Constructive Methods of Invariant Manifolds for Kinetic Problems

Alexander N. Gorban[1,2,3*], Iliya V. Karlin[1,2**], and Andrei Yu. Zinovyev[2,3***]

[1] ETH-Zentrum, Department of Materials, Institute of Polymers, Sonneggstr. 3, ML J19, CH-8092 Zürich, Switzerland;

[2] Institute of Computational Modeling SB RAS, Akademgorodok, Krasnoyarsk 660036, Russia;

[3] Institut des Hautes Etudes Scientifiques, Le Bois-Marie, 35, route de Chartres, F-91440, Bures-sur-Yvette, France

Abstract

We present the Constructive Methods of Invariant Manifolds for model reduction in physical and chemical kinetics, developed during last two decades. The physical problem of reduced description is studied in a most general form as a problem of constructing the slow invariant manifold. The invariance conditions are formulated as the differential equation for a manifold immersed in the phase space (*the invariance equation*). The equation of motion for immersed manifolds is obtained (*the film extension of the dynamics*). Invariant manifolds are fixed points for this equation, and slow invariant manifolds are Lyapunov stable fixed points, thus *slowness is presented as stability*. A collection of methods for construction of slow invariant manifolds is presented, in particular, the Newton method subject to incomplete linearization is the analogue of *KAM methods for dissipative systems*. The systematic use of thermodynamics structures and of the quasi-chemical representation allow to construct approximations which are in concordance with physical restrictions. We systematically consider a discrete analogue of the slow (stable) positively invariant manifolds for dissipative systems, *invariant grids*. Dynamic and static *postprocessing procedures* give us the opportunity to estimate the accuracy of obtained approximations, and to improve this accuracy significantly.

The following examples of applications are presented: Nonperturbative deviation of physically consistent hydrodynamics from the Boltzmann equation and from

*agorban@mat.ethz.ch, **ikarlin@mat.ethz.ch, ***zinovyev@ihes.fr

the reversible dynamics, for Knudsen numbers $Kn \sim 1$; construction of the moment equations for nonequilibrium media and their dynamical correction (instead of extension of list of variables) to gain more accuracy in description of highly nonequilibrium flows; determination of molecules dimension (as diameters of equivalent hard spheres) from experimental viscosity data; invariant grids for a two-dimensional catalytic reaction and a four-dimensional oxidation reaction (six species, two balances); universal continuous media description of dilute polymeric solution; the limits of macroscopic description for polymer molecules, etc.

Keywords: Model Reduction; Invariant Manifold; Entropy; Kinetics; Boltzmann Equation; Fokker-Planck Equation; Postprocessing.

Contents

1 Introduction

In this paper, we present a collection of constructive methods to study slow (stable) positively invariant manifolds of dynamic systems. The main object of our study are dissipative dynamic systems (finite or infinite) which arise in various problems of kinetics. Some of the results and methods presented herein might have a more general applicability, and can be useful not only for dissipative systems but also, for example, for conservative systems.

Nonequilibrium statistical physics is a collection of ideas and methods to extract slow invariant manifolds. Reduction of description for dissipative systems assumes (explicitly or implicitly) the following picture: There exists a manifold of slow motions in the phase space of the system. From the initial conditions the system goes quickly in a small neighborhood of the manifold, and after that moves slowly along it. The manifold of slow motion must be positively invariant: if the motion starts on at t_0, the it stays on the manifold at $t > t_0$. Frequently using wording "invariant manifold" is not truly exact: For the dissipative systems the possibility of extending the solutions (in a meaningful way) backwards in time is limited. So, in noneqiulibrium statistical physics we study *positively invariant* slow manifolds. The invariance condition can be written in explicit form as the differential equation for the manifold immersed into the phase space.

A dissipative system may have many closed positively invariant sets. For every set of initial conditions K, unification of all the trajectories $\{x(t), t \geq 0\}$ with initial conditions $x(0) \in K$ is positively invariant. Thus, selection of the slow (stable) positively invariant manifolds becomes a very important problem.

One of the difficulties in the problem of reducing the description is pertinent to the fact that there exist no commonly accepted formal definition of slow (and stable) positively invariant manifolds. We consider manifolds immersed into a phase space and study their motion along trajectories. We subtract from this motion the motion of immersed manifolds along themselves, and obtain new a equation for dynamics of manifolds in phase space: *the film extension of the dynamics*. Invariant manifolds are fixed points for this extended dynamics, and **slow** invariant manifolds are **Lyapunov stable fixed points**.

Here we present three approaches to constructing slow (stable) positively invariant manifolds.

- *Iteration method* (Newton method subject to incomplete linearization);
- *Relaxation methods* based on a film extension of the original dynamic system;
- *The method of natural projector*

The Newton method (with incomplete linearization) is convenient for obtaining the explicit formulas - even one iteration can give a good approximation.

Relaxation methods are oriented (in higher degree) at the numerical implementation. Nevertheless, several first steps also can give appropriate analytical approximations, competitive with other methods.

Finally, the method of natural projector constructs not the manifold itself but a projection of slow dynamics from the slow manifold onto some set of variables.

The Newton method subject to incomplete linearization was developed for the construction of slow (stable) positively invariant manifolds for the following problems:

- Derivation of the post-Navier-Stokes hydrodynamics from the Boltzmann equation [1, 3, 4].
- Description of the dynamics of polymers solutions [5].
- Correction of the moment equations [6].
- Reduced description for the chemical kinetics [7, 8], etc.

Relaxation methods based on a film extension of the original dynamic system were applied for the analysis of the Fokker-Planck equation [9]. Applications of these methods in the theory of the Boltzmann equation can benefit from the estimations, obtained in the papers [11, 12].

The method of natural projector was initially applied to derivation of the dissipative equations of macroscopic dynamics from the conservative equations of microscopic dynamics [13, 14, 15, 16, 17, 19, 18]. Using the method, new equations were obtained for the post-Navier-Stokes hydrodynamics, equations of plasma hydrodynamics and others [14, 18]. This short-memory approximation is applied to the Wigner formulation of quantum mechanics. The dissipative dynamics of a single quantum particle in a confining external potential is shown to take the form of a damped oscillator whose effective frequency and damping coefficients depend on the shape of the quantum-mechanical potential [19]. The method of natural projector can also be applied effectively for the dissipative systems: instead of Chapman-Enskog method in theory of the Boltzmann equation, etc.

A natural initial approximation for the methods under consideration is a quasiequilibrium manifold. It is the manifold of conditional maxima of the entropy. Most of the works on nonequilibrium thermodynamics deal with corrections to quasi-equilibrium approximations, or with applications of these approximations (with or without corrections). The construction of the quasi-equilibrium allows for the following generalization: Almost every manifold can be represented as a set of minimizers of the entropy under linear constrains. However, in contrast to the standard quasiequilibrium, these linear constrains will depend on the point on the manifold. We describe the quasiequilibrium manifold and a quasiequilibrium projector on the tangent space of this manifold. This projector is orthogonal with respect to entropic scalar product (the bilinear form defined by the negative second differential of the entropy). We construct the thermodynamical projector, which transforms the arbitrary vector field equipped with the given Lyapunov function (the entropy) into a vector field with the same Lyapunov function for an arbitrary anzatz manifold which is not tangent to the level of the Lyapunov function. The uniqueness of this construction is demonstrated.

We must define the status of most the statements in this text. Just like the absolute majority of all claims concerning such things as general solutions of the Navier-Stokes and Boltzmann equations, etc., they have the status of being plausible. They can become theorems only if one restricts essentially the set of the objects under consideration. Among such restrictions we should mention cases of exact reduction, i.e. exact derivation of the hydrodynamics from the kinetics [20, 21]. In these (still infinite-dimensional) examples one can compare different methods, for example, the Newton method with the methods of series summation in the perturbation theory [21, 22].

Also, it is necessary to stress here, that even if in the limit all the methods lead to the same results, they can give rather different approximations "on the way".

The rigorous grounds of the constructive methods of invariant manifolds should, in particular, include the theorems concerning *persistence of invariant manifolds under perturbations*. The most known result of this type is the Kolmogorov-Arnold-Moser theory about persistence of almost all invariant tori of completely integrable system under small perturbation [25, 26, 27]. Such theorems exist for some classes of infinite dimensional dissipative systems too [28]. Unfortunately, it is not proven now that many important systems (the Boltzmann equation, 3D Navier-Stokes equations, Grad equations, etc.) belong to these classes. So, it is necessary to act with these systems without rigorous basis.

Two approaches are widely known to the construction of the invariant manifolds: the *Taylor series expansion* [29, 30] and the method of *renormalization group* [34, 35, 36, 37]. The advantages and disadvantages of the Taylor expansion are well-known: constructivity against the absence of physical meaning for the high-order terms (often) and divergence in the most interesting cases (often).

In the paper [34] a geometrical formulation of the renormalization group method for global analysis was given. It was shown that the renormalization group equation can be interpreted as an envelope equation. Recently [35] the renormalization group method was formulated in terms of the notion of invariant manifolds. This method was applied to derive kinetic and transport equations from the respective microscopic equations [36]. The derived equations include Boltzmann equation in classical mechanics (see also the paper [33], where was shown for the first time that kinetic equations such as the Boltzmann equation can be understood naturally as renormalization group equations), Fokker-Planck equation, a rate equation in a quantum field theoretical model. The renormalization group approach was applied to the stochastic Navier-Stokes equation that describes fully developed fluid turbulence [38, 39, 40]. For the evaluation of the relevant degrees of freedom the renormalization group technique was revised for discrete systems in the recent paper [37].

The new quantum field theory formulation of the problem of persistence of invariant tori in perturbed completely integrable systems was obtained, and the new proof of the KAM theorem for analytic Hamiltonians based on the renormalization group method was given [41].

From the authors of the paper [33] point of view, the relation of renormalization group theory and reductive perturbation theory has simultaneously been recognized: renormalization group equations are actually the slow-motion equations which are usually obtained by reductive perturbation methods.

The first systematic and (at least partially) successfull method of constructing invariant manifolds for dissipative systems was the celebrated *Chapman-Enskog method* [43] for the Boltzmann kinetic equation[1]. The Chapman-Enskog method results in a series development of the so-called normal solution (the notion introduced by Hilbert [44]) where the one-body distribution function depends on time and space through its locally conserved moments. To the first approximation, the Chapman-Enskog series leads to hydrodynamic equations with transport coefficients expressed in terms of molecular scattering cross-sections. However, next terms of the Chapman-Enskog bring in the "ltra-violet catastrophy" (noticed first by Bobylev [45]) and negative viscosity. These drawbacks pertinent to the Taylor-series expansion disappear as soon as the Newton method is used to construct the invariant manifold [3].

The Chapman-Enskog method gave rise to a host of subsequent works and methods, such as the famous method of the *quasi-steady state* in chemical kinetics, pioneered by Bodenstein and Semenov and explored in considerable detail by many authors (see, for example, [46, 47, 48, 49, 50, 7]), and the theory of *singularly perturbed* differential equations [46, 51, 52, 53, 54, 55, 56].

There exist a group of methods to construct an ansatz for the invariant manifold based on the spectral decomposition of the Jacobian. The idea to use the spectral decomposition of Jacobian fields in the problem of separating the motions into fast and slow originates from methods of analysis of stiff systems [57], and from methods of sensitivity analysis in control theory [58, 59]. One of the currently most popular methods based on the spectral decomposition of Jacobian fields is the construction of the so-called *intrinsic low-dimensional manifold* (ILDM) [60].

The Newton method with incomplete linearization as well as the relaxation method allow us to find an approximate slow invariant manifolds without the preliminary stage of Jacobian field spectral decomposition. Moreover, a necessary slow invariant subspace of Jacobian in equilibrium point appears as a by-product of the Newton iterations (with incomplete linearization), or of the relaxation method.

Past decade witnessed a rapid development of the so-called *set oriented* numerical methods [61]. The purpose of these methods is to compute attractors, invariant manifolds (often, computation of stable and unstable manifolds in hyperbolic systems [62, 63, 64]). Also, one of the central tasks of these methods is to gain statistical information, i. e. computations of physically observable invariant measures. The distinguished feature of the modern set-oriented methods of numerical dynamics is the use of ensembles of trajectories within a relatively short propagation time instead of a long time single trajectory.

In this paper we systematically consider a discrete analogue of the slow (stable) positively invariant manifolds for dissipative systems, *invariant grids*. These invariant grids

[1]Nonlinear kinetic equations and methods of reduced description are reviewed for a wide audience of specialists and postgraduate students in physics, mathematical physics, material science, chemical engineering and interdisciplinary research in the paper [42].

were introduced in [7]. Here we will describe the Newton method subject to incomplete linearization and the relaxation methods for the invariant grids [65].

It is worth to mention, that the problem of the grid correction is fully decomposed into the tasks of the grid's nodes correction. The edges between the nodes appears only in the calculation of the tangent spaces at the nodes. This fact determines high computational efficiency of the invariant grids method.

Let the (approximate) slow invariant manifold for a dissipative system be found. *What for have we constructed it?* One important part of the answer to this question is: *We have constructed it to create models of open system dynamics in the neighborhood of this manifold.* Different approaches for this modeling are described. We apply these methods to the problem of reduced description in polymer dynamics and derive the universal limit in dynamics of dilute polymeric solutions. It is represented by the *revised Oldroyd 8 constants* constitutive equation for the polymeric stress tensor. Coefficients of this constitutive equation are expressed in terms of the microscopic parameters. This limit of dynamics of dilute polymeric solutions is universal in the same sense, as Korteweg-De-Vries equation is universal in the description of the dispersive dissipative nonlinear waves: any physically consistent equation should contain the obtained equation as a limit.

The phenomenon of *invariant manifold explosion* in driven open systems is demonstrated on the example of dumbbell models of dilute polymeric solutions [66]. This explosion gives us a possible mechanism of drug reduction in dilute polymeric solutions [67].

Suppose that for the kinetic system the approximate invariant manifold has been constructed and the slow motion equations have been derived. Suppose that we have solved the slow motion system and obtain $x_{sl}(t)$. We consider the following two questions:

- How well this solution approximates the real solution $x(t)$ given the same initial conditions?
- How is it possible to use the solution $x_{sl}(t)$ for it's refinement without solving the slow motion system (or it's modifications) again?

These two questions are interconnected. The first question states the problem of the *accuracy estimation*. The second one states the problem of *postprocessing*. We propose various algorithms for postprocessing and accuracy estimation, and give an example of application.

The present paper comprises sections of the two kinds. Numbered sections contain basic notions, methods and algorithmic realizations. Sections entitled "Examples" contain various case studies where the methods are applied to specific equations. Exposition in the "Examples" sections is not as consequent as in the numbered sections. In some of the examples we use notions not readily introduced in the preceding numbered sections. Most of the examples can be read more or less independently.

The list of cited literature is by no means complete although we spent effort in order to reflect at least the main directions of studies related to computations of the invariant manifolds. We assume that this list is more or less exhaustive in the second-order approximation.

Acknowledgements. First of all, we are grateful to our coauthors: Prof V. I. Bykov (Krasnoyarsk), Prof. M. Deville (Lausanne), Dr. G. Dukek (Ulm), Dr. P. Ilg (Zürich-Berlin), Prof. T. F. Nonnenmacher (Ulm), Prof. H. C. Öttinger (Zürich), Prof. S. Succi (Roma), Dr. L. L. Tatarinova (Krasnoyarsk-Zürich), Prof. G. S. Yablonskii (Novosibirsk-Saint-Louis), Dr. V. B. Zmievskii (Krasnoyarsk-Lausanne-Montreal) for years of collaboration, stimulating discussion and support. We thank Prof M. Grmela (Montreal) for detailed and encouraging discussion of the geometrical foundations of nonequilibrium thermodynamics. Prof. M. Shubin (Moscow-Boston) explained us some important chapters of the pseudodifferential operators theory. Finally, it is our pleasure to thank Prof. Misha Gromov (IHES, Bures-sur-Yvette) for encouragement and the spirit of Geometry.

2 The source of examples

2.1 The Boltzmann equation

2.1.1 The equation

The **Boltzmann equation** is the first and the most celebrated nonlinear kinetic equation introduced by the great Austrian physicist Ludwig Boltzmann in 1872 [68]. This equation describes the dynamics of a moderately rarefied gas, taking into account the two processes, the free flight of the particles, and their collisions. In its original version, the Boltzmann equation has been formulated for particles represented by hard spheres. The physical condition of rarefaction means that only pair collisions are taken into account, a mathematical specification of which is given by the **Grad-Boltzmann limit**: If N is the number of particles, and σ is the diameter of the hard sphere, then the Boltzmann equation is expected to hold when N tends to infinity, σ tends to zero, $N\sigma^3$ (the volume occupied by the particles) tends to zero, while $N\sigma^2$ (the total collision cross section) remains constant. The microscopic state of the gas at time t is described by the one-body distribution function $P(\boldsymbol{x}, \boldsymbol{v}, t)$, where $\boldsymbol{x}$ is the position of the center of the particle, and $\boldsymbol{v}$ is the velocity of the particle. The distribution function is the probability density of finding the particle at time t within the infinitesimal phase space volume centered at the phase point $(\boldsymbol{x}, \boldsymbol{v})$. The collision mechanism of two hard spheres is presented by a relation between the velocities of the particles before [$\boldsymbol{v}$ and $\boldsymbol{w}$] and after [$\boldsymbol{v}'$ and $\boldsymbol{w}'$] their impact:

$$\begin{aligned} \boldsymbol{v}' &= \boldsymbol{v} - \boldsymbol{n}(\boldsymbol{n}, \boldsymbol{v} - \boldsymbol{w}), \\ \boldsymbol{w}' &= \boldsymbol{w} + \boldsymbol{n}(\boldsymbol{n}, \boldsymbol{v} - \boldsymbol{w}), \end{aligned}$$

where $\boldsymbol{n}$ is the unit vector along $\boldsymbol{v} - \boldsymbol{v}'$. Transformation of the velocities conserves the total momentum of the pair of colliding particles ($\boldsymbol{v}' + \boldsymbol{w}' = \boldsymbol{v} + \boldsymbol{w}$), and the total kinetic energy ($\boldsymbol{v}'^2 + \boldsymbol{w}'^2 = \boldsymbol{v}^2 + \boldsymbol{w}^2$) The Boltzmann equation reads:

$$\begin{aligned} &\frac{\partial P}{\partial t} + \left(\boldsymbol{v}, \frac{\partial P}{\partial \boldsymbol{x}}\right) = \qquad (1) \\ &N\sigma^2 \int_R \int_{B^-} (P(\boldsymbol{x}, \boldsymbol{v}', t)P(\boldsymbol{x}, \boldsymbol{w}', t) - P(\boldsymbol{x}, \boldsymbol{v}, t)P(\boldsymbol{x}, \boldsymbol{w}, t)) \mid (\boldsymbol{w} - \boldsymbol{v}, \boldsymbol{n}) \mid d\boldsymbol{w} d\boldsymbol{n}, \end{aligned}$$

where integration in $\boldsymbol{n}$ is carried over the unit sphere R^3, while integration in $\boldsymbol{w}$ goes over a hemisphere $B^- = \{\boldsymbol{w} \mid (\boldsymbol{w} - \boldsymbol{v}, \boldsymbol{n}) < 0\}$. This hemisphere corresponds to the particles entering the collison. The nonlinear integral operator in the right hand side of Eq. (1) is nonlocal in the velocity variable, and local in space. The Boltzmann equation for arbitrary hard-core interaction is a generalization of the Boltzmann equation for hard spheres under the proviso that the true infinite-range interaction potential between the particles is cut-off at some distance. This generalization amounts to a replacement,

$$\sigma^2 \mid (\boldsymbol{w} - \boldsymbol{v}, \boldsymbol{n}) \mid d\boldsymbol{n} \to B(\theta, \mid \boldsymbol{w} - \boldsymbol{v} \mid) d\theta d\varepsilon, \qquad (2)$$

where function B is determined by the interaction potential, and vector $\boldsymbol{n}$ is identified with two angles, θ and ε. In particular, for potentials proportional to the n-th inverse power of the distance, the function B reads,

$$B(\theta, \mid \boldsymbol{v}-\boldsymbol{w} \mid) = \beta(\theta) \mid \boldsymbol{v}-\boldsymbol{w} \mid^{\frac{n-5}{n-1}} . \tag{3}$$

In the special case $n = 5$, function B is independent of the magnitude of the relative velocity (Maxwell molecules). Maxwell molecules occupy a distinct place in the theory of the Boltzmann equation, they provide exact results. Three most important findings for the Maxwell molecules are mentioned here: 1. The exact spectrum of the linearized Boltzmann collision integral, found by Truesdell and Muncaster, 2. Exact transport coefficients found by Maxwell even before the Boltzmann equation was formulated, 3. Exact solutions to the space-free model version of the nonlinear Boltzmann equation. Pivotal results in this domain belong to Galkin who has found the general solution to the system of moment equations in a form of a series expansion, to Bobylev, Krook and Wu who have found an exact solution of a particular elegant closed form, and to Bobylev who has demonstrated the complete integrability of this dynamic system.

The broad review of the Boltzmann equation and analysis of analytical solutions to kinetic models is presented in the book of Cercignani [69] A modern account of rigorous results on the Boltzmann equation is given in the book [70]. Proof of the existence theorem for the Boltzmann equation was done by DiPerna and Lions [74].

It is customary to write the Boltzmann equation using another normalization of the distribution function, $f(\boldsymbol{x}, \boldsymbol{v}, t)d\boldsymbol{x}d\boldsymbol{v}$, taken in such a way that the function f is compliant with the definition of the hydrodynamic fields: the mass density ρ, the momentum density $\rho\boldsymbol{u}$, and the energy density ε:

$$\begin{aligned} \int f(\boldsymbol{x}, \boldsymbol{v}, t) m d\boldsymbol{v} &= \rho(\boldsymbol{x}, t), \\ \int f(\boldsymbol{x}, \boldsymbol{v}, t) m \boldsymbol{v} d\boldsymbol{v} &= \rho\boldsymbol{u}(\boldsymbol{x}, t), \\ \int f(\boldsymbol{x}, \boldsymbol{v}, t) m \frac{v^2}{2} d\boldsymbol{v} &= \varepsilon(\boldsymbol{x}, t). \end{aligned} \tag{4}$$

Here m is the particle's mass.

The Boltzmann equation for the distribution function f reads,

$$\frac{\partial f}{\partial t} + \left(\boldsymbol{v}, \frac{\partial}{\partial \boldsymbol{x}} f\right) = Q(f, f), \tag{5}$$

where the nonlinear integral operator in the right hand side is the Boltzmann collision integral,

$$Q = \int_{R^3} \int_{B^-} (f(\boldsymbol{v}')f(\boldsymbol{w}') - f(\boldsymbol{v})f(\boldsymbol{w}))B(\theta, \boldsymbol{v}) d\boldsymbol{w} d\theta d\varepsilon. \tag{6}$$

Finally, we mention the following form of the Boltzmann collision integral (sometimes referred to as the scattering or the quasi-chemical representation),

$$Q = \int W(\boldsymbol{v}, \boldsymbol{w} \mid \boldsymbol{v}', \boldsymbol{w}')[(f(\boldsymbol{v}')f(\boldsymbol{w}') - f(\boldsymbol{v})f(\boldsymbol{w}))] d\boldsymbol{w} d\boldsymbol{w}' d\boldsymbol{v}', \tag{7}$$

where W is a generalized function which is called the probability density of the elementary event,

$$W = w(\boldsymbol{v}, \boldsymbol{w} \mid \boldsymbol{v}', \boldsymbol{w}')\delta(\boldsymbol{v} + \boldsymbol{w} - \boldsymbol{v}' - \boldsymbol{w}')\delta(v^2 + w^2 - v'^2 - w'^2). \tag{8}$$

2.1.2 The basic properties of the Boltzmann equation

Generalized function W has the following symmetries:

$$W(\boldsymbol{v}', \boldsymbol{w}' \mid \boldsymbol{v}, \boldsymbol{w}) \equiv W(\boldsymbol{w}', \boldsymbol{v}' \mid \boldsymbol{v}, \boldsymbol{w}) \equiv W(\boldsymbol{v}', \boldsymbol{w}' \mid \boldsymbol{w}, \boldsymbol{v}) \equiv W(\boldsymbol{v}, \boldsymbol{w} \mid \boldsymbol{v}', \boldsymbol{w}'). \tag{9}$$

The first two identities reflect the symmetry of the collision process with respect to labeling the particles, whereas the last identity is the celebrated **detail balance** condition which is underpinned by the time-reversal symmetry of the microscopic (Newton's) equations of motion. The basic properties of the Boltzmann equation are:

1. **Additive invariants of collision operator**:

$$\int Q(f, f)\{1, \boldsymbol{v}, v^2\} d\boldsymbol{v} = 0, \tag{10}$$

for any function f, assuming integrals exist. Equality (10) reflects the fact that the number of particles, the three components of particle's momentum, and the particle's energy are conserved by the collision. Conservation laws (10) imply that the local hydrodynamic fields (4) can change in time only due to redistribution in the space.

2. Zero point of the integral ($Q = 0$) satisfy the equation (which is also called **the detail balance**): For almost all velocities,

$$f(\boldsymbol{v}', \boldsymbol{x}, t) f(\boldsymbol{w}', \boldsymbol{x}, t) = f(\boldsymbol{v}, \boldsymbol{x}, t) f(\boldsymbol{w}, \boldsymbol{x}, t).$$

3. Boltzmann's **local entropy production inequality**:

$$\sigma(\boldsymbol{x}, t) = -k_B \int \ln f Q(f, f) d\boldsymbol{v} \geq 0, \tag{11}$$

for any function f, assuming integrals exist. Dimensional **Boltzmann's constant** ($k_B \approx 6 \cdot 10^{-23} J/K$) in this expression serves for a recalculation of the energy units into the absolute temperature units. Moreover, equality sign takes place if $\ln f$ is a linear combination of the additive invariants of collision.

Distribution functions f whose logarithm is a linear combination of additive collision invariants, with coefficients dependent on x, are called **local Maxwell distribution functions** f_{LM},

$$f_{LM} = \frac{\rho}{m} \left(\frac{2\pi k_B T}{m} \right)^{-3/2} \exp\left(\frac{-m(\boldsymbol{v} - \boldsymbol{u})^2}{2k_B T} \right). \tag{12}$$

Local Maxwellians are parametrized by values of five scalar functions, ρ , $\boldsymbol{u}$ and T. This parametrization is consistent with the definitions of the hydrodynamic fields

(4), $\int f_{LM}(m, m\boldsymbol{v}, mv^2/2) = (\rho, \rho\boldsymbol{u}, \varepsilon)$ provided the relation between the energy and the kinetic temperature T, holds, $\varepsilon = \frac{3\rho}{2mk_BT}$.

4. Boltzmann's ***H* theorem**: The function

$$S[f] = -k_B \int f \ln f d\boldsymbol{v}, \tag{13}$$

is called the **entropy density**. The **local *H* theorem** for distribution functions independent of space states that the rate of the entropy density increase is equal to the nonnegative entropy production,

$$\frac{dS}{dt} = \sigma \geq 0. \tag{14}$$

Thus, if no space dependence is concerned, the Boltzmann equation describes relaxation to the unique global Maxwellian (whose parameters are fixed by initial conditions), and the entropy density grows monotonically along the solutions. Mathematical specifications of this property has been initialized by Carleman, and many estimations of the entropy growth were obtained over the past two decades. In the case of space-dependent distribution functions, the local entropy density obeys the **entropy balance equation**:

$$\frac{\partial S(\boldsymbol{x}, t)}{\partial t} + \left(\frac{\partial}{\partial \boldsymbol{x}}, \mathbf{J}_s(\boldsymbol{x}, t)\right) = \sigma(\boldsymbol{x}, t) \geq 0, \tag{15}$$

where $\mathbf{J}_s$ is the entropy flux, $\mathbf{J}_s(\boldsymbol{x}, t) = -k_B \int \ln f(\boldsymbol{x}, t)\boldsymbol{v} f(\boldsymbol{x}, t) d\boldsymbol{v}$. For suitable boundary conditions, such as, specularly reflecting or at the infinity, the entropy flux gives no contribution to the equation for the **total entropy**, $S_{tot} = \int S(\boldsymbol{x}, t) d\boldsymbol{x}$ and its rate of changes is then equal to the nonnegative total entropy production $\sigma_{tot} = \int \sigma(\boldsymbol{x}, t) d\boldsymbol{x}$ (the **global *H* theorem**). For more general boundary conditions which maintain the entropy influx the global H theorem needs to be modified. A detailed discussion of this question is given by Cercignani. The local Maxwellian is also specified as the maximizer of the Boltzmann entropy function (13), subject to fixed hydrodynamic constraints (4). For this reason, the local Maxwellian is also termed as the local equilibrium distribution function.

2.1.3 Linearized collision integral

Linearization of the Boltzmann integral around the local equilibrium results in the linear integral operator,

$$Lh(\boldsymbol{v}) = \int W(\boldsymbol{v}, \boldsymbol{w} \mid \boldsymbol{v}', \boldsymbol{w}') f_{LM}(\boldsymbol{v}) f_{LM}(\boldsymbol{w}) \left[\frac{h(\boldsymbol{v}')}{f_{LM}(\boldsymbol{v}')} + \frac{h(\boldsymbol{w}')}{f_{LM}(\boldsymbol{w}')} - \frac{h(\boldsymbol{v})}{f_{LM}(\boldsymbol{v})} - \frac{h(\boldsymbol{w})}{f_{LM}(\boldsymbol{w})}\right] d\boldsymbol{w}' d\boldsymbol{v}' d\boldsymbol{w}.$$

Linearized collision integral is symmetric with respect to scalar product defined by the second derivative of the entropy functional,

$$\int f_{LM}^{-1}(\boldsymbol{v}) g(\boldsymbol{v}) Lh(\boldsymbol{v}) d\boldsymbol{v} = \int f_{LM}^{-1}(\boldsymbol{v}) h(\boldsymbol{v}) Lg(\boldsymbol{v}) d\boldsymbol{v},$$

it is nonpositively definite,

$$\int f_{LM}^{-1}(\boldsymbol{v})h(\boldsymbol{v})Lh(\boldsymbol{v})d\boldsymbol{v} \leq 0,$$

where equality sign takes place if the function hf_{LM}^{-1} is a linear combination of collision invariants, which characterize the null-space of the operator L. Spectrum of the linearized collision integral is well studied in the case of the small angle cut-off.

