

11 Method of Natural Projector

P. and T. Ehrenfest introduced in 1911 a model of dynamics with a coarse-graining of the original conservative system in order to introduce irreversibility [15]. Ehrenfests considered a partition of the phase space into small cells, and they have suggested to combine the motions of the phase space ensemble due to the reversible dynamics with the coarse-graining (“shaking”) steps – averaging of the density of the ensemble over the phase cells. This generalizes to the following: alternations of the motion of the phase ensemble due to the microscopic equations with returns to the quasiequilibrium manifold while preserving the values of the macroscopic variables. We here develop a formalism of nonequilibrium thermodynamics based on this generalization. The Ehrenfests’ coarse-graining can be treated as a result of interaction of the system with a generalized thermostat. There are many ways for introduction of thermostat in computational statistical physics [283], but the Ehrenfests’ approach remains the basic for understanding the irreversibility phenomenon.

11.1 Ehrenfests’ Coarse-Graining Extended to a Formalism of Nonequilibrium Thermodynamics

The idea of the Ehrenfests is the following: One partitions the phase space of the Hamiltonian system into cells. The density distribution of the ensemble over the phase space evolves in time according to the Liouville equation within the time segments $n\tau < t < (n+1)\tau$, where τ is the fixed coarse-graining time step. Coarse-graining is executed at discrete times $n\tau$, densities are averaged over each cell. This alternation of the regular flow with the averaging describes the irreversible behavior of the system.

The most general construction extending the Ehrenfests’ idea is given below. Let us stay with notation of Chap. 3, and let a submanifold $F(W)$ be defined in the phase space U . Furthermore, we assume a map (a projection) is defined, $\Pi : U \rightarrow W$, with the properties:

$$\Pi \circ F = 1, \quad \Pi(F(y)) = y. \quad (11.1)$$

In addition, one requires some mild properties of regularity, in particular, surjectivity of the differential, $D_x \Pi : E \rightarrow L$, in each point $x \in U$.

Let us fix the coarse-graining time $\tau > 0$, and consider the following problem: Find a vector field Ψ in W ,

$$\frac{dy}{dt} = \Psi(y), \quad (11.2)$$

such that, for every $y \in W$,

$$\Pi(T_\tau F(y)) = \Theta_\tau y, \quad (11.3)$$

where T_τ is the shift operator for the system (3.1), and Θ_τ is the (yet unknown!) shift operator for the system in question (11.2).

Equation (11.3) means that one projects not the vector fields but segments of trajectories. The resulting vector field $\Psi(y)$ is called *the natural projection* of the vector field $J(x)$.

Let us assume that there is a very stiff hierarchy of relaxation times in the system (3.1): The motions of the system tend very rapidly to a slow manifold, and next proceed slowly along it. Then there is a smallness parameter, the ratio of these times. Let us take F for the initial condition to the film equation (4.5). If the solution F_t relaxes to the positively invariant manifold F_∞ , then in the limit of a very stiff decomposition of motions, the natural projection of the vector field $J(x)$ tends to the usual infinitesimal projection of the restriction of J on F_∞ , as $\tau \rightarrow \infty$:

$$\Psi_\infty(y) = D_x \Pi|_{x=F_\infty(y)} J(F_\infty(y)). \quad (11.4)$$

For stiff dynamic systems, the limit (11.4) is qualitatively almost obvious: After some relaxation time τ_0 (for $t > \tau_0$), the motion $T_\tau(x)$ is located in an ϵ -neighborhood of $F_\infty(W)$. Thus, for $\tau \gg \tau_0$, the natural projection Ψ (equations (11.2) and (11.3)) is defined by the vector field attached to F_∞ with any predefined accuracy. Rigorous proofs of (11.4) requires existence and uniqueness theorems, as well as uniform continuous dependence of solutions on the initial conditions and right hand sides of equations.

The method of natural projector is applied not only to dissipative systems but also (and even mostly) to conservative systems. One of the methods to study the natural projector is based on series expansion¹ in powers of τ . Various other approximation schemes like the Padé approximation are possible too.

The construction of the natural projector was rediscovered in a rather different context by Chorin, Hald and Kupferman [282]. They constructed the optimal prediction methods for an estimation of the solution of nonlinear time-dependent problems when that solution is too complex to be fully

¹ In the well-known work of Lewis [281], this expansion was executed incorrectly (terms of different orders were matched on the left and on the right hand sides of equation (11.3)). This created an obstacle in the development of the method. See a more detailed discussion in the example below.

resolved or when data are missing. The initial conditions for the unresolved components of the solution are drawn from a probability distribution, and their effect on a small set of variables that are actually computed is evaluated via statistical projection. The formalism resembles the projection methods of irreversible statistical mechanics, supplemented by the systematic use of conditional expectations and methods of solution for the fast dynamics equation, needed to evaluate a non-Markovian memory term. The authors claim [282] that result of the computations is close to the best possible estimate that can be obtained given the partial data.

The majority of the methods of invariant manifold can be discussed as development of the Chapman–Enskog method. The central idea is to construct the manifold of distribution functions, where the slow dynamics occurs. The (implicit) change-over from solving the Boltzmann equation to construction of invariant manifold was the crucial idea of Enskog and Chapman. On the other hand, the method of natural projector gives development to the ideas of the Hilbert method. The Hilbert method was historically the first in the solution of the Boltzmann equation. This method is not very popular nowadays, nevertheless, for some purposes it may be more convenient than the Chapman–Enskog method, for example, for a study of stationary solutions [284]. In the method of natural projector we are looking for solutions of kinetic equations with the quasiequilibrium initial state (and in the Hilbert method we start from the local equilibrium too). The main new element in the method of natural projector with respect to the Hilbert method is the construction of the macroscopic equation (11.3). In the next Example the solution for the matching condition (11.3) will be found in a form of Taylor series expansion.

11.2 Example: From Reversible Dynamics to Navier–Stokes and Post-Navier–Stokes Hydrodynamics by Natural Projector

The starting point of our construction are microscopic equations of motion. A traditional example of the microscopic description is the Liouville equation for classical particles. However, we need to stress that the distinction between “micro” and “macro” is always context dependent. For example, Vlasov’s equation describes the dynamics of the one-particle distribution function. In one statement of the problem, this is a microscopic dynamics in comparison to the evolution of hydrodynamic moments of the distribution function. In a different setting, this equation itself is a result of reducing the description from the microscopic Liouville equation.

The problem of reducing the description includes a definition of the microscopic dynamics, and of the macroscopic variables of interest, for which equations of the reduced description must be found. The next step is the construction of the initial approximation. This is the well known quasiequilibrium

approximation, which is the solution to the variational problem, $S \rightarrow \max$, where S is the entropy, under given constraints. This solution assumes that the microscopic distribution functions depend on time only through their dependence on the macroscopic variables. Direct substitution of the quasiequilibrium distribution function into the microscopic equation of motion gives the initial approximation to the macroscopic dynamics. All further corrections can be obtained from a more precise approximation of the microscopic as well as of the macroscopic trajectories within a given time interval τ which is the parameter of the method of natural projector.

The method described here has several clear advantages:

(i) It allows to derive complicated macroscopic equations, instead of writing them *ad hoc*. This fact is especially significant for the description of complex fluids. The method gives explicit expressions for relevant variables with one unknown parameter (τ). This parameter can be obtained from the experimental data.

(ii) Another advantage of the method is its simplicity. For example, in the case where the microscopic dynamics is given by the Boltzmann equation, the approach avoids evaluation of the Boltzmann collision integral.

(iii) The most significant advantage of this formalism is that it is applicable to nonlinear systems. Usually, in the classical approaches to reduced description, the microscopic equation of motion is linear. In that case, one can formally write the evolution operator in the exponential form. Obviously, this does not work for nonlinear systems, such as, for example, systems with mean field interactions. The method which we are presenting here is based on mapping the expanded microscopic trajectory into the consistently expanded macroscopic trajectory. This does not require linearity. Moreover, the order-by-order recurrent construction can be, in principle, enhanced by restoring to other types of approximations, like Padé approximation, for example, but we do not consider these options here.

