$

With (4.4) and the discretization procedure for functional integrals introduced previously to evaluate the normalization integral we have

$$\boldsymbol{C}(\boldsymbol{r},\boldsymbol{r}') = \boldsymbol{C}_i = \frac{\int \boldsymbol{\sigma}_i\boldsymbol{\sigma}_i \left[\det\left(\mathbf{1}+\boldsymbol{\sigma}_i/p_i\right)\right]^{N_i} d\boldsymbol{\sigma}_i}{\int \left[\det\left(\mathbf{1}+\boldsymbol{\sigma}_i/p_i\right)\right]^{N_i} d\boldsymbol{\sigma}_i}, \tag{4.32}$$

if $\boldsymbol{r}$ and $\boldsymbol{r}'$ belong to the same cell i, and $\boldsymbol{C}(\boldsymbol{r},\boldsymbol{r}') = 0$ otherwise. In the continuum limit, these two cases can be summarized by

$$\boldsymbol{C}(\boldsymbol{r},\boldsymbol{r}') = V_i\delta(\boldsymbol{r}-\boldsymbol{r}')\boldsymbol{C}_i = 2\frac{m}{\rho}N_i\boldsymbol{C}_i\delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{4.33}$$

The fourth-rank tensor $\boldsymbol{C}_i$ is determined by the covariance matrix (4.10), and we thus find

$$C_{ij,kl}(\boldsymbol{r},\boldsymbol{r}') = \frac{m}{\rho}p^2\delta(\boldsymbol{r}-\boldsymbol{r}')\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\frac{2}{3}\delta_{ij}\delta_{kl}\right). \tag{4.34}$$

If we switch from the notation with two arguments $\boldsymbol{r}$ and $\boldsymbol{r}'$, for which a matrix multiplication implies an integration over $\boldsymbol{r}'$, to the operator notation without integration, then we obtain the coarse graining contribution to the friction operator for conventional hydrodynamics in the form

$$\bar{\bar{M}}' = \begin{pmatrix} 0 & 0 & 0 \\ 0 & M_{22} & M_{23} \\ 0 & M_{32} & M_{33} \end{pmatrix}, \tag{4.35}$$

where the matrix elements are differential operators,

$$M_{22} = -\frac{1}{\rho}\left[\left(\frac{\partial}{\partial\boldsymbol{r}}\eta T\frac{\partial}{\partial\boldsymbol{r}} + \mathbf{1}\frac{\partial}{\partial\boldsymbol{r}}\cdot\eta T\frac{\partial}{\partial\boldsymbol{r}}\right)^T - \frac{2}{3}\frac{\partial}{\partial\boldsymbol{r}}\eta T\frac{\partial}{\partial\boldsymbol{r}}\right]\frac{1}{\rho}, \tag{4.36}$$

$$M_{23} = \frac{1}{\rho}\frac{\partial}{\partial\boldsymbol{r}}\cdot\eta T\left(\dot{\boldsymbol{\gamma}} - \frac{1}{3}\mathbf{1}\mathrm{tr}\dot{\boldsymbol{\gamma}}\right)\frac{2m}{3\rho k_{\mathrm{B}}}, \tag{4.37}$$

$$M_{32} = -\frac{2m}{3\rho k_{\mathrm{B}}}\eta T\left(\dot{\boldsymbol{\gamma}} - \frac{1}{3}\mathbf{1}\mathrm{tr}\dot{\boldsymbol{\gamma}}\right)\cdot\frac{\partial}{\partial\boldsymbol{r}}\frac{1}{\rho}, \tag{4.38}$$

and

$$M_{33} = \frac{\eta T}{2}\left[\dot{\boldsymbol{\gamma}}:\dot{\boldsymbol{\gamma}} - \frac{1}{3}(\mathrm{tr}\dot{\boldsymbol{\gamma}})^2\right]\left(\frac{2m}{3\rho k_{\mathrm{B}}}\right)^2, \tag{4.39}$$

with the deformation rate tensor $\dot{\boldsymbol{\gamma}} = \boldsymbol{\kappa} + \boldsymbol{\kappa}^T$ and the viscosity $\eta = \tau p$. In summary, the systematic coarse graining procedure for hydrodynamics with diffusion resulted in the known energy (4.13), entropy (4.15), Poisson operator (4.17), and friction operator with contributions (4.26) and (4.35). We thus obtain the expected set of hydrodynamic equations (3.18)–(3.20) with

$$\boldsymbol{\pi} = p\mathbf{1} - \eta\left(\dot{\boldsymbol{\gamma}} - \frac{1}{3}\mathbf{1}\mathrm{tr}\dot{\boldsymbol{\gamma}}\right). \tag{4.40}$$