2.2 Phenomenology and Quasi-chemical representation of the Boltzmann equation

Boltzmann's original derivation of his collision integral was based on a phenomenological "bookkeeping" of the gain and of the loss of probability density in the collision process. This derivation postulates that the rate of gain G equals

$$G = \int W^{+}(\boldsymbol{v}, \boldsymbol{w} \mid \boldsymbol{v}', \boldsymbol{w}')f(\boldsymbol{v})f(\boldsymbol{w})d\boldsymbol{v}'d\boldsymbol{w}'d\boldsymbol{w},$$

while the rate of loss is

$$L = \int W^{-}(\boldsymbol{v}, \boldsymbol{w} \mid \boldsymbol{v}', \boldsymbol{w}')f(\boldsymbol{w})f(\boldsymbol{w})d\boldsymbol{v}'d\boldsymbol{w}'d\boldsymbol{w}.$$

The form of the gain and of the loss, containing products of one-body distribution functions in place of the two-body distribution, constitutes the famous Stosszahlansatz. The Boltzmann collision integral follows now as $(G - L)$, subject to the detail balance for the rates of individual collisions,

$$W^{+}(\boldsymbol{v}, \boldsymbol{w} \mid \boldsymbol{v}', \boldsymbol{w}') = W^{-}(\boldsymbol{v}', \boldsymbol{w}' \mid \boldsymbol{v}, \boldsymbol{w}).$$

This representation for interactions different from hard spheres requires also the cut-off of functions β (3) at small angles. The gain-loss form of the collision integral makes it evident that the detail balance for the rates of individual collisions is sufficient to prove the local H theorem. A weaker condition which is also sufficient to establish the H theorem was first derived by Stueckelberg (so-called **semi-detailed balance**), and later generalized **to inequalities of concordance**:

$$\int d\boldsymbol{v}' \int d\boldsymbol{w}'(W^{+}(\boldsymbol{v}, \boldsymbol{w} \mid \boldsymbol{v}', \boldsymbol{w}') - W^{-}(\boldsymbol{v}, \boldsymbol{w} \mid \boldsymbol{v}', \boldsymbol{w}')) \geq 0,$$
$$\int d\boldsymbol{v} \int d\boldsymbol{w}(W^{+}(\boldsymbol{v}, \boldsymbol{w} \mid \boldsymbol{v}', \boldsymbol{w}') - W^{-}(\boldsymbol{v}, \boldsymbol{w} \mid \boldsymbol{v}', \boldsymbol{w}')) \leq 0.$$

The semi-detailed balance follows from these expressions if the inequality signes are replaced by equalities.

The pattern of Boltzmann's phenomenological approach is often used in order to construct nonlinear kinetic models. In particular, **nonlinear equations of chemical kinetics** are based on this idea: If n chemical species A_i participate in a complex chemical reaction,

$$\sum_i \alpha_{si} A_i \leftrightarrow \sum_i \beta_{si} A_i,$$

where α_{si} and β_{si} are nonnegative integers (stoichiometric coefficients) then equations of chemical kinetics for the concentrations of species c_j are written

$$\frac{dc_i}{dt} = \sum_{s=1}^{n} (\beta_{si} - \alpha_{si}) \left[\varphi_s^+ \exp\left(\sum_{j=1}^{n} \frac{\partial G}{\partial c_j} \alpha_{sj} \right) - \varphi_s^- \exp\left(\sum_{j=1}^{n} \frac{\partial G}{\partial c_j} \beta_{sj} \right) \right].$$

Functions φ_s^+ and φ_s^- are interpreted as constants of the direct and of the inverse reactions, while the function G is an analog of the Boltzmann's H-function. Modern derivation of the Boltzmann equation, initialized by the seminal work of N.N.Bogoliubov, seek a replacement condition, and which would be more closely related to many-particle dynamics. Such conditions are applied to the N-particle Liouville equation should factorize in the remote enough past, as well as in the remote infinity (the hypothesis of weakening of correlations). Different conditions has been formulated by D.N.Zubarev, J.Lewis and others. The advantage of these formulations is the possibility to systematically find corrections not included in the Stosszahlansatz.

2.3 Kinetic models

Mathematical complications caused by the nonlinearly Boltzmann collision integral are traced back to the Stosszahlansatz. Several approaches were developed in order to simplify the Boltzmann equation. Such simplifications are termed kinetic models. Various kinetic models preserve certain features of the Boltzmann equation, while scarifying the rest of them. The most well known kinetic model which preserve the H theorem is the nonlinear Bhatnagar-Gross-Krook model (BGK) [71]. The BGK collision integral reads:

$$Q_{BGK} = -\frac{1}{\tau}(f - f_{LM}(f)).$$

The time parameter $\tau > 0$ is interpreted as a characteristic relaxation time to the local Maxwellian. The BGK is a nonlinear operator: Parameters of the local Maxwellian are identified with the values of the corresponding moments of the distribution function f. This nonlinearly is of "lower dimension" than in the Boltzmann collision integral because $f_{LM}(f)$ is a nonlinear function of only the moments of f whereas the Boltzmann collision integral is nonlinear in the distribution function f itself. This type of simplification introduced by the BGK approach is closely related to the family of so-called mean-field approximations in statistical mechanics. By its construction, the BGK collision integral preserves the following three properties of the Boltzmann equation: additive invariants of collision, uniqueness of the equilibrium, and the H theorem. A class of kinetic models which generalized the BGK model to quasiequilibrium approximations of a general form is described as follows: The quasiequilibrium f^* for the set of linear functionales $M(f)$

is a distribution function $f^*(M)(\boldsymbol{x}, \boldsymbol{v})$ which maximizes the entropy under fixed values of functions M. The Quasiequilibrium (QE) models are characterized by the collision integral [72],

$$Q_{QE}(f) = -\frac{1}{\tau}[f - f^*(M(f))] + Q_B(f^*(M(f)), f^*(M(f))).$$

Same as in the case of the BGK collision integral, operator Q_{QE} is nonlinear in the moments M only. The QE models preserve the following properties of the Boltzmann collision operator: additive invariants, uniqueness of the equilibrium, and the H theorem, provided the relaxation time τ to the quasiequilibrium is sufficiently small. A different nonlinear model was proposed by Lebowitz, Frisch and Helfand [73]:

$$Q_D = D\left(\frac{\partial}{\partial \boldsymbol{v}}\frac{\partial}{\partial \boldsymbol{v}}f + \frac{m}{k_B T}\frac{\partial}{\partial \boldsymbol{v}}(\boldsymbol{v} - \boldsymbol{u}(f))f\right).$$

The collision integral has the form of the self-consistent Fokker-Planck operator, describing diffusion (in the velocity space) in the self-consistent potential. Diffusion coefficient $D > 0$ may depend on the distribution function f. Operator Q_D preserves the same properties of the Boltzmann collision operator as the BGK model. Kinetic BGK model has been used for obtaining exact solutions of gasdynamic problems, especially its linearized form for stationary problems. Linearized B GK collision model has been extended to model more precisely the linearized Boltzmann collision integral.

2.4 Methods of reduced description

One of the major issues raised by the Boltzmann equation is the problem of the reduced description. Equations of hydrodynamics constitute a closet set of equations for the hydrodynamic field (local density, local momentum, and local temperature). From the standpoint of the Boltzmann equation, these quantities are low-order moments of the one-body distribution function, or, in other words, the macroscopic variables. The problem of the reduced description consists in giving an answer to the following two questions:

1. What are the conditions under which the macroscopic description sets in?
2. How to derive equations for the macroscopic variables from kinetic equations?

The classical methods of reduced description for the Boltzmann equation are: the Hilbert method, the Chapman-Enskog method, and the Grad moment method.

2.4.1 The Hilbert method

In 1911, David Hilbert introduced the notion of normal solutions,

$$f_H(\boldsymbol{v}, n(\boldsymbol{r}, t), \boldsymbol{u}(\boldsymbol{r}, t), T(\boldsymbol{r}, t)),$$

that is, solution to the Boltzmann equation which depends on space and time only through five hydrodynamic fields [44].

The normal solutions are found from a singularly perturbed Boltzmann equation,

$$D_t f = \frac{1}{\varepsilon} Q(f, f), \tag{16}$$

where ε is a small parameter, and

$$D_t f \equiv \frac{\partial}{\partial t} f + (\boldsymbol{v}, \frac{\partial}{\partial \boldsymbol{r}}) f.$$

Physically, parameter ε corresponds to the Knudsen number, the ratio between the mean free path of the molecules between collisions, and the characteristic scale of variation of the hydrodynamic fields. In the Hilbert method, one seeks functions $n(\boldsymbol{r}, t)$, $\boldsymbol{u}(\boldsymbol{r}, t)$, $T(\boldsymbol{r}, t)$, such that the normal solution in the form of the Hilbert expansion,

$$f_H = \sum_{i=0}^{\infty} \varepsilon^i f_H^{(i)} \tag{17}$$

satisfies the Eq. (16) order by order. Hilbert was able to demonstrate that this is formally possible. Substituting (17) into (16), and matching various order in ε, we have the sequence of integral equations

$$Q(f_H^{(0)}, f_H^{(0)}) = 0, \tag{18}$$

$$L f_H^{(1)} = D_t f_H^{(0)}, \tag{19}$$

$$L f_H^{(2)} = D_t f_H^{(1)} - Q(f_H^{(0)}, f_H^{(1)}), \tag{20}$$

and so on for higher orders. Here L is the linearized collision integral. From Eq.(18), it follows that $f_H^{(0)}$ is the local Maxwellian with parameters not yet determined. The Fredholm alternative, as applied to the second Eq. (19) results in

a) Solvability condition,

$$\int D_t f_H^{(0)} \{1, \boldsymbol{v}, v^2\} d\boldsymbol{v} = 0,$$

which is the set of compressible Euler equations of the non-viscous hydrodynamics. Solution to the Euler equation determine the parameters of the Maxwellian f_H^0.

b) General solution $f_H^{(1)} = f_H^{(1)1} + f_H^{(1)2}$, where $f_H^{(1)1}$ is the special solution to the linear integral equation (19), and $f_H^{(1)2}$ is yet undetermined linear combination of the additive invariants of collision.

c) Solvability condition to the next equation (19) determines coefficients of the function $f_H^{(1)2}$ in terms of solutions to the linear hyperbolic differential equations,

$$\int D_t (f_H^{(1)1} + f_H^{(1)2}) \{1, \boldsymbol{v}, v^2\} d\boldsymbol{v} = 0.$$

Hilbert was able to demonstrate that this procedure of constructing the normal solution can be carried out to arbitrary order n, where the function $f_H^{(n)}$ is determined from the solvability condition at the next, $(n+1)$-th order. In order to summarize, implementation of the Hilbert method requires solutions for the function $n(\boldsymbol{r}, t)$, $\boldsymbol{u}(\boldsymbol{r}, t)$, and $T(\boldsymbol{r}, t)$ obtained from a sequence of partial differential equations.

2.4.2 The Chapman-Enskog method

A completely different approach to the reduced description was invented in 1917 by David Enskog [75], and independently by Sidney Chapman [43]. The key innovation was to seek an expansion of the time derivatives of the hydrodynamic variables rather than seeking the time-space dependencies of these functions as in the Hilbert method.

The Chapman-Enskog method starts also with the singularly perturbed Boltzmann equation, and with the expansion

$$f_{CE} = \sum_{n=0}^{\infty} \varepsilon^n f_{CE}^{(n)}.$$

However, the procedure of evaluation of the functions $f_{CE}^{(n)}$ differs from the Hilbert method:

$$Q(f_{CE}^{(0)}, f_{CE}^{(0)}) = 0, \tag{21}$$

$$Lf_{CE}^{(1)} = -Q(f_{CE}^{(0)}, f_{CE}^{(0)}) + \frac{\partial^{(0)}}{\partial t} f_{CE}^{(0)} - \left(\boldsymbol{v}, \frac{\partial}{\partial \boldsymbol{r}}\right) f_{CE}^{(0)}. \tag{22}$$

Operator $\partial^{(0)}/\partial t$ is defined from the expansion of the right hand side of hydrodynamic equation,

$$\frac{\partial^{(0)}}{\partial t}\{\rho, \rho\boldsymbol{u}, e\} \equiv -\int \left\{m, m\boldsymbol{v}, \frac{mv^2}{2}\right\} \left(\boldsymbol{v}, \frac{\partial}{\partial \boldsymbol{r}}\right) f_{CE}^{(0)} d\boldsymbol{v}. \tag{23}$$

From Eq. (21), function $f_{CE}^{(0)}$ is again the local Maxwellian, whereas (23) is the Euler equations, and $\partial^{(0)}/\partial t$ acts on various functions $g(\rho, \rho\boldsymbol{u}, e)$ according to the chain rule,

$$\frac{\partial^{(0)}}{\partial t} g = \frac{\partial g}{\partial \rho}\frac{\partial^{(0)}}{\partial t}\rho + \frac{\partial g}{\partial(\rho\boldsymbol{u})}\frac{\partial^{(0)}}{\partial t}\rho\boldsymbol{u} + \frac{\partial g}{\partial e}\frac{\partial^{(0)} e}{\partial t},$$

while the time derivatives $\frac{\partial^{(0)}}{\partial t}$ of the hydrodynamic fields are expressed using the right hand side of Eq. (23).

The result of the Chapman-Enskog definition of the time derivative $\frac{\partial^{(0)}}{\partial t}$, is that the Fredholm alternative is satisfied by the right hand side of Eq. (22). Finally, the solution to the homogeneous equation is set to be zero by the requirement that the hydrodynamic variables as defined by the function $f^{(0)} + \varepsilon f^{(1)}$ coincide with the parameters of the local Maxwellian $f^{(0)}$:

$$\int \{1, \boldsymbol{v}, v^2\} f_{CE}^{(1)} d\boldsymbol{v} = 0.$$

The first correction $f_{CE}^{(1)}$ of the Chapman-Enskog method adds the terms

$$\frac{\partial^{(1)}}{\partial t}\{\rho, \rho\boldsymbol{u}, e\} = -\int \left\{m, m\boldsymbol{v}, \frac{mv^2}{2}\right\} \left(\boldsymbol{v}, \frac{\partial}{\partial \boldsymbol{r}}\right) f_{CE}^{(1)} d\boldsymbol{v}$$

to the time derivatives of the hydrodynamic fields. These terms correspond to the dissipative hydrodynamics where viscous momentum transfer and heat transfer are in the

Navier-Stokes and Fourier form. The Chapman-Enskog method was the first true success of the Boltzmann equation since it had made it possible to derive macroscopic equation without a priori guessing (the generalization of the Boltzmann equation onto mixtures predicted existence of the thermodiffusion before it has been found experimentally), and to express the kinetic coefficient in terms of microscopic particle's interaction.

However, higher-order corrections of the Chapman-Enskog method, resulting in hydrodynamic equations with derivatives (Burnett hydrodynamic equations) face serve difficulties both from the theoretical, as well as from the practical sides. In particular, they result in unphysical instabilities of the equilibrium.

2.4.3 The Grad moment method

In 1949, Harold Grad extended the basic assumption behind the Hilbert and the Chapman-Enskog methods (the space and time dependence of the normal solutions is mediated by the five hydrodynamic moments) [113]. A physical rationale behind the Grad moment method is an assumption of the decomposition of motions:
(i). During the time of order τ, a set of distinguished moments M' (which include the hydrodynamic moments and a subset of higher-order moment) does not change significantly as compared to the rest of the moments M'' (the fast evolution).
(ii). Towards the end of the fast evolution, the values of the moments M'' become unambiguously determined by the values of the distinguished moments M'.
(iii). On the time of order $\theta \gg \tau$, dynamics of the distribution function is determined by the dynamics of the distinguished moments while the rest of the moments remain to be determined by the distinguished moments (the slow evolution period).

Implementation of this picture requires an ansatz for the distribution function in order to represent the set of states visited in the course of the slow evolution. In Grad's method, these representative sets are finite-order truncations of an expansion of the distribution functions in terms of Hermit velocity tensors:

$$f_G(M', \boldsymbol{v}) = f_{LM}(\rho, \boldsymbol{u}, E, \boldsymbol{v})[1 + \sum_{(\alpha)}^{N} a_{(\alpha)}(M')H_{(\alpha)}(\boldsymbol{v} - \boldsymbol{u})], \tag{24}$$

where $H_{(\alpha)}(\boldsymbol{v}-\boldsymbol{u})$ are various Hermit tensor polynomials, orthogonal with the weight f_{LM}, while coefficient $a_{(\alpha)}(M')$ are known functions of the distinguished moments M', and N is the highest order of M'. Other moments are functions of M': $M'' = M''(f_G(M'))$.

Slow evolution of distinguished moments is found upon substitution of Eq. (24) into the Boltzmann equation and finding the moments of the resulting expression (Grad's moment equations). Following Grad, this extremely simple approximation can be improved by extending the list of distinguished moments. The most well known is Grad's thirteen-moment approximation where the set of distinguished moments consists of five hydrodynamic moments, five components of the traceless stress tensor $\sigma_{ij} = \int m[(v_i - u_i)(v_j - u_j) - \delta_{ij}(\boldsymbol{v} - \boldsymbol{u})^2/3]f d\boldsymbol{v}$, and of the three components of the heat flux vector $q_i = \int (v_i - u_i)m(\boldsymbol{v} - \boldsymbol{u})^2/2 f d\boldsymbol{v}$.

The time evolution hypothesis cannot be evaluated for its validity within the framework of Grad's approach. It is not surprising therefore that Grad's methods failed to work in situations where it was (unmotivatedly) supposed to, primarily, in the phenomena with sharp time-space dependence such as the strong shock wave. On the other hand, Grad's method was quite successful for describing transition between parabolic and hyperbolic propagation, in particular, the second sound effect in massive solids at low temperatures, and, in general, situations slightly deviating from the classical Navier-Stokes- Fourier domain. Finally, the Grad method has been important background for development of phenomenological nonequilibrium thermodynamics based on hyperbolic first-order equation, the so-called EIT (extended irreversible thermodynamics).

2.4.4 Special approximations

Special approximation of the solutions to the Boltzmann equation has been found for several problems, and which perform better than results of "regular" procedures. The most well known is the ansatz introduced independently by Mott-Smith and Tamm for the strong shock wave problem: The (stationary) distribution function is thought as

$$f_{TMS}(a(x)) = (1 - a(x))f_+ + a(x)f_-, \tag{25}$$

where $f_\pm$ are upstream and downstream Maxwell distribution functions, whereas $a(x)$ is an undetermined scalar function of the coordinate along the shock tube.

Equation for function $a(x)$ has to be found upon substitution of Eq.(25) into the Bolltzmann equation, and upon integration with some velocity-dependent function $\varphi(\boldsymbol{v})$. Two general problems arise with the special approximation thus constructed: Which function $\varphi(\boldsymbol{v})$ should be taken, and how to find correction to the ansatz like Eq. (25).

2.4.5 The method of invariant manifold

The general approach to the problem of reduced description for dissipative system was recognized as the problem of finding stable invariant manifolds in the space of distribution function [1, 2, 3]. The notion of invariant manifold generalizes the normal solution in the Hilbert and in the Chapman-Enskog method, and the finite-moment sets of distribution function in the Grad method: If Ω is a smooth manifold in the space of distribution function, and if f_Ω is an element of Ω, then Ω is invariant with respect to the dynamic system,

$$\frac{\partial f}{\partial t} = J(f), \tag{26}$$

$$\text{if } J(f_\Omega) \in T\Omega, \text{ for all } f_\Omega \in \Omega, \tag{27}$$

where $T\Omega$ is the tangent bundle of the manifold Ω. Application of the invariant manifold idea to dissipative systems is based on iterations, progressively improving the initial approximation, involves the following steps:

Thermodynamic projector Given a manifold Ω (not obligatory invariant), the macroscopic dynamics on this manifold is defined by the macroscopic vector field, which is the result of a projection of vectors $J(f_\Omega)$ onto the tangent bundle $T\Omega$. The thermodynamic projector $P^*_{f_\Omega}$ takes advantage of dissipativity:

$$\ker P^*_{f_\Omega} \subseteq \ker D_f S\mid_{f_\Omega}, \tag{28}$$

where $D_f S\mid_{f_\Omega}$ is the differential of the entropy evaluated in f_Ω.

This condition of thermodynamicity means that each state of the manifold Ω is regarded as the result of decomposition of motions occurring near Ω: The state f_Ω is the maximum entropy state on the set of states $f_\Omega + \ker P^*_{f_\Omega}$. Condition of thermodynamicity does not define projector completely; rather, it is the condition that should be satisfied by any projector used to define the macroscopic vector field, $J'_\Omega = P^*_{f_\Omega} J(f_\Omega)$. For, once the condition (28) is met, the macroscopic vector field preserves dissipativity of the original microscopic vector field $J(f)$:

$$D_f S\mid_{f_\Omega} \cdot P^*_{f_\Omega}(J(f_\Omega)) \geq 0 \text{ for all } f_\Omega \in \Omega.$$

The thermodynamic projector is the formalization of the assumption that Ω is the manifold of slow motion: If a fast relaxation takes place at least in a neighborhood of Ω, then the states visited in this process before arriving at f_Ω belong to $\ker P^*_{f_\Omega}$. In general, $P^*_{f_\Omega}$ depends in a non-trivial way on f_Ω.

Iterations for the invariance condition The invariance condition for the manifold Ω reads,

$$P_\Omega(J(f_\Omega)) - J(f_\Omega) = 0,$$

here P_Ω is arbitrary (not obligatory thermodynamic) projector onto the tangent bundle of Ω. The invariance condition is considered as an equation which is solved iteratively, starting with initial approximation Ω_0. On the $(n+1)-$th iteration, the correction $f^{(n+1)} = f^{(n)} + \delta f^{(n+1)}$ is found from linear equations,

$$\begin{aligned} D_f J^*_n \delta f^{(n+1)} &= P^*_n J(f^{(n)}) - J(f^{(n)}), \\ P^*_n \delta f^{(n+1)} &= 0, \end{aligned} \tag{29}$$

here $D_f J^*_n$ is the linear selfajoint operator with respect to the scalar product by the second differential of the entropy $D^2_f S\mid_{f^{(n)}}$.

Together with the above-mentioned principle of thermodynamic projecting, the selfadjoint linearization implements the assumption about the decomposition of motions around the n'th approximation. The selfadjoint linearization of the Boltzmann collision integral Q (7) around a distribution function f is given by the formula,

$$\begin{aligned} D_f Q^* \delta f &= \int W(\boldsymbol{v}, \boldsymbol{w}, \mid \boldsymbol{v}', \boldsymbol{w}') \frac{f(\boldsymbol{v})f(\boldsymbol{w}) + f(\boldsymbol{v}')f(\boldsymbol{w}')}{2} \times \\ &\left[\frac{\delta f(\boldsymbol{v}')}{f(\boldsymbol{v}')} + \frac{\delta f(\boldsymbol{w}')}{f(\boldsymbol{w}')} - \frac{\delta f(\boldsymbol{v})}{f(\boldsymbol{v})} - \frac{\delta f(\boldsymbol{w})}{f(\boldsymbol{w})}\right] d\boldsymbol{w}' d\boldsymbol{v}' d\boldsymbol{w}. \end{aligned} \tag{30}$$

If $f = f_{LM}$, the selfadjoint operator (30) becomes the linearized collision integral.

The method of invariant manifold is the iterative process:

$$(f^{(n)}, P_n^*) \to (f^{(n+1)}, P_n^*) \to (f^{(n+1)}, P_{n+1}^*)$$

On the each 1-st part of the iteration, the linear equation (29) is solved with the projector known from the previous iteration. On the each 2-nd part, the projector is updated, following the thermodynamic construction.

The method of invariant manifold can be further simplified if smallness parameters are known.

The proliferation of the procedure in comparison to the Chapman-Enskog method is essentially twofold:

First, the projector is made dependent on the manifold. This enlarges the set of admissible approximations.

Second, the method is based on iteration rather than a series expansion in a smallness parameter. Importance of iteration procedures is well understood in physics, in particular, in the renormalization group approach to reducing the description in equilibrium statistical mechanics, and in the Kolmogorov- Arnold-Moser theory of finite-dimensional Hamiltonian systems.

2.4.6 Quasiequilibrium approximations

Important generalization of the Grad moment method is the concept of the quasiequilibrium approximations already mentioned above (we will discuss this approximation in detail in a separate section). The quasiequilibrium distribution function for a set of distinguished moment M maximizes the entropy density S for fixed M. The quasiequilibrium manifold $\Omega^*(M)$ is the collection of the quasiequilibrium distribution functions for all admissible values of M. The quasiequilibrium approximation is the simplest and extremely useful (not only in the kinetic theory itself) implementation of the hypothesis about a decomposition of motions: If M are considered as slow variables, then states which could be visited in the course of rapid motion in the vicinity of $\Omega^*(M)$ belong to the planes $\Gamma_M = \{f \mid m(f - f^*(M)) = 0\}$. In this respect, the thermodynamic construction in the method of invariant manifold is a generalization of the quasiequilibrium approximation where the given manifold is equipped with a quasiequilibrium structure by choosing appropriately the macroscopic variables of the slow motion. In contrast to the quasiequilibrium, the macroscopic variables thus constructed are not obligatory moments. A text book example of the quasiequilibrium approximation is the generalized Gaussian function for $M = \{\rho, \rho\boldsymbol{u}, P\}$ where $P_{ij} = \int v_i v_j f d\boldsymbol{v}$ is the pressure tensor.

The thermodynamic projector P^* for a quasiequilibrium approximation was first introduced by B. Robertson [77] (in a different context of conservative dynamics and for a special case of the Gibbs-Shannon entropy). It acts on a function Ψ as follows

$$P_M^*\Psi = \sum_i \frac{\partial f^*}{\partial M_i} \int m_i \Psi d\boldsymbol{v},$$

where $M = \int m_i f d\boldsymbol{v}$. The quasiequilibrium approximation does not exist if the highest order moment is an odd polynomial of velocity (therefore, there exists no quasiequilibrium for thirteen Grad's moments). Otherwise, the Grad moment approximation is the first-order expansion of the quasiequilibrium around the local Maxwellian.

2.5 Discrete velocity models

If the number of microscopic velocities is reduced drastically to only a finite set, the resulting discrete velocity, continuous time and continuous space models can still mimic the gas-dynamic flows. This idea was introduced in Broadwell's paper in 1963 to mimic the strong shock wave [76].

Further important development of this idea was due to Cabannes and Gatignol in the seventies who introduced a systematic class of discrete velocity models [79]. The structure of the collision operators in the discrete velocity models mimics the polynomial character of the Boltzmann collision integral. Discrete velocity models are implemented numerically by using the natural operator splitting in which each update due to free flight is followed by the collision update, the idea which dates back to Grad. One of the most important recent results is the proof of convergence of the discrete velocity models with pair collisions to the Boltzmann collision integral.

2.6 Direct simulation

Besides the analytical approach, direct numerical simulation of Boltzmann-type nonlinear kinetic equations have been developed since mid of 1960s [78]. The basis of the approach is a representation of the Boltzmann gas by a set of particles whose dynamics is modeled as a sequence of free propagation and collisions. The modeling of collisions uses a random choice of pairs of particles inside the cells of the space, and changing the velocities of these pairs in such a way as to comply with the conservation laws, and in accordance with the kernel of the Boltzmann collision integral. At present, there exists a variety of this scheme known under the common title of the Direct Simulation Monte-Carlo method. The DSMC, in particular, provides data to test various analytical theories.

2.7 Lattice Gas and Lattice Boltzmann models

Since mid of 1980s, the kinetic theory based approach to simulation of complex macroscopic phenomena such as hydrodynamics has been developed. The main idea of the approach is construction of minimal kinetic system in such a way that their long-time and large-scale limit matches the desired macroscopic equations. For this purpose, the fully discrete (in time- space-velocity) nonlinear kinetic equations are considered on sufficiently isotropic lattices, where the links represent the discrete velocities of fictitious particles. In the earlier version of the lattice methods, the particle-based picture has been exploited, subject to the exclusion rule (one or zero particle per lattice link) [the Lattice gas model [80]]. Most of the present versions use the distribution function picture, where populations of the links are non-integer [the Lattice Boltzmann model [81, 82, 83]]. Discrete-time dynamics consists of a propagation step where populations are transmitted to adjacent links and collision step where populations of the links at each node of the lattice are equilibrated by a certain rule. Most of the present versions use the BGK-type equilibration, where the local equilibrium is constructed in such a way as to match desired macroscopic equations. The Lattice Boltzmann method is a useful approach for computational fluid dynamics, effectively compliant with parallel architectures. The proof of the H theorem for the Lattice gas models is based on the semi-detailed (or Stueckelberg's) balance principle. The proof of the H theorem in the framework of the Lattice Boltzmann method has been only very recently achieved [83].

2.8 Other kinetic equations

2.8.1 The Enskog equation for hard spheres

The Enskog equation for hard spheres is an extension of the Boltzmann equation to moderately dense gases. The Enskog equation explicitly takes into account the nonlocality of collisions through a two-fold modification of the Boltzmann collision integral: First, the one-particle distribution functions are evaluated at the locations of the centers of spheres, separated by the non- zero distance at the impact. This makes the collision integral nonlocal in space. Second, the equilibrium pair distribution function at the contact of the spheres enhances the scattering probability. The proof of the H theorem for the Enskog equation has posed certain difficulties, and has led to a modification of the collision integral.

Methods of solution of the Enskog equation are immediate generalizations of those developed for the Boltzmann equation.

2.8.2 The Vlasov equation

The Vlasov equation (or kinetic equation for a self-consistent force) is the nonlinear equation for the one-body distribution function, which takes into account a long-range interaction between particles:

$$\frac{\partial}{\partial t} f + \left(\boldsymbol{v}, \frac{\partial}{\partial \boldsymbol{r}} f\right) + \left(\mathbf{F}, \frac{\partial}{\partial \boldsymbol{v}} f\right) = 0,$$

where $\mathbf{F} = \int \Phi(\mid \boldsymbol{r} - \boldsymbol{r}' \mid) \frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|} n(\boldsymbol{r}') d\boldsymbol{r}'$ is the self-consistent force. In this expression $\Phi(\mid \boldsymbol{r} - \boldsymbol{r}' \mid) \frac{\boldsymbol{r}-\boldsymbol{r}'}{|\boldsymbol{r}-\boldsymbol{r}'|}$ is the microscopic force between the two particles, and $n(\boldsymbol{r}')$ is the density of particles, defined self-consistently, $n(\boldsymbol{r}') = \int f(\boldsymbol{r}', \boldsymbol{v}) d\boldsymbol{v}$.

The Vlasov equation is used for a description of collisionless plasmas in which case it is completed by a set of Maxwell equation for the electromagnetic field [91]. It is also used for a description of the gravitating gas.

The Vlasov equation is an infinite-dimensional Hamiltonian system. Many special and approximate (wave-like) solutions to the Vlasov equation are known and they describe important physical effects. One of the most well known effects is the Landau damping: The energy of a volume element dissipates with the rate

$$Q \approx - \mid E \mid^2 \frac{\omega(k)}{k^2} \left. \frac{df_0}{dv} \right|_{v=\frac{\omega}{k}},$$

where f_0 is the Maxwell distribution function, $\mid E \mid$ is the amplitude of the applied monochromatic electric field with the frequency $\omega(k)$, k is the wave vector. The Landau damping is thermodynamically reversible effect, and it is not accompanied with an entropy increase. Thermodynamically reversed to the Landau damping is the plasma echo effect.

2.8.3 The Fokker-Planck equation

The Fokker-Planck equation (FPE) is a familiar model in various problems of nonequilibrium statistical physics [84, 85]. We consider the FPE of the form

$$\frac{\partial W(\boldsymbol{x},t)}{\partial t} = \frac{\partial}{\partial \boldsymbol{x}} \left\{ D \left[W \frac{\partial}{\partial \boldsymbol{x}} U + \frac{\partial}{\partial \boldsymbol{x}} W \right] \right\}. \tag{31}$$

Here $W(\boldsymbol{x},t)$ is the probability density over the configuration space x, at the time t, while $U(\boldsymbol{x})$ and $D(\boldsymbol{x})$ are the potential and the positively semi-definite $((\boldsymbol{y}, D\boldsymbol{y}) \geq 0)$ diffusion matrix.