In the present section we discuss in detail applications of the method of natural projector [29, 30, 34] to derivations of macroscopic equations, and demonstrate how computations are performed in the higher orders of the expansion. The structure of the Example is as follows: In the next subsection, we describe the formalization of Ehrenfest's approach [29, 30]. We stress the role of the quasiequilibrium approximation as the starting point for the constructions to follow. We derive explicit expressions for the correction to the quasiequilibrium dynamics, and conclude this section with the entropy production formula and its discussion. After that, we use the present formalism in order to derive hydrodynamic equations. Zeroth approximation of the scheme is the Euler equations of the compressible nonviscous fluid. The first approximation leads to the Navier–Stokes equations. Moreover, the approach allows to obtain the next correction, so-called post-Navier–Stokes equations. The latter example is of particular interest. Indeed, it is well known that the post-Navier–Stokes equations as derived from the Boltzmann kinetic equation

by the Chapman–Enskog method (the Burnett and the super-Burnett hydrodynamics) suffer from unphysical instability already in the linear approximation [72]. We demonstrate it by the explicit computation that the linearized higher-order hydrodynamic equations derived within the method of natural projector are free from this drawback.

11.2.1 General Construction

Let us consider a microscopic dynamics given by an equation,

$$\dot{f} = J(f), \quad (11.5)$$

where $f(x, t)$ is a distribution function over the phase space x at time t , and where operator $J(f)$ may be linear or nonlinear. We consider linear macroscopic variables $M_k = \mu_k(f)$, where operator μ_k maps f into M_k . The problem is to obtain closed macroscopic equations of motion, $\dot{M}_k = \phi_k(M)$. This is achieved in two steps: First, we construct an initial approximation to the macroscopic dynamics and, second, this approximation is further corrected on the basis of the coarse-gaining.

The initial approximation is the quasiequilibrium approximation, and it is based on the entropy maximum principle under fixed constraints (Chap. 5:

$$S(f) \rightarrow \max, \quad \mu(f) = M, \quad (11.6)$$

where S is the entropy functional, which is assumed to be strictly concave, and M is the set of the macroscopic variables $\{M_k\}$, and μ is the set of the corresponding operators. If the solution to the problem (11.6) exists, it is unique thanks to the concavity of the entropy functional. The solution to equation (11.6) is called the quasiequilibrium state, and it will be denoted as $f^*(M)$. The classical example is the local equilibrium of the ideal gas: f is the one-body distribution function, S is the Boltzmann entropy, μ are five linear operators, $\mu(f) = \int \{1, \mathbf{v}, v^2\} f d\mathbf{v}$, with \mathbf{v} the particle's velocity; the corresponding $f^*(M)$ is called the local Maxwell distribution function.

If the microscopic dynamics is given by equation (11.5), then the quasiequilibrium dynamics of the variables M reads:

$$\dot{M}_k = \mu_k(J(f^*(M))) = \phi_k^*. \quad (11.7)$$

The quasiequilibrium approximation has important property, it conserves the type of the dynamics: If the entropy monotonically increases (or not decreases) due to equation (11.5), then the same is true for the quasiequilibrium entropy, $S^*(M) = S(f^*(M))$, due to the quasiequilibrium dynamics (11.7). That is, if

$$\dot{S} = \frac{\partial S(f)}{\partial f} \dot{f} = \frac{\partial S(f)}{\partial f} J(f) \geq 0,$$

then

$$\dot{S}^* = \sum_k \frac{\partial S^*}{\partial M_k} \dot{M}_k = \sum_k \frac{\partial S^*}{\partial M_k} \mu_k(J(f^*(M))) \geq 0. \quad (11.8)$$

Summation in k always implies summation or integration over the set of labels of the macroscopic variables.

Conservation of the type of dynamics by the quasiequilibrium approximation is a simple yet a general and useful fact. If the entropy S is an integral of motion of equation (11.5) then $S^*(M)$ is the integral of motion for the quasiequilibrium equation (11.7). Consequently, if we start with a system which conserves the entropy (for example, with the Liouville equation) then we end up with the quasiequilibrium system which conserves the quasiequilibrium entropy. For instance, if M is the one-body distribution function, and (11.5) is the (reversible) Liouville equation, then (11.7) is the Vlasov equation which is reversible, too. On the other hand, if the entropy was monotonically increasing on the solutions of equation (11.5), then the quasiequilibrium entropy also increases monotonically on the solutions of the quasiequilibrium dynamic equations (11.7). For instance, if equation (11.5) is the Boltzmann equation for the one-body distribution function, and M is a finite set of moments (chosen in such a way that the solution to the problem (11.6) exists), then (11.7) are closed moment equations for M which increase the quasiequilibrium entropy (this is the essence of a well known generalization of Grad's moment method, Chap. 5).

11.2.2 Enhancement of Quasiequilibrium Approximations for Entropy-Conserving Dynamics

The goal of the present subsection is to describe the simplest analytic implementation, the microscopic motion with periodic coarse-graining. The notion of coarse-graining was introduced by P. and T. Ehrenfest in their seminal work [15]: The phase space is partitioned into cells, the coarse-grained variables are the amounts of the phase density inside the cells. Dynamics is described by the two processes, by the Liouville equation for f , and by periodic coarse-graining, replacement of $f(x)$ in each cell by its average value in this cell. The coarse-graining operation means forgetting the microscopic details, or of the history.

From the perspective of the general quasiequilibrium approximations, periodic coarse-graining amounts to the return of the true microscopic trajectory on the quasiequilibrium manifold with the preservation of the macroscopic variables. The motion starts at the quasiequilibrium state f_i^* . Then the true solution $f_i(t)$ of the microscopic equation (11.5) with the initial condition $f_i(0) = f_i^*$ is coarse-grained at a fixed time $t = \tau$, solution $f_i(\tau)$ is replaced by the quasiequilibrium function $f_{i+1}^* = f^*(\mu(f_i(\tau)))$. This process is sketched in Fig. 11.1.

From the features of the quasiequilibrium approximation it follows that for the motion with the periodic coarse-graining, the inequality is valid,

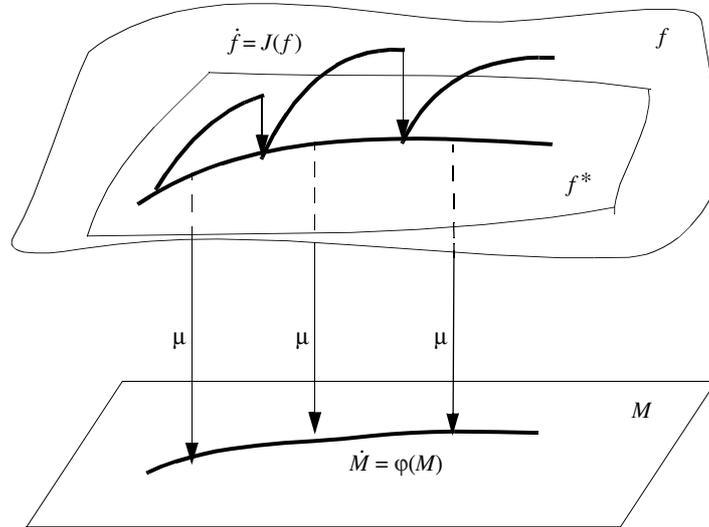


Fig. 11.1. Coarse-graining scheme. f is the space of microscopic variables, M is the space of the macroscopic variables, f^* is the quasiequilibrium manifold, μ is the mapping from the microscopic to the macroscopic space

$$S(f_i^*) \leq S(f_{i+1}^*) , \quad (11.9)$$

the equality occurs if and only if the quasiequilibrium is the invariant manifold of the dynamic system (11.5). Whenever the quasiequilibrium is *not* the solution to equation (11.5), the strict inequality in (11.9) demonstrates the entropy increase. Following Ehrenfests, the sequence of the quasiequilibrium states is called the *H-curve*.