5. Conclusions and perspectives. The derivation of hydrodynamics from Grad's moment equations can be achieved by a systematic coarse graining procedure rooted in statistical mechanics. This procedure manifestly preserves the thermodynamic structure of the evolution equations, known as GENERIC, and it gives the same results as the usual asymptotic perturbation approach.

For general problems, the statistically founded coarse graining procedure guarantees the preservation of all properties of the GENERIC structure, except for the Jacobi identity for the coarse grained bracket. It is hence useful to establish this identity by Lie–Poisson reduction [17, 24]. If the space of independent variables is the dual of the Lie algebra of a Lie group, then a Poisson structure is generally obtained by reduction of the canonical symplectic structure on the cotangent bundle of the Lie group. For example, in describing fluids, the basic Lie group is the group of space transformations and the Lie algebra consists of velocity fields, with momentum density fields as the natural duals. Further independent variables are included through semidirect products if it is known how the group of space transformations acts on the vector space of further thermodynamic or structural variables. The coarse grained Poisson bracket, which automatically satisfies the Jacobi identity, can be obtained by finding the inherited transformation behavior of the coarse grained variables under space transformations.

Coarse graining usually changes the nature of the equations and hence the required set of boundary conditions. It is hence important to include the boundary conditions into the formulation of the GENERIC structure [26]. In the ideal case, the thermodynamic building blocks imply a set of boundary conditions that lead to uniquely solvable equations.

We have emphasized that the GENERIC structure should be preserved by all coarse graining and approximation procedures. This is crucial to keep a proper separation of reversible and irreversible terms with all their characteristic features. An issue of great practical importance is the preservation of the thermodynamic structure under time discretization, in the spirit of symplectic integrators for Hamiltonian systems [29]. A perturbative analysis inspired by the classical work of Moser [21] for Hamiltonian systems suggests that, for time-discrete systems, the Hamiltonian and the friction operator should be modified by terms of the order of the time step, whereas the Poisson bracket and the entropy should remain unchanged. However, there is a clear need to characterize the structure-preserving time-discrete schemes by a nonperturbative criterion in the spirit of canonical transformations for symplectic structures. In the absence of a variational principle [18] for dissipative dynamic systems, this is a serious challenge. Clearly, to avoid artificial irreversible effects due to time discretization, dissipative schemes should become canonical in the limit of vanishing friction operator.

Appendix. Ehrenfest-type coarse graining. Inspired by the ideas of Paul and Tatyana Ehrenfest, a microscopic motion with regularly repeated coarse graining has been constructed by matching Taylor series [7, 8]. In the present notation, the coarser variables are of the form $y = \int \Pi(x) f(x) \mathcal{D}x$, where the evolution of the probability density is governed by

$$\frac{df}{dt} = J(f) = \mathcal{K}f. \tag{A.1}$$

The notation indicates that the Fokker–Planck operator $\mathcal{K}$ is the adjoint of the operator $\mathcal{K}^+$ occurring in Kolmogorov's backward equation. In the Ehrenfest-type approach to coarse graining, the irreversible contribution to the time evolution of the variables is given by [7, 8]

$$\dot{y}_{\rm cg} = \tau \int \Pi \mathcal{K}(1 - \mathcal{P}^+)\mathcal{K} f^*_y \mathcal{D}x, \tag{A.2}$$

where the period of the coarse graining steps is taken as 2τ. The operator $\mathcal{P}^+$ is a projector to the quasi-equilibrium manifold of probability densities $f^*_y(x)$ obtained by maximizing the entropy $S(f)$ for given averages y of Π. For arbitrary functionals $A(x)$ and $B(x)$, the projection operator $\mathcal{P}^+$ is defined by

$$\mathcal{P}^+ A = \frac{\delta f^*_y}{\delta y} \cdot \int \Pi A \, \mathcal{D}x, \tag{A.3}$$

which is the adjoint of the operator with the definition

$$\mathcal{P} B = \Pi \cdot \int B \frac{\delta f^*_y}{\delta y} \, \mathcal{D}x. \tag{A.4}$$