The FPE (31) is particularly important in studies of polymer solutions [86, 87, 88]. Let us recall the two properties of the FPE (31), important to what will follow: (i). Conservation of the total probability: $\int W(\boldsymbol{x},t)dx = 1$. (ii). Dissipation: The equilibrium distribution, $W_{eq} \propto \exp(-U)$, is the unique stationary solution to the FPE (31). The entropy,

$$S[W] = - \int W(\boldsymbol{x},t) \ln \left[\frac{W(\boldsymbol{x},t)}{W_{eq}(\boldsymbol{x})} \right] dx, \tag{32}$$

is a monotonically growing function due to the FPE (31), and it arrives at the global maximum in the equilibrium. These properties are most apparent when the FPE (31) is rewritten as follows:

$$\partial_t W(\boldsymbol{x},t) = \hat{M}_W \frac{\delta S[W]}{\delta W(\boldsymbol{x},t)}, \tag{33}$$

where

$$\hat{M}_W = -\frac{\partial}{\partial \boldsymbol{x}} \left[W(\boldsymbol{x},t) D(\boldsymbol{x}) \frac{\partial}{\partial \boldsymbol{x}} \right]$$

is a positive semi–definite symmetric operator with kernel 1. The form (33) is the dissipative part of a structure termed GENERIC (the dissipative vector field is a metric transform of the entropy gradient) [89, 90].

***

Basic introductory textbook on physical kinetics of the Landau L.D. and Lifshitz E.M. Course of Theoretical Physics [91] contains many further examples and their applications.

Modern development of kinetics follows the route of specific numerical methods, such as direct simulations. An opposite tendency is also clearly observed, and the kinetic theory based schemes are increasingly used for the development of numerical methods and models in mechanics of continuous media.

3 Invariance equation in the differential form

Definition of the invariance in terms of motions and trajectories assumes, at least, existence and uniqueness theorems for solutions of the original dynamic system. This prerequisite causes difficulties when one studies equations relevant to physical and chemical kinetics, such as, for example, equations of hydrodynamics. Nevertheless, there exists a necessary *differential condition of invariance*: The vector field of the original dynamic system touches the manifold in every point. Let us write down this condition in order to set up notation.

Let E be a linear space, let U, the phase space, be a domain in E, and let a vector field $J:\ U \to E$ be defined in U. This vector field defines the original dynamic system,

$$\frac{dx}{dt} = J(x),\ x \in U. \tag{34}$$

In the sequel, we consider submanifolds in U which are parameterized with a given set of parameters. Let a linear space of parameters L be defined, and let W be a domain in L. We consider differentiable maps, $F:\ W \to U$, such that, for every $y \in W$, the differential of F, $D_yF:\ \ L \to E$, is an isomorphism of L on a subspace of E. That is, F are the manifolds, immersed in the phase space of the dynamic system (34), and parametrized by parameter set W.

Remark: One never discusses the choice of norms and topologies is such a general setting. It is assumed that the corresponding choice is made appropriately in each specific case.

We denote T_y the tangent space in the point y, $T_y = (D_yF)(L)$. *The differential condition of invariance* has the following form: For every $y \in W$,

$$J(F(y)) \in T_y. \tag{35}$$

Let us rewrite the differential condition of invariance (35) in a form of a differential equation. In order to achieve this, one needs to define a projector $P_y:\ E \to T_y$ for every $y \in W$. Once a projector P_y is defined, then condition (35) takes the form:

$$\Delta_y = (1 - P_y)J(F(y)) = 0. \tag{36}$$

Obviously, by $P_y^2 = P_y$ we have, $P_y\Delta_y = 0$. We refer to the function Δ_y as *the defect of invariance* in the point y. The defect of invariance will be encountered oft in what will follow.

Equation (36) is the first-order differential equation for the function $F(y)$. Projectors P_y should be tailored to the specific physical features of the problem at hand. A separate section below is devoted to the construction of projectors. There we shall demonstrate how to construct a projector, $P(x,T):\ \ E \to T$, given a point $x \in U$ and a specified subspace T. We then set $P_y = P(F(y),T_y)$ in equation (36) [2].

[2]One of the main routes to define the field of projectors $P(x,T)$ would be to make use of a Riemannian

structure. To this end, one defines a scalar product in E for every point $x \in U$, that is, a bilinear form $\langle p|q\rangle_x$ with a positive definite quadratic form, $\langle p|p\rangle_x > 0$, if $p \neq 0$. A good candidate for such a scalar product is the bilinear form defined by the negative second differential of the entropy in the point x, $-D^2S(x)$. As we demonstrate it later in this paper, this choice is essentially the only correct one close to the equilibrium. However, far from the equilibrium, an improvement is required in order to guarantee the thermodymamicity condition, $\ker P_y \subset \ker(D_xS)_{x=F(y)}$, for the field of projectors, $P(x,T)$, defined for any x and T, if $T \not\subset \ker D_xS$. The thermodymamicity condition provides the preservation of the type of dynamics: if $dS/dt > 0$ for initial vector field (34) in point $x = F(y)$, then $dS/dt > 0$ in this point x for projected vector field $P_y(J(F(y)))$ too.

4 Film extension of the dynamics: Slowness as stability

4.1 Equation for the film motion

One of the difficulties in the problem of reducing the description is pertinent to the fact that there exist no commonly accepted formal definition of slow (and stable) positively invariant manifolds. Classical definitions of stability and of the asymptotic stability of the invariant sets sound as follows: Let a dynamic system be defined in some metric space, and let $x(t, x_0)$ be a motion of this system at time t with the initial condition $x(0) = x_0$ at time $t = 0$. The subset S of the phase space is called *invariant* if it is made of whole trajectories, that is, if $x_0 \in S$ then $x(t, x_0) \in S$ for all $t \in (-\infty, \infty)$.

Let us denote as $\rho(x, y)$ the distance between the points x and y. The distance from x to the closed set S is defined as usual: $\rho(x, S) = \inf\{\rho(x, y)|y \in S\}$. The closed invariant subset S is called *stable*, if for every $\epsilon > 0$ there exists $\delta > 0$ such that if $\rho(x_0, S) < \delta$ then for every $t > 0$ it holds $\rho(x(t, x_0), S) < \epsilon$. A closed invariant subset S is called *asymptotically stable* if it is stable and attractive, that is, there exists $\epsilon > 0$ such that if $\rho(x_0, S) < \epsilon$ then $\rho(x(t, x_0), S) \to 0$ as $t \to \infty$.

Formally, one can reiterate the definitions of stability and of the asymptotic stability for positively invariant subsets. Moreover, since in the definitions mentioned above it goes only about $t \geq 0$ or $t \to \infty$, it might seem that positively invariant subsets can be a natural object of study for the stability. Such conclusion is misleading, however. The study of the classical stability of the positively invariant subsets reduces essentially to the notion of stability of invariant sets - maximal attractors.

Let Y be a closed positively invariant subset of the phase space. *The maximal attractor* for Y is the set M_Y,

$$M_Y = \bigcap_{t\geq 0} T_t(Y), \tag{37}$$

where T_t is the shift operator for the time t:

$$T_t(x_0) = x(t, x_0).$$

The maximal attractor M_Y is invariant, and the stability of Y defined classically is equivalent to the stability of M_Y under any sensible assumption about homogeneous continuity (for example, this is evident for a compact phase space).

For systems which relax to a stable equilibrium, the maximal attractor is simply one and the same for any bounded positively invariant subset, and it consists of a single stable point.

It is important to note that in the definition (37) one considers motions of a positively invariant subset to equilibrium *along itself*: $T_tY \subset Y$ for $t \geq 0$. It is precisely this motion which is uninteresting from the perspective of the comparison of stability of positively invariant subsets. If one subtracts this *motion along itself* out of the vector field $J(x)$ (34), one obtains a less trivial picture.

We again assume submanifolds in U parameterized with a single parameter set $F : W \to U$. Note that there exist a wide class of transformations which do not alter the geometric picture of motion: For a smooth diffeomorphism $\varphi : W \to W$ (a smooth coordinate transform), maps F and $F \circ \varphi$ define the same geometric pattern in the phase space.

Let us consider motions of the manifold $F(W)$ along solutions of equation (34). Denote as F_t the time-dependent map, and write equation of motion for this map:

$$\frac{dF_t(y)}{dt} = J(F_t(y)). \tag{38}$$

Let us now subtract the component of the vector field responsible for the motion of the map $F_t(y)$ along itself from the right hand side of equation (38). In order to do this, we decompose the vector field $J(x)$ in each point $x = F_t(y)$ as

$$J(x) = J_{||}(x) + J_{\perp}(x), \tag{39}$$

where $J_{||}(x) \in T_{t,y}$ $(T_{t,y} = (D_y F_t(y)(L))$. If projectors are defined, $P_{t,y} = P(F_t(y), T_{t,y})$, then decomposition (39) has the form:

$$J(x) = P_{t,y}J(x) + (1 - P_{t,y})J(x). \tag{40}$$

Subtracting the component $J_{||}$ from the right hand side of equation (38), we obtain,

$$\frac{dF_t(y)}{dt} = (1 - P_{t,y})J(F_t(y)). \tag{41}$$

Note that the geometric pictures of motion corresponding to equations (38) and (41) are identical *locally* in y and t. Indeed, the infinitesimal shift of the manifold W along the vector field is easily computed:

$$(D_y F_t(y))^{-1} J_{||}(F_t(y)) = (D_y F_t(y))^{-1}(P_{t,y}J(F_t(y))). \tag{42}$$

This defines a smooth change of the coordinate system (assuming all solutions exist). In other words, the component $J_{\perp}$ defines the motion of the manifold in U, while we can consider (locally) the component $J_{||}$ as a component which locally defines motions in W (a coordinate transform).

Very recently, the notion of exponential stability of invariants manifold for ODEs was revised by splitting motions into tangent and transversal (orthogonal) components in the work [92].

We further refer to equation (41) as *the film extension* of the dynamic system (34). The phase space of the dynamic system (41) is the set of maps F (films). Fixed points of equation (41) are solutions to the invariance equation in the differential form (36). These include, in particular, all positively invariant manifolds. Stable or asymptotically stable fixed points of equation (41) are slow manifolds we are interested in. It is the notion of stability associated with the film extension of the dynamics which is relevant to our study. Below in section 8, we consider relaxation methods for constructing slow positively invariant manifolds on the basis of the film extension (41).

4.2 Stability of analytical solutions

When studying the Cauchy problem for equation (41), one must ask a question of how to choose the boundary conditions: Which conditions the function F must satisfy at the boundary of W? Without fixing the boundary conditions, the general solution of the Cauchy problem for the film extension equations (41) in the class of smooth functions on W, is essentially ambiguous.

The boundary of W, ∂W splits on two pieces: $W = \partial W_+ \bigcup \partial W_-$. For smooth boundary these parts can be defined as

$$\begin{aligned} \partial W_+ &= \{y \in \partial W | (\nu(y), (DF(y))^{-1}(P_y J(F(y)))) < 0\}, \\ \partial W_- &= \{y \in \partial W | (\nu(y), (DF(y))^{-1}(P_y J(F(y)))) \geq 0\}. \end{aligned} \tag{43}$$

where $\nu(y)$ denotes the unitary outer normal vector in the boundary point y, $(DF(y))^{-1}$ is the isomorphism of the tangent space T_y on the linear space of parameters L.

One can understand the boundary splitting (43) in such a way: The projected vector field $P_y J(F(y))$ defines dynamics on the manifold $F(W)$, this dynamics is the image of some dynamics on W. The corresponding vector field on W is $v(y) = (DF(y))^{-1}(P_y J(F(y)))$. The boundary part ∂W_+ consists of points y, where velocity vector $v(y)$ is directed into W, and for $y \in \partial W_-$ this vector $v(y)$ is directed out of W (or is tangent to ∂W). The splitting $W = \partial W_+ \bigcup \partial W_-$ depends on t with the vector field $v(y)$.

If we would like to derive a solution of the film extension (41) $F(y,t)$ for $(y,t) \in W \times [0,\tau]$, for some time $\tau > 0$, then it is necessary to fix some boundary conditions on ∂W_+ (for "incoming from abroad" part of the function $F(y)$).

Nevertheless, there is a way to study equation (41) without introducing any boundary conditions. It is in the spirit of the classical Cauchy-Kovalevskaya theorem [93, 94, 95] about analytical Cauchy problem solutions with analytical data, as well as in the spirit of the classical Lyapunov auxilary theorem about analytical invariant manifolds in the neighborhood of fixed point [98, 30] and H. Poincaré Lya2 theorem about analytical linearization of analytical non-resonant contractions (see [100]).

We note in passing that recently, the interest to the classical analytical Caughy problem revived in the mathematical physics literature [96, 97]. In particular, analogs of the Caughy-Kovalevskaja theorem were obtained for generalized Euler equations [96]. A technique to estimate the convergence radii of the series emerging therein was also developed.

Analytical solutions to equation (41) do not require boundary conditions on the boundary of W. The analycity condition itself allows finding unique analytical solutions of the equation (41) with analytical right hand side $(1-P)J$ for analytical initial conditions F_0 in W (assuming that such solutions exist). Of course, the analytical continuation without additional regularity conditions is an ill-posed problem. However, it may be useful to go from functions to germs: we can solve chains of ordinary differential equations for Tailor coefficients instead of partial differential equations for functions (41), and after that it may be possible to prove the convergence of the Tailor series thus obtained. This is the way to prove the Lyapunov auxilary theorem [98], and one of the known ways to prove the Cauchy-Kovalevskaya theorem.

Let us consider the system (1) with stable equilibrium point x^*, real analytical right hand side J, and real analytical projector field $P(x,T): \ E \to T$. We shall study real analytical sub-manifolds, which include the equilibrium point point x^* ($0 \in W, F(0)=x^*$). Let us expand F in a Taylor series in the neighborhood of zero:

$$F(y) = x^* + A_1(y) + A_2(y,y) + \ldots + A_k(y,y,\ldots,y) + \ldots, \tag{44}$$

where $A_k(y,y,\ldots,y)$ is a symmetric k-linear operator ($k=1,2,\ldots$).

Let us expand also the right hand side of the film equation (41). Matching operators of the same order, we obtain a chain of equations for $A_1,\ldots,A_k,\ldots$:

$$\frac{dA_k}{dt} = \Psi_k(A_1,\ldots,A_k). \tag{45}$$

It is crucially important, that the dynamics of A_k does not depend on $A_{k+1},\ldots$, and equations (45) can be studied in the following order: we first study the dynamics of A_1, then the dynamics of A_2 with the A_1 motion already given, then A_3 and so on.

Let the projector P_y in equation (41) be an analytical function of the derivative $D_yF(y)$ and of the deviation $x-x^*$. Let the correspondent Tailor expansion in the point $(A_1^0(\bullet), x^*)$ have the form:

$$D_yF(y)(\bullet) = A_1(\bullet) + \sum_{k=2}^{\infty} kA_k(y,\ldots,\bullet), \tag{46}$$

$$P_y = \sum_{k,m=0}^{\infty} P_{k,m}(\underbrace{D_yF(y)(\bullet) - A_1^0(\bullet),\ldots,D_yF(y)(\bullet) - A_1^0(\bullet)}_{k};\underbrace{F(y)-x^*,\ldots,F(y)-x^*}_{m}),$$

where $A_1^0(\bullet)$, $A_1(\bullet)$, $A_k(y,\ldots,\bullet)$ are linear operators. $P_{k,m}$ is a $k+m$-linear operator ($k,m=0,1,2,\ldots$) with values in the space of linear operators $E \to E$. The operators $P_{k,m}$ depend on the operator $A_1^0(\bullet)$ as on a parameter. Let the point of expansion $A_1^0(\bullet)$ be the linear part of F: $A_1^0(\bullet) = A_1(\bullet)$.

Let us represent the analytical vector field $J(x)$ as a power series:

$$J(x) = \sum_{k=1}^{\infty} J_k(x-x^*,\ldots,x-x^*), \tag{47}$$

where J_k is a symmetric k-linear operator ($k=1,2,\ldots$).

Let us write, for example, the first two equations of the equation chain (45):

$$\begin{aligned}\frac{dA_1(y)}{dt} &= (1-P_{0,0})J_1(A_1(y)),\\ \frac{dA_2(y,y)}{dt} &= (1-P_{0,0})[J_1(A_2(y,y))+J_2(A_1(y),A_1(y))]-\\ &\quad [2P_{1,0}(A_2(y,\bullet))+P_{0,1}(A_1(y))]J_1(A_1(y)).\end{aligned}\tag{48}$$

Here operators $P_{0,0}$, $P_{1,0}(A_2(y,\bullet))$, $P_{0,1}(A_1(y))$ parametrically depend on the operator $A_1(\bullet)$, hence, the first equation is nonlinear, and the second is linear with respect to $A_2(y,y)$. The leading term in the right hand side has the same form for all equations of the sequence (45):

$$\frac{dA_n(y,\dots,y)}{dt}=(1-P_{0,0})J_1(A_n(y,\dots,y))-nP_{1,0}(A_n(\underbrace{y,\dots,y}_{n-1},\bullet))J_1(A_1(y))+\dots. \tag{49}$$

There are two important conditions on P_y and $D_yF(y)$: $P_y^2=P_y$, because P_y is a projector, and $\mathrm{Im}P_y=\mathrm{Im}D_yF(y)$, because P_y projects on the image of $D_yF(y)$. If we expand these conditions in the power series, then we get the conditions on the coefficients. For example, from the first condition we get:

$$\begin{aligned}&P_{0,0}^2=P_{0,0},\\ &P_{0,0}[2P_{1,0}(A_2(y,\bullet))+P_{0,1}(A_1(y))]+[2P_{1,0}(A_2(y,\bullet))+P_{0,1}(A_1(y))]P_{0,0}=\\ &2P_{1,0}(A_2(y,\bullet))+P_{0,1}(A_1(y)),\dots .\end{aligned}\tag{50}$$

After multiplication the second equation in (50) with $P_{0,0}$ we get

$$P_{0,0}[2P_{1,0}(A_2(y,\bullet))+P_{0,1}(A_1(y))]P_{0,0}=0. \tag{51}$$

Similar identities can be obtained for any oder of the expansion. These equalities allow us to simplify the stationary equation for the sequence (45). For example, for the first two equations of this sequence (48) we obtain the following stationary equations:

$$\begin{aligned}&(1-P_{0,0})J_1(A_1(y))=0,\\ &(1-P_{0,0})[J_1(A_2(y,y))+J_2(A_1(y),A_1(y))]-\\ &[2P_{1,0}(A_2(y,\bullet))+P_{0,1}(A_1(y))]J_1(A_1(y))=0.\end{aligned}\tag{52}$$

The operator $P_{0,0}$ is the projector on the space $\mathrm{Im}A_1$ (the image of A_1), hence, from the first equation in (52) it follows: $J_1(\mathrm{Im}A_1)\subseteq \mathrm{Im}A_1$. So, $\mathrm{Im}A_1$ is a J_1-invariant subspace in E ($J_1=D_xJ(x)|_{x^*}$) and $P_{0,0}(J_1(A_1(y))\equiv J_1(A_1(y)$. It is equivalent to the first equation of (52). Let us multiply the second equation of (52) with $P_{0,0}$ from the left. As a result we obtain the condition:

$$P_{0,0}[2P_{1,0}(A_2(y,\bullet))+P_{0,1}(A_1(y))]J_1(A_1(y))=0,$$

for solution of equations (52), because $P_{0,0}(1 - P_{0,0}) \equiv 0$. If $A_1(y)$ is a solution of the first equation of (52), then this condition becomes an identity, and we can write the second equation of (52) in the form

$$
\begin{aligned}
&(1 - P_{0,0}) \times \qquad (53)\\
&[J_1(A_2(y,y)) + J_2(A_1(y), A_1(y)) - (2P_{1,0}(A_2(y, \bullet)) + P_{0,1}(A_1(y)))J_1(A_1(y))] = 0.
\end{aligned}
$$

It should be stressed, that the choice of projector field P_y (46) has impact only on the $F(y)$ parametrization, whereas the invariant geometrical properties of solutions of (41) do not depend of projector field if some transversality and analycity conditions hold. The conditions of thermodynamic structures preservation significantly reduce ambiguousness of the projector choice. One of the most important condition is $\ker P_y \subset \ker D_x S$, where $x = F(y)$ and S is the entropy (see the section about the entropy below). The thermodynamic projector is the unique operator which transforms the arbitrary vector field equipped with the given Lyapunov function into a vector field with the same Lyapunov function on the arbitrary submanifold which is not tangent to the level of the Lyapunov function. For the thermodynamic projectors P_y the entropy $S(F(y))$ conserves on solutions $F(y,t)$ of the equation (41) for any $y \in W$.

If projectors P_y in equations (46)-(53) are thermodynamic, then $P_{0,0}$ is the orthogonal projector with respect to the entropic scalar product[3]. For orthogonal projectors the operator $P_{1,0}$ has a simple explicit form. Let $A : L \to E$ be a isomorphic injection, and $P : E \to E$ be the orthogonal projector on the image of A. The orthogonal projector on the image of perturbed operator $A + \delta A$ is $P + \delta P$,

$$
\begin{aligned}
\delta P &= (1 - P)\delta A A^{-1} P + (\delta A A^{-1} P)^{+}(1 - P) + o(\delta A),\\
P_{1,0}(\delta A(\bullet)) &= (1 - P)\delta A(\bullet) A^{-1} P + (\delta A(\bullet) A^{-1} P)^{+}(1 - P).
\end{aligned} \qquad (54)
$$

Here, in (54), the operator A^{-1} is defined on ImA, ImA = ImP, the operator $A^{-1}P$ acts on E.

Formula for δP (54) follows from the three conditions:

$$
(P + \delta P)(A + \delta A) = A + \delta A,\ (P + \delta P)^2 = P + \delta P,\ (P + \delta P)^{+} = P + \delta P. \qquad (55)
$$

Every A_k is driven by $A_1, \ldots, A_{k-1}$. Stability of the germ of the positively invariant analytical manifold $F(W)$ in the point 0 ($F(0) = x^*$) is defined as stability of the solution of corresponding equations sequence (45). Moreover, the notion of the k-jet stability can be useful: let's call k-jet stable such a germ of positively invariant manifold $F(M)$ in the point 0 ($F(0) = x^*$), if the corresponding solution of the equations sequence (45) is stable for $k = 1, \ldots, n$. The simple "triangle" structure of the equation sequence (45) with the form (49) of main linear part makes the problem of jets stability very similar for all orders $n > 1$.

[3]This scalar product is the bilinear form defined by the negative second differential of the entropy in the point x^*, $-D^2S(x)$.

Let us demonstrate the stability conditions for the 1-jets in a n-dimensional space E. Let the Jacobian matrix $J_1 = D_x J(x)|_{x^*}$ be selfadjoint with a simple spectrum $\lambda_1, \dots, \lambda_n$, and the projector $P_{0,0}$ be orthogonal (this is typical "thermodynamic" situation). Eigenvectors of J_1 form a basis in E: $\{e_i\}_{i=1}^n$. Let a linear space of parameters L be a k-dimensional real space, $k < n$. We shall study stability of a operator A_1^0 which is a fixed point for the first equation of the sequence (45). The operator A_1^0 is a fixed point of this equation, if $\mathrm{Im}A_1^0$ is a J_1-invariant subspace in E. We discuss full-rang operators, so, for some order of $\{e_i\}_{i=1}^n$ numbering, the matrix of A_1^0 should have a form: $a_{1ij}^0 = 0$, if $i > k$. Let us choose the basis in L: $l_j = (A_1^0)^{-1} e_j$, $(j = 1, \dots, k)$. For this basis $a_{1ij}^0 = \delta_{ij}$, $(i = 1, \dots, n,\ j = 1, \dots, k,\ \delta_{ij}$ is the Kronecker symbol). The corresponding projectors P and $1 - P$ have the matrices:

$$P = \mathrm{diag}(\underbrace{1, \dots, 1}_{k}, \underbrace{0, \dots, 0}_{n-k}),\ 1 - P = \mathrm{diag}(\underbrace{0, \dots, 0}_{k}, \underbrace{1, \dots, 1}_{n-k}), \tag{56}$$

where $\mathrm{diag}(\alpha_1, \dots, \alpha_n)$ is the $n \times n$ diagonal matrix with numbers $\alpha_1, \dots, \alpha_n$ on the diagonal.

The linear approximation equations for dynamics of deviations δA reads:

$$\frac{d\delta A}{dt} = \mathrm{diag}(\underbrace{0, \dots, 0}_{k}, \underbrace{1, \dots, 1}_{n-k})[\mathrm{diag}(\lambda_1, \dots, \lambda_n)\delta A - \delta A \mathrm{diag}(\underbrace{\lambda_1, \dots, \lambda_k}_{k})]. \tag{57}$$

The time derivative of A is orthogonal to A: for any $y, z \in L$ the equality $(\dot{A}(y), A(x)) = 0$ holds, hence, for stability analysis it is necessary and sufficient to study δA with $\mathrm{Im}\delta A_1^0 \perp \mathrm{Im}A$. The matrix for the such δA has a form:

$$\delta a_{ij} = 0, \text{ if } i \leq k.$$

For $i = k + 1, \dots, n$, $j = 1, \dots, k$ equation (57) gives:

$$\frac{d\delta a_{ij}}{dt} = (\lambda_i - \lambda_j)\delta a_{ij}. \tag{58}$$

From equation (58) the stability condition follows:

$$\lambda_i - \lambda_j < 0 \text{ for all } i > k,\ j \leq k. \tag{59}$$

It means that the relaxation to $\mathrm{Im}A$ (with spectrum of relaxation times $|\lambda_i|^{-1}$ $(i = k + 1, \dots, n)$) is faster, then the relaxation along $\mathrm{Im}A$ (with spectrum of relaxation times $|\lambda_j|^{-1}$ $(j = 1, \dots, k)$).

Let this condition (59) hold. The relaxation time for the film (in the first approximation) is:

$$\tau = 1/(min_{i>k}|\lambda_i| - max_{j \leq k}|\lambda_j|),$$

thus it depends on the **spectral gap** between the spectrum of the operator $J_1 = D_x J(x)|_{x^*}$ restriction on the J_1-invariant subspace $\mathrm{Im}A_1^0$ (it is the tangent space to the slow invariant manifold in the point x^*).

The stability condition (59) demonstrates that our formalization of manifold slowness as stability of fixed points for the film extension (41) of initial dynamics met the intuitive expectations.

For the analysis of the system (45) in the neighborhood of some manifold F_0 ($F_0(0) = x^*$), the following parametrization can be convenient. Let's consider $F_0(y) = A_1(y) + ...$, $T_0 = A_1(L)$ is a tangent space for $F_0(W)$ in the point x^*, $E = T_0 \bigoplus H$ is the direct sum decomposition.

We shall consider analytical sub-manifolds in the form

$$x = x^* + (y, \Phi(y)), \tag{60}$$

where $y \in W_0 \subset T_0$, W_0 is neighborhood of zero in T_0, $\Phi(y)$ is an analytical map of W_0 in H, $\Phi(0) = 0$.

Any analytical manifold close to F_0 can be represented in this form.

Let us define projector P_y, that corresponds to the decomposition (60) as the projector on T_y parallel to H. Furthermore, let us introduce the corresponding decomposition of the vector field $J = J_y \bigoplus J_z$, $J_y \in T_0$, $J_z \in H$. Then

$$P_y(J) = (J_y, (D_y\Phi(y))J_y). \tag{61}$$

The corresponding equation of motion of the film (41) has the following form:

$$\frac{d\Phi(y)}{dt} = J_z(y, \Phi(y)) - (D_y\Phi(y))J_y(y, \Phi(y)). \tag{62}$$

If J_y and J_z depend analytically on their arguments, then from (62) one can easily obtain the hierarchy of equations of the form (45) (of course, $J_y(x^*) = 0,\ J_z(x^*) = 0$).

Using these notions, it is convenient to formulate the Lyapunov Auxiliary Theorem [98]. Let $T_0 = R^m, H = R^p$, and in U an analytical vector field is defined $J(y, z) = J_y(y, z) \bigoplus J_z(y, z)$, ($y \in T_0, z \in H$), and the following conditions are satisfied:

1) $J(0, 0) = 0$;

2) $D_z J_y(y, z)|_{(0,0)} = 0$;

3) $0 \notin conv\{k_1, .., k_m\}$, where $k_1, .., k_m$ are the eigenvalues of $D_y J_y(y, z)|_{(0.0)}$, and $conv\{k_1, .., k_m\}$ is the convex envelope of $\{k_1, .., k_m\}$;

4) the numbers k_i and λ_j are not related by any equation of the form

$$\sum_{i=1}^{m} m_i k_i = \lambda_j, \tag{63}$$

where λ_j ($j = 1, .., p$) are eigenvalues of $D_z J_z(y, z)|_{(0,0)}$, and $m_i \geq 0$ are integers, $\sum_{i=1}^{m} m_i > 0$.

Let us consider analytical manifold $(y, \Phi(y))$ in U in the neighborhood of zero ($\Phi(0) = 0$) and write for it the differential invariance equation with the projector (61):

$$(D_y\Phi(y))J_y(y, \Phi(y)) = J_z(y, \Phi(y)). \tag{64}$$

Lyapunov Auxiliary theorem. Given conditions 1-4, the equation (60) has unique analytical in the neighborhood of zero solution, satisfying condition $\Phi(0) = 0$.

Recently new generalizations and applications of this theorem [30, 101, 102, 103] were developed.

Studying germs of invariant manifolds using Taylor expansion is definitely useful from the theoretical as well as from the practical perspective. But the well known difficulties pertinent to this approach, of convergence, small denominators (connected with proximity to the resonances (63)) and others call for development of different methods. A hint can be found in the famous **KAM** theory: one should use iterative methods instead of Taylor expansion [25, 26, 27]. Further we present two such methods:

- Newton method subject to incomplete linearization;
- Relaxation method which is the Galerkin-type approximation to Newton's method with projection on defect of invariance (36), i.e. on the right hand side of equation (41).

5 Entropy, quasiequilibrium and projectors field

Projector operators P_y contribute both to the invariance equation (35), and to the film extension of the dynamics (41). Limiting results, exact solutions, etc. depend only weakly on the particular choice of projectors, or do not depend at all on it. However, the validity of approximations obtained in each iteration step towards the limit does strongly depend on the choice of the projector. Moreover, if we want that each approximate solution should be consistent with such physically crucial conditions as the second law of thermodynamics (the entropy of the isolated systems increases), then the choice of the projector becomes practically unique.

In this section we consider the main ingredients for constructing the projector, based on two additional structures: (a) The moment parameterization, and (b) The entropy and the entropic scalar product.

5.1 Moment parameterization

Same as in the previous section, let a regular map (projection) is defined, $\Pi : U \to W$. We consider only maps $F : W \to U$ which satisfy $\Pi \circ F = 1$. We seek slow invariant manifolds among such maps (a natural remark is in order here: Sometimes one has to consider F which are defined not on the whole W but only on some subset of it). In this case, the unique projector consistent with the given structure is the superposition of the differentials:

$$P_y J = (D_y F)_y \circ (D_x \Pi)_{F(y)}. \tag{65}$$

In the language of differential equations, formula (65) has the following significance: First, equation (34) is projected,

$$\frac{dy}{dt} = (D_x \Pi)_{F(y)} J(F(y), \tag{66}$$

second, the latter equation is lifted back to U with the help of F and its differential,

$$x(t) = F(y(t)),\ \left.\frac{dx}{dt}\right|_{x=F(y)} = (D_y F)_y J. \tag{67}$$

The most standard example of the construction just described is as follows: x is the distribution density, $y = \Pi(x)$ is the set of selected moments of this density, $F : y \to x$ is a "closure assumption", which constructs a distribution density parameterized by the values of the moments y. Another standard example is relevant to problems of chemical kinetics: x is a detailed description of the reacting species (including all the intermediates and radicals), y are concentrations of stable reactants and products of the reaction.