In other words, let us assume that the trajectory begins at the quasiequilibrium manifold, then it takes off from this manifold according to the microscopic evolution equations. Then, after some time τ , the trajectory is coarse-grained, that is the, state is brought back on the quasiequilibrium manifold while keeping the current values of the macroscopic variables. The irreversibility is born in the latter process, and this construction clearly rules out quasiequilibrium manifolds which are invariant with respect to the microscopic dynamics, as candidates for a coarse-graining.

The coarse-graining indicates the way to derive equations for the macroscopic variables from the condition that the macroscopic trajectory, $M(t)$, which governs the motion of the quasiequilibrium states, $f^*(M(t))$, should match precisely the same points on the quasiequilibrium manifold, $f^*(M(t + \tau))$, and this matching should be independent of both the initial time, t , and the initial condition, $M(t)$. The problem is then how to derive the continuous time macroscopic dynamics which would be consistent with this picture. The simplest realization suggested in [29, 30] is based on matching

an expansion of both the microscopic and the macroscopic trajectories. Here we present this construction to the third order accuracy [29, 30].

Let us write down the solution to the microscopic equation (11.5), and approximate this solution by the polynomial of the third order in τ . Introducing notation, $J^* = J(f^*(M(t)))$, we write,

$$f(t + \tau) = f^* + \tau J^* + \frac{\tau^2}{2} \frac{\partial J^*}{\partial f} J^* + \frac{\tau^3}{3!} \left(\frac{\partial J^*}{\partial f} \frac{\partial J^*}{\partial f} J^* + \frac{\partial^2 J^*}{\partial f^2} J^* J^* \right) + o(\tau^3). \quad (11.10)$$

Evaluation of the macroscopic variables on the function (11.10) gives

$$\begin{aligned} M_k(t + \tau) &= M_k + \tau \phi_k^* + \frac{\tau^2}{2} \mu_k \left(\frac{\partial J^*}{\partial f} J^* \right) \\ &+ \frac{\tau^3}{3!} \left\{ \mu_k \left(\frac{\partial J^*}{\partial f} \frac{\partial J^*}{\partial f} J^* \right) + \mu_k \left(\frac{\partial^2 J^*}{\partial f^2} J^* J^* \right) \right\} + o(\tau^3), \end{aligned} \quad (11.11)$$

where $\phi_k^* = \mu_k(J^*)$ is the quasiequilibrium macroscopic vector field (the right hand side of equation (11.7)), and all the functions and derivatives are taken in the quasiequilibrium state at time t .

We shall now establish the macroscopic dynamic by matching the macroscopic and the microscopic dynamics. Specifically, the macroscopic dynamic equations (11.7) with the right-hand side not yet defined, give the following third-order result:

$$\begin{aligned} M_k(t + \tau) &= M_k + \tau \phi_k + \frac{\tau^2}{2} \sum_j \frac{\partial \phi_k}{\partial M_j} \phi_j \\ &+ \frac{\tau^3}{3!} \sum_{ij} \left(\frac{\partial^2 \phi_k}{\partial M_i \partial M_j} \phi_i \phi_j + \frac{\partial \phi_k}{\partial M_i} \frac{\partial \phi_i}{\partial M_j} \phi_j \right) + o(\tau^3). \end{aligned} \quad (11.12)$$

Expanding functions ϕ_k into a series

$$\phi_k = R_k^{(0)} + \tau R_k^{(1)} + \tau^2 R_k^{(2)} + \dots \quad (R_k^{(0)} = \phi_k^*),$$

and requiring that the microscopic and the macroscopic dynamics coincide to the order of τ^3 , we obtain the sequence of approximations to the right-hand side of the equation for the macroscopic variables. Zeroth order is the quasiequilibrium approximation to the macroscopic dynamics. The first-order correction gives:

$$R_k^{(1)} = \frac{1}{2} \left\{ \mu_k \left(\frac{\partial J^*}{\partial f} J^* \right) - \sum_j \frac{\partial \phi_k^*}{\partial M_j} \phi_j^* \right\}. \quad (11.13)$$

The next, second-order correction has the following explicit form:

$$\begin{aligned}
 R_k^{(2)} = & \frac{1}{3!} \left\{ \mu_k \left(\frac{\partial J^*}{\partial f} \frac{\partial J^*}{\partial f} J^* \right) + \mu_k \left(\frac{\partial^2 J^*}{\partial f^2} J^* J^* \right) \right\} - \frac{1}{3!} \sum_{ij} \left(\frac{\partial \phi_k^*}{\partial M_i} \frac{\partial \phi_i^*}{\partial M_j} \phi_j^* \right) \\
 & - \frac{1}{3!} \sum_{ij} \left(\frac{\partial^2 \phi_k^*}{\partial M_i \partial M_j} \phi_i^* \phi_j^* \right) - \frac{1}{2} \sum_j \left(\frac{\partial \phi_k^*}{\partial M_j} R_j^{(1)} + \frac{\partial R_j^{(1)}}{\partial M_j} \phi_j^* \right). \quad (11.14)
 \end{aligned}$$

Further corrections are found by the same token. Equations (11.13)–(11.14) give explicit closed expressions for corrections to the quasiequilibrium dynamics to the order of accuracy specified above.

11.2.3 Entropy Production

The most important consequence of the above construction is that the resulting continuous time macroscopic equations retain the dissipation property of the discrete time coarse-graining (11.9) on each order of approximation $n \geq 1$. Let us first consider the entropy production formula for the first-order approximation. In order to shorten notations, it is convenient to introduce the quasiequilibrium projection operator,

$$P^* g = \sum_k \frac{\partial f^*}{\partial M_k} \mu_k(g). \quad (11.15)$$

It has been demonstrated in [30] that the entropy production,

$$\dot{S}_{(1)}^* = \sum_k \frac{\partial S^*}{\partial M_k} (R_k^{(0)} + \tau R_k^{(1)}),$$

equals

$$\dot{S}_{(1)}^* = -\frac{\tau}{2} (1 - P^*) J^* \left. \frac{\partial^2 S^*}{\partial f \partial f} \right|_{f^*} (1 - P^*) J^*. \quad (11.16)$$

Expression (11.16) is nonnegative definite due to concavity of the entropy. The entropy production (11.16) is equal to zero only if the quasiequilibrium approximation is the true solution to the microscopic dynamics, that is, if $(1 - P^*) J^* \equiv 0$. While quasiequilibrium approximations which solve the Liouville equation are uninteresting objects (except, of course, for the equilibrium itself), vanishing of the entropy production in this case is a simple test of consistency of the theory. Note that the entropy production (11.16) is proportional to τ . Note also that the projection operator does not appear in our consideration a priori, rather, it is the result of exploring the coarse-graining condition in the previous subsection.

Though equation (11.16) looks very natural, its existence is rather subtle. Indeed, equation (11.16) is a difference of the two terms, $\sum_k \mu_k (J^* \partial J^* / \partial f)$

(contribution of the second-order approximation to the microscopic trajectory), and $\sum_{ik} R_i^{(0)} \partial R_k^{(0)} / \partial M_i$ (contribution of the derivative of the quasi-equilibrium vector field). Each of these expressions separately gives a positive contribution to the entropy production, and equation (11.16) is the difference of the two positive definite expressions. In the higher order approximations, these subtractions are more involved, and explicit demonstration of the entropy production formulae becomes a formidable task. Yet, it is possible to demonstrate the increase-in-entropy without explicit computation, though at a price of smallness of τ . Indeed, let us denote $\dot{S}_{(n)}^*$ the time derivative of the entropy on the n th order approximation. Then

$$\int_t^{t+\tau} \dot{S}_{(n)}^*(s) ds = S^*(t+\tau) - S^*(t) + O(\tau^{n+1}),$$

where $S^*(t+\tau)$ and $S^*(t)$ are true values of the entropy at the adjacent states of the H -curve. The difference $\delta S = S^*(t+\tau) - S^*(t)$ is strictly positive for any fixed τ , and, by equation (11.16), $\delta S \sim \tau^2$ for small τ . Therefore, if τ is small enough, the right hand side in the above expression is positive, and

$$\tau \dot{S}_{(n)}^*(\theta_{(n)}) > 0,$$

where $t \leq \theta_{(n)} \leq t + \tau$. Finally, since $\dot{S}_{(n)}^*(t) = \dot{S}_{(n)}^*(s) + O(\tau^n)$ for any s on the segment $[t, t + \tau]$, we can replace $\dot{S}_{(n)}^*(\theta_{(n)})$ in the latter inequality by $\dot{S}_{(n)}^*(t)$. The sense of this consideration is as follows: Since the entropy production formula (11.16) is valid in the leading order of the construction, the entropy production will not collapse in the higher orders at least if the coarse-graining time is small enough. More refined estimations can be obtained only from the explicit analysis of the higher-order corrections.