Before we extract a friction operator from (A.2), we need to introduce a number of related second-order differential operators. So far, we have considered the Fokker–Planck operator

$$\mathcal{K} = -\frac{\delta}{\delta x} \cdot \left(L \cdot \frac{\delta E}{\delta x} + M \cdot \frac{\delta S}{\delta x} \right) + k_{\rm B} \frac{\delta}{\delta x} \cdot M \cdot \frac{\delta}{\delta x} \tag{A.5}$$

and its adjoint

$$\mathcal{K}^+ = \left(L \cdot \frac{\delta E}{\delta x} + M \cdot \frac{\delta S}{\delta x} \right) \cdot \frac{\delta}{\delta x} + k_{\rm B} \frac{\delta}{\delta x} \cdot M \cdot \frac{\delta}{\delta x}. \tag{A.6}$$

Whereas $\mathcal{K}^+$ characterizes the mean forward derivative associated with a stochastic differential equation [22], the mean backward derivative is described by the operator

$$\mathcal{K}^- = \left(L \cdot \frac{\delta E}{\delta x} + M \cdot \frac{\delta S}{\delta x} - 2k_{\rm B} M \cdot \frac{\delta \ln f}{\delta x} \right) \cdot \frac{\delta}{\delta x} - k_{\rm B} \frac{\delta}{\delta x} \cdot M \cdot \frac{\delta}{\delta x}. \tag{A.7}$$

Without any reference to stochastic differential equations, the definition of the operator $\mathcal{K}^-$ can be motivated by the following product or Leibniz rule:

$$\int AB\mathcal{K}f \, \mathcal{D}x = \int f \mathcal{K}^+(AB) \mathcal{D}x = \int f (A\mathcal{K}^+ B + B\mathcal{K}^- A) \mathcal{D}x. \tag{A.8}$$

A further second-order differential operator is associated with any factorization of the solution of the Fokker–Planck equation in the form $f = f_0 e^R$. One then has

$$\frac{1}{f}\mathcal{K}f = \frac{1}{f_0}\mathcal{K}f_0 - \tilde{\mathcal{K}}R, \tag{A.9}$$

with

$$\tilde{\mathcal{K}} = \mathcal{K}^- + 2k_\mathrm{B}\frac{\delta R}{\delta x} \cdot M \cdot \frac{\delta}{\delta x}. \tag{A.10}$$

We now consider the situation where the evolution of f_0 can be neglected, that is, $\mathcal{K}f_0 = 0$, and where the factorization arises from maximization of the entropy under constraints, that is,

$$R = -\frac{1}{k_\mathrm{B}}\Pi \cdot \frac{\delta S'}{\delta y} + \text{const.} \tag{A.11}$$

Equation (A.2) can then be rewritten as

$$\dot{y}_\mathrm{cg} = \frac{\tau}{k_\mathrm{B}} \int f_y^* \left[(1-\mathcal{P})\mathcal{K}^+\Pi\right] \left[(1-\mathcal{P})\tilde{\mathcal{K}}\Pi\right] \mathcal{D}x \cdot \frac{\delta S'}{\delta y}, \tag{A.12}$$

where we have used the identity $(1-\mathcal{P}^+)f_y^* = f_y^*(1-\mathcal{P})$. We thus identify a friction operator which is identical to the approximate expression (4.25), except that one of the factors $\mathcal{K}^\mathrm{f}\Pi$ is formed with $\tilde{\mathcal{K}}$ instead of $\mathcal{K}^+$. When fluctuation terms are neglected, as recommended here, then we have $\tilde{\mathcal{K}} = \mathcal{K}^+ = \mathcal{K}^- = \mathcal{K}_0$.

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