The moment parameterization and moment projectors (65) are mostly encountered in the applications. However, they have a set of shortcomings. In particular, it is by far not always that the moment projection *transforms a dissipative system into another dissipative system.* Of course, for invariant $F(y)$ *any* projector transforms the dissipative system into the dissipative system. However, for various approximations to invariant manifolds (closure assumptions) this is already not the case [4]. The property of projectors to *preserve the type of the dynamics* will be taken below for one of the requirements.

5.2 Entropy and quasiequilibrium

The dissipation properties of the system (34) are described by specifying the *entropy* S, the distinguished *Lyapunov function* which monotonically increases along solutions to equation (34). In a certain sense, this Lyapunov function is more fundamental than the system (34). That is, usually, the entropy is known much better than the right hand side of equation (34). For example, in chemical kinetics, the entropy is obtained from the *equilibrium* data. The same holds for other Lyapunov functions, which are defined by the entropy and by specification of the reaction conditions (the free energy, $U - TS$, for the isothermal isochoric processes, the free enthalpy, $U - TH$, for the isothermal isobaric processes etc.). On physical grounds, all these entropic Lyapunov functions are proportional (up to additive constants) to the entropy of the minimal isolated system which includes the system under study [107]. In general, with some abuse of language, we term the Lyapunov functional S the entropy elsewhere below, although it is a different functional for non-isolated systems.

Thus, we assume that a concave functional S is defined in U, such that it takes maximum in an inner point $x^* \in U$. This point is termed the equilibrium.

For any dissipative system (34) under consideration in U, the derivative of S due to equation (34) must be nonnegative,

$$\left.\frac{dS}{dt}\right|_x = (D_x S)(J(x)) \geq 0, \tag{68}$$

where $D_x S$ is the linear functional, the differential of the entropy, while the equality in (68) is achieved only in the equilibrium $x = x^*$.

Most of the works on nonequilibrium thermodynamics deal with corrections to quasiequilibrium approximations, or with applications of these approximations (with or without corrections). This viewpoint is not the only possible but it proves very efficient for the construction of a variety of useful models, approximations and equations, as well as methods to solve them [5]

[4] See, e. g. a discussion of this problem for the Tamm–Mott-Smith approximation for the strong shock wave in

[5] From time to time it is discussed in the literature, who was the first to introduce the quasiequilibrium approximations, and how to interpret them. At least a part of the discussion is due to a different rôle the quasiequilibrium plays in the entropy–conserving and the dissipative dynamics. The very first use of the entropy maximization dates back to the classical work of G. W. Gibbs [121], but it was first claimed for a principle by E. T. Jaynes [108]. Probably the first explicit and systematic use of quasiequilibria to derive dissipation from entropy–conserving systems is due to the works of D. N. Zubarev. Recent detailed exposition is given in [110]. For dissipative systems, the use of the quasiequilibrium to reduce description can be traced to the works of H. Grad on the Boltzmann equation [113]. The viewpoint of two of the present authors (ANG and IVK) was influenced by the papers by L. I. Rozonoer and co-workers, in particular, [122, 123, 124]. A detailed exposition of the quasiequilibrium approximation for Markov

Let a *linear* moment parameterization, $\Pi : E \to L$, where Π is a linear operator, be defined in U, and let $W = \Pi(U)$. *Quasiequilibrium* (or restricted equilibrium, or conditional equilibrium) is the embedding, $F^* : W \to U$, which puts into correspondence to each $y \in W$ the solution to the entropy maximization problem:

$$S(x) \to \max, \ \Pi(x) = y. \tag{69}$$

We assume that, for each $y \in \mathrm{int}\, W$, there exists the unique solution $F^*(y) \in \mathrm{int}\, U$ to the problem (69). This solution, $F^*(y)$, is called the quasiequilibrium, corresponding to the value y of the macroscopic variables. The set of quasiequilibria $F^*(y)$, $y \in W$, forms a manifold in $\mathrm{int} U$, parameterized by the values of the macroscopic variables $y \in W$.

Let us specify some notations: E^T is the adjoint to the E space. Adjoint spaces and operators will be indicated by ^{T}, whereas notation * is earmarked for equilibria and quasiequilibria.

Furthermore, $[l, x]$ is the result of application of the functional $l \in E^T$ to the vector $x \in E$. We recall that, for an operator $A : E_1 \to E_2$, the adjoint operator, $A^T : E_1^T \to E_2^T$ is defined by the following relation: For any $l \in E_2^T$ and $x \in E_1$,

$$[l, Ax] = [A^T l, x].$$

Next, $D_x S(x) \in E^T$ is the differential of the entropy functional $S(x)$, $D_x^2 S(x)$ is the second differential of the entropy functional $S(x)$. The corresponding quadratic functional $D_x^2 S(x)(z, z)$ on E is defined by the Taylor formula,

$$S(x + z) = S(x) + [D_x S(x), z] + \frac{1}{2} D_x^2 S(x)(z, z) + o(\|z\|^2). \tag{70}$$

We keep the same notation for the corresponding symmetric bilinear form, $D_x^2 S(x)(z, p)$, and also for the linear operator, $D_x^2 S(x) : E \to E^T$, defined by the formula,

$$[D_x^2 S(x) z, p] = D_x^2 S(x)(z, p).$$

In the latter formula, on the left hand side, there is the operator, on the right hand side there is the bilinear form. Operator $D_x^2 S(x)$ is symmetric on E, $D_x^2 S(x)^T = D_x^2 S(x)$.

Concavity of the entropy S means that, for any $z \in E$, the inequality holds, $D_x^2 S(x)(z, z) \leq 0$; in the restriction onto the affine subspace parallel to $\ker \Pi$ we assume the strict concavity, $D_x^2 S(x)(z, z) < 0$, if $z \in \ker \Pi$, and if $z \neq 0$.

In the remainder of this subsection we are going to derive the important object, projector onto the tangent space of the quasiequilibrium manifold.

---

chains is given in the book [107] (Chapter 3, *Quasiequilibrium and entropy maximum*, pp. 92-122), and for the BBGKY hierarchy in the paper [125]. We have applied maximum entropy principle to the description the universal dependence the 3-particle distribution function F_3 on the 2-particle distribution function F_2 in classical systems with binary interactions [126]. For a recent discussion the quasiequilibrium moment closure hierarchies for the Boltzmann equation [123] see the paper of C. D. Levermore [127]. A very general discussion of the maximum entropy principle with applications to dissipative kinetics is given in the review [128].

Let us compute the derivative $D_y F^*(y)$. For this purpose, let us apply the method of Lagrange multipliers: There exists such a linear functional $\Lambda(y) \in (E/L)^T$, that

$$D_x S(x)|_{F^*(y)} = \Lambda(y) \cdot \Pi, \ \Pi(F^*(y)) = y, \tag{71}$$

or

$$D_x S(x)|_{F^*(y)} = \Pi^T \cdot \Lambda(y), \ \Pi(F^*(y)) = y. \tag{72}$$

From equation (72) we get,

$$\Pi(D_y F^*(y)) = 1_{(E/L)}, \tag{73}$$

where we have indicated the space in which the unit operator acts. Next, using the latter expression, we transform the differential of the equation (71),

$$D_y \Lambda = (\Pi (D_x^2 S)^{-1}_{F^*(y)} \Pi^T)^{-1}, \tag{74}$$

and, consequently,

$$D_y F^*(y) = (D_x^2 S)^{-1}_{F^*(y)} \Pi^T (\Pi (D_x^2 S)^{-1}_{F^*(y)} \Pi^T)^{-1}. \tag{75}$$

Notice that, elsewhere in equation (75), operator $(D_x^2 S)^{-1}$ acts on the linear functionals from $\mathrm{Im}\Pi^T$. These functionals are precisely those which become zero on L (that is, on $\ker\Pi$), or, which is the same, those which can be represented as linear functionals of macroscopic variables.

The tangent space to the quasiequilibrium manifold in the point $F^*(y)$ is the image of the operator $D_y F^*(y)$:

$$\mathrm{Im}\,(D_y F^*(y)) = (D_x^2 S)^{-1}_{F^*(y)} \mathrm{Im}\Pi^T = (D_x^2 S)^{-1}_{F^*(y)} \mathrm{Ann}(\ker \Pi) \tag{76}$$

where $\mathrm{Ann}(\ker \Pi)$ is the set of linear functionals which become zero on $\ker \Pi$. Another way to write equation (76) is the following:

$$x \in \mathrm{Im}\,(D_y F^*(y)) \Leftrightarrow (D_x^2 S)_{F^*(y)}(z, p) = 0, \ p \in \ker \Pi \tag{77}$$

This means that $\mathrm{Im}\,(D_y F^*(y))$ is the orthogonal completement of $\ker \Pi$ in E with respect to the scalar product,

$$\langle z|p \rangle_{F^*(y)} = -(D_x^2 S)_{F^*(y)}(z, p). \tag{78}$$

The entropic scalar product (78) appears often in the constructions below. (Usually, IT becomes the scalar product indeed after the conservation laws are excluded). Let us denote as $T_y = \mathrm{Im}(D_y F^*(y))$ the tangent space to the quasiequilibrium manifold in the point $F^*(y)$. Important role in the construction of quasiequilibrium dynamics and its generalizations is played by the quasiequilibrium projector, an operator which projects

E on T_y parallel to $\ker \Pi$. This is the orthogonal projector with respect to the entropic scalar product, $P^*_y : E \to T_y$:

$$P^*_y = D_y F^*(y) \cdot \Pi = \left(D^2_x S|_{F^*(y)} \right)^{-1} \Pi^T \left(m \left(D^2_x S|_{F^*(y)} \right)^{-1} \Pi^T \right)^{-1} \Pi. \tag{79}$$

It is straightforward to check the equality $P^{*2}_y = P^*_y$, and the self-adjointness of P^*_y with respect to entropic scalar product (78). Thus, we have introduced the basic constructions: Quasiequilibrium manifold, entropic scalar product, and quasiequilibrium projector.

The construction of the quasiequilibrium allows for the following generalization: Almost every manifold can be represented as a set of minimizers of the entropy under linear constrains. However, in contrast to the standard quasiequilibrium, these linear constrains will depend, generally speaking, on the point on the manifold.

So, let the manifold $\Omega = F(W) \subset U$ be given. This is a parametric set of distribution function, however, now macroscopic variables y are not functionals on R or U but just parameters defining points on the manifold. The problem is how to extend definitions of y onto a neighborhood of $F(W)$ in such a way that $F(W)$ will appear as the solution to the variational problem:

$$S(x) \to \max, \ \Pi(x) = y. \tag{80}$$

For each point $F(y)$, we identify $T_y \in E$, the tangent space to the manifold Ω in F_y, and subspace $Y_y \subset E$, which depends smoothly on y, and which has the property, $Y_y \bigoplus T_y = E$. Let us define $\Pi(x)$ in the neighborhood of $F(W)$ in such a way, that

$$\Pi(x) = y, \ \text{if} \ x - F(y) \in Y_y. \tag{81}$$

The point $F(y)$ will be the solution of the quasiequilibrium problem (80) if and only if

$$D_x S(x)|_{F(y)} \in \text{Ann } Y_y. \tag{82}$$

That is, if and only if $Y_y \subset \ker D_x S(x)|_{F(y)}$. It is always possible to construct subspaces Y_y with the properties just specified, at least locally, if the functional $D_x S|_{F(y)}$ is not identically equal to zero on T_y.

The construction just described allows to consider practically any manifold as a quasiequilibrium. This construction is required when one seeks the induced dynamics on a given manifold. Then the vector fields are projected on T_y parallel to Y_y, and this preserves intact the basic properties of the quasiequilibrium approximations.

Let us return to usual linear moment parametrization. *Quasiequilibrium entropy* $S(y)$ is a functional on W. It is defined as the value of the entropy on the corresponding quasiequilibrium $x = F^*(y)$:

$$S(y) = S(F^*(y)) \tag{83}$$

Quasiequilibrium dynamics is a dynamics on W, defined by the equation (66) for the quasiequilibrium $F^*(y)$:

$$\frac{dy}{dt} = \Pi J(F^*(y)). \tag{84}$$

Here Π is constant linear operator (in general case (66 it may be nonlinear). The corresponding quasiequilibrium dynamics on the quasiequilibrium manifold $F^*(W)$ is defined using the projector (65):

$$\frac{dx}{dt} = P_y^*|_{x=F^*(y)} J(x) = (D_y F^*)_{x=F^*(y)} \Pi J(x),\ x \in F^*(W). \tag{85}$$

The orthogonal projector P_y^* in the right hand side of equation (85) can be explicitly written using the second derivative of S and the operator Π (79). Let's remind that the only distinguished scalar product in E is the entropic scalar product (78):

$$\langle z, p \rangle_x = -(D_x^2 S)_x(z,p) \tag{86}$$

It depends on the point $x \in U$. This dependence $\langle | \rangle_x$ determines in U the structure of Riemann space.

The most important property of the quasiequilibrium system (85) is given by the *conservation of the dynamics type* theorem: if for the original dynamic system (34) $\frac{dS}{dt} \geq 0$, then for the quasiequilibrium dynamics $\frac{dS}{dt} \geq 0$. If for the original dynamic system (34) $\frac{dS}{dt} = 0$ (conservative system), then for the quasiequilibrium dynamics $\frac{dS}{dt} = 0$ as well.

5.3 Thermodynamic projector without a priori parameterization

Quasiequilibrium manifolds is a place where entropy and moment parameterization meet each other. Projectors P_y for a quasiequilibrium manifold is nothing but the orthogonal projector with respect to the entropic scalar product $\langle | \rangle_x$ projector (79). The quasiequilibrium projector preserves the type of dynamics. Note that in order to preserve the type of dynamics we needed only one condition to be satisfied,

$$\ker P_y \subset \ker (D_x S)_{x=F(y)}. \tag{87}$$

Let us require that the field of projectors, $P(x,T)$, is defined for any x and T, if

$$T \not\subset \ker D_x S. \tag{88}$$

It follows immediately from these conditions that in the equilibrium, $P(x^*, T)$ is the orthogonal projector onto T (ortogonality with respect to entropic scalar product $\langle | \rangle_{x^*}$).

The field of projectors is constructed in the neighborhood of the equilibrium based on the requirement of maximal smoothness of P as a function of $g_x = D_x S$ and x. It turns out that to the first order in the deviations $x - x^*$ and $g_x - g_{x^*}$, the projector is defined uniquely. Let us first describe the construction of the projector, and next discuss its uniqueness.

Let the subspace $T \subset E$, the point x, and the differential of the entropy in this point, $g = D_x S$, be defined such that the transversality condition (88) is satisfied. Let us define $T_0 = T \bigcap \ker g_x$. By the condition (88), $T_0 \neq T$. Let us denote, $e_g = e_g(T) \in T$ the vector in T, such that e_g is orthogonal to T_0, and is normalized by the condition $g(e_g) = 1$. Vector e_g is defined unambiguously. Projector $P_{S,x} = P(x, T)$ is defined as follows: For any $z \in E$,

$$P_{S,x}(z) = P_0(z) + e_g g_x(z), \tag{89}$$

where P_0 is the orthogonal projector on T_0 (orthogonality with respect to the entropic scalar product $\langle|\rangle_x$). Entropic projector (89) depends on the point x through the x-dependence of the scalar product $\langle|\rangle_x$, and also through the differential of S in x, the functional g_x.

Obviously, $P(z) = 0$ implies $g(z) = 0$, that is, the thermodynamicity requirement (87) is satisfied. Uniqueness of the thermodynamic projector (89) is supported by the requirement of the *maximal smoothness* (analyticity) [7] of the projector as a function of g_x and $\langle|\rangle_x$, and is done in two steps which we sketch here:

1. Considering the expansion of the entropy in the equilibrium up to the quadratic terms, one shows that in the equilibrium the thermodynamic projector is the orthogonal projector with respect to the scalar product $\langle|\rangle_{x^*}$.

2. For a given g, one considers auxiliary dissipative dynamic systems (34), which satisfy the condition: For every $x' \in U$, it holds, $g_x(J(x')) = 0$, that is, g_x defines an additional linear conservation law for the auxiliary systems. For the auxiliary systems, the point x is the equilibrium. Eliminating the linear conservation law g_x, and using the result of the previous point, we end up with the formula (89).

Thus, the entropic structure defines unambiguously the field of projectors (89), for which the dynamics of *any* dissipative system (34) projected on *any* closure assumption remains dissipative.

Example 1: Quasiequilibrium projector and defect of invariance for the Local Maxwellians manifold for the Boltzmann equation

The Boltzmann equation is one of the everlasting equations. It remains the important source for the model reduction problems. By this subsection we start the series of examples for the Boltzmann equation.

Difficulties of classical methods of the Boltzmann equation theory

As was mentioned above, the first systematic and (at least partially) successful method of constructing invariant manifolds for dissipative systems was the celebrated *Chapman-Enskog method* [43] for the Boltzmann kinetic equation. The main difficulty of the Chapman-Enskog method [43] are "nonphysical" properties of high-order approximations. This was stated by a number of authors and was discussed in detail in [69]. In particular, as it was noted in [45], the Burnett approximation results in a short-wave instability of the acoustic spectra. This fact contradicts the H-theorem (cf. in [45]). The Hilbert expansion contains secular terms [69]. The latter contradicts the H-theorem.

The other difficulties of both of these methods are: the restriction upon the choice of initial approximation (the local equilibrium approximation), the demand for a small parameter, and the usage of slowly converging Taylor expansion. These difficulties never allow a direct transfer of these methods on essentially nonequilibrium situations.

The main difficulty of the Grad method [113] is the uncontrollability of the chosen approximation. An extension of the list of moments can result in a certain success, but it can also give nothing. Difficulties of moment expansion in the problems of shock waves and sound propagation can be seen in [69].

Many attempts were made to make these methods more perfect. For the Chapman-Enskog and Hilbert methods these attempts are based in general on some "good" rearrangement of expansions (e.g. neglecting high-order derivatives [69], reexpanding [69], Pade approximations and partial summing [22, 129, 120], etc.). This type of work with formal series is wide spread in physics. Sometimes the results are surprisingly good - from the renormalization theory in quantum fields to the Percus-Yevick equation and the ring-operator in statistical mechanics. However, one should realize that a success is not at all guaranteed. Moreover, rearrangements never remove the restriction upon the choice of the initial local equilibrium approximation.

Attempts to improve the Grad method are based on quasiequilibrium approximations [122, 123]. It was found in [123] that Grad distributions are linearized versions of appropriate quasiequilibrium approximations (see also the late papers [129, 130, 127]). A method which treats fluxes (e.g. moments with respect to collision integrals) as independent variables in a quasiequilibrium description was introduced in [140, 129, 142, 130].

An important feature of quasiequilibrium approximations is that they are always thermodynamic, i.e. they are concordant with the H-theorem due to their construction. However, quasiequilibrium approximations do not remove the uncontrollability of the Grad method.

Boltzmann Equation (BE)

The phase space E consists of distribution functions $f(\boldsymbol{v}, \boldsymbol{x})$ which depend on the spatial variable $\boldsymbol{x}$ and on velocity variable $\boldsymbol{v}$. The variable $\boldsymbol{x}$ spans an open domain $\Omega^3_{\boldsymbol{x}} \subseteq \mathbf{R}_{\boldsymbol{x}}$, and the variable $\boldsymbol{v}$ spans the space $\mathbf{R}^3_{\boldsymbol{v}}$. We require that $f(\boldsymbol{v}, \boldsymbol{x}) \in F$ are nonnegative functions, and also that the following integrals are finite for every $\boldsymbol{x} \in \Omega_{\boldsymbol{x}}$ (the existence of moments and of the entropy):

$$I^{(i_1 i_2 i_3)}_{\boldsymbol{x}}(f) = \int v_1^{i_1} v_2^{i_2} v_3^{i_3} f(\boldsymbol{v}, \boldsymbol{x}) d^3\boldsymbol{v}, i_1 \geq 0, i_2 \geq 0, i_3 \geq 0; \tag{90}$$

$$H_{\boldsymbol{x}}(f) = \int f(\boldsymbol{v}, \boldsymbol{x})(\ln f(\boldsymbol{v}, \boldsymbol{x}) - 1) d^3\boldsymbol{v}, H(f) = \int H_{\boldsymbol{x}}(f) d^3\boldsymbol{x} \tag{91}$$

Here and below integration in $\boldsymbol{v}$ is made over $\mathbf{R}^3_{\boldsymbol{v}}$, and it is made over $\Omega_{\boldsymbol{x}}$ in $\boldsymbol{x}$. For every fixed $x \in \Omega_{\boldsymbol{x}}$, $I^{(\dots)}_{\boldsymbol{x}}$ and $H_{\boldsymbol{x}}$ might be treated as functionals defined in F.

We write BE in the form of (34) using standard notations [69]:

$$\frac{\partial f}{\partial t} = J(f),\ J(f) = -v_s \frac{\partial f}{\partial x_s} + Q(f, f) \tag{92}$$

Here and further a summation in two repeated indices is assumed, and $Q(f, f)$ stands for the Boltzmann collision integral [1]. The latter represents the dissipative part of the vector field $J(f)$ (92).

In this paper we consider the case when boundary conditions for equation (92) *are relevant to the local with respect to* $\boldsymbol{x}$ *form of the* H*-theorem.*

For every fixed $\boldsymbol{x}$, we denote as $H^0_{\boldsymbol{x}}(f)$ the space of linear functionals $\sum_{i=0}^4 a_i(\boldsymbol{x}) \int \psi_i(\boldsymbol{v}) f(\boldsymbol{v}, \boldsymbol{x}) d^3\boldsymbol{v}$, where $\psi_i(\boldsymbol{v})$ represent summational invariants of a collision $[1, 2](\psi_0 = 1, \psi_i = v_i, i = 1, 2, 3, \psi_4 = v^2)$. We write $(\mathrm{mod} H^0_{\boldsymbol{x}}(f))$ if an expression is valid within the accuracy of adding a functional from $H^0_{\boldsymbol{x}}(f)$. The local H-theorem states: for any functional

$$H_{\boldsymbol{x}}(f) = \int f(\boldsymbol{v}, \boldsymbol{x})(\ln f(\boldsymbol{v}, \boldsymbol{x}) - 1) d^3\boldsymbol{v}\ (\mathrm{mod} H^0_{\boldsymbol{x}}(f)) \tag{93}$$

the following inequality is valid:

$$dH_{\boldsymbol{x}}(f)/dt \equiv \int Q(f, f)|_{f = f(\boldsymbol{v}, \boldsymbol{x})} \ln f(\boldsymbol{v}, \boldsymbol{x}) d^3\boldsymbol{v} \leq 0 \tag{94}$$

Expression (94) is equal to zero if and only if $\ln f = \sum_{i=0}^4 a_i(\boldsymbol{x}) \psi_i(\boldsymbol{v})$.

Although all functionals (93) are equivalent in the sense of the H-theorem, it is convenient to deal with the functional

$$H_{\boldsymbol{x}}(f) = \int f(\boldsymbol{v}, \boldsymbol{x})(\ln f(\boldsymbol{v}, \boldsymbol{x}) - 1) d^3\boldsymbol{v}.$$

All what was said in previous sections can be applied to BE (92). Now we will discuss some specific points.

Local manifolds

Although the general description of manifolds $\Omega \subset F$ (Section 2.1) holds as well for BE, a specific class of manifolds might be defined due to the different character of spatial and of velocity dependencies in BE vector field (92). These manifolds will be called **local manifolds**, and they are constructed as follows. Denote as $F_{\rm loc}$ the set of functions $f(\boldsymbol{v})$ with finite integrals

$$
\begin{aligned}
&a) I^{(i_1 i_2 i_3)}(f) = \int v_1^{i_1} v_2^{i_2} v_3^{i_3} f(\boldsymbol{v}) d^3\boldsymbol{v}, i_1 \geq 0, i_2 \geq 0, i_3 \geq 0; \\
&b) H(f) = \int f(\boldsymbol{v}) \ln f(\boldsymbol{v}) d^3\boldsymbol{v} \qquad (95)
\end{aligned}
$$

In order to construct a local manifold in F, we, firstly, consider a manifold in $F_{\rm loc}$. Namely, we define a domain $A \subset B$, where B is a linear space, and consider a smooth immersion $A \to F_{\rm loc}$: $a \to f(a, \boldsymbol{v})$. The set of functions $f(a, \boldsymbol{v}) \in F_{\rm loc}$, where a spans the domain A, is a manifold in $F_{\rm loc}$. Secondly, we consider *all* bounded and sufficiently smooth functions $a(\boldsymbol{x})$: $\Omega_{\boldsymbol{x}} \to A$, and we define the local manifold in F as the set of functions $f(a(\boldsymbol{x}), \boldsymbol{v})$. Roughly speaking, the local manifold is a set of functions which are parameterized with $\boldsymbol{x}$-dependent functions $a(\boldsymbol{x})$. A local manifold will be called a **locally finite-dimensional** manifold if B is a finite- dimensional linear space.

Locally finite-dimensional manifolds are a natural source of initial approximations for constructing dynamic invariant manifolds in BE theory. For example, the Tamm-Mott-Smith (TMS) approximation gives us locally two-dimensional manifold $\{f(a_-, a_+)\}$ which consists of distributions

$$f(a_-, a_+) = a_- f_- + a_+ f_+ \qquad (96)$$

Here a_- and a_+ (the coordinates on the manifold $\Omega_{\rm TMS} = \{f(a_-, a_+)\}$) are non-negative real functions of the position vector $\boldsymbol{x}$, and f_- and f_+ are fixed Maxwellians.

Next example is locally five-dimensional manifold $\{f(n, \boldsymbol{u}, T)\}$ which consists of local Maxwellians (LM). The LM manifold consists of distributions f_0 which are labeled with parameters $n, \boldsymbol{u}$, and T:

$$f_0(n, \boldsymbol{u}, T) = n \left(\frac{2\pi k_B T}{m} \right)^{-3/2} \exp \left(- \frac{m(\boldsymbol{v} - \boldsymbol{u})^2}{2 k_B T} \right) \qquad (97)$$

Parameters $n, \boldsymbol{u}$, and T in (97) are functions depending on $\boldsymbol{x}$. In this section we will not indicate this dependency explicitly.

Distribution $f_0(n, \boldsymbol{u}, T)$ is the unique solution of the variational problem:

$$
\begin{aligned}
& H(f) = \int f \ln f d^3\boldsymbol{v} \to \min \\
\text{for:} \quad & \\
& M_0(f) = \int 1 \cdot f d^3\boldsymbol{v};
\end{aligned}
$$

$$M_i(f) = \int v_i f d^3\boldsymbol{v} = nu_i, i = 1, 2, 3;$$
$$M_4(f) = \int v^2 f d^3\boldsymbol{v} = \frac{3nk_BT}{m} + nu^2 \tag{98}$$

Hence, the LM manifold is a quasiequilibrium manifold. Considering $n, \boldsymbol{u}$, and T as five scalar parameters (see the remark on locality in Section 3), we see that LM manifold is parameterized with the values of $M_s(f), s = 0, \ldots, 4$, which are defined in the neighborhood of LM manifold. It is sometimes convenient to consider the variables $M_s(f_0), s = 0, \ldots, 4$, as new coordinates on LM manifold. The relationship between the sets $\{M_s(f_0)\}$ and $\{n, \boldsymbol{u}, T\}$ is:

$$n = M_0; u_i = M_0^{-1}M_i, i = 1, 2, 3; T = \frac{m}{3k_B}M_0^{-1}(M_4 - M_0^{-1}M_iM_i) \tag{99}$$

This is a standard moment parametrization of a quasiequilibrium manifold.

Thermodynamic quasiequilibrium projector

Thermodynamic quasiequilibrium projector $P_{f_0(n,\boldsymbol{u},T)}(J)$ onto the tangent space $T_{f_0(n,\boldsymbol{u},T)}$ is defined as:

$$P_{f_0(n,\boldsymbol{u},T)}(J) = \sum_{s=0}^{4} \frac{\partial f_0(n, \boldsymbol{u}, T)}{\partial M_s} \int \psi_s J d^3\boldsymbol{v} \tag{100}$$

Here we have assumed that $n, \boldsymbol{u}$, and T are functions of $M_0, \ldots, M_4$ (see relationship (99)), and

$$\psi_0 = 1, \psi_i = v_i, i = 1, 2, 3, \psi_4 = v^2 \tag{101}$$

Calculating derivatives in (100), and next returning to variables $n, \boldsymbol{u}$, and T, we obtain:

$$\begin{aligned} P_{f_0(n,\boldsymbol{u},T)}(J) = f_0(n, \boldsymbol{u}, T) \Bigg\{ \Bigg[\frac{1}{n} - \frac{mu_i}{nk_BT}(v_i - u_i) + \left(\frac{mu^2}{3nk_B} - \frac{T}{n}\right)\Bigg(\frac{m(\boldsymbol{v} - \boldsymbol{u})^2}{2k_BT^2} - \\ - \frac{3}{2T}\Bigg)\Bigg] \int 1 \cdot J d^3\boldsymbol{v} + \left[\frac{m}{nk_BT}(v_i - u_i) - \frac{2mu_i}{3nk_B}\left(\frac{m(\boldsymbol{v} - \boldsymbol{u})^2}{2k_BT^2} - \frac{3}{2T}\right)\right] \int v_i J d^3\boldsymbol{v} + \\ + \frac{m}{3nk_B}\left(\frac{m(\boldsymbol{v} - \boldsymbol{u})^2}{2k_BT^2} - \frac{3}{2T}\right) \int \boldsymbol{v}^2 J d^3\boldsymbol{v} \Bigg\} \end{aligned} \tag{102}$$

It is sometimes convenient to rewrite (102) as:

$$P_{f_0(n,\boldsymbol{u},T)}(J) = f_0(n, \boldsymbol{u}, T) \sum_{s=0}^{4} \psi^{(s)}_{f_0(n,\boldsymbol{u},T)} \int \psi^{(s)}_{f_0(n,\boldsymbol{u},T)} J d^3\boldsymbol{v} \tag{103}$$

Here

$$\psi^{(0)}_{f_0(n,\boldsymbol{u},T)} = n^{-1/2}, \qquad \psi^{(i)}_{f_0(n,\boldsymbol{u},T)} = (2/n)^{1/2}c_i, i = 1, 2, 3,$$
$$\psi^{(4)}_{f_0(n,\boldsymbol{u},T)} = (2/3n)^{1/2}(c^2 - (3/2)); \qquad c_i = (m/2k_BT)^{1/2}(v_i - u_i) \tag{104}$$

It is easy to check that

$$\int f_0(n,\boldsymbol{u},T)\psi^{(k)}_{f_0(n,\boldsymbol{u},T)}\psi^{(l)}_{f_0(n,\boldsymbol{u},T)}d^3\boldsymbol{v} = \delta_{kl} \tag{105}$$

Here δ_{kl} is the Kronecker delta.