11.2.4 Relation to the Work of Lewis

Among various realizations of the coarse-graining procedures, the work of Lewis [281] appears to be most close to our approach. It is therefore pertinent to discuss the differences. Both methods are based on the coarse-graining condition,

$$M_k(t + \tau) = \mu_k(T_\tau f^*(M(t))), \quad (11.17)$$

where T_τ is the formal solution operator of the microscopic dynamics. Above, we applied a consistent expansion of both, the left hand side and the right hand side of the coarse-graining condition (11.17), in terms of the coarse-graining time τ . In the work of Lewis [281], it was suggested, as a general way to exploring the condition (11.17), to write the first-order equation for M in the form of the differential pursuit,

$$M_k(t) + \tau \frac{dM_k(t)}{dt} \approx \mu_k(T_\tau f^*(M(t))). \quad (11.18)$$

In other words, in the work of Lewis [281], the expansion to the first order was considered on the left (macroscopic) side of equation (11.17), whereas the right hand side containing the microscopic trajectory $T_\tau f^*(M(t))$ was not treated on the same footing. Clearly, expansion of the right hand side to first order in τ is the only equation which is common in both approaches, and this is the quasiequilibrium dynamics. However, the difference occurs already in the next, second-order term (see [29,30] for details). Namely, the expansion to the second order of the right hand side of Lewis' equation (11.18) results in a dissipative equation (in the case of the Liouville equation, for example) which remains dissipative even if the quasiequilibrium approximation is the exact solution to the microscopic dynamics, that is, when microscopic trajectories once started on the quasiequilibrium manifold belong to it in all the later times, and thus no dissipation can be born by any coarse-graining.

On the other hand, our approach assumes a certain smoothness of trajectories so that the application of the low-order expansion bears physical significance. For example, while using lower-order truncations it is not possible to derive the Boltzmann equation because in that case the relevant quasiequilibrium manifold (N -body distribution function is proportional to the product of one-body distributions, or uncorrelated states) is almost invariant during the long time (of the order of the mean free flight of particles), while the trajectory steeply leaves this manifold during the short-time pair collision. It is clear that in such a case lower-order expansions of the microscopic trajectory do not lead to useful results. It has been clearly stated by Lewis [281], that the exploration of the condition (11.17) depends on the physical situation, and how one makes approximations. In fact, derivation of the Boltzmann equation given by Lewis on the basis of the condition (11.17) does not follow the differential pursuit approximation: As is well known, the expansion in terms of particle's density of the solution to the BBGKY hierarchy is singular, and begins with the *linear* in time term. Assuming the quasiequilibrium approximation for the N -body distribution function under fixed one-body distribution function, and that collisions are well localized in space and time, one gets on the right hand side of equation (11.17),

$$f(t + \tau) = f(t) + n\tau J_B(f(t)) + o(n) ,$$

where n is particle's density, f is the one-particle distribution function, and J_B is the Boltzmann's collision integral. Next, using the mean-value theorem on the left hand side of the equation (11.17), the Boltzmann equation is derived (see also a recent elegant renormalization-group argument for this derivation [55]).

Our approach of matched expansions for exploring the coarse-graining condition (11.17) is, in fact, the exact (formal) statement that the unknown macroscopic dynamics which causes the shift of M_k on the left hand side of equation (11.17) can be reconstructed order-by-order to any degree of accuracy, whereas the low-order truncations may be useful for certain physical

situations. A thorough study of the cases beyond the lower-order truncations is of great importance which is left for Chap. 12.

11.2.5 Equations of Hydrodynamics

The method discussed above enables one to establish in a simple way the form of equations of the macroscopic dynamics to various degrees of approximation.

In this subsection, the microscopic dynamics is given by the simplest one-particle Liouville equation (the equation of free flight). For the macroscopic variables we take the density, average velocity, and temperature (average kinetic energy) of the fluid. Under this condition the solution to the quasi-equilibrium problem (11.6) is the local Maxwell distribution. For the hydrodynamic equations, the zeroth (quasiequilibrium) approximation is given by Euler's equations of compressible nonviscous fluid. The next order approximation are the Navier–Stokes equations which have dissipative terms.

Higher-order approximations to the hydrodynamic equations, when they are derived from the Boltzmann kinetic equation (the so-called Burnett approximation), are subject to various difficulties, in particular, they exhibit an instability of acoustic waves at sufficiently short wave length (see, e.g. [42] for a recent review). Here we demonstrate how model hydrodynamic equations, including the post-Navier–Stokes approximations, can be derived on the basis of the coarse-graining idea, and study the linear stability of the obtained equations. We found that the resulting equations are stable.

Two points need a clarification before we proceed further [30]. First, below we consider the simplest Liouville equation for the one-particle distribution, describing freely moving particles without interactions. The procedure of coarse-graining we use is an implementation of collisions leading to dissipation. If we had used the full interacting N -particle Liouville equation, the result would be different, in the first place, in the expression for the local equilibrium pressure. Whereas in the present case we have the ideal gas pressure, in the N -particle case the non-ideal gas pressure would arise.

Second, and more essential is that, to the order of the Navier–Stokes equations, the *result* of our method is identical to the lowest-order Chapman–Enskog method as applied to the Boltzmann equation with a single relaxation time model collision integral (the Bhatnagar–Gross–Krook model [116]). However, this happens only at this particular order of approximation, because already the next, post-Navier–Stokes approximation, is different from the Burnett hydrodynamics as derived from the BGK model (the latter is unstable).

11.2.6 Derivation of the Navier–Stokes Equations

Let us assume that reversible microscopic dynamics is given by the one-particle Liouville equation,

$$\frac{\partial f}{\partial t} = -v_i \frac{\partial f}{\partial r_i}, \quad (11.19)$$

where $f = f(\mathbf{r}, \mathbf{v}, t)$ is the one-particle distribution function, and index i runs over spatial components $\{x, y, z\}$. Subject to appropriate boundary conditions which we assume, this equation conserves the Boltzmann entropy $S = -k_B \int f \ln f \, d\mathbf{v} \, d\mathbf{r}$.

We introduce the following hydrodynamic moments as the macroscopic variables: $M_0 = \int f \, d\mathbf{v}$, $M_i = \int v_i f \, d\mathbf{v}$, $M_4 = \int v^2 f \, d\mathbf{v}$. These variables are related to the more conventional density, average velocity and temperature, n , \mathbf{u} , T as follows:

$$\begin{aligned} M_0 &= n, & M_i &= nu_i, & M_4 &= \frac{3nk_B T}{m} + nu^2, \\ n &= M_0, & u_i &= M_0^{-1} M_i, & T &= \frac{m}{3k_B M_0} (M_4 - M_0^{-1} M_i M_i). \end{aligned} \quad (11.20)$$

The quasiequilibrium distribution function (local Maxwellian) reads:

$$f_0 = n \left(\frac{m}{2\pi k_B T} \right)^{3/2} \exp \left(\frac{-m(v - u)^2}{2k_B T} \right). \quad (11.21)$$

Here and below, n , \mathbf{u} , and T depend on \mathbf{r} and t .