Defect of invariance for the LM manifold

The defect of invariance for the LM manifold at the point $f_0(n,\boldsymbol{u},T)$ for the BE is:

$$\begin{aligned}\Delta(f_0(n,\boldsymbol{u},T)) &= P_{f_0(n,\boldsymbol{u},T)}\left(-(v_s-u_s)\frac{\partial f_0(n,\boldsymbol{u},T)}{\partial x_s} + Q(f_0(n,\boldsymbol{u},T))\right) - \\ &\quad -\left(-(v_s-u_s)\frac{\partial f_0(n,\boldsymbol{u},T)}{\partial x_s} + Q(f_0(n,\boldsymbol{u},T))\right) = \\ &= P_{f_0(n,\boldsymbol{u},T)}\left(-(v_s-u_s)\frac{\partial f_0(n,\boldsymbol{u},T)}{\partial x_s}\right) + (v_s-u_s)\frac{\partial f_0(n,\boldsymbol{u},T)}{\partial x_s}\end{aligned} \tag{106}$$

Substituting (102) into (106), we obtain:

$$\begin{aligned}\Delta(f_0(n,\boldsymbol{u},T)) &= f_0(n,\boldsymbol{u},T)\left\{\left(\frac{m(\boldsymbol{v}-\boldsymbol{u})^2}{2k_BT} - \frac{5}{2}\right)(v_i-u_i)\frac{\partial \ln T}{\partial x_i} + \right. \\ &\quad \left. + \frac{m}{k_BT}(((v_i-u_i)(v_s-u_s) - \frac{1}{3}\delta_{is}(\boldsymbol{v}-\boldsymbol{u})^2)\frac{\partial u_s}{\partial x_i}\right\}\end{aligned} \tag{107}$$

The LM manifold is not a dynamic invariant manifold of the Boltzmann equation and the defect (107) is not identical to zero.

Example 2: Scattering rates versus moments: alternative Grad equations

In this subsection scattering rates (moments of collision integral) are treated as new independent variables, and as an alternative to moments of the distribution function, to describe the rarefied gas near local equilibrium. A version of entropy maximum principle is used to derive the Grad-like description in terms of a finite number of scattering rates. New equations are compared to the Grad moment system in the heat non-conductive case. Estimations for hard spheres demonstrate, in particular, some 10% excess of the viscosity coefficient resulting from the scattering rate description, as compared to the Grad moment estimation.

In 1949, Harold Grad [113] has extended the basic assumption behind the Hilbert and Chapman-Enskog method (the space and time dependence of the normal solutions is mediated by the five hydrodynamic moments [43]). A physical rationale behind the Grad moment method is an assumption of the decomposition of motion (i). During the time of order τ, a set of distinguished moments M' (which include the hydrodynamic moments and a subset of higher-order moment) does not change significantly as compared to the rest of the moments M'' (the fast evolution) (ii). Towards the end of the fast evolution, the values of the moments M'' become unambiguously determined by the values of the distinguished moments M', and (iii). On the time of order $\theta \gg \tau$, dynamics of the distribution function is determined by the dynamics of the distinguished moments while the rest of the moments remains to be determined by the distinguished moments (the slow evolution period).

Implementation of this picture requires an ansatz for the distribution function in order to represent the set of states visited in the course of the slow evolution. In Grad's method, these representative sets are finite-order truncations of an expansion of the distribution functions in terms of Hermit velocity tensors:

$$f_C(M', \boldsymbol{v}) = f_{LM}(\rho, \boldsymbol{u}, E, \boldsymbol{v})[1 + \sum_{(\alpha)}^{N} a_\alpha(M') H_{(\alpha)}(\boldsymbol{v} - \boldsymbol{u})], \tag{108}$$

where $H_{(\alpha)}(\boldsymbol{v}-\boldsymbol{u})$ are various Hermit tensor polynomials, orthogonal with the weight f_{LM}, while coefficient $a_{(\alpha)}(M')$ are known functions of the distinguished moments M', and N is the highest order of M'. Other moments are functions of M': $M'' = M''(f_C(M'))$.

Slow evolution of distinguished moments is found upon substitution of Eq. (108) into the Boltzmann equation and finding the moments of the resulting expression (Grad's moment equations). Following Grad, this extremely simple approximation can be improved by extending the list of distinguished moments. The most well known is Grad's thirteen-moment approximation where the set of distinguished moments consists of five hydrodynamic moments, five components of the traceless stress tensor $\sigma_{ij} = \int m[(v_i - u_i)(v_j - u_j) - \delta_{ij}(\boldsymbol{v} - \boldsymbol{u})^2/3] f d\boldsymbol{v}$, and of the three components of the heat flux vector $q_i = \int (v_i - u_i) m (\boldsymbol{v} - \boldsymbol{u})^2/2 f d\boldsymbol{v}$.

The time evolution hypothesis cannot be evaluated for its validity within the framework of Grad's approach. It is not surprising therefore that Grad's methods failed to work in situations where it was (unmotivatedly) supposed to, primarily, in the phenomena with sharp time-space dependence such as the strong shock wave. On the other hand, Grad's method was quite successful for describing transition between parabolic and hyperbolic propagation, in particular the second sound effect in massive solids at low temperatures, and, in general, situations slightly deviating from the classical Navier-Stokes- Fourier domain. Finally, the Grad method has been important background for development of phenomenological nonequilibrium thermodynamics based on hyperbolic first-order equation, the so-called EIT (extended irreversible thermodynamics [131]).

Important generalization of the Grad moment method is the concept of quasiequilibrium approximations already mentioned above. The quasiequilibrium distribution function for a set of distinguished moment M' maximizes the entropy density S for fixed M'. The quasiequilibrium manifold $\Omega^3(M)$ is the collection of the quasiequilibrium distribution functions for all admissible values of M. The quasiequilibrium approximation is the simplest and extremely useful (not only in the kinetic theory itself) implementation of the hypothesis about a decomposition: If M' are considered as slow variables, then states which could be visited in the course of rapid motion in the neighbored of $\Omega^*(M')$ belong to the planes $\Gamma_{M'} = \{f \mid m'(f - f^*(M')) = 0\}$. In this respect, the thermodynamic construction in the method of invariant manifold is a generalization of the quasiequilibrium approximation where the given manifold is equipped with a quasiequilibrium structure by choosing appropriately the macroscopic variables of the slow motion. In contrast to the quasiequilibrium, the macroscopic variables thus constructed are not obligatory moments. A text book example of the quasiequilibrium approximation is the generalized Gaussian function for $M' = \{\rho, \rho\boldsymbol{u}, P\}$ where $P_{ij} = \int v_i v_j f d\boldsymbol{v}$ is the pressure tensor. The quasiequilibrium approximation does not exist if the highest order moment is an odd polynomial of velocity (therefore, there exists no quasiequilibrium for thirteen Grad's moments). Otherwise, the Grad moment approximation is the first-order expansion of the quasiequilibrium around the local Maxwellian.

The classical Grad moment method [113] provides an approximate solution to the Boltzmann equation, and leads to a closed system of equations where hydrodynamic variables ρ, $\boldsymbol{u}$, and P (density, mean flux, and pressure) are coupled to a finite set of non-hydrodynamic variables. The latter are usually the stress tensor σ and the heat flux $\mathbf{q}$ constituting 10 and 13 moment Grad systems. The Grad method was originally introduced for diluted gases to describe regimes beyond the normal solutions [43], but later it was used, in particular, as a prototype of certain phenomenological schemes in nonequilibrium thermodynamics [131].

However, the moments do not constitute the unique system of non-hydrodynamic variables, and the exact dynamics might be equally expressed in terms of other infinite sets of variables (possibly, of a non-moment nature). Moreover, as long as one shortens the description to only a finite subset of variables, the advantage of the moment description above other systems is not obvious.

Nonlinear functionals instead of moments in the closure problem

Here we consider a new system of non-hydrodynamic variables, *scattering rates* $M^w(f)$:

$$\begin{aligned} M^w_{i_1 i_2 i_3}(f) &= \int \mu_{i_1 i_2 i_3} Q^w(f) d\boldsymbol{v}; \\ \mu_{i_1 i_2 i_3} &= m v_1^{i_1} v_2^{i_2} v_3^{i_3}, \end{aligned} \tag{109}$$

which, by definition, are the moments of the Boltzmann collision integral $Q^w(f)$:

$$Q^w(f) = \int w(\boldsymbol{v}', \boldsymbol{v}'_1, \boldsymbol{v}, \boldsymbol{v}_1) \left\{ f(\boldsymbol{v}')f(\boldsymbol{v}'_1) - f(\boldsymbol{v})f(\boldsymbol{v}_1) \right\} d\boldsymbol{v}' d\boldsymbol{v}'_1 d\boldsymbol{v}_1.$$

Here w is the probability density of a change of the velocities, $(\boldsymbol{v}, \boldsymbol{v}_1) \to (\boldsymbol{v}', \boldsymbol{v}'_1)$, of the two particles after their encounter, and w is defined by a model of pair interactions. The description in terms of the scattering rates M^w (109) is alternative to the usually treated description in terms of the moments M: $M_{i_1 i_2 i_3}(f) = \int \mu_{i_1 i_2 i_3} f d\boldsymbol{v}$.

A reason to consider scattering rates instead of the moments is that M^w (109) reflect features of the interactions because of the w incorporated in their definition, while the moments do not. For this reason we can expect that, in general, a description with a *finite* number of scattering rates will be more informative than a description provided by the same number of their moment counterparts.

To come to the Grad-like equations in terms of the scattering rates, we have to complete the following two steps:

i). To derive a hierarchy of transport equations for ρ, $\boldsymbol{u}$, P, and $M^w_{i_1 i_2 i_3}$ in a neighborhood of the local Maxwell states $f_0(\rho, \boldsymbol{u}, P)$.

ii). To truncate this hierarchy, and to come to a closed set of equations with respect to ρ, $\boldsymbol{u}$, P, and a finite number of scattering rates.

In the step (i), we derive a description with infinite number of variables, which is formally equivalent both to the Boltzmann equation near the local equilibrium, and to the description with an infinite number of moments. The approximation comes into play in the step (ii) where we reduce the description to a finite number of variables. The difference between the moment and the alternative description occurs at this point.

The program (i) and (ii) is similar to what is done in the Grad method [113], with the only exception (and this is important) that we should always use scattering rates as independent variables and not to expand them into series in moments. Consequently, we will use a method of a closure in the step (ii) that does not refer to the moment expansions. Major steps of the computation will be presented below.

Linearization

To complete the step (i), we represent f as $f_0(1+\varphi)$, where f_0 is the local Maxwellian, and we linearize the scattering rates (109) with respect to φ:

$$\begin{aligned} \Delta M^w_{i_1 i_2 i_3}(\varphi) &= \int \Delta \mu^w_{i_1 i_2 i_3} f_0 \varphi d\boldsymbol{v}; \\ \Delta \mu^w_{i_1 i_2 i_3} &= L^w(\mu_{i_1 i_2 i_3}). \end{aligned} \tag{110}$$

Here L^w is the usual linearized collision integral, divided by f_0. Though ΔM^w are linear in φ, they are not moments because their microscopic densities, $\Delta\mu^w$, are not velocity polynomials for a general case of w.

It is not difficult to derive the corresponding hierarchy of transport equations for variables $\Delta M^w_{i_1 i_2 i_3}$, ρ, $\boldsymbol{u}$, and P (we will further refer to this hierarchy as to the alternative chain): one has to calculate the time derivative of the scattering rates (109) due to the Boltzmann equation, in the linear approximation (110), and to complete the system with the five known balance equations for the hydrodynamic moments (scattering rates of the hydrodynamic moments are equal to zero due to conservation laws). The structure of the alternative chain is quite similar to that of the usual moment transport chain, and for this reason we do not reproduce it here (details of calculations can be found in [132]). One should only keep in mind that the stress tensor and the heat flux vector in the balance equations for $\boldsymbol{u}$ and P are no more independent variables, and they are expressed in terms of $\Delta M^w_{i_1 i_2 i_3}$, ρ, $\boldsymbol{u}$, and P.

Truncating the chain

To truncate the alternative chain (step (ii)), we have, first, to choose a finite set of "essential" scattering rates (110), and, second, to obtain the distribution functions which depend parametrically only on ρ, $\boldsymbol{u}$, P, and on the chosen set of scattering rates. We will restrict our consideration to a single non-hydrodynamic variable, σ^w_{ij}, which is the counterpart of the stress tensor σ_{ij}. This choice corresponds to the polynomial mv_iv_j in the expressions (109) and (110), and the resulting equations will be alternative to the 10 moment Grad system [6]. For a spherically symmetric interaction, the expression for σ^w_{ij} may be written:

$$
\begin{aligned}
\sigma^w_{ij}(\varphi) &= \int \Delta\mu^w_{ij} f_0 \varphi d\boldsymbol{v}; \qquad (111)\\
\Delta\mu^w_{ij} = L^w(mv_iv_j) &= \frac{P}{\eta^w_0(T)} S^w(c^2)\left\{c_ic_j - \frac{1}{3}\delta_{ij}c^2\right\}.
\end{aligned}
$$

Here $\eta^w_0(T)$ is the first Sonine polynomial approximation of the Chapman-Enskog viscosity coefficient (VC) [43], and, as usual, $\mathbf{c} = \sqrt{\frac{m}{2kT}}(\boldsymbol{v}-\boldsymbol{u})$. The scalar dimensionless function S^w depends only on c^2, and its form depends on the choice of interaction w.

Entropy maximization

Next, we find the functions $f^*(\rho, \boldsymbol{u}, P, \sigma^w_{ij}) = f_0(\rho, \boldsymbol{u}, P)(1 + \varphi^*(\rho, \boldsymbol{u}, P, \sigma^w_{ij}))$ which maximize the Boltzmann entropy $S(f)$ in a neighborhood of f_0 (the quadratic approximation to the entropy is valid within the accuracy of our consideration), for fixed values of σ^w_{ij}. That is, φ^* is a solution to the following conditional variational problem:

[6] To get the alternative to the 13 moment Grad equations, one should take into account the scattering counterpart of the heat flux, $q^w_i = m\int v_i \frac{v^2}{2} Q^w(f) d\boldsymbol{v}$.

$$\Delta S(\varphi) = -\frac{k_B}{2}\int f_0 \varphi^2 d\boldsymbol{v} \to \max, \tag{112}$$
$$\text{i)} \int \Delta\mu^w_{ij} f_0 \varphi d\boldsymbol{v} = \sigma^w_{ij}; \quad \text{ii)} \int \left\{1, \boldsymbol{v}, v^2\right\} f_0 \varphi d\boldsymbol{v} = 0.$$

The second (homogeneous) condition in (112) reflects that a deviation φ from the state f_0 is due only to non-hydrodynamic degrees of freedom, and it is straightforwardly satisfied for $\Delta\mu^w_{ij}$ (111).

Notice, that if we turn to the usual moment description, then condition (i) in (112) would fix the stress tensor σ_{ij} instead of its scattering counterpart σ^w_{ij}. Then the resulting function $f^*(\rho, \boldsymbol{u}, P, \sigma_{ij})$ will be exactly the 10 moment Grad approximation. It can be shown that a choice of any finite set of higher moments as the constraint (i) in (112) results in the corresponding Grad approximation. In that sense our method of constructing f^* is a direct generalization of the Grad method onto the alternative description.

The Lagrange multipliers method gives straightforwardly the solution to the problem (112). After the alternative chain is closed with the functions $f^*(\rho, \boldsymbol{u}, P, \sigma^w_{ij})$, the step (ii) is completed, and we arrive at a set of equations with respect to the variables ρ, $\boldsymbol{u}$, P, and σ^w_{ij}. Switching to the variable $\zeta_{ij} = n^{-1}\sigma^w_{ij}$, we have:

$$\partial_t n + \partial_i(n u_i) = 0; \tag{113}$$
$$\rho(\partial_t u_k + u_i \partial_i u_k) + \partial_k P + \partial_i \left\{\frac{\eta^w_0(T) n}{2 r^w P}\zeta_{ik}\right\} = 0; \tag{114}$$
$$\frac{3}{2}(\partial_t P + u_i \partial_i P) + \frac{5}{2}P\partial_i u_i + \left\{\frac{\eta^w_0(T) n}{2 r^w P}\zeta_{ik}\right\}\partial_i u_k = 0; \tag{115}$$
$$\begin{aligned}\partial_t \zeta_{ik} + \partial_s(u_s \zeta_{ik}) + \{\zeta_{ks}\partial_s u_i + \zeta_{is}\partial_s u_k - \frac{2}{3}\delta_{ik}\zeta_{rs}\partial_s u_r\} \\ + \left\{\gamma^w - \frac{2\beta^w}{r^w}\right\}\zeta_{ik}\partial_s u_s - \frac{P^2}{\eta^w_0(T) n}(\partial_i u_k + \partial_k u_i \\ -\frac{2}{3}\delta_{ik}\partial_s u_s) - \frac{\alpha^w P}{r^w \eta^w_0(T)}\zeta_{ik} = 0.\end{aligned} \tag{116}$$

Here $\partial_t = \partial/\partial t, \partial_i = \partial/\partial x_i$, summation in two repeated indices is assumed, and the coefficients r^w, β^w, and α^w are defined with the aid of the function S^w (111) as follows:

$$r^w = \frac{8}{15\sqrt{\pi}}\int_0^\infty \mathrm{e}^{-c^2} c^6 \left(S^w(c^2)\right)^2 dc; \tag{117}$$
$$\beta^w = \frac{8}{15\sqrt{\pi}}\int_0^\infty \mathrm{e}^{-c^2} c^6 S^w(c^2)\frac{dS^w(c^2)}{d(c^2)}dc;$$
$$\alpha^w = \frac{8}{15\sqrt{\pi}}\int_0^\infty \mathrm{e}^{-c^2} c^6 S^w(c^2) R^w(c^2) dc.$$

The function $R^w(c^2)$ in the last expression is defined due to the action of the operator L^w on the function $S^w(c^2)(c_i c_j - \frac{1}{3}\delta_{ij}c^2)$:

$$\frac{P}{\eta^w_0}R^w(c^2)(c_i c_j - \frac{1}{3}\delta_{ij}c^2) = L^w(S^w(c^2)(c_i c_j - \frac{1}{3}\delta_{ij}c^2)). \tag{118}$$

Finally, the parameter γ^w in (113-117) reflects the temperature dependence of the VC:

$$\gamma^w = \frac{2}{3}\left(1 - \frac{T}{\eta_0^w(T)}\left(\frac{d\eta_0^w(T)}{dT}\right)\right).$$

The set of ten equations (113-117) is alternative to the 10 moment Grad equations.

A new determination of molecular dimensions (revisit)

The first observation to be made is that for Maxwellian molecules we have: $S^{MM} \equiv 1$, and $\eta_0^{MM} \propto T$; thus $\gamma^{MM} = \beta^{MM} = 0$, $r^{MM} = \alpha^{MM} = \frac{1}{2}$, and (113-117) becomes the 10 moment Grad system under a simple change of variables $\lambda\zeta_{ij} = \sigma_{ij}$, where λ is the proportionality coefficient in the temperature dependence of η_0^{MM}.

These properties (the function S^w is a constant, and the VC is proportional to T) are true only for Maxwellian molecules. For all other interactions, the function S^w is not identical to one, and the VC $\eta_0^w(T)$ is not proportional to T. Thus, the shortened alternative description is not equivalent indeed to the Grad moment description. In particular, for hard spheres, the exact expression for the function S^{HS} (111) reads:

$$S^{HS} = \frac{5\sqrt{2}}{16}\int_0^1 \exp(-c^2t^2)(1-t^4)\left(c^2(1-t^2)+2\right)dt, \tag{119}$$

$$\eta_0^{HS} \propto \sqrt{T}.$$

Thus, $\gamma^{HS} = \frac{1}{3}$, and $\frac{\beta^{HS}}{r^{HS}} \approx 0.07$, and the equation for the function ζ_{ik} (117) contains a nonlinear term,

$$\theta^{HS}\zeta_{ik}\partial_s u_s, \tag{120}$$

where $\theta^{HS} \approx 0.19$. This term is missing in the Grad 10 moment equation.

Finally, let us evaluate the VC which results from the alternative description (113-117). Following Grad's arguments [113], we see that, if the relaxation of ζ_{ik} is fast compared to the hydrodynamic variables, then the two last terms in the equation for ζ_{ik} (113-117) become dominant, and the equation for $\boldsymbol{u}$ casts into the standard Navier-Stokes form with an effective VC η_{eff}^w:

$$\eta_{\mathrm{eff}}^w = \frac{1}{2\alpha^w}\eta_0^w. \tag{121}$$

For Maxwellian molecules, we easily derive that the coefficient α^w in eq. (121) is equal to $\frac{1}{2}$. Thus, as one expects, the effective VC (121) is equal to the Grad value, which, in turn, is equal to the exact value in the frames of the Chapman-Enskog method for this model.

For all interactions different from the Maxwellian molecules, the VC η_{eff}^w (121) is not equal to η_0^w. For hard spheres, in particular, a computation of the VC (121) requires information about the function R^{HS} (118). This is achieved upon a substitution of the function S^{HS} (119) into the eq. (118). Further, we have to compute the action of the operator L^{HS} on the function $S^{HS}(c_ic_j - \frac{1}{3}\delta_{ij}c^2)$, which is rather complicated. However,

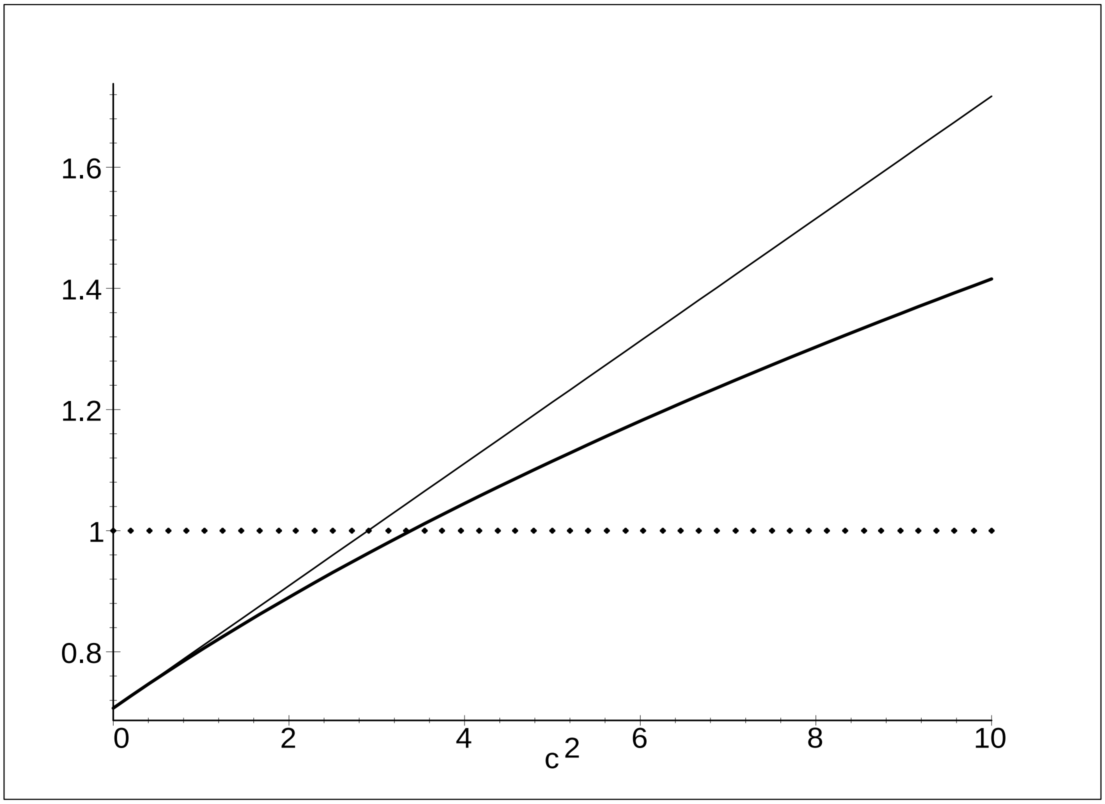


Figure 1: Approximations for hard spheres: bold line - function S^{HS}, solid line - approximation S_a^{HS}, dotted line - Grad moment approximation.

the VC η_{eff}^{HS} can be relatively easily estimated by using a function $S_a^{HS} = \frac{1}{\sqrt{2}}(1 + \frac{1}{7}c^2)$, instead of the function S^{HS}, in eq. (118). Indeed, the function S_a^{HS} is tangent to the function S^{HS} at $c^2 = 0$, and is its majorant (see Fig. 1). Substituting S_a^{HS} into eq. (118), and computing the action of the collision integral, we find the approximation R_a^{HS}; thereafter we evaluate the integral α^{HS} (117), and finally come to the following expression:

$$\eta_{\mathrm{eff}}^{HS} \geq \frac{75264}{67237}\eta_0^{HS} \approx 1.12\eta_0^{HS}. \tag{122}$$

Thus, for hard spheres, the description in terms of scattering rates results in the VC of more than 10% higher than in the Grad moment description.

A discussion of the results concerns the following two items.

1. Having two not equivalent descriptions which were obtained within one method, we may ask: which is more relevant? A simple test is to compare characteristic times of an approach to hydrodynamic regime. We have $\tau_G \sim \eta_0^{HS}/P$ for 10-moment description, and $\tau_a \sim \eta_{\mathrm{eff}}^{HS}/P$ for alternative description. As $\tau_a > \tau_G$, we see that scattering rate decay slower than corresponding moment, hence, at least for rigid spheres, alternative description is more relevant. For Maxwellian molecules both the descriptions are, of course, equivalent.

2. The VC η_{eff}^{HS} (122) has the same temperature dependence as η_0^{HS}, and also the same dependence on a scaling parameter (a diameter of the sphere). In th classical book [43]

Table 1: Three virial coefficients: experimental $B_{\rm exp}$, classical B_0 [133], and reduced $B_{\rm eff}$ for three gases at $T = 500K$

	$B_{\rm exp}$	B_0	$B_{\rm eff}$
Argon	8.4	60.9	50.5
Helium	10.8	21.9	18.2
Nitrogen	168	66.5	55.2

(pp. 228-229), "sizes" of molecules are presented, assuming that a molecule is represented with an equivalent sphere and VC is estimated as η_0^{HS}. Since our estimation of VC differs only by a dimensionless factor from η_0^{HS}, it is straightforward to conclude that effective sizes of molecules will be reduced by the factor b, where

$$b = \sqrt{\eta_0^{HS}/\eta_{\rm eff}^{HS}} \approx 0.94.$$

Further, it is well known that sizes of molecules estimated via viscosity in [43] disagree with the estimation via the virial expansion of the equation of state. In particular, in book [133], p. 5 the measured second virial coefficient $B_{\rm exp}$ was compared with the calculated B_0, in which the diameter of the sphere was taken from the viscosity data. The reduction of the diameter by factor b gives $B_{\rm eff} = b^3 B_0$. The values $B_{\rm exp}$ and B_0 [133] are compared with $B_{\rm eff}$ in the Table 1 for three gases at $T = 500K$. The results for argon and helium are better for $B_{\rm eff}$, while for nitrogen $B_{\rm eff}$ is worth than B_0. However, both B_0 and $B_{\rm eff}$ are far from the experimental values.

Hard spheres is, of course, an oversimplified model of interaction, and the comparison presented does not allow for a decision between η_0^{HS} and $\eta_{\rm eff}^{HS}$. However, this simple example illustrates to what extend the correction to the VC can affect a comparison with experiment. Indeed, as is well known, the first-order Sonine polynomial computation for the Lennard-Jones (LJ) potential gives a very good fit of the temperature dependence of the VC for all noble gases [134], subject to a proper choice of the two unknown scaling parameters of the LJ potential [7]. We may expect that a dimensionless correction of the VC for the LJ potential might be of the same order as above for rigid spheres. However, the functional character of the temperature dependence will not be affected, and a fit will be obtained subject to a different choice of the molecular parameters of the LJ potential.

There remains, however, a general question how the estimation of the VC (121) responds to the exact value [43], [135]. Since the analysis performed above does not immediately appeal to the exact Chapman-Enskog expressions just mentioned, this question remains open for a further work.

[7] A comparison of molecular parameters of the LJ potential, as derived from the viscosity data, to those obtained from independent sources, can be found elsewhere, e.g. in Ref. [43], p. 237.

6 Newton method with incomplete linearization

Let us come back to the invariance equation (36),

$$\Delta_y = (1 - P_y)J(F(y)) = 0.$$

One of the most efficient methods to solve this equation is the Newton method with incomplete linearization. Let us linearize the vector field J around $F(y)$:

$$J(F(y) + \delta F(y)) = J(F(y)) + (DJ)_{F(y)}\delta F(y) + o(\delta F(y)). \quad (123)$$

Equation of the Newton method with incomplete linearization makes it possible to determine $\delta F(y)$:

$$\begin{cases} P_y \delta F(y) = 0 \\ (1 - P_y)(DJ)_{F(y)}\delta F(y) = (1 - P_y)J(F(y)). \end{cases} \quad (124)$$

The crucial point here is that the same projector P_y is used as in the equation (36), that is, without computing the variation of the projector δP (hence, the linearization of equation (36) is incomplete). We recall that projector P_y depends on the tangent space $T_y = \mathrm{Im}(DF)_y$. If the thermodynamic projector (89) is used here, then P_y depends also on $\langle | \rangle_{F(y)}$ and on $g = (DS)_{F(y)}$.

Equations of the Newton method with incomplete linearization (124) are not differential equations in y anymore, they do not contain derivatives of the unknown $\delta F(y)$ with respect to y (which would be the case if the variation of the projector δP has been taken into account). The absence of the derivatives in equation (124) significantly simplifies its solving. However, even this is not the main advantage of the incomplete linearization. More essential is the fact that iterations of the Newton method with incomplete linearization is expected to converge to slow invariant manifolds, unlike the usual Newton method. This has been demonstrated in [3] in the linear approximation.

In order to illustrate the nature of the Eq. (124), let us consider the case of linear manifolds for linear systems. Let a linear evolution equation be given in the finite-dimensional real space: $\dot{\boldsymbol{x}} = \mathbf{A}\boldsymbol{x}$, where $\mathbf{A}$ is negatively definite symmetric matrix with a simple spectrum. Let us further assume quadratic Lyapunov function, $S(\boldsymbol{x}) = \langle \boldsymbol{x}, \boldsymbol{x} \rangle$. The manifolds we consider are lines, $\boldsymbol{l}(y) = y\boldsymbol{e}$, where $\boldsymbol{e}$ is the unit vector, and y is a scalar. The invariance equation for such manifolds reads: $\boldsymbol{e}\langle \boldsymbol{e}, \mathbf{A}\boldsymbol{e} \rangle - \mathbf{A}\boldsymbol{e} = 0$, and is simply the eigenvalue problem for the operator $\mathbf{A}$. Solutions to the latter equation are eigenvectors $\boldsymbol{e}_i$, corresponding to eigenvalues λ_i.