Based on the microscopic dynamics (11.19), the set of macroscopic variables (11.20), and the quasiequilibrium (11.21), we can derive the equations of the macroscopic motion.

A specific feature of the present example is that the quasiequilibrium equation for the density (the continuity equation),

$$\frac{\partial n}{\partial t} = -\frac{\partial nu_i}{\partial r_i}, \quad (11.22)$$

should be excluded out of the further corrections. This rule should be applied generally: If a part of the chosen macroscopic variables (momentum flux nu here) correspond to fluxes of other macroscopic variables, then the quasiequilibrium equation for the latter is already exact, and has to be exempted of corrections.

The quasiequilibrium approximation for the rest of the macroscopic variables is derived in the usual way. In order to derive the equation for the velocity, we substitute the local Maxwellian into the one-particle Liouville equation, and act with the operator $\mu_k = \int v_k \cdot d\mathbf{v}$ on both the sides of the equation (11.19). We have:

$$\frac{\partial nu_k}{\partial t} = -\frac{\partial}{\partial r_k} \frac{nk_B T}{m} - \frac{\partial nu_k u_j}{\partial r_j}.$$

Similarly, we derive the equation for the energy density, and the complete system of equations of the quasiequilibrium approximation reads (compressible Euler equations):

$$\begin{aligned}
\frac{\partial n}{\partial t} &= -\frac{\partial nu_i}{\partial r_i}, \\
\frac{\partial nu_k}{\partial t} &= -\frac{\partial}{\partial r_k} \frac{nk_B T}{m} - \frac{\partial nu_k u_j}{\partial r_j}, \\
\frac{\partial \varepsilon}{\partial t} &= -\frac{\partial}{\partial r_i} \left(\frac{5k_B T}{m} nu_i + u^2 nu_i \right).
\end{aligned} \tag{11.23}$$

where $varepsilon = \frac{3}{2}nk_B T$ is the energy density.

Now we are going to derive the next order approximation to the macroscopic dynamics (first order in the coarse-graining time τ). For the velocity equation we have:

$$R_{nu_k} = \frac{1}{2} \left(\int v_k v_i v_j \frac{\partial^2 f_0}{\partial r_i \partial r_j} d\mathbf{v} - \sum_j \frac{\partial \phi_{nu_k}}{\partial M_j} \phi_j \right),$$

where ϕ_j are the corresponding right hand sides of the Euler equations (11.23). In order to take derivatives with respect to macroscopic moments $\{M_0, M_i, M_4\}$, we need to rewrite equations (11.23) in terms of these variables instead of $\{n, u_i, T\}$. After some computation, we obtain:

$$R_{nu_k} = \frac{1}{2} \frac{\partial}{\partial r_j} \left(\frac{nk_B T}{m} \left[\frac{\partial u_k}{\partial r_j} + \frac{\partial u_j}{\partial r_k} - \frac{2}{3} \frac{\partial u_n}{\partial r_n} \delta_{kj} \right] \right). \tag{11.24}$$

For the energy we obtain:

$$\begin{aligned}
R_\varepsilon &= \frac{1}{2} \left(\int v^2 v_i v_j \frac{\partial^2 f_0}{\partial r_i \partial r_j} d\mathbf{v} - \sum_j \frac{\partial \phi_\varepsilon}{\partial M_j} \phi_j \right) \\
&= \frac{5}{2} \frac{\partial}{\partial r_i} \left(\frac{nk_B^2 T}{m^2} \frac{\partial T}{\partial r_i} \right).
\end{aligned} \tag{11.25}$$

Thus, we get the system of the Navier–Stokes equations in the following form:

$$\begin{aligned}
\frac{\partial n}{\partial t} &= -\frac{\partial nu_i}{\partial r_i}, \\
\frac{\partial nu_k}{\partial t} &= -\frac{\partial}{\partial r_k} \frac{nk_B T}{m} - \frac{\partial nu_k u_j}{\partial r_j} \\
&\quad + \frac{\tau}{2} \frac{\partial}{\partial r_j} \frac{nk_B T}{m} \left(\frac{\partial u_k}{\partial r_j} + \frac{\partial u_j}{\partial r_k} - \frac{2}{3} \frac{\partial u_n}{\partial r_n} \delta_{kj} \right), \\
\frac{\partial \varepsilon}{\partial t} &= -\frac{\partial}{\partial r_i} \left(\frac{5k_B T}{m} nu_i + u^2 nu_i \right) + \tau \frac{5}{2} \frac{\partial}{\partial r_i} \left(\frac{nk_B^2 T}{m^2} \frac{\partial T}{\partial r_i} \right).
\end{aligned} \tag{11.26}$$

We see that the kinetic coefficients (viscosity and heat conductivity) are proportional to the coarse-graining time τ . Note that they are identical with kinetic coefficients as derived from the Bhatnagar–Gross–Krook model [116] in the first approximation of the Chapman–Enskog method [70].

11.2.7 Post-Navier–Stokes Equations

Now we are going to obtain the second-order approximation to the hydrodynamic equations in the framework of the present approach. We shall compare qualitatively the result with the Burnett approximation. The comparison concerns stability of the hydrodynamic modes near the global equilibrium. Stability of the global equilibrium is violated in the Burnett approximation. Though the derivation is straightforward also in the general, nonlinear case, we shall consider only the linearized equations which is appropriate to our purpose here.

Linearizing the local Maxwell distribution function, we obtain:

$$\begin{aligned} f &= n_0 \left(\frac{m}{2\pi k_B T_0} \right)^{3/2} \left(\frac{n}{n_0} + \frac{mv_n}{k_B T_0} u_n + \left(\frac{mv^2}{2k_B T_0} - \frac{3}{2} \right) \frac{T}{T_0} \right) e^{-\frac{mv^2}{2k_B T_0}} \\ &= \left\{ (M_0 + 2M_i c_i + \left(\frac{2}{3} M_4 - M_0 \right) \left(c^2 - \frac{3}{2} \right)) \right\} e^{-c^2}, \end{aligned} \quad (11.27)$$

where we have introduced dimensionless variables:

$$c_i = \frac{v_i}{v_T}, \quad M_0 = \frac{\delta n}{n_0}, \quad M_i = \frac{\delta u_i}{v_T}, \quad M_4 = \frac{3}{2} \frac{\delta n}{n_0} + \frac{\delta T}{T_0},$$

$v_T = \sqrt{2k_B T_0/m}$ is the thermal velocity, Note that δn , and δT determine deviations of these variables from their equilibrium values, n_0 , and T_0 .

The linearized Navier–Stokes equations read:

$$\begin{aligned} \frac{\partial M_0}{\partial t} &= -\frac{\partial M_i}{\partial r_i}, \\ \frac{\partial M_k}{\partial t} &= -\frac{1}{3} \frac{\partial M_4}{\partial r_k} + \frac{\tau}{4} \frac{\partial}{\partial r_j} \left(\frac{\partial M_k}{\partial r_j} + \frac{\partial M_j}{\partial r_k} - \frac{2}{3} \frac{\partial M_n}{\partial r_n} \delta_{kj} \right), \\ \frac{\partial M_4}{\partial t} &= -\frac{5}{2} \frac{\partial M_i}{\partial r_i} + \tau \frac{5}{2} \frac{\partial^2 M_4}{\partial r_i \partial r_i}. \end{aligned} \quad (11.28)$$

Let us first compute the post-Navier–Stokes correction to the velocity equation. In accordance with the equation (11.14), the first part of this term in the linear approximation is:

$$\begin{aligned} &\frac{1}{3!} \mu_k \left(\frac{\partial J^*}{\partial f} \frac{\partial J^*}{\partial f} J^* \right) - \frac{1}{3!} \sum_{ij} \left(\frac{\partial \phi_k^*}{\partial M_i} \frac{\partial \phi_i^*}{\partial M_j} \phi_j^* \right) = -\frac{1}{6} \int c_k \frac{\partial^3}{\partial r_i \partial r_j \partial r_n} c_i c_j c_n \\ &\times \left\{ (M_0 + 2M_i c_i + \left(\frac{2}{3} M_4 - M_0 \right) \left(c^2 - \frac{3}{2} \right)) \right\} e^{-c^2} d^3 c \\ &+ \frac{5}{108} \frac{\partial}{\partial r_i} \frac{\partial}{\partial r_s} \frac{\partial^2 M_4}{\partial r_s \partial r_s} = \frac{1}{6} \frac{\partial}{\partial r_k} \left(\frac{3}{4} \frac{\partial^2 M_0}{\partial r_s \partial r_s} - \frac{\partial^2 M_4}{\partial r_s \partial r_s} \right) + \frac{5}{108} \frac{\partial}{\partial r_k} \frac{\partial}{\partial r_s} \frac{\partial^2 M_4}{\partial r_s \partial r_s} \\ &= \frac{1}{8} \frac{\partial}{\partial r_k} \frac{\partial^2 M_0}{\partial r_s \partial r_s} - \frac{13}{108} \frac{\partial}{\partial r_k} \frac{\partial^2 M_4}{\partial r_s \partial r_s}. \end{aligned} \quad (11.29)$$

The part of equation (11.14) proportional to the first-order correction is:

$$-\frac{1}{2} \sum_j \left(\frac{\partial \phi_k^*}{\partial M_j} R_j^{(1)} + \frac{\partial R_k^{(1)}}{\partial M_j} \phi_j^* \right) = \frac{5}{6} \frac{\partial}{\partial r_k} \frac{\partial^2 M_4}{\partial r_s \partial r_s} + \frac{1}{9} \frac{\partial}{\partial r_k} \frac{\partial^2 M_4}{\partial r_s \partial r_s}. \quad (11.30)$$

Combining together terms (11.29), and (11.30), we obtain:

$$R_{M_k}^{(2)} = \frac{1}{8} \frac{\partial}{\partial r_k} \frac{\partial^2 M_0}{\partial r_s \partial r_s} + \frac{89}{108} \frac{\partial}{\partial r_k} \frac{\partial^2 M_4}{\partial r_s \partial r_s}.$$

Similar calculation for the energy equation leads to the following result:

$$\int c^2 \frac{\partial^3}{\partial r_i \partial r_j \partial r_k} c_i c_j c_k \left\{ (M_0 + 2M_i c_i + \left(\frac{2}{3}M_4 - M_0\right) \left(c^2 - \frac{3}{2}\right) \right\} e^{-c^2} d^3 c \\ - \frac{25}{72} \frac{\partial}{\partial r_i} \frac{\partial^2 M_i}{\partial r_s \partial r_s} = \frac{1}{6} \left(\frac{21}{4} \frac{\partial}{\partial r_i} \frac{\partial^2 M_i}{\partial r_s \partial r_s} + \frac{25}{12} \frac{\partial}{\partial r_i} \frac{\partial^2 M_i}{\partial r_s \partial r_s} \right) = \frac{19}{36} \frac{\partial}{\partial r_i} \frac{\partial^2 M_i}{\partial r_s \partial r_s}.$$

The term proportional to the first-order corrections gives:

$$\frac{5}{6} \left(\frac{\partial^2}{\partial r_s \partial r_s} \frac{\partial M_i}{\partial r_i} \right) + \frac{25}{4} \left(\frac{\partial^2}{\partial r_s \partial r_s} \frac{\partial M_i}{\partial r_i} \right).$$

Thus, we obtain:

$$R_{M_4}^{(2)} = \frac{59}{9} \left(\frac{\partial^2}{\partial r_s \partial r_s} \frac{\partial M_i}{\partial r_i} \right). \quad (11.31)$$

Finally, combining together all the terms, we obtain the following system of linearized hydrodynamic equations:

$$\begin{aligned} \frac{\partial M_0}{\partial t} &= -\frac{\partial M_i}{\partial r_i}, \\ \frac{\partial M_k}{\partial t} &= -\frac{1}{3} \frac{\partial M_4}{\partial r_k} + \frac{\tau}{4} \frac{\partial}{\partial r_j} \left(\frac{\partial M_k}{\partial r_j} + \frac{\partial M_j}{\partial r_k} - \frac{2}{3} \frac{\partial M_n}{\partial r_n} \delta_{kj} \right) + \\ &\quad \tau^2 \left\{ \frac{1}{8} \frac{\partial}{\partial r_k} \frac{\partial^2 M_0}{\partial r_s \partial r_s} + \frac{89}{108} \frac{\partial}{\partial r_k} \frac{\partial^2 M_4}{\partial r_s \partial r_s} \right\}, \\ \frac{\partial M_4}{\partial t} &= -\frac{5}{2} \frac{\partial M_i}{\partial r_i} + \tau \frac{5}{2} \frac{\partial^2 M_4}{\partial r_i \partial r_i} + \tau^2 \frac{59}{9} \left(\frac{\partial^2}{\partial r_s \partial r_s} \frac{\partial M_i}{\partial r_i} \right). \end{aligned} \quad (11.32)$$

Now we are in a position to investigate the dispersion relation of this system. Substituting $M_i = \tilde{M}_i \exp(\omega t + i(\mathbf{k}, \mathbf{r}))$ ($i = 0, k, 4$) into equation (11.32), we reduce the problem to finding the spectrum of the matrix:

$$\begin{pmatrix} 0 & -ik_x & -ik_y \\ -ik_x \frac{k^2}{8} & -\frac{1}{4}k^2 - \frac{1}{12}k_x^2 & -\frac{k_x k_y}{12} \\ -ik_y \frac{k^2}{8} & -\frac{k_x k_y}{12} & -\frac{1}{4}k^2 - \frac{1}{12}k_y^2 \\ -ik_z \frac{k^2}{8} & -\frac{k_x k_z}{12} & -\frac{k_y k_z}{12} \\ 0 & -ik_x \left(\frac{5}{2} + \frac{59k^2}{9} \right) & -ik_y \left(\frac{5}{2} + \frac{59k^2}{9} \right) \end{pmatrix}$$

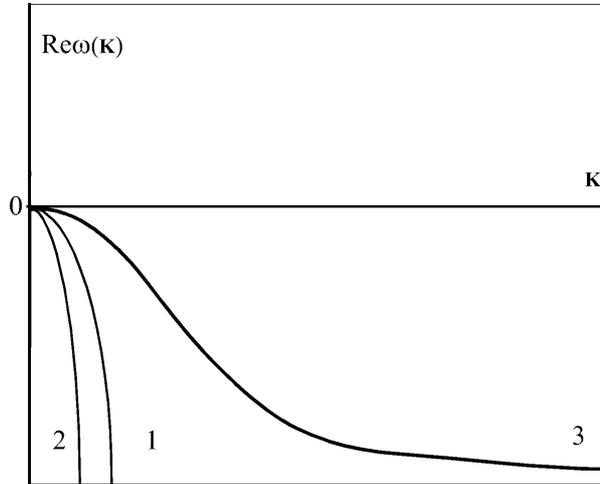


Fig. 11.2. Attenuation rates of various modes of the post-Navier–Stokes equations as functions of the wave vector. Attenuation rate of the twice degenerated shear mode is curve 1. Attenuation rate of the two sound modes is curve 2. Attenuation rate of the diffusion mode is curve 3

$$\begin{pmatrix} -ik_z & 0 \\ -\frac{k_x k_z}{12} & -ik_x \left(\frac{1}{3} + \frac{89k^2}{108} \right) \\ -\frac{k_y k_z}{12} & -ik_y \left(\frac{1}{3} + \frac{89k^2}{108} \right) \\ -\frac{1}{4}k^2 - \frac{1}{12}k_z^2 & -ik_z \left(\frac{1}{3} + \frac{89k^2}{108} \right) \\ -ik_z \left(\frac{5}{2} + \frac{59k^2}{9} \right) & -\frac{5}{2}k^2 \end{pmatrix}$$

This matrix has five eigenvalues. The real parts of these eigenvalues responsible for the decay rate of the corresponding modes are shown in Fig.11.2 as functions of the wave vector k . We see that *all real parts of all the eigenvalues are non-positive for any wave vector*. In other words, this means that the present system is linearly stable. For the Burnett hydrodynamics as derived from the Boltzmann or from the single relaxation time Bhatnagar–Gross–Krook model, it is well known that the decay rate of the acoustic branch becomes positive after some value of the wave vector [42, 72], which leads to the instability. While the method suggested here is clearly semi-phenomenological (coarse-graining time τ remains unspecified), the consistency of the expansion with the entropy requirements, and especially the latter result of the linear stable limit of the post-Navier–Stokes correction strongly indicates that it might be more suited to establishing models of highly nonequilibrium hydrodynamics.