Assume that we have chosen a line, $\boldsymbol{l}_0 = y\boldsymbol{e}_0$, defined by the unit vector $\boldsymbol{e}_0$, and that $\boldsymbol{e}_0$ is not an eigenvector of $\mathbf{A}$. We seek another line, $\boldsymbol{l}_1 = a\boldsymbol{e}_1$, where $\boldsymbol{e}_1$ is another unit vector, $\boldsymbol{e}_1 = \boldsymbol{x}_1/\|\boldsymbol{x}_1\|$, $\boldsymbol{x}_1 = \boldsymbol{e}_0 + \delta\boldsymbol{x}$. The additional condition in (124) reads: $P_y\delta F(y) = 0$, i.e. $\langle \boldsymbol{e}_0, \delta\boldsymbol{x} \rangle = 0$. Then the Eq. (124) becomes $[1 - \boldsymbol{e}_0\langle \boldsymbol{e}_0, \cdot \rangle]\mathbf{A}[\boldsymbol{e}_0 + \delta\boldsymbol{x}] = 0$. Subject to the additional condition, the unique solution is as follows: $\boldsymbol{e}_0 + \delta\boldsymbol{x} = \langle \boldsymbol{e}_0, \mathbf{A}^{-1}\boldsymbol{e}_0 \rangle^{-1}\mathbf{A}^{-1}\boldsymbol{e}_0$. Rewriting the latter expression in the eigen–basis of $\mathbf{A}$, we have: $\boldsymbol{e}_0 + \delta \boldsymbol{y} \propto \sum_i \lambda_i^{-1} \boldsymbol{e}_i \langle \boldsymbol{e}_i, \boldsymbol{e}_0 \rangle$. The leading term in this sum corresponds to the eigenvalue with the minimal absolute value. The example indicates that the method (124) seeks the direction of the *slowest relaxation*. For this reason, the Newton method with incomplete linearization (124) can be recognized as the basis of an iterative construction of the manifolds of slow motions.

In an attempt to simplify computations, the question which always can be asked is as follows: To what extend is the choice of the projector essential in the equation (124)? This question is a valid one, because, if we accept that iterations converge to a relevant slow manifold, and also that the projection on the true invariant manifold is insensible to the choice of the projector, then should one care of the projector on each iteration? In particular, for the moment parameterizations, can one use in equation (124) the projector (65)? Experience gained from some of the problems studied by this method indicates that this is possible. However, in order to derive physically meaningful equations of motion along the approximate slow manifolds, one has to use the thermodynamic projector (89). Otherwise we are not guaranteed from violating the dissipation properties of these equations of motion.

Example 3: Non-perturbative correction of Local Maxwellian manifold and derivation of nonlinear hydrodynamics from Boltzmann equation (1D)

This section is a continuation of **Example 1**. Here we apply the method of invariant manifold to a particular situation when the initial manifold consists of local Maxwellians (97) (the LM manifold). This manifold and its corrections play the central role in the problem of derivation of hydrodynamics from BE. Hence, any method of approximate investigation of BE should be tested with the LM manifold. Classical methods (Chapman-Enskog and Hilbert methods) use Taylor-type expansions into powers of a small parameter (Knudsen number expansion). However, as we have mentioned above, the method of invariant manifold, generally speaking, assumes no small parameters, at least in its formal part where convergency properties are not discussed. We will develop an appropriate technique to consider the invariance equation of the first iteration. This involves ideas of parametrics expansions of the theory of pseudodifferential and Fourier integral operators [143, 144]. This approach will make it possible to reject the restriction of using small parameters.

We search for a correction to the LM manifold as:

$$f_1(n, \boldsymbol{u}, T) = f_0(n, \boldsymbol{u}, T) + \delta f_1(n, \boldsymbol{u}, T). \tag{125}$$

We will use the Newton method with incomplete linearization for obtaining the correction $\delta f_1(n, \boldsymbol{u}, T)$, because we search for a manifold of slow (hydrodynamic) motions. We introduce the representation:

$$\delta f_1(n, \boldsymbol{u}, T) = f_0(n, \boldsymbol{u}, T)\varphi(n, \boldsymbol{u}, T). \tag{126}$$

Positivity and normalization

When searching for a correction, we should be ready to face two problems that are typical for any method of successive approximations in BE theory. Namely, the first of this problems is that the correction

$$f_{\Omega_{k+1}} = f_{\Omega_k} + \delta f_{\Omega_{k+1}}$$

obtained from the linearized invariance equation of the $k+1$-th iteration may be not a non-negatively defined function and thus it can not be used directly to define the thermodynamic projector for the $k+1$-th approximation. In order to overcome this difficulty, we can treat the procedure as a process of correcting the dual variable $\mu_f = D_f H(f)$ rather than the process of immediate correcting the distribution functions.

The dual variable μ_f is:

$$\mu_f|_{f=f(\boldsymbol{x},\boldsymbol{v})} = D_f H(f)|_{f=f(\boldsymbol{x},\boldsymbol{v})} = D_f H_{\boldsymbol{x}}(f)|_{f=f(\boldsymbol{x},\boldsymbol{v})} = \ln f(\boldsymbol{v}, \boldsymbol{x}). \tag{127}$$

Then, at the $k+1$-th iteration, we search for new dual variables $\mu_f|_{\Omega_{k+1}}$:

$$\mu_f|_{\Omega_{k+1}} = \mu_f|_{\Omega_k} + \delta\mu_f|_{\Omega_{k+1}}. \tag{128}$$

Due to the relationship $\mu_f \longleftrightarrow f$, we have:

$$\delta\mu_f|_{\Omega_{k+1}} = \varphi_{\Omega_{k+1}} + O(\delta f^2_{\Omega_{k+1}}), \varphi_{\Omega_{k+1}} = f^{-1}_{\Omega_k} \delta f_{\Omega_{k+1}}. \tag{129}$$

Thus, solving the linear invariance equation of the k-th iteration with respect to the unknown function $\delta f_{\Omega_{k+1}}$, we find a correction to the dual variable $\varphi_{\Omega_{k+1}}$(129), and we derive the corrected distributions $f_{\Omega_{k+1}}$ as

$$f_{\Omega_{k+1}} = \exp(\mu_f|_{\Omega_k} + \varphi_{\Omega_{k+1}}) = f_{\Omega_k} \exp(\varphi_{\Omega_{k+1}}). \tag{130}$$

Functions (130) are positive, and they satisfy the invariance equation and the additional conditions within the accuracy of $\varphi_{\Omega_{k+1}}$.

However, the second difficulty which might occur is that functions (130) might have no finite integrals (91). In particular, this difficulty can be a result of some approximations used in solving equations. Hence, we have to "regularize" the functions (130). A sketch of an approach to make this regularization might be as follows: instead of $f_{\Omega_{k+1}}$(130), we consider functions:

$$f^{(\beta)}_{\Omega_{k+1}} = f_{\Omega_k} \exp(\varphi_{\Omega_{k+1}} + \varphi^{\mathrm{reg}}(\beta)). \tag{131}$$

Here $\varphi^{\mathrm{reg}}(\beta)$ is a function labeled with $\beta \in B$, and B is a linear space. Then we derive β_* from the condition of coincidence of macroscopic parameters. Further consideration of this procedure [3] remains out of frames of this paper.

The two difficulties mentioned here are not specific for the approximate method developed. For example, corrections to the LM distribution in the Chapman-Enskog method [43] and the thirteen-moment Grad approximation [113] are not non-negatively defined functions, while the thirteen-moment quasiequilibrium approximation [123] has no finite integrals (90) and (91).

Galilean invariance of invariance equation

In some cases, it is convenient to consider BE vector field in a reference system which moves with the flow velocity. In this reference system, we define the BE vector field as:

$$\frac{df}{dt} = J_u(f), \frac{df}{dt} = \frac{\partial f}{\partial t} + u_{\boldsymbol{x},s}(f)\frac{\partial f}{\partial x_s}; J_u(f) = -(v_s - u_{\boldsymbol{x},s}(f))\frac{\partial f}{\partial x_s} + Q(f,f). \tag{132}$$

Here $u_{\boldsymbol{x},s}(f)$ stands for the s-th component of the flow velocity:

$$u_{\boldsymbol{x},s}(f) = n^{-1}_{\boldsymbol{x}}(f) \int v_s f(\boldsymbol{v},\boldsymbol{x}) d^3\boldsymbol{v};\ n_{\boldsymbol{x}}(f) = \int f(\boldsymbol{v},\boldsymbol{x}) d^3\boldsymbol{v}. \tag{133}$$

In particular, this form of BE vector field is convenient when the initial manifold Ω_0 consists of functions f_{Ω_0} which depend explicitly on $(\boldsymbol{v}-u_{\boldsymbol{x}}(f))$ (i.e., if functions $f_{\Omega_0}\in\Omega_0$ do not change under velocity shifts: $\boldsymbol{v}\to\boldsymbol{v}+c$, where c is a constant vector).

Substituting $J_u(f)$ (132) instead of $J(f)$ (92) into all expressions which depend on the BE vector field, we transfer all procedures developed above into the moving reference system. In particular, we obtain the following analog of the invariance equation of the first iteration:

$$
\begin{aligned}
(P^{0*}_{a(\boldsymbol{x})}(\cdot)-1)J^0_{u,\mathrm{lin},a(\boldsymbol{x})}(\delta f_1(a(\boldsymbol{x}),\boldsymbol{v}))+\Delta(f_0(a(\boldsymbol{x}),\boldsymbol{v}))=0;\\
J^0_{u,\mathrm{lin},a(\boldsymbol{x})}(g)=\Big\{n_{\boldsymbol{x}}^{-1}(f_0(a(\boldsymbol{x})))\int v_s g d^3\boldsymbol{v}+\\
+u_{\boldsymbol{x},s}(f_0(a(\boldsymbol{x})))n_{\boldsymbol{x}}^{-1}(f_0(a(\boldsymbol{x})))\int g d^3\boldsymbol{v}\Big\}\frac{\partial f_0(a(\boldsymbol{x}),\boldsymbol{v})}{\partial x_s}-\\
-(v_s-u_{\boldsymbol{x},s}(f_0(a(\boldsymbol{x}))))\frac{\partial g}{\partial x_s}+L_{f_0(a(\boldsymbol{x}),\boldsymbol{v})}(g);\\
\Delta(f_0(a(\boldsymbol{x}),\boldsymbol{v}))=(P^{*}_{a(\boldsymbol{x})}(\cdot)-1)J_u(f_0(a(\boldsymbol{x}),\boldsymbol{v})).
\end{aligned}\tag{134}
$$

Additional conditions do not depend on the vector field, and thus they remain valid for equation (134).

The equation of the first iteration

The equation of the first iteration in the form of (129) for the correction $\varphi(n,\boldsymbol{u},T)$ is:

$$
\begin{aligned}
\{P_{f_0(n,\boldsymbol{u},T)}(\cdot)-1\}\Big\{-(v_s-u_s)\frac{\partial f_0(n,\boldsymbol{u},T)}{\partial x_s}+f_0(n,\boldsymbol{u},T)L_{f_0(n,\boldsymbol{u},T)}(\varphi)-\\
-(v_s-u_s)\frac{\partial(f_0(n,\boldsymbol{u},T)\varphi)}{\partial x_s}-n^{-1}\Big(f_0(n,\boldsymbol{u},T)\Big)\Big(\int v_s f_0(n,\boldsymbol{u},T)\varphi d^3\boldsymbol{v}+\\
+u_s(f_0(n,\boldsymbol{u},T))\int f_0(n,\boldsymbol{u},T)\varphi d^3\boldsymbol{v}\Big)\frac{\partial f_0(n,\boldsymbol{u},T)}{\partial x_s}\Big\}=0.
\end{aligned}\tag{135}
$$

Here $f_0(n,\boldsymbol{u},T)L_{f_0(n,\boldsymbol{u},T)}(\varphi)$ is the linearized Boltzmann collision integral:

$$
\begin{aligned}
f_0(n,\boldsymbol{u},T)L_{f_0(n,\boldsymbol{u},T)}(\varphi)=\int w(\mathbf{v}',\boldsymbol{v}|\boldsymbol{v},\boldsymbol{v}_1)f_0(n,\boldsymbol{u},T)\times\\
\times\{\varphi'+\varphi_1'-\varphi_1-\varphi\}d^3\mathbf{v}'d^3\mathbf{v}_1'd^3\boldsymbol{v}_1.
\end{aligned}\tag{136}
$$

and $w(\mathbf{v}',\boldsymbol{v}_1'|\boldsymbol{v},\boldsymbol{v}_1)$ is the kernel of the Boltzmann collision integral, standard notations label the velocities before and after a collision.

Additional condition for equation (135) has the form:

$$
P_{f_0(n,\boldsymbol{u},T)}(f_0(n,\boldsymbol{u},T)\varphi)=0.\tag{137}
$$

In detail notation:

$$\int 1 \cdot f_0(n, \boldsymbol{u}, T)\varphi d^3\boldsymbol{v} = 0, \qquad \int v_i f_0(n, \boldsymbol{u}, T)\varphi d^3\boldsymbol{v} = 0,\ i = 1, 2, 3,$$
$$\int \boldsymbol{v}^2 f_0(n, \boldsymbol{u}, T)\varphi d^3\boldsymbol{v} = 0. \tag{138}$$

Eliminating in (135) the terms containing $\int v_s f_0(n, \boldsymbol{u}, T)\varphi d^3\boldsymbol{v}$ and $\int f_0(n, \boldsymbol{u}, T)\varphi d^3\boldsymbol{v}$ with the aid of (138), we obtain the following form of equation (135):

$$\{P_{f_0(n,\boldsymbol{u},T)}(\cdot) - 1\} \times \tag{139}$$
$$\left(-(v_s - u_s)\frac{\partial f_0(n, \boldsymbol{u}, T)}{\partial x_s} + f_0(n, \boldsymbol{u}, T)L_{f_0(n,\boldsymbol{u},T)}(\varphi) - (v_s - u_s)\frac{\partial (f_0(n, \boldsymbol{u}, T)\varphi)}{\partial x_s}\right) = 0.$$

In order to consider the properties of equation (139), it is useful to introduce real Hilbert spaces $G_{f_0(n,\boldsymbol{u},T)}$ with scalar products:

$$(\varphi, \psi)_{f_0(n,\boldsymbol{u},T)} = \int f_0(n, \boldsymbol{u}, T)\varphi\psi d^3\boldsymbol{v}. \tag{140}$$

Each Hilbert space is associated with the corresponding LM distribution $f_0(n, \boldsymbol{u}, T)$.

The projector $P_{f_0(n,\boldsymbol{u},T)}$ (103) is associated with a projector $\Pi_{f_0(n,\boldsymbol{u},T)}$ which acts in the space $G_{f_0(n,\boldsymbol{u},T)}$:

$$\Pi_{f_0(n,\boldsymbol{u},T)}(\varphi) = f_0^{-1}(n, \boldsymbol{u}, T)P_{f_0(n,\boldsymbol{u},T)}(f_0(n, \boldsymbol{u}, T)\varphi). \tag{141}$$

It is an orthogonal projector, because

$$\Pi_{f_0(n,\boldsymbol{u},T)}(\varphi) = \sum_{s=0}^{4} \psi^{(s)}_{f_0(n,\boldsymbol{u},T)}(\psi^{(s)}_{f_0(n,\boldsymbol{u},T)}, \varphi)_{f_0(n,\boldsymbol{u},T)}. \tag{142}$$

Here $\psi^{(s)}_{f_0(n,\boldsymbol{u},T)}$ are given by the expression (104).

We can rewrite the equation of the first iteration (139) in the form:

$$L_{f_0(n,\boldsymbol{u},T)}(\varphi) + K_{f_0(n,\boldsymbol{u},T)}(\varphi) = D_{f_0(n,\boldsymbol{u},T)}. \tag{143}$$

Notations used here are:

$$D_{f_0(n,\boldsymbol{u},T)} = f_0^{-1}(n, \boldsymbol{u}, T)\Delta(f_0(n, \boldsymbol{u}, T)); \tag{144}$$
$$K_{f_0(n,\boldsymbol{u},T)}(\varphi) = \left\{\Pi_{f_0(n,\boldsymbol{u},T)}(\cdot) - 1\right\} f_0^{-1}(n, \boldsymbol{u}, T)(v_s - u_s)\frac{\partial (f_0(n, \boldsymbol{u}, T)\varphi)}{\partial x_s}.$$

The additional condition for equation (143) is:

$$(\psi^{(s)}_{f_0(n,\boldsymbol{u},T)}, \varphi)_{f_0(n,\boldsymbol{u},T)} = 0, s = 0, \ldots, 4. \tag{145}$$

Now we will list the properties of the equation (143) for usual models of a collision [43]:

a) The linear integral operator $L_{f0(n,\boldsymbol{u},T)}$ is selfadjoint with respect to the scalar product $(\cdot,\cdot)_{f0(n,\boldsymbol{u},T)}$, and the quadratic form $(\varphi, L_{f0(n,\boldsymbol{u},T)}(\varphi))$ is negatively defined in $\mathrm{Im}_{f0(n,\boldsymbol{u},T)}$.
b) The kernel of $L_{f0(n,\boldsymbol{u},T)}$ does not depend on $f_0(n,\boldsymbol{u},T)$, and it is the linear envelope of the polynomials $\psi_0 = 1, \psi_i = v_i, i = 1,2,3$, and $\psi_4 = v^2$.
c) The RHS $D_{f0(n,\boldsymbol{u},T)}$ is orthogonal to $\ker L_{f0(n,\boldsymbol{u},T)}$ in the sense of the scalar product $(\cdot,\cdot)_{f0(n,\boldsymbol{u},T)}$.
d) The projecting operator $\Pi_{f0(n,\boldsymbol{u},T)}$ is the selfadjoint projector onto $\ker L_{f0(n,\boldsymbol{u},T)}$:

$$\Pi_{f0(n,\boldsymbol{u},T)}(\varphi) \in \ \ker L_{f0(n,\boldsymbol{u},T)} \tag{146}$$

Projector $\Pi_{f0(n,\boldsymbol{u},T)}$ projects orthogonally.
e) The image of the operator $K_{f0(n,\boldsymbol{u},T)}$ is orthogonal to $\ker L_{f0(n,\boldsymbol{u},T)}$.
f) Additional condition (145) require the solution of equation (143) to be orthogonal to $\ker L_{f0(n,\boldsymbol{u},T)}$.

These properties result in the *necessity condition* for solving the equation (143) with the additional constraint (145). This means the following: equation (143), provided with constraint (145), satisfies the necessary condition for to have an unique solution in $\mathrm{Im} L_{f0(n,\boldsymbol{u},T)}$.
Remark. Because of the *differential* part of the operator $K_{f0(n,\boldsymbol{u},T)}$, we are not able to apply the Fredholm alternative to obtain the *necessary and sufficient* conditions for solvability of equation (145). Thus, the condition mentioned here is, rigorously speaking, only the necessity condition. Nevertheless, we will still develop a formal procedure for solving the equation (143).

To this end, we paid no attention to the dependency of all functions, spaces, operators, etc, on $\boldsymbol{x}$. It is useful to rewrite once again the equation (143) in order to separate the local in $\boldsymbol{x}$ operators from those differential. Furthermore, we shall replace the subscript $f_0(n,\boldsymbol{u},T)$ with the subscript $\boldsymbol{x}$ in all expressions. We represent (143) as:

$$\begin{aligned}
A_{\mathrm{loc}}(\boldsymbol{x},\boldsymbol{v})\varphi - A_{\mathrm{diff}}\left(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v}\right)\varphi &= -D(\boldsymbol{x},\boldsymbol{v});\\
A_{\mathrm{loc}}(\boldsymbol{x},\boldsymbol{v})\varphi &= -\left\{L_{\boldsymbol{x}}(\boldsymbol{v})\varphi + (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}}\varphi\right\};\\
A_{\mathrm{diff}}\left(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v}\right)\varphi &= (\Pi_{\boldsymbol{x}}(\cdot) - 1)\left((v_s - u_s)\frac{\partial}{\partial x_s}\varphi\right);\\
\Pi_{\boldsymbol{x}}(\boldsymbol{v})g &= \sum_{s=0}^{4} \psi_{\boldsymbol{x}}^{(s)}(\psi_{\boldsymbol{x}}^{(s)}, g);\\
\psi_{\boldsymbol{x}}^{(0)} = n^{-1/2}, \qquad \psi_{\boldsymbol{x}}^{(s)} &= (2/n)^{1/2}c_s(\boldsymbol{x},\boldsymbol{v}),\ s = 1,2,3,\\
\psi_{\boldsymbol{x}}^{(4)} = (2/3n)^{1/2}(c^2(\boldsymbol{x},\boldsymbol{v}) - 3/2); \qquad c_i(\boldsymbol{x},\boldsymbol{v}) &= (m/2k_BT(\boldsymbol{x}))^{1/2}(v_i - u_i(\boldsymbol{x})),\\
r_{\boldsymbol{x}} = (v_s - u_s)\left(\frac{\partial \ln n}{\partial x_s} + \frac{m}{k_BT}(v_i - u_i)\frac{\partial u_i}{\partial x_s}\right. &+ \left.\left(\frac{m(\boldsymbol{v}-\boldsymbol{u})^2}{2k_BT} - \frac{3}{2}\right)\frac{\partial \ln T}{\partial x_s}\right);\\
D(\boldsymbol{x},\boldsymbol{v}) &= \left\{\left(\frac{m(\boldsymbol{v}-\boldsymbol{u})^2}{2k_BT} - \frac{5}{2}\right)(v_i - u_i)\frac{\partial \ln T}{\partial x_i} + \right.\\
&\left. + \frac{m}{k_BT}\left(((v_i - u_i)(v_s - u_s) - \frac{1}{3}\delta_{is}(\boldsymbol{v}-\boldsymbol{u})^2\right)\frac{\partial u_s}{\partial x_i}\right\}.
\end{aligned} \tag{147}$$

Here we have omitted the dependence on $\boldsymbol{x}$ in the functions $n(\boldsymbol{x})$, $u_i(\boldsymbol{x})$, and $T(\boldsymbol{x})$. Further, if no discrepancy might occur, we will always assume this dependence, and we will not indicate it explicitly.

The additional condition for this equation is:

$$\Pi_{\boldsymbol{x}}(\varphi) = 0. \tag{148}$$

Equation (147) is linear in φ. However, the main difficulty in solving this equation is caused with the differential in $\boldsymbol{x}$ operator A_{diff} which does not commutate with the local in $\boldsymbol{x}$ operator A_{loc}.

Parametrics Expansion

In this subsection we introduce a procedure to construct approximate solutions of equation (146). This procedure involves an expansion similar to the parametrics expansion in the theory of pseudo-differential (PDO) and Fourier integral operators (FIO).

Considering $\varphi \in \mathrm{Im} L_{\boldsymbol{x}}$, we write a formal solution of equation (147) as:

$$\varphi(\boldsymbol{x},\boldsymbol{v}) = \left(A_{\text{loc}}(\boldsymbol{x},\boldsymbol{v}) - A_{\text{diff}}\left(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v}\right)\right)^{-1} (-D(\boldsymbol{x},\boldsymbol{v})) \tag{149}$$

It is useful to extract the differential operator $\frac{\partial}{\partial \boldsymbol{x}}$ from the operator $A_{\text{diff}}(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v})$:

$$\varphi(\boldsymbol{x},\boldsymbol{v}) = \left(1 - B_s(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_s}\right)^{-1} \varphi_{\text{loc}}(\boldsymbol{x},\boldsymbol{v}). \tag{150}$$

Notations used here are:

$$\begin{aligned}
\varphi_{\text{loc}}(\boldsymbol{x},\boldsymbol{v}) &= A_{\text{loc}}^{-1}(\boldsymbol{x},\boldsymbol{v})(-D(\boldsymbol{x},\boldsymbol{v})) = \\
&= [-L_{\boldsymbol{x}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}}]^{-1}(-D(\boldsymbol{x},\boldsymbol{v})); \\
B_s(\boldsymbol{x},\boldsymbol{v}) &= A_{\text{loc}}^{-1}(\boldsymbol{x},\boldsymbol{v})(\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)(v_s - u_s) = \\
&= [-L_{\boldsymbol{x}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}}]^{-1}(\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)(v_s - u_s).
\end{aligned} \tag{151}$$

We will now discuss in more detail the character of expressions in (151).

For every $\boldsymbol{x}$, the function $\varphi_{\text{loc}}(\boldsymbol{x},\boldsymbol{v})$, considered as a function of $\boldsymbol{v}$, is an element of the Hilbert space $G_{\boldsymbol{x}}$. It gives a solution to the integral equation:

$$-L_{\boldsymbol{x}}(\boldsymbol{v})\varphi_{\text{loc}} - (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)(r_{\boldsymbol{x}}\varphi_{\text{loc}}) = (-D(\boldsymbol{x},\boldsymbol{v})) \tag{152}$$

This latter linear integral equation has an unique solution in $\mathrm{Im} L_{\boldsymbol{x}}(\boldsymbol{v})$. Indeed,

$$\begin{aligned}
\ker A_{\text{loc}}^{+}(\boldsymbol{x},\boldsymbol{v}) &= \ker(L_{\boldsymbol{x}}(\boldsymbol{v}) + (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}})^{+} = \\
&= \ker(L_{\boldsymbol{x}}(\boldsymbol{v}))^{+} \bigcap \ker((\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}})^{+} =
\end{aligned}$$

$$\ker(L_{\boldsymbol{x}}(\boldsymbol{v}))^{+} \bigcap \ker(r_{\boldsymbol{x}}(\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)), \text{ and } G_{\boldsymbol{x}} \bigcap \Pi_{\boldsymbol{x}}(\boldsymbol{v})G_{\boldsymbol{x}} = \{0\}\,. \tag{153}$$

Thus, the existence of the unique solution of equation (152) follows from the Fredholm alternative.

Let us consider the operator $R(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v})$:

$$R\left(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v}\right) = \left(1 - B_s(\boldsymbol{x}, \boldsymbol{v})\frac{\partial}{\partial x_s}\right)^{-1}. \tag{154}$$

One can represent it as a formal series:

$$R\left(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v}\right) = \sum_{m=0}^{\infty}\left[B_s(\boldsymbol{x}, \boldsymbol{v})\frac{\partial}{\partial x_s}\right]^m. \tag{155}$$

Here

$$\left[B_s(\boldsymbol{x}, \boldsymbol{v})\frac{\partial}{\partial x_s}\right]^m = B_{s_1}(\boldsymbol{x}, \boldsymbol{v})\frac{\partial}{\partial x_{s_1}} \dots B_{s_m}(\boldsymbol{x}, \boldsymbol{v})\frac{\partial}{\partial x_{s_m}}. \tag{156}$$

Every term of the type (156) can be represented as a finite sum of operators which are superpositions of the following two operations: of the integral in $\boldsymbol{v}$ operations with kernels depending on $\boldsymbol{x}$, and of differential in $\boldsymbol{x}$ operations.

Our goal is to obtain an explicit representation of the operator $R(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v})$(154) as an integral operator. If the operator $B_s(\boldsymbol{x}, \boldsymbol{v})$ would not depend on $\boldsymbol{x}$(i.e., if no dependence on spatial variables would occur in kernels of integral operators, in $B_s(\boldsymbol{x}, \boldsymbol{v})$), then we could reach our goal via usual Fourier transformation. However, operators $B_s(\boldsymbol{x}, \boldsymbol{v})$ and $\frac{\partial}{\partial x_k}$ do not commutate, and thus this elementary approach does not work. We will develop a method to obtain the required explicit representation using the ideas of PDO and IOF technique.

We start with the representation (155). Our strategy is to transform every summand (156) in order to place integral in $\boldsymbol{v}$ operators $B_s(\boldsymbol{x}, \boldsymbol{v})$ left to differential operators $\frac{\partial}{\partial x_k}$. The transposition of every pair $\frac{\partial}{\partial x_k}B_s(\boldsymbol{x}, \boldsymbol{v})$ yields an elementary transform:

$$\frac{\partial}{\partial x_k}B_s(\boldsymbol{x}, \boldsymbol{v}) \to B_s(\boldsymbol{x}, \boldsymbol{v})\frac{\partial}{\partial x_k} - \left[B_s(\boldsymbol{x}, \boldsymbol{v}), \frac{\partial}{\partial x_k}\right]. \tag{157}$$

Here $[M, N] = MN - NM$ denotes the commutator of operators M and N. We can represent (156) as:

$$\begin{aligned}\left[B_s(\boldsymbol{x}, \boldsymbol{v})\frac{\partial}{\partial x_s}\right]^m = B_{s_1}(\boldsymbol{x}, \boldsymbol{v}) \dots B_{s_m}(\boldsymbol{x}, \boldsymbol{v})\frac{\partial}{\partial x_{s_1}} \dots \frac{\partial}{\partial x_{s_m}} +\\ +O\left(\left[B_{s_i}(\boldsymbol{x}, \boldsymbol{v}), \frac{\partial}{\partial x_{s_k}}\right]\right).\end{aligned} \tag{158}$$

Here $O([B_{s_i}(\boldsymbol{x}, \boldsymbol{v}), \frac{\partial}{\partial x_{s_k}}])$ denotes the terms which contain one or more pairs of brackets $[\cdot, \cdot]$. The first term in (158) contains no these brackets. We can continue this process of selection and extract the first-order in the number of pairs of brackets terms, the second-order terms, etc. Thus, we arrive at the **expansion into powers of commutator** of the expressions (156).

In this paper we will consider explicitly the zeroth-order term of this commutator expansion. Neglecting all terms with brackets in (158), we write:

$$\left[B_s(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_s}\right]_0^m = B_{s_1}(\boldsymbol{x},\boldsymbol{v})\dots B_{s_m}(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_{s_1}}\dots\frac{\partial}{\partial x_{s_m}}. \tag{159}$$

Here the subscript zero indicates the zeroth order with respect to the number of brackets.

We now substitute expressions $[B_s(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_s}]_0^m$ (159) instead of expressions $[B_s(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_s}]^m$ (156) into the series (155):

$$R_0\left(\boldsymbol{x},\frac{\partial}{\partial x},\boldsymbol{v}\right) = \sum_{m=0}^{\infty}\left[B_s(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_s}\right]_0^m. \tag{160}$$

The action of every summand (159) might be defined via the Fourier transform with respect to spatial variables.

Denote as F the direct Fourier transform of a function $g(\boldsymbol{x},\boldsymbol{v})$:

$$Fg(\boldsymbol{x},\boldsymbol{v}) \equiv \hat{g}(\boldsymbol{k},\boldsymbol{v}) = \int g(\boldsymbol{x},\boldsymbol{v})\exp(-ik_sx_s)d^p\boldsymbol{x}. \tag{161}$$

Here p is the spatial dimension. Then the inverse Fourier transform is:

$$g(x,\boldsymbol{v}) \equiv F^{-1}\hat{g}(\boldsymbol{k},\boldsymbol{v}) = (2\pi)^{-p}\int \hat{g}(\boldsymbol{k},\boldsymbol{v})\exp(ik_sx_s)d^p\boldsymbol{k}. \tag{162}$$

The action of the operator (159) on a function $g(\boldsymbol{x},\boldsymbol{v})$ is defined as:

$$\begin{aligned}\left[B_s(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_s}\right]_0^m g(\boldsymbol{x},\boldsymbol{v}) &= \\ = \left(B_{s_1}(\boldsymbol{x},\boldsymbol{v})\dots B_{s_m}(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_{s_1}}\dots\frac{\partial}{\partial x_{s_m}}\right)(2\pi)^{-p}\int \hat{g}(\boldsymbol{k},\boldsymbol{v})e^{ik_sx_s}d^p\boldsymbol{k} &= \\ = (2\pi)^{-p}\int \exp(ik_sx_s)[ik_lB_l(\boldsymbol{x},\boldsymbol{v})]^m\hat{g}(\boldsymbol{k},\boldsymbol{v})d^p\boldsymbol{k}.\end{aligned} \tag{163}$$

The account of (163) in the formula (160) yields the following definition of the operator R_0:

$$R_0g(\boldsymbol{x},\boldsymbol{v}) = (2\pi)^{-p}\int e^{ik_sx_s}(1-ik_lB_l(\boldsymbol{x},\boldsymbol{v}))^{-1}\hat{g}(\boldsymbol{k},\boldsymbol{v})d^p\boldsymbol{k}. \tag{164}$$

This is the **Fourier integral operator** (note that the kernel of this integral operator depends on $\boldsymbol{k}$ and on $\boldsymbol{x}$). The commutator expansion introduced above is a version of the **parametrics expansion** [143, 144], while expression (164) is the leading term of this expansion. The kernel $(1-ik_lB_l(\boldsymbol{x},\boldsymbol{v}))^{-1}$ is called the **main symbol of the parametrics**.

The account of (164) in the formula (150) yields the zeroth-order term of parametrics expansion $\varphi_0(\boldsymbol{x},\boldsymbol{v})$:

$$\varphi_0(\boldsymbol{x},\boldsymbol{v}) = F^{-1}(1-ik_lB_l(\boldsymbol{x},\boldsymbol{v}))^{-1}F\varphi_{\mathrm{loc}}. \tag{165}$$

In detail notation:

$$\varphi_0(\boldsymbol{x},\boldsymbol{v}) = (2\pi)^{-p}\int\int \exp(ik_s(x_s - y_s))\times$$
$$\times(1 - ik_s[-L_{\boldsymbol{x}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}}]^{-1}(\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)(v_s - u_s(\boldsymbol{x})))^{-1}\times$$
$$\times[-L_{\boldsymbol{y}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{y}}(\boldsymbol{v}) - 1)r_{\boldsymbol{y}}]^{-1}(-D(\boldsymbol{y},\boldsymbol{v}))d^p\boldsymbol{y}d^p\boldsymbol{k}. \quad (166)$$

We now will list the steps to calculate the function $\varphi_0(\boldsymbol{x},\boldsymbol{v})$ (166).
Step 1. Solve the linear integral equation

$$[-L_{\boldsymbol{x}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}}]\varphi_{\text{loc}}(\boldsymbol{x},\boldsymbol{v}) = -D(\boldsymbol{x},\boldsymbol{v}). \quad (167)$$

and obtain the function $\varphi_{\text{loc}}(\boldsymbol{x},\boldsymbol{v})$.
Step 2. Calculate the Fourier transform $\hat{\varphi}_{\text{loc}}(\boldsymbol{k},\boldsymbol{v})$:

$$\hat{\varphi}_{\text{loc}}(\boldsymbol{k},\boldsymbol{v}) = \int \varphi_{\text{loc}}(\boldsymbol{y},\boldsymbol{v})\exp(-ik_s y_s)d^p\boldsymbol{y}. \quad (168)$$

Step 3. Solve the linear integral equation

$$[-L_{\boldsymbol{x}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)(r_{\boldsymbol{x}} + ik_s(v_s - u_s(\boldsymbol{x}))]\hat{\varphi}_0(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v}) = -\hat{D}(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v});$$
$$-\hat{D}(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v}) = [-L_{\boldsymbol{x}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}}]\hat{\varphi}_{\text{loc}}(\boldsymbol{k},\boldsymbol{v}). \quad (169)$$

and obtain the function $\hat{\varphi}_0(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v})$.
Step 4. Calculate the inverse Fourier transform $\varphi_0(\boldsymbol{x},\boldsymbol{v})$:

$$\varphi_0(\boldsymbol{x},\boldsymbol{v}) = (2\pi)^{-p}\int \hat{\varphi}_0(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v})\exp(ik_s x_s)d^p\boldsymbol{k}. \quad (170)$$

Completing these four steps, we obtain an explicit expression for the zeroth-order term of parametrics expansion $\varphi_0(\boldsymbol{x},\boldsymbol{v})$(165).

As we have already mentioned it above, equation (167) of Step 1 has an unique solution in $\text{Im}L_{\boldsymbol{x}}(\boldsymbol{v})$. Equation (169) of Step 3 has the same property. Indeed, for every $\boldsymbol{k}$, the right hand side $-\hat{D}(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v})$ is orthogonal to $\text{Im}\Pi_{\boldsymbol{x}}(\boldsymbol{v})$, and thus the existence and the uniqueness of formal solution $\hat{\varphi}_0(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v})$ follows again from the Fredholm alternative.

Thus, in Step 3, we obtain the unique solution $\hat{\varphi}_0(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v})$. For every $\boldsymbol{k}$, this is a function which belongs to $\text{Im}L_{\boldsymbol{x}}(\boldsymbol{v})$. Accounting that $f_0(\boldsymbol{x},\boldsymbol{v}) = f_0(n(\boldsymbol{x}),\boldsymbol{u}(\boldsymbol{x}),T(\boldsymbol{x}),\boldsymbol{v})$ expose no explicit dependency on $\boldsymbol{x}$, we see that the inverse Fourier transform of Step 4 gives $\varphi_0(\boldsymbol{x},\boldsymbol{v}) \in \text{Im}L_{\boldsymbol{x}}(\boldsymbol{v})$.

Equations (167)-(170) provide us with the scheme of constructing the zeroth-order term of parametrics expansion. Finishing this section, we will outline briefly the way to calculate the first-order term of this expansion.

Consider a formal operator $R = (1 - AB)^{-1}$. Operator R is defined by a formal series:

$$R = \sum_{m=0}^{\infty}(AB)^m. \quad (171)$$

In every term of this series, we want to place operators A left to operators B. In order to do this, we have to commutate B with A from left to right. The commutation of every pair BA yields the elementary transform $BA \to AB - [A,B]$ where $[A,B] = AB - BA$. Extracting the terms with no commutators $[A,B]$ and with a single commutator $[A,B]$, we arrive at the following representation:

$$R = R_0 + R_1 + (\text{terms with more than two brackets}). \tag{172}$$

Here

$$R_0 = \sum_{m=0}^{\infty} A^m B^m; \tag{173}$$

$$R_1 = -\sum_{m=2}^{\infty}\sum_{i=2}^{\infty} iA^{m-i}[A,B]A^{i-1}B^{i-1}B^{m-i}. \tag{174}$$

Operator R_0 (173) is the zeroth-order term of parametrics expansion derived above. Operator R_1 (the **first-order term of parametrics expansion**) can be represented as follows:

$$R_1 = -\sum_{m=1}^{\infty} mA^m[A,B](\sum_{i=0}^{\infty} A^i B^i)B^m = -\sum_{m=1}^{\infty} mA^m C B^m, \quad C = [A,B]R_0. \tag{175}$$

This expression can be considered as an *ansatz* for the formal series (171), and it gives the most convenient way to calculate R_1. Its structure is similar to that of R_0. Continuing in this manner, we can derive the second-order term R_2, etc. We will not discuss these questions in this paper.

In the next subsection we will consider in more detail the first-order term of parametrics expansion.

Finite-Dimensional Approximations to Integral Equations

Dealing further only with the zeroth-order term of parametrics expansion (166), we have to solve two linear integral equations, (167) and (169). These equations satisfy the Fredholm alternative, and thus they have unique solutions. The problem we face here is exactly of the same level of complexity as that of the Chapman-Enskog method [43]. The usual approach is to replace integral operators with some appropriate finite-dimensional operators.

First we will recall standard objectives of finite- dimensional approximations, considering equation (167). Let $p_i(\boldsymbol{x},\boldsymbol{v})$, where $i = 1, 2, \ldots$, be a basis in $\mathrm{Im}L_{\boldsymbol{x}}(\boldsymbol{v})$. Every function $\varphi(\boldsymbol{x},\boldsymbol{v}) \in \mathrm{Im}L_{\boldsymbol{x}}(\boldsymbol{v})$ might be represented in this basis as:

$$\varphi(\boldsymbol{x},\boldsymbol{v}) = \sum_{i=1}^{\infty} a_i(\boldsymbol{x}) p_i(\boldsymbol{x},\boldsymbol{v}); a_i(\boldsymbol{x}) = (\varphi(\boldsymbol{x},\boldsymbol{v}), p_i(\boldsymbol{x},\boldsymbol{v}))_{\boldsymbol{x}}. \tag{176}$$

Equation (167) is equivalent to an infinite set of linear algebraic equations with respect to unknowns $a_i(\boldsymbol{x})$:

$$\sum_{i=1}^{\infty} m_{ki}(\boldsymbol{x}) a_i(\boldsymbol{x}) = d_k(\boldsymbol{x}), \quad k = 1, 2, \dots. \tag{177}$$

Here

$$\begin{aligned} m_{ki}(\boldsymbol{x}) &= (p_k(\boldsymbol{x}, \boldsymbol{v}), A_{\mathrm{loc}}(\boldsymbol{x}, \boldsymbol{v}) p_i(\boldsymbol{x}, \boldsymbol{v}))_{\boldsymbol{x}}; \\ d_k(\boldsymbol{x}) &= -(p_k(\boldsymbol{x}, \boldsymbol{v}), D(\boldsymbol{x}, \boldsymbol{v}))_{\boldsymbol{x}}. \end{aligned} \tag{178}$$

For a finite-dimensional approximation of equation (177) we use a projection onto a finite number of basis elements $p_i(\boldsymbol{x}, \boldsymbol{v}), i = i_1, \dots, i_n$. Then, instead of (176), we search for the function φ_{fin}:

$$\varphi_{\mathrm{fin}}(\boldsymbol{x}, \boldsymbol{v}) = \sum_{s=1}^{n} a_{i_s}(\boldsymbol{x}) p_{i_s}(\boldsymbol{x}, \boldsymbol{v}). \tag{179}$$

Infinite set of equations (177) is replaced with a finite set of linear algebraic equations with respect to $a_{i_s}(\boldsymbol{x})$, where $s = 1, \dots, n$:

$$\sum_{l=1}^{n} m_{i_s i_l}(\boldsymbol{x}) a_{i_l}(\boldsymbol{x}) = d_{i_s}(\boldsymbol{x}), \quad s = 1, \dots, n. \tag{180}$$

There are no a priori restrictions upon the choice of the basis, as well as upon the choice of its finite-dimensional approximations. In this paper we use the standard basis of unreducible Hermite tensors (see, for example, [69, 113]. The simplest appropriate version of a finite-dimensional approximation occurs if the finite set of Hermite tensors is chosen as:

$$\begin{aligned} p_k(\boldsymbol{x}, \boldsymbol{v}) &= c_k(\boldsymbol{x}, \boldsymbol{v})(c^2(\boldsymbol{x}, \boldsymbol{v}) - (5/2)), k = 1, 2, 3; \\ p_{ij}(\boldsymbol{x}, \boldsymbol{v}) &= c_i(\boldsymbol{x}, \boldsymbol{v}) c_j(\boldsymbol{x}, \boldsymbol{v}) - \frac{1}{3}\delta_{ij} c^2(\boldsymbol{x}, \boldsymbol{v}), \quad i, j = 1, 2, 3; \\ c_i(\boldsymbol{x}, \boldsymbol{v}) &= \boldsymbol{v}_T^{-1}(\boldsymbol{x})(v_i - u_i(\boldsymbol{x})), \quad v_T(\boldsymbol{x}) = (2k_B T(\boldsymbol{x})/m)^{1/2}. \end{aligned} \tag{181}$$

It is important to stress here that "good" properties of orthogonality of Hermite tensors, as well as of other similar polynomial systems in BE theory, have the local in $\boldsymbol{x}$ character, i.e. when these functions are treated as polynomials in $c(\boldsymbol{x}, \boldsymbol{v})$ rather than polynomials in $\boldsymbol{v}$. For example, functions $p_k(\boldsymbol{x}, \boldsymbol{v})$ and $p_{ij}(\boldsymbol{x}, \boldsymbol{v})$(181) are orthogonal in the sense of the scalar product $(\cdot, \cdot)_{\boldsymbol{x}}$:

$$(p_k(\boldsymbol{x}, \boldsymbol{v}), p_{ij}(\boldsymbol{x}, \boldsymbol{v}))_{\boldsymbol{x}} \propto \int e^{-c^2(\boldsymbol{x}, \boldsymbol{v})} p_k(\boldsymbol{x}, \boldsymbol{v}) p_{ij}(\boldsymbol{x}, \boldsymbol{v}) d^3 c(\boldsymbol{x}, \boldsymbol{v}) = 0. \tag{182}$$

On contrary, functions $p_k(\boldsymbol{y}, \boldsymbol{v})$ and $p_{ij}(\boldsymbol{x}, \boldsymbol{v})$ are not orthogonal neither in the sense of the scalar product $(\cdot, \cdot)_{\boldsymbol{y}}$, nor in the sense of the scalar product $(\cdot, \cdot)_{\boldsymbol{x}}$, if $\boldsymbol{y} \neq \boldsymbol{x}$. This distinction is important for constructing the parametrics expansion. Further, we will omit the dependencies on $\boldsymbol{x}$ and $\boldsymbol{v}$ in the dimensionless velocity $c_i(\boldsymbol{x}, \boldsymbol{v})$(181) if no misunderstanding might occur.

In this section we will consider the case of one-dimensional in $\boldsymbol{x}$ equations. We assume that:

$$u_1(\boldsymbol{x}) = u(x_1), \quad u_2 = u_3 = 0, \quad T(\boldsymbol{x}) = T(x_1), \quad n(\boldsymbol{x}) = n(x_1). \tag{183}$$

We write x instead of x_1 below. Finite-dimensional approximation (181) requires only two functions:

$$p_3(x,\boldsymbol{v}) = c_1^2(x,\boldsymbol{v}) - \frac{1}{3}c^2(x,\boldsymbol{v}), \quad p_4(x,\boldsymbol{v}) = c_1(x,\boldsymbol{v})(c^2(x,\boldsymbol{v}) - (5/2)),$$
$$c_1(x,\boldsymbol{v}) = v_T^{-1}(x)(v_1 - u(x)), c_{2,3}(x,\boldsymbol{v}) = v_T^{-1}(x)v_{2,3}. \tag{184}$$

We now will make a step-by-step calculation of the zeroth-order term of parametrics expansion, in the one-dimensional case, for the finite-dimensional approximation (184).

Step 1. *Calculation of* $\varphi_{\mathrm{loc}}(x,\boldsymbol{v})$ *from equation* (167).

We search for the function $\varphi_{\mathrm{loc}}(x,\boldsymbol{v})$ in the approximation (184) as:

$$\varphi_{\mathrm{loc}}(x,\boldsymbol{v}) = a_{\mathrm{loc}}(x)(c_1^2 - (1/3)c^2) + b_{\mathrm{loc}}(x)c_1(c^2 - (5/2)). \tag{185}$$

Finite-dimensional approximation (180) of integral equation (167) in the basis (184) yields:

$$m_{33}(x)a_{\mathrm{loc}}(x) + m_{34}(x)b_{\mathrm{loc}}(x) = \alpha_{\mathrm{loc}}(x);$$
$$m_{43}(x)a_{\mathrm{loc}}(x) + m_{44}(x)b_{\mathrm{loc}}(x) = \beta_{\mathrm{loc}}(x). \tag{186}$$

Notations used are:

$$m_{33}(x) = n(x)\lambda_3(x) + \frac{11}{9}\frac{\partial u}{\partial x}; \qquad m_{44}(x) = n(x)\lambda_4(x) + \frac{27}{4}\frac{\partial u}{\partial x};$$
$$m_{34}(x) = m_{43}(x) = \frac{v_T(x)}{3}\left(\frac{\partial \ln n}{\partial x} + \frac{11}{2}\frac{\partial \ln T}{\partial x}\right);$$
$$\lambda_{3,4}(x) = -\frac{1}{\pi^{3/2}}\int e^{-c^2(\boldsymbol{x},\boldsymbol{v})}p_{3,4}(x,\boldsymbol{v})L_{\boldsymbol{x}}(\boldsymbol{v})p_{3,4}(\boldsymbol{x},\boldsymbol{v})d^3c(\boldsymbol{x},\boldsymbol{v}) > 0;$$
$$\alpha_{\mathrm{loc}}(x) = -\frac{2}{3}\frac{\partial u}{\partial x}; \qquad \beta_{\mathrm{loc}}(x) = -\frac{5}{4}v_T(x)\frac{\partial \ln T}{\partial x}. \tag{187}$$

Parameters $\lambda_3(x)$ and $\lambda_4(x)$ are easily expressed via Enskog integral brackets, and they are calculated in [43] for a wide class of molecular models.

Solving equation (186), we obtain coefficients $a_{\mathrm{loc}}(x)$ and $b_{\mathrm{loc}}(x)$ in the expression (185):

$$a_{\mathrm{loc}} = \frac{A_{\mathrm{loc}}(x)}{Z(x,0)}; \qquad b_{\mathrm{loc}} = \frac{B_{\mathrm{loc}}(x)}{Z(x,0)}; \qquad Z(x,0) = m_{33}(x)m_{44}(x) - m_{34}^2(x);$$
$$A_{\mathrm{loc}}(x) = \alpha_{\mathrm{loc}}(x)m_{44}(x) - \beta_{\mathrm{loc}}(x)m_{34}(x);$$
$$B_{\mathrm{loc}}(x) = \beta_{\mathrm{loc}}(x)m_{33}(x) - \alpha_{\mathrm{loc}}(x)m_{34}(x);$$
$$a_{\mathrm{loc}} = \frac{-\frac{2}{3}\frac{\partial u}{\partial x}\left(n\lambda_4 + \frac{27}{4}\frac{\partial u}{\partial x}\right) + \frac{5}{12}v_T^2\frac{\partial \ln T}{\partial x}\left(\frac{\partial \ln n}{\partial x} + \frac{11}{2}\frac{\partial \ln T}{\partial x}\right)}{\left(n\lambda_3 + \frac{11}{9}\frac{\partial u}{\partial x}\right)\left(n\lambda_4 + \frac{27}{4}\frac{\partial u}{\partial x}\right) - \frac{v_T^2}{9}\left(\frac{\partial \ln n}{\partial x} + \frac{11}{2}\frac{\partial \ln T}{\partial x}\right)^2};$$

$$b_{\mathrm{loc}} = \frac{-\frac{5}{4}v_T\frac{\partial \ln T}{\partial x}\left(n\lambda_3 + \frac{11}{9}\frac{\partial u}{\partial x}\right) + \frac{2}{9}v_T\frac{\partial u}{\partial x}\left(\frac{\partial \ln n}{\partial x} + \frac{11}{2}\frac{\partial \ln T}{\partial x}\right)}{\left(n\lambda_3 + \frac{11}{9}\frac{\partial u}{x}\right)\left(n\lambda_4 + \frac{27}{4}\frac{\partial u}{\partial x}\right) - \frac{v_T^2}{9}\left(\frac{\partial \ln n}{x} + \frac{11}{2}\frac{\partial \ln T}{x}\right)^2}. \tag{188}$$

These expressions complete Step 1.

Step 2. *Calculation of Fourier transform of $\varphi_{loc}(x, \boldsymbol{v})$ and its expression in the local basis.*

In this step we make two operations:
i) The Fourier transformation of the function $\varphi_{\mathrm{loc}}(x, \boldsymbol{v})$:

$$\hat{\varphi}_{\mathrm{loc}}(k, \boldsymbol{v}) = \int_{-\infty}^{+\infty} \exp(-iky)\varphi_{\mathrm{loc}}(y, \boldsymbol{v})dy. \tag{189}$$

ii) The representation of $\hat{\varphi}_{\mathrm{loc}}(k, \boldsymbol{v})$ in the local basis $\{p_0(x, \boldsymbol{v}), \ldots, p_4(x, \boldsymbol{v})\}$:

$$\begin{gathered} p_0(x, \boldsymbol{v}) = 1, p_1(x, \boldsymbol{v}) = c_1(x, \boldsymbol{v}), p_2(x, \boldsymbol{v}) = c^2(x, \boldsymbol{v}) - (3/2), \\ p_3(x, \boldsymbol{v}) = c_1^2(x, \boldsymbol{v}) - (1/3)c^2(x, \boldsymbol{v}), p_4(x, \boldsymbol{v}) = c_1(x, \boldsymbol{v})(c^2(x, \boldsymbol{v}) - (5/2)). \end{gathered} \tag{190}$$

Operation (ii) is necessary for completing Step 3 because there we deal with x-dependent operators. Obviously, the function $\hat{\varphi}_{\mathrm{loc}}(k, \boldsymbol{v})$ (189) is a finite-order polynomial in $\boldsymbol{v}$, and thus the operation (ii) is exact.

We obtain in (ii):

$$\hat{\varphi}_{\mathrm{loc}}(x, k, \boldsymbol{v}) \equiv \hat{\varphi}_{\mathrm{loc}}(x, k, c(x, \boldsymbol{v})) = \sum_{i=0}^{4} \hat{h}_i(x, k)p_i(x, \boldsymbol{v}). \tag{191}$$

Here

$$\hat{h}_i(x, k) = (p_i(x, \boldsymbol{v}), p_i(x, \boldsymbol{v}))_x^{-2}(\hat{\varphi}_{\mathrm{loc}}(k, \boldsymbol{v}), p_i(x, \boldsymbol{v}))_x \tag{192}$$

. Let us introduce notations:

$$\vartheta \equiv \vartheta(x, y) = (T(x)/T(y))^{1/2}, \gamma \equiv \gamma(x, y) = \frac{u(x) - u(y)}{v_T(y)}. \tag{193}$$

Coefficients $\hat{h}_i(x, k)$(192) have the following explicit form:

$$\begin{aligned} \hat{h}_i(x, k) = \int_{-\infty}^{+\infty} \exp(-iky)h_i(x, y)dy; h_i(x, y) = Z^{-1}(y, 0)g_i(x, y) \\ g_0(x, y) = B_{\mathrm{loc}}(y)(\gamma^3 + \frac{5}{2}\gamma(\vartheta^2 - 1)) + \frac{2}{3}A_{\mathrm{loc}}(y)\gamma^2; \\ g_1(x, y) = B_{\mathrm{loc}}(y)(3\vartheta\gamma^2 + \frac{5}{2}\vartheta(\vartheta^2 - 1)) + \frac{4}{3}A_{\mathrm{loc}}(y)\vartheta\gamma; \\ g_2(x, y) = \frac{5}{3}B_{\mathrm{loc}}(y)\vartheta^2\gamma; \\ g_3(x, y) = B_{\mathrm{loc}}(y)2\vartheta\gamma + A_{\mathrm{loc}}(y)\vartheta^2; \\ g_4(x, y) = B_{\mathrm{loc}}(y)\vartheta^3. \end{aligned} \tag{194}$$

Here $Z(y,0), B_{\rm loc}(y)$ and $A_{\rm loc}(y)$ are functions defined in (188)

Step 3. *Calculation of the function* $\hat{\varphi}_0(x,k,\boldsymbol{v})$ *from equation* (169).

Linear integral equation (169) has character similar to that of equation (167). We search for the function $\hat{\varphi}_0(x,k,\boldsymbol{v})$ in the basis (184) as:

$$\hat{\varphi}_0(x,k,\boldsymbol{v}) = \hat{a}_0(x,k)p_3(x,\boldsymbol{v}) + \hat{b}_0(x,k)p_4(x,\boldsymbol{v}). \tag{195}$$

Finite-dimensional approximation of the integral equation (169) in the basis (184) yields the following equations for unknowns $\hat{a}_0(x,k)$ and $\hat{b}_0(x,k)$:

$$\begin{gathered} m_{33}(x)\hat{a}_0(x,k) + \left[m_{34}(x) + \frac{1}{3}ikv_T(x)\right]\hat{b}_0(x,k) = \hat{\alpha}_0(x,k); \\ \left[m_{43}(x) + \frac{1}{3}ikv_T(x)\right]\hat{a}_0(x,k) + m_{44}(x)\hat{b}_0(x,k) = \hat{\beta}_0(x,k). \end{gathered} \tag{196}$$

Notations used here are:

$$\begin{gathered} \hat{\alpha}_0(x,k) = m_{33}(x)\hat{h}_3(x,k) + m_{34}(x)\hat{h}_4(x,k) + \hat{s}_\alpha(x,k); \\ \hat{\beta}_0(x,k) = m_{43}(x)\hat{h}_3(x,k) + m_{44}(x)\hat{h}_4(x,k) + \hat{s}_\beta(x,k); \\ \hat{s}_{\alpha,\beta}(x,k) = \textstyle\int_{-\infty}^{+\infty} \exp(-iky)s_{\alpha,\beta}(x,y)dy; \end{gathered}$$

$$s_\alpha(x,y) = \tfrac{1}{3}v_T(x)\left(\tfrac{\partial \ln n}{\partial x} + 2\tfrac{\partial \ln T}{\partial x}\right)h_1(x,y) + \tfrac{2}{3}\tfrac{\partial u}{\partial x}(h_0(x,y) + 2h_2(x,y)); \tag{197}$$

$$s_\beta(x,y) = \tfrac{5}{4}v_T(x)\left(\tfrac{\partial \ln n}{\partial x}h_2(x,y) + \tfrac{\partial \ln T}{\partial x}(3h_2(x,y) + h_0(x,y))\right) + \tfrac{2\partial u}{3\partial x}h_1(x,y). \tag{198}$$

Solving equations (196), we obtain functions $\hat{a}_0(x,k)$ and $\hat{b}_0(x,k)$ in (195):

$$\begin{aligned} \hat{a}_0(x,k) &= \frac{\hat{\alpha}_0(x,k)m_{44}(x) - \hat{\beta}_0(x,k)(m_{34}(x) + \frac{1}{3}ikv_T(x))}{Z(x,\frac{1}{3}ikv_T(x))}; \\ \hat{b}_0(x,k) &= \frac{\hat{\beta}_0(x,k)m_{33}(x) - \hat{\alpha}_0(x,k)(m_{34}(x) + \frac{1}{3}ikv_T(x))}{Z(x,\frac{1}{3}ikv_T(x))}. \end{aligned} \tag{199}$$

Here

$$\begin{aligned} Z(x,\frac{1}{3}ikv_T(x)) &= Z(x,0) + \frac{k^2v_T^2(x)}{9} + \frac{2}{3}ikv_T(x)m_{34}(x) = \\ = \left(n\lambda_3 + \frac{11\partial u}{9\partial x}\right)&\left(n\lambda_4 + \frac{27\partial u}{4\partial x}\right) - \frac{v_T^2(x)}{9}\left(\frac{\partial \ln n}{\partial x} + \frac{11\partial \ln T}{2\partial x}\right)^2 + \frac{k^2v_T^2(x)}{9} + \\ &+\frac{2}{9}ikv_T^2(x)\left(\frac{\partial \ln n}{\partial x} + \frac{11\partial \ln T}{2\partial x}\right). \end{aligned} \tag{200}$$

Step 4. *Calculation of the inverse Fourier transform of the function* $\hat{\varphi}_0(x,k,\boldsymbol{v})$.

The inverse Fourier transform of the function $\hat{\varphi}_0(x,k,\boldsymbol{v})$ (195) yields:

$$\varphi_0(x,\boldsymbol{v}) = a_0(x)p_3(x,\boldsymbol{v}) + b_0(x)p_4(x,\boldsymbol{v}). \tag{201}$$

Here

$$a_0(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \exp(ikx)\hat{a}_0(x,k)dk,$$
$$b_0(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \exp(ikx)\hat{b}_0(x,k)dk. \tag{202}$$

Taking into account expressions (188), (197)-(200), and (194), we obtain the explicit expression for the **finite-dimensional approximation of the zeroth-order term of parametrics expansion** (201):

$$\begin{aligned} a_0(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dk \exp(ik(x-y))Z^{-1}(x, \frac{1}{3}ikv_T(x)) \times \\ \times \{Z(x,0)h_3(x,y) + [s_\alpha(x,y)m_{44}(x) - s_\beta(x,y)m_{34}(x)] - \\ -\frac{1}{3}ikv_T(x)[m_{34}(x)h_3(x,y) + m_{44}(x)h_4(x,y) + s_\beta(x,y)]\Big\}; \\ b_0(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dk \exp(ik(x-y))Z^{-1}(x, \frac{1}{3}ikv_T(x)) \times \\ \times \{Z(x,0)h_4(x,y) + [s_\beta(x,y)m_{33}(x) - s_\alpha(x,y)m_{34}(x)] - \\ -\frac{1}{3}ikv_T(x)[m_{34}(x)h_4(x,y) + m_{33}(x)h_3(x,y) + s_\alpha(x,y)]\Big\}. \end{aligned} \tag{203}$$

Hydrodynamic Equations

Now we will discuss briefly the utility of obtained results for hydrodynamics.

The correction to LM functions $f_0(n,\boldsymbol{u},T)$(97) obtained has the form:

$$f_1(n,\boldsymbol{u},T) = f_0(n,\boldsymbol{u},T)(1+\varphi_0(n,\boldsymbol{u},T)) \tag{204}$$

Here the function $\varphi_0(n,\boldsymbol{u},T)$ is given explicitly with expressions (201)-(203).

The usual form of closed hydrodynamic equations for $n, \boldsymbol{u}$, and T, where the traceless tension tensor σ_{ik} and the heat flux vector q_i are expressed via hydrodynamic variables, will be obtained if we substitute the function (204) into balance equations of the density, of the momentum, and of the energy. For LM approximation, these balance equations result in Euler equation of the nonviscid liquid (i.e. $\sigma_{ik}(f_0) \equiv 0$, and $q_i(f_0) \equiv 0$). For the correction f_1 (204), we obtain the following expressions of $\sigma = \sigma_{xx}(f_1)$ and $q = q_x(f_1)$ (all other components are equal to zero in the one- dimensional situation under consideration):

$$\sigma = \frac{1}{3}na_0,\ q = \frac{5}{4}nb_0. \tag{205}$$

Here a_0 and b_0 are given by expression (203).

From the geometrical viewpoint, hydrodynamic equations with the tension tensor and the heat flux vector (205) have the following interpretation: we take the corrected manifold Ω_1 which consists of functions f_1 (204), and we project the BE vectors $J_{\boldsymbol{u}}(f_1)$ onto the tangent spaces T_{f_1} using the LM projector P_{f_0} (102).

Although a detailed investigation of these hydrodynamic equations is a subject of a special study and it is not the goal of this paper, some points should be mentioned.

Nonlocality

Expressions (203) expose a nonlocal spatial dependency, and, hence, the corresponding hydrodynamic equations are nonlocal. This nonlocality appears through two contributions. The first of these contributions might be called a *frequency-response* contribution, and it comes through explicit non- polynomial k-dependency of integrands in (203). This latter dependency has the form:

$$\int_{-\infty}^{+\infty} \frac{A(x,y)+ikB(x,y)}{C(x,y)+ikD(x,y)+k^2E(x,y)} \exp(ik(x-y))dk. \tag{206}$$

Integration over k in (206) can be completed via auxiliary functions.

The second nonlocal contribution might be called *correlative*, and it is due to relationships via $(u(x)-u(y))$ (the difference of flow velocities in points x and y) and via $T(x)/T(y)$ (the ratio of temperatures in points x and y).