11.3 Example: Natural Projector for the Mc Kean Model

In this section the fluctuation–dissipation formula derived by the method of natural projector [31] is illustrated by the explicit computation for McKean’s kinetic model [285]. 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 solution of the invariance equation. The equality between all the three results holds up to the crossover from the hydrodynamic to the kinetic domain.

11.3.1 General Scheme

Let us consider a microscopic dynamics (3.1) given by an equation for the distribution function $f(x, t)$ over a configuration space x :

$$\partial_t f = J(f) , \quad (11.33)$$

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,

$$\mathbf{m}(f(\mathbf{M})) = \mathbf{M} . \quad (11.34)$$

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 the condition (11.34) only.

Given a finite time interval τ , it is possible to reconstruct uniquely the macroscopic dynamics from a single condition of the coarse-graining. 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 equation (11.33) at the time t . Then the condition for the reconstruction of the macroscopic dynamics reads as follows: For every initial condition $\{\mathbf{M}(t), t\}$, solution to the macroscopic dynamic equations at the time $t + \tau$ is equal to the value of the macroscopic variables on the solution to equation (11.33) with the initial condition $\{f(\mathbf{M}(t), x), t\}$:

$$\mathbf{M}(t + \tau) = \mathbf{m}(T_\tau f(\mathbf{M}(t))) , \quad (11.35)$$

where T_τ is the formal solution operator of the microscopic equation (11.33). The right hand side of equation (11.35) represents an operation on trajectories of the microscopic equation (11.33), introduced in a particular form by Ehrenfest’s [15] (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 equation (11.35) 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 [29,30]: Seeking the macroscopic equations in the form,

$$\partial_t \mathbf{M} = \mathbf{R}(\mathbf{M}, \tau), \quad (11.36)$$

we proceed with the Taylor expansion of the unknown functions \mathbf{R} in terms of powers τ^n , where $n = 0, 1, \dots$, and require that each approximation, $\mathbf{R}^{(n)}$, of the order n , is such that the resulting macroscopic solutions satisfy the condition (11.36) to the order τ^{n+1} . This process of successive approximation is solvable. Thus, the unknown macroscopic equation (11.36) can be reconstructed to any given accuracy.

Coming back to the problem of choosing the distribution function $f(\mathbf{M}, x)$, we recall that many physically relevant cases of the microscopic dynamics (11.33) are characterized by existence of a concave functional $S(f)$ (the entropy functional; discussions of S can be found in [115,191,192]). Traditionally, two cases are distinguished, the conservative [$dS/dt \equiv 0$ due to equation (11.33)], and the dissipative [$dS/dt \geq 0$ due to equation (11.33), where equality sign corresponds to the stationary solution]. The approach (11.35) and (11.36) is applicable to both these 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 quasiequilibrium approximations, $f^*(\mathbf{M}, x)$, which are maximizers of the functional $S(f)$ for fixed \mathbf{M} . We recall that, due to convexity of the functional S , if such maximizer exists then it is unique.

The special role of the quasiequilibrium approximations is due to the fact that they preserve the type of dynamics (Chap. 5): If $dS/dt \geq 0$ due to equation (11.33), then $dS^*/dt \geq 0$ due to the quasiequilibrium dynamics, where $S^*(\mathbf{M}) = S(f^*(\mathbf{M}))$ is the quasiequilibrium entropy, and where the quasiequilibrium dynamics coincides with the zeroth order in the above construction, $\mathbf{R}^{(0)} = \mathbf{m}(J(f^*(\mathbf{M})))$.

In particular, the strict increase in the quasiequilibrium entropy has been demonstrated for the first and higher order approximations (see preceding sections of this chapter and [30]). Examples have been provided 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 method of natural projector 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 phenomenological device which makes it possible to infer the form of the macroscopic equations by a

non-complicated 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 (see previous example).

Going away from the limitations imposed by the finite coarse graining time [29, 30] can be recognized as the major problem of a consistent formulation of the nonequilibrium statistical thermodynamics. Intuitively, this requires taking the limit $\tau \rightarrow \infty$, allowing for all the relevant correlations to be developed by the microscopic dynamics, rather than to be cut off at the finite τ (see Chap. 12).

11.3.2 Natural Projector for Linear Systems

However, there is one important exception when the “ $\tau \rightarrow \infty$ problem” is readily solved [30, 31]. This is the case where equation (11.33) is linear,

$$\partial_t f = Lf , \quad (11.37)$$

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

$$\partial_t \mathbf{M} = \mathbf{R}\mathbf{M} , \quad (11.38)$$

where the linear operator \mathbf{R} is determined by the coarse-graining condition (11.35) in the limit $\tau \rightarrow \infty$:

$$\mathbf{R} = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \ln [\mathbf{m}(e^{\tau L} f^{\text{eq}} \mathbf{m}^\dagger)] . \quad (11.39)$$

Formula (11.39) has been already briefly mentioned in [30], and its relation to the Green-Kubo formula has been demonstrated in [31]. The Green-Kubo formula reads:

$$\mathbf{R}_{\text{GK}} = \int_0^\infty \langle \dot{\mathbf{m}}(0) \dot{\mathbf{m}}(t) \rangle dt , \quad (11.40)$$

where angular brackets denote equilibrium averaging, and where $\dot{\mathbf{m}} = L^\dagger \mathbf{m}$. The difference between the formulae (11.39) and (11.40) stems from the fact that condition (11.35) does not use an a priori hypothesis about the separation of the macroscopic and the microscopic time scales. For the classical N -particle dynamics, equation (11.39) is a very complicated expression, involving a logarithm of non-commuting operators. It is therefore desirable to gain its understanding in simple model situations.

11.3.3 Explicit Example of the Fluctuation–Dissipation Formula

In this subsection we want to give an explicit example of the formula (11.39). 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 [285] for the purpose of testing various ideas in kinetic theory. In the dissipative case with a clear separation of time scales, existence of the formula (11.39) is underpinned by the entropy growth in both the fast and slow 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 [16], and has been discussed by many authors, e.g. . [112, 197, 201]. Case studies for linear kinetic equation help clarifying the concept of this extraction [202, 203, 285].

Therefore, since 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 the formula (11.39). Specifically, we compare the result with the exact sum of the Chapman–Enskog expansion [70], and with the exact solution in the framework of the method of invariant manifold. We demonstrate that both the 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 $\mathbf{f}(r, t) = (f_+(r, t), f_-(r, t))^\dagger$:

$$\begin{aligned} \partial_t f_+ &= -\partial_r f_+ + \epsilon^{-1} \left(\frac{f_+ + f_-}{2} - f_+ \right) , \\ \partial_t f_- &= \partial_r f_- + \epsilon^{-1} \left(\frac{f_+ + f_-}{2} - f_- \right) . \end{aligned} \quad (11.41)$$

Equation (11.41) describes the one-dimensional kinetics of particles with velocities $+1$ and -1 as a combination of the 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’s density, where $\mathbf{n} = (1, 1)$], and $j(r, t) = (\mathbf{j}, \mathbf{f})$ [the local momentum density, where $\mathbf{j} = (1, -1)$]. Equation (11.41) can be equivalently written in terms of the moments,

$$\begin{aligned} \partial_t n &= -\partial_r j , \\ \partial_t j &= -\partial_r n - \epsilon^{-1} j . \end{aligned} \quad (11.42)$$

The local equilibrium,

$$\mathbf{f}^*(n) = \frac{n}{2} \mathbf{n} , \quad (11.43)$$

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 quasiequilibrium manifold (11.43) is linear in our example, as well as the kinetic equation.

The problem of reducing the description for the model (11.41) 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 Chapman–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 (11.39), and other methods, extend this result.

Because of the linearity of the equation (11.41) and of the local equilibrium, it is natural to use the Fourier transform, $h_k = \int \exp(ikr) h(r) dr$. Equation (11.41) is then written,

$$\partial_t \mathbf{f}_k = \mathbf{L}_k \mathbf{f}_k, \quad (11.44)$$

where

$$\mathbf{L}_k = \begin{pmatrix} -ik - \frac{1}{2\epsilon} & \frac{1}{2\epsilon} \\ \frac{1}{2\epsilon} & ik - \frac{1}{2\epsilon} \end{pmatrix}. \quad (11.45)$$

Derivation of the fluctuation-dissipation formula (11.39) in our example goes as follows: We seek the macroscopic dynamics of the form,

$$\partial_t n_k = R_k n_k, \quad (11.46)$$

where the function R_k is yet unknown. In the left-hand side of equation (11.35) we have:

$$n_k(t + \tau) = e^{\tau R_k} n_k(t). \quad (11.47)$$

In the right-hand side of equation (11.35) we have:

$$\left(\mathbf{n}, e^{\tau \mathbf{L}_k} \mathbf{f}^*(n_k(t)) \right) = \frac{1}{2} \left(\mathbf{n}, e^{\tau \mathbf{L}_k} \mathbf{n} \right) n_k(t). \quad (11.48)$$

After equating the expressions (11.47) and (11.48), we require that the resulting equality holds in the limit $\tau \rightarrow \infty$ independently of the initial data $n_k(t)$. Thus, we arrive at the formula (11.39):

$$R_k = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \ln \left[\left(\mathbf{n}, e^{\tau \mathbf{L}_k} \mathbf{n} \right) \right]. \quad (11.49)$$

Equation (11.49) defines the macroscopic dynamics (11.46) within the present approach. Explicit evaluation of the expression (11.49) is straightforward in the present model. Indeed, operator \mathbf{L}_k has two eigenvalues, Λ_k^\pm , where

$$\Lambda_k^\pm = -\frac{1}{2\epsilon} \pm \sqrt{\frac{1}{4\epsilon^2} - k^2} \quad (11.50)$$

Let us denote as \mathbf{e}_k^\pm two (arbitrary) eigenvectors of the matrix \mathbf{L}_k , corresponding to the eigenvalues Λ_k^\pm . Vector \mathbf{n} has a representation, $\mathbf{n} = \alpha_k^+ \mathbf{e}_k^+ +$

$\alpha_k^- \mathbf{e}_k^-$, where α_k^\pm are complex-valued coefficients. With this, we obtain in equation (11.49),

$$R_k = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \ln \left[\alpha_k^+ (\mathbf{n}, \mathbf{e}_k^+) e^{\tau A_k^+} + \alpha_k^- (\mathbf{n}, \mathbf{e}_k^-) e^{\tau A_k^-} \right]. \quad (11.51)$$

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

$$R_k = A_k^+, \text{ for } k < k_c. \quad (11.52)$$

As was expected, formula (11.39) in our case results in the exact hydrodynamic branch of the spectrum of the kinetic equation (11.41). The standard diffusion approximation is recovered from equation (11.52) as the first non-vanishing 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 $\text{Re} A_k^+ = \text{Re} A_k^-$. However, we may still extend the function R_k for $k \geq k_c$ on the basis of the formula (11.49):

$$R_k = \text{Re } A_k^+ \text{ for } k \geq k_c \quad (11.53)$$

Notice that the function R_k as given by equations (11.52) and (11.53) is continuous but non-analytic at the crossover.

11.3.4 Comparison with the Chapman–Enskog Method and Solution of the Invariance Equation

Let us now compare this result with the Chapman–Enskog method. Since the exact Chapman–Enskog solution for the systems like equation (11.43) has been recently discussed in detail elsewhere [40, 42, 205, 219–221], we shall be brief here. Following the Chapman–Enskog method, we seek the momentum variable j in terms of an expansion,

$$j^{\text{CE}} = \sum_{n=0}^{\infty} \epsilon^{n+1} j^{(n)} \quad (11.54)$$

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

$$j^{(n)} = - \sum_{m=0}^{n-1} \partial_t^{(m)} j^{(n-1-m)}, \quad (11.55)$$

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

$$\partial_t^{(m)} n = -\partial_r j^{(m)}. \quad (11.56)$$

The recurrence equations (11.54), (11.55), and (11.56), become well defined as soon as the aforementioned zero-order approximation $j^{(0)}$ is specified,

$$j^{(0)} = -\partial_r n . \quad (11.57)$$

From equations (11.55), (11.56), and (11.57), it follows that the Chapman–Enskog coefficients $j^{(n)}$ have the following structure:

$$j^{(n)} = b_n \partial_r^{2n+1} n , \quad (11.58)$$

where coefficients b_n are found from the recurrence equation,

$$b_n = \sum_{m=0}^{n-1} b_{n-1-m} b_m , \quad b_0 = -1 . \quad (11.59)$$

Notice that coefficients (11.59) 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,

$$j_k^{\text{CE}} = ik B_k^{\text{CE}} n_k , \quad (11.60)$$

where

$$B_k^{\text{CE}} = \sum_{n=0}^{\infty} b_n (-\epsilon k^2)^n . \quad (11.61)$$

Equation for the function B (11.61) is easily found upon multiplying equation (11.59) by $(-k^2)^n$, and summing in n from zero to infinity:

$$\epsilon k^2 B_k^2 + B_k + 1 = 0 . \quad (11.62)$$

Solution to the latter equation which respects condition (11.57), and which constitutes the exact Chapman–Enskog solution (11.61) is:

$$B_k^{\text{CE}} = \begin{cases} k^{-2} A_k^+ , & k < k_c \\ \text{none} , & k \geq k_c \end{cases} \quad (11.63)$$

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

$$\partial_t n_k = -ik j_k^{\text{CE}} = R_k^{\text{CE}} n_k , \quad (11.64)$$

where

$$R_k^{\text{CE}} = \begin{cases} A_k^+ , & k < k_c \\ \text{none} , & k \geq k_c \end{cases} \quad (11.65)$$

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 the diffusion approximation, whereas formula (11.49) is not based on such an extension.

Finally, let us discuss briefly the comparison with the solution within the method of invariant manifold [9, 11, 14]. Specifically, the momentum variable

$j_k^{\text{inv}} = ikB_k^{\text{inv}}n_k$ 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,

$$\frac{\partial j_k^{\text{inv}}}{\partial n_k} \partial_t n_k = ikB_k^{\text{inv}}(-ik)[ikB_k^{\text{inv}}], \quad (11.66)$$

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

$$\partial_t j_k^{\text{inv}} = -ikn_k - \epsilon^{-1}ikB_k^{\text{inv}}n_k, \quad (11.67)$$

and that the equality of the derivatives (11.66) and (11.67) 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 equation (11.62), and it is straightforward to show that the same selection procedure of the hydrodynamic root as above in the Chapman–Enskog case results in equation (11.65).

In conclusion, in this Example we have given the explicit illustration for the formula (11.39). The example demonstrates that the fluctuation-dissipation formula (11.39) 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, the formula (11.39) demonstrates a non-analytic extension.