Acoustic spectra

The purely frequency-response contribution to hydrodynamic equations is relevant to small perturbations of equilibria. The tension tensor σ and the heat flux q(205) are:

$$\sigma = -(2/3)n_0T_0R\left(2\varepsilon\frac{\partial u'}{\partial\xi} - 3\varepsilon^2\frac{\partial^2 T}{\partial\xi^2}\right);$$

$$q = -(5/4)T_0^{3/2}n_0R\left(3\varepsilon\frac{\partial T'}{\partial\xi} - (8/5)\varepsilon^2\frac{\partial^2 u}{\partial\xi^2}\right). \tag{207}$$

Here

$$R = \left(1-(2/5)\varepsilon^2\frac{\partial^2}{\partial\xi^2}\right)-1. \tag{208}$$

In (207), we have expressed parameters λ_3 and λ_4 via the viscosity coefficient μ of the Chapman-Enskog method [43] (it is easy to see from (187) that $\lambda_3 = \lambda_4 \propto \mu^{-1}$ for spherically symmetric models of a collision), and we have used the following notations: T_0 and n_0 are the equilibrium temperature and density, $\xi = (\eta T_0^{1/2})^{-1}n_0x$ is the dimensionless coordinate, $\eta = \mu(T_0)/T_0, u' = T_0^{-1/2}\delta u, T' = \delta T/T_0, n' = \delta n/n_0$, and $\delta u, \delta T, \delta n$ are the deviations of the flux velocity, of the temperature and of the density from their equilibrium values $u=0, T=T_0$ and $n=n_0$. We also use the system of units with $k_B = m = 1$.

In the linear case, the parametrics expansion degenerates, and its zeroth-order term (170) gives the solution of equation (147).

The dispersion relationship for the approximation (207) is:

$$\omega^3 + (23k^2/6D)\omega^2 + \left\{k^2 + (2k^4/D^2) + (8k^6/5D^2)\right\}\omega + (5k^4/2D) = 0;$$
$$D = 1 + (4/5)k^2. \tag{209}$$

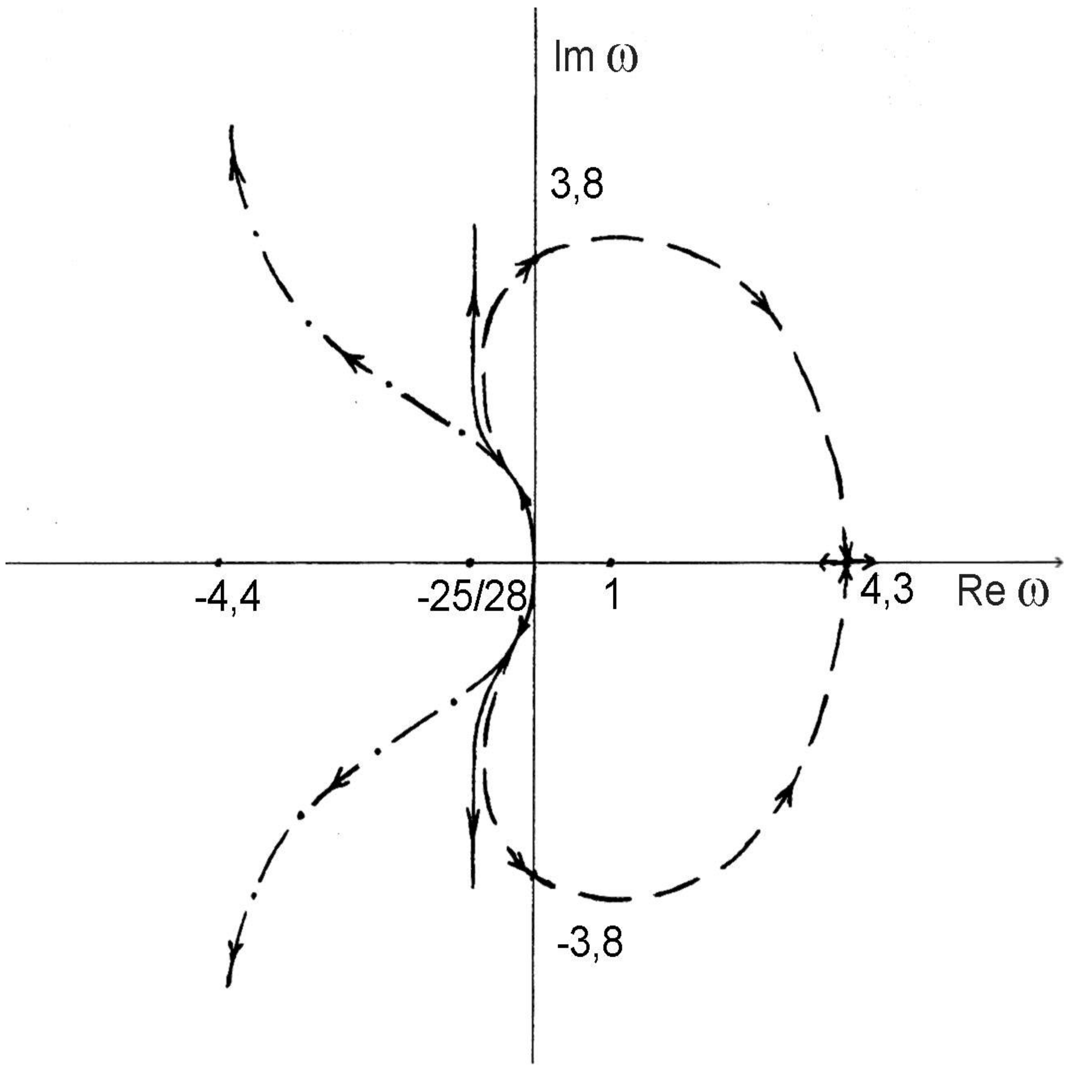


Figure 2: Acoustic dispersion curves for approximation 207 (solid line), for second (the Burnett) approximation of the Chapman-Enskog expansion [45] (dashed line) and for the regularization of the Burnett approximation via partial summing of the Chapman-Enskog expansion [22, 23] (punctuated dashed line). Arrows indicate an increase of k^2.

Here k is the wave vector.

Acoustic spectra given by dispersion relationship (209) contains no nonphysical short-wave instability characteristic to the Burnett approximation (Fig. 2). The regularization of the Burnett approximation [22, 23] has the same feature. Both of these approximations predict a limit of the decrement Reω for short waves.

Nonlinearity

Nonlinear dependency on $\frac{\partial u}{\partial x}$, on $\frac{\partial \ln T}{\partial x}$, and on $\frac{\partial \ln n}{\partial x}$ appears already in the local approximation $\varphi_{\rm loc}$(188). In order to outline some peculiarities of this nonlinearity, we represent the zeroth-order term of the expansion of $a_{\rm loc}$(188) into powers of $\frac{\partial \ln T}{\partial x}$ and $\frac{\partial \ln n}{\partial x}$:

$$a_{\rm loc} = -\frac{2}{3}\frac{\partial u}{\partial x}\left(n\lambda_3 + \frac{11}{9}\frac{\partial u}{\partial x}\right)^{-1} + O\left(\frac{\partial \ln T}{\partial x}, \frac{\partial \ln n}{\partial x}\right). \tag{210}$$

This expression describes the asymptotic of the "purely nonlinear" contribution to the tension tensor σ(205) for a strong divergency of a flow. The account of nonlocality yields instead of (207):

$$\begin{aligned} a_0(x) = -\frac{1}{2\pi}\int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dk \exp(ik(x-y))\frac{2}{3}\frac{\partial u}{\partial y}\left(n\lambda_3 + \frac{11}{9}\frac{\partial u}{\partial y}\right)^{-1} \times \\ \times \left[\left(n\lambda_3 + \frac{11}{9}\frac{\partial u}{\partial x}\right)\left(n\lambda_4 + \frac{27}{4}\frac{\partial u}{\partial x}\right) + \frac{k^2 v_T^2}{9}\right]^{-1}\left[\left(n\lambda_3 + \frac{11}{9}\frac{\partial u}{\partial x}\right)\left(n\lambda_4 + \frac{27}{4}\frac{\partial u}{\partial x}\right) + \right. \\ \left. + \frac{4}{9}\left(n\lambda_4 + \frac{27}{4}\frac{\partial u}{dy}\right)\frac{\partial u}{\partial x} v_T^{-2}(u(x)-u(y))^2 - \frac{2}{3}ik\frac{\partial u}{\partial x}(u(x)-u(y))\right] + \\ + O\left(\frac{\partial \ln T}{\partial x}, \frac{\partial \ln n}{\partial x}\right). \end{aligned} \tag{211}$$

Both expressions, (210) and (211) become singular when

$$\frac{\partial u}{\partial y} \to \left(\frac{\partial u}{\partial y}\right)^{*} = -\frac{9n\lambda_3}{11}. \tag{212}$$

Hence, the tension tensor (206) becomes infinite if $\frac{\partial u}{\partial y}$ tends to $\frac{\partial u}{\partial y}^{*}$ in any point y. In other words, the flow becomes infinitely viscid when $\frac{\partial u}{\partial y}$ approaches the negative value $-\frac{9n\lambda_3}{11}$. This infinite viscosity threshold prevents a transfer of the flow into nonphysical region of negative viscosity if $\frac{\partial u}{\partial y} > \frac{\partial u}{\partial y}^{*}$ because of the infinitely strong dumping at $\frac{\partial u}{\partial y}^{*}$. This peculiarity was detected in [22, 23] as a result of partial summing of the Chapman-Enskog expansion. In particular, partial summing for the simplest nonlinear situation [24, 129] yields the following expression for the tension tensor σ:

$$\begin{aligned} \sigma = \sigma_{{\rm I}R} + \sigma_{{\rm II}R}; \quad \sigma_{{\rm I}R} = -\frac{4}{3}\left(1 - \frac{5}{3}\varepsilon^2\frac{\partial^2}{\partial\xi^2}\right)^{-1}\left(\varepsilon\frac{\partial u'}{\partial \xi} + \varepsilon^2\frac{\partial^2\theta'}{\partial\xi^2}\right); \quad \theta' = T' + n'; \\ \sigma_{{\rm II}R} = \frac{28}{9}\left(1 + \frac{7}{3}\varepsilon\frac{\partial u'}{\partial\xi}\right)^{-1}\frac{\partial^2 u'}{\partial\xi^2}. \end{aligned} \tag{213}$$

Notations here follow (207) and (208). Expression (213) might be considered as a "rough draft" of the "full" tension tensor defined by a_0(203). It accounts both the frequency-response and the nonlinear contributions ($\sigma_{\mathrm{I}R}$ and $\sigma_{\mathrm{II}R}$, respectively) in a simple form of a sum. However, the superposition of these contributions in (203) is more complicated. Moreover, the explicit correlative nonlocality of expression (203) was never detected neither in [24], nor in numerous examples of partial summing [129].

Nevertheless, approximation (213) contains the peculiarity of viscosity similar to that in (210) and (211). In dimensionless variables and $\varepsilon = 1$, expression (213) predicts the infinite threshold at velocity divergency equal to -(3/7), rather than $-(9/11)$ in (210) and (211). Viscosity tends to zero as the divergency tends to positive infinity in both approximations. Physical interpretation of these phenomena was given in [24]: large *positive* values of $\frac{\partial u}{\partial x}$ means that the gas diverges rapidly, and the flow becomes nonviscid because the particles retard to exchange their momentum. On contrary, its *negative* values (such as -(3/7) for (213) and -(9/11)) for (210) and (211)) describe a strong compression of the flow. Strong deceleration results in "solid fluid" limit with an infinite viscosity (Fig. 3).

Thus, hydrodynamic equations for approximation (204) are both nonlinear and nonlocal. This result is not surprising, accounting the integro-differential character of equation (147).

It is important that no small parameters were used neither when we were deriving equation (147) nor when we were obtaining the correction (204).

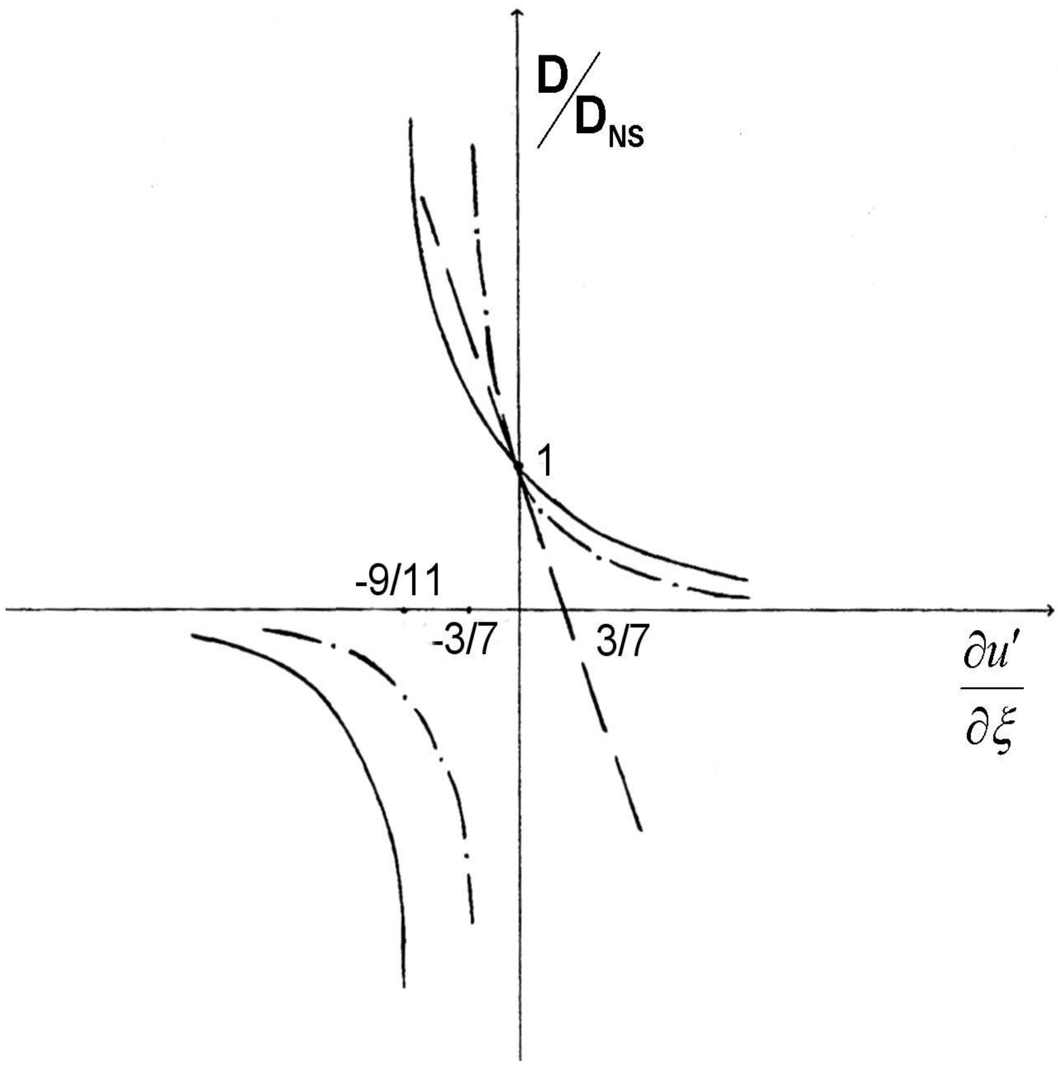


Figure 3: Dependency of viscosity on compression for approximation (210) (solid line), for partial summing (213) (punctuated dashed line), and for the Burnett approximation [24, 129] (dashed line). The latter changes the sign at a regular point and, hence, nothing prevents the flow to transfer into the nonphysical region.

Example 4: Non-perturbative derivation of linear hydrodynamics from Boltzmann equation (3D)

Using Newton method instead of power series, a model of linear hydrodynamics is derived from the Boltzmann equation for regimes where Knudsen number is of order unity. The model demonstrates no violation of stability of acoustic spectra in contrast to Burnett hydrodynamics.

Knudsen number ε (a ratio between the mean free path, l_c, and a scale of hydrodynamic flows, l_h) is a recognized order parameter when hydrodynamics is derived from the Boltzmann equation [134]. The Chapman–Enskog method [43] establishes Navier-Stokes hydrodynamic equations as the first-order correction to Euler hydrodynamics at $\varepsilon \to 0$, and it also derives formal corrections of order ε^2, ε^3, ... (known as Burnett and super-Burnett corrections). These corrections are important outside the strictly hydrodynamic domain $\varepsilon \ll 1$, and has to be considered for an exension of hydrodynamic description into a highly nonequilidrium domain $\varepsilon \leq 1$. Not much is known about high-order in ε hydrodynamics, especially in a nonlinear case. Nonetheless, in a linear case, some definite information can be obtained. On the one hand, experiments on sound propagation in noble gases are considerably better explained with Burnett and super-Burnett hydrodynamics rather than with Navier-Stokes approximation alone [136]. On the other hand, a direct calculation shows a non-physical behavior of Burnett hydrodynamics for ultra-short waves: acoustic waves increase instead of decay [45]. The latter failure of Burnett approximation cannot be rejected on a basis that for such regimes they might be not applicable because for Navier-Stokes approximation, which is formally still less valid, no such violation is observed.

These two results indicate that, at least in a linear regime, it makes sense to consider hydrodynamics at $\varepsilon \leq 1$, but Enskog way of deriving such hydrodynamics is problematic. The problem of constructing solutions to the Boltzmann equation valid when ε is of order unity is one of the main open problems of classical kinetic theory [134].

In this Example we suggest a new approach to derive a hydrodynamics at $\varepsilon \leq 1$. The main idea is to pose a problem of a finding a correction to Euler hydrodynamics in such a fashion that expansions in ε do not appear as a necessary element of analysis. This will be possible by using Newton method instead of Taylor expansions to get such correction. We restrict our consideration to a linear case. Resulting hydrodynamic equations do not exhibit the mentioned violation.

The starting point is the set of local Maxwell distribution functions (LM) $f_0(n, \boldsymbol{u}, T; \boldsymbol{v})$, where $\boldsymbol{v}$ is the particle's velocity, and n, $\boldsymbol{u}$, and T are local number density, average velocity, and temperature. We write the Boltzmann equation as:

$$\frac{df}{dt} = J(f), \quad J(f) = -(\boldsymbol{v} - \boldsymbol{u}) \cdot \nabla f + Q(f), \tag{214}$$

where $d/dt = \partial/\partial t + \boldsymbol{u} \cdot \nabla$ is the material derivative, while Q is the Boltzmann collision integral [134].

On the one hand, calculating r.h.s. of eq. (214) in LM-states, we obtain $J(f_0)$, a time derivative of LM-states due to Boltzmann equation. On the other hand, calculating a time derivative of LM-states due to Euler dynamics, we obtain $P_0 J(f_0)$, where P_0 is a projector operator onto the LM manifold (see [3]):

$$P_0 J = \frac{f_0}{n}\left\{\int J d\boldsymbol{c} + 2\boldsymbol{c}\cdot\int \boldsymbol{c} J d\boldsymbol{c} + \frac{2}{3}\left(c^2-\frac{3}{2}\right)\int\left(c^2-\frac{3}{2}\right) J d\boldsymbol{c}\right\}, \tag{215}$$

Since the LM functions are not solutions to the Boltzmann equation (214) (except for constant n, $\boldsymbol{u}$, and T), a difference of $J(f_0)$ and $P_0 J(f_0)$ is not equal to zero:

$$\Delta(f_0) = J(f_0) - P_0 J(f_0) = -f_0\left\{2\nabla\boldsymbol{u} : \left(\boldsymbol{cc} - \frac{1}{3}\mathrm{I}c^2\right) + v_T\frac{\nabla T}{T}\cdot\boldsymbol{c}\left(c^2-\frac{5}{2}\right)\right\}. \tag{216}$$

here $\boldsymbol{c} = v_T^{-1}(\boldsymbol{v}-\boldsymbol{u})$, and $v_T = \sqrt{2k_B T/m}$ is a heat velocity. Note that the latter expression gives a complete non-exactness of the linearized local Maxwell approximation, and it is neither big nor small in itself. An unknown hydrodynamic solution of eq.(214), $f_\infty(n,\boldsymbol{u},T;\boldsymbol{v})$, satisfies the following equation:

$$\Delta(f_\infty) = J(f_\infty) - P_\infty J(f_\infty) = 0, \tag{217}$$

where P_∞ is an unknown projecting operator. Both P_∞ and f_∞ are unknown in eq. (217), but, nontheless, one is able to consider a sequence of corrections $\{f_1, f_2, \ldots\}$, $\{P_1, P_2, \ldots\}$ to the initial approximation f_0 and P_0. A method to deal with equations of a form (217) was developed in [3] for a general case of dissipative systems. In particular, it was shown, how to ensure the H-theorem on every step of approximations by choosing appropriate projecting operators P_n. In the present illustrative example we will not consider projectors other than P_0, rather, we will use an iterative procedure to find f_1.

Let us apply the Newton method with incomplete linearization to eq. (217) with f_0 as initial approximation for f_∞ and with P_0 as an initial approximation for P_∞. Writing $f_1 = f_0 + \delta f$, we get the first Newton iterate:

$$L(\delta f/f_0) + (P_0 - 1)(\boldsymbol{v}-\boldsymbol{u})\cdot\nabla\delta f + \Delta(f_0) = 0, \tag{218}$$

where L is a linearized collision integral.

$$L(g) = f_0(\boldsymbol{v})\int w(\boldsymbol{v}_1', \boldsymbol{v}'; \boldsymbol{v}_1, \boldsymbol{v}) f_0(\boldsymbol{v}_1)\{g(\boldsymbol{v}_1') + g(\boldsymbol{v}') - g(\boldsymbol{v}_1) - g(\boldsymbol{v})\} d\boldsymbol{v}_1' d\boldsymbol{v}' d\boldsymbol{v}_1. \tag{219}$$

Here w is a probability density of a change of velocities, $(\boldsymbol{v},\boldsymbol{v}_1)\leftrightarrow(\boldsymbol{v}',\boldsymbol{v}_1')$, of a pair of molecules after their encounter. When deriving (218), we have accounted $P_0 L = 0$, and an additional condition which fixes the same values of n, $\boldsymbol{u}$, and T in states f_1 as in LM states f_0:

$$P_0 \delta f = 0. \tag{220}$$

Equation (218) is basic in what follows. Note that it contains no Knudsen number explicitly. Our strategy will be to treat equation (218) in such a way that the Knudsen number will appear explicitly only at the latest stage of computations.

The two further approximations will be adopted. The first concerns a linearization of eq. (218) about a global equilibria F_0. The second concerns a finite-dimensional approximation of integral operator in (218) in velocity space. It is worthwhile noting here that none of these approximations concerns an assumption about the Knudsen number.

Following the first of the approximations mentioned, denote as δn, $\delta \boldsymbol{u}$, and δT deviations of hydrodynamic variables from their equilibrium values n_0, $\boldsymbol{u}_0 = 0$, and T_0. Introduce also not-dimensional variables $\Delta n = \delta n / n_0$, $\Delta \boldsymbol{u} = \delta \boldsymbol{u} / v_T^0$, and $\Delta T = \delta T / T_0$, where v_T^0 is a heat velocity in equilibria, and a not-dimensional relative velocity $\boldsymbol{\xi} = \boldsymbol{v} / v_T^0$. Correction f_1 in a linear in deviations from F_0 approximation reads: $f_1 = F_0(1 + \varphi_0 + \varphi_1)$, where $\varphi_0 = \Delta n + 2\Delta \boldsymbol{u} \cdot \boldsymbol{\xi} + \Delta T(\xi^2 - 3/2)$ is a linearized deviation of LM from F_0, and φ_1 is an unknown function. The latter is to be obtained from a linearized version of eq.(218).

Following the second approximation, we search for φ_1 in a form:

$$\varphi_1 = A(\boldsymbol{x}) \cdot \boldsymbol{\xi} \left(\xi^2 - \frac{5}{2}\right) + B(\boldsymbol{x}) : \left(\boldsymbol{\xi}\boldsymbol{\xi} - \frac{1}{3} I \xi^2\right) + \dots \tag{221}$$

where dots denote terms of an expansion of φ_1 in velocity polynomials, orthogonal to $\boldsymbol{\xi}$ $(\xi^2 - 5/2)$ and $\boldsymbol{\xi}\boldsymbol{\xi} - 1/3 I \xi^2$, as well as to 1, to $\boldsymbol{\xi}$, and to ξ^2. These terms do not contribute to shear stress tensor and heat flux vector in hydrodynamic equations. Independency of functions A and B from ξ^2 amounts to a first Sonine polynomial approximation of viscosity and heat transfer coefficients. Put another way, we consider a projection onto a finite-dimensional subspace spanned by $\boldsymbol{\xi}(\xi^2 - 5/2)$ and $\boldsymbol{\xi}\boldsymbol{\xi} - (1/3) I \xi^2$. Our goal is to derive functions A and B from a linearized version of eq.(218). Knowing A and B, we get the following expressions for shear stress tensor $\boldsymbol{\sigma}$ and heat flux vector $\boldsymbol{q}$:

$$\sigma = p_0 B, \ \boldsymbol{q} = \frac{5}{4} p_0 v_T^0 A, \tag{222}$$

where p_0 is equilibrium pressure of ideal gas.

Linearizing eq.(218) near F_0, using an ansatz for φ_1 cited above, and turning to Fourier transform in space, we derive:

$$\begin{aligned} \frac{5 p_0}{3 \eta_0} \boldsymbol{a}_k + i v_T^0 \boldsymbol{b}_k \cdot \boldsymbol{k} &= -\frac{5}{2} i v_T^0 \boldsymbol{k} \tau_k; \\ \frac{p_0}{\eta_0} \boldsymbol{b}_k + i v_T^0 \overline{\boldsymbol{k}\boldsymbol{a}_k} &= -2 i v_T^0 \overline{\boldsymbol{k}\boldsymbol{\gamma}_k}, \end{aligned} \tag{223}$$

where $i = \sqrt{-1}$, $\boldsymbol{k}$ is a wave vector, η_0 is the first Sonine polynomial approximation of shear viscosity coefficient, $\boldsymbol{a}_k$, $\boldsymbol{b}_k$, τ_k and $\boldsymbol{\gamma}_k$ are Fourier transforms of $\boldsymbol{A}$, $\boldsymbol{B}$, ΔT, and $\Delta \boldsymbol{u}$, respectively, and the over-bar denotes a symmetric traceless dyad. Introducing dimensionless wave vector $\boldsymbol{f} = [(v_T^0 \eta_0)/(p_0)] \boldsymbol{k}$, solution to Eq. (223) may be written:

$$\boldsymbol{b}_k = -\frac{10}{3} i \overline{\boldsymbol{\gamma}_k \boldsymbol{f}} [(5/3) + (1/2) f^2]^{-1} + \frac{5}{3} i (\boldsymbol{\gamma}_k \cdot \boldsymbol{f}) \overline{\boldsymbol{f}\boldsymbol{f}} [(5/3) + (1/2) f^2]^{-1} [5 + 2 f^2]^{-1} \tag{224}$$

$$
\begin{aligned}
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad -\frac{15}{2}\tau_k\overline{\boldsymbol{f}\boldsymbol{f}}[5+2f^2]^{-1}\\
\boldsymbol{a}_k &= -\frac{15}{2}i\boldsymbol{f}\tau_k[5+2f^2]^{-1}-[5+2f^2]^{-1}[(5/3)+(1/2)f^2]^{-1}[(5/3)\boldsymbol{f}(\boldsymbol{\gamma}_k\cdot\boldsymbol{f})\\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad +\boldsymbol{\gamma}_k f^2(5+2f^2)]
\end{aligned}
$$

Considering z-axis as a direction of propagation and denoting k_z as k, γ as γ_z, we obtain from (223) the k-dependence of $a=a_z$ and $b=b_{zz}$:

$$
\begin{aligned}
a_k &= -\frac{\frac{3}{2}p_0^{-1}\eta_0 v_T^0 ik\tau_k+\frac{4}{5}p_0^{-2}\eta_0^2(v_T^0)^2k^2\gamma_k}{1+\frac{2}{5}p_0^{-2}\eta_0^2(v_T^0)^2k^2}, \\
b_k &= -\frac{\frac{4}{3}p_0^{-1}\eta_0 v_T^0 ik\gamma_k+p_0^{-2}\eta_0^2(v_T^0)^2k^2\tau_k}{1+\frac{2}{5}p_0^{-2}\eta_0^2(v_T^0)^2k^2}.
\end{aligned}
\tag{225}
$$

Using expressions for σ and $\mathbf{q}$ cited above, and also using (225), it is an easy matter to close the linearized balance equations (given in Fourier terms):

$$
\begin{aligned}
\frac{1}{v_T^0}\partial_t\nu_k+ik\gamma_k &= 0, \\
\frac{2}{v_T^0}\partial_t\gamma_k+ik(\tau_k+\nu_k)+ikb_k &= 0, \\
\frac{3}{2v_T^0}\partial\tau+ik\gamma_k+\frac{5}{4}ika_k &= 0.
\end{aligned}
\tag{226}
$$

Eqs. (226), together with expressions (225), complete our derivation of hydrodynamic equations.

To this end, the Knudsen number was not penetrating our derivations. Now it is worthwhile to introduce it. The Knudsen number will appear most naturally if we turn to dimensionless form of eq. (225). Taking $l_c=v_T^0\eta_0/p_0$ (l_c is of order of a mean free path), and introducing a hydrodynamic scale l_h, so that $k=\kappa/l_h$, where κ is a not-dimensional wave vector, we obtain in (225):

$$
\begin{aligned}
a_\kappa &= -\frac{\frac{3}{2}i\varepsilon\kappa\tau_\kappa+\frac{4}{5}\varepsilon^2\kappa^2\gamma_\kappa}{1+\frac{2}{5}\varepsilon^2\kappa^2}, \\
b_\kappa &= -\frac{\frac{4}{3}i\varepsilon\kappa\gamma_\kappa+\varepsilon^2\kappa^2\tau_\kappa}{1+\frac{2}{5}\varepsilon^2\kappa^2},
\end{aligned}
\tag{227}
$$

where $\varepsilon=l_c/l_h$. Considering a limit $\varepsilon\to 0$ in (227), we come back to familiar Navier-Stokes expressions: $\sigma_{zz}^{NS}=-\frac{4}{3}\eta_0\partial_z\delta u_z$, $q_z^{NS}=-\lambda_0\partial_z\delta T$, where $\lambda_0=15k_B\eta_0/4m$ is the first Sonine polynomial approximation of heat conductivity coefficient.

Since we were not assuming smallness of the Knudsen number ε while deriving (227), we are completely legal to put $\varepsilon=1$. With all the approximations mentioned above, eqs. (226) and (225) (or, equivalently, (226) and (227)) may be considered as a model of a linear hydrodynamics at ε of order unity. The most interesting feature of this model is a non-polynomial dependence on κ. This amounts to that share stress tensor and heat flux vector depend on spatial derivatives of $\delta\boldsymbol{u}$ and of δT of an arbitrary high order.

To find out a result of non-polynomial behavior (227), it is most informative to calculate a dispersion relation for planar waves. It is worthwhile introducing dimensionless frequency $\lambda = \omega l_h / v_T^0$, where ω is a complex variable of a wave $\sim \exp(\omega t + ikz)$ (Reω is a damping rate, and Imω is a circular frequency). Making use of eqs. (226) and (227), writing $\varepsilon = 1$, we obtain the following dispersion relation $\lambda(\kappa)$:

$$12(1+\frac{2}{5}\kappa^2)^2\lambda^3 + 23\kappa^2(1+\frac{2}{5}\kappa^2)\lambda^2 + 2\kappa^2(5+5\kappa^2+\frac{6}{5}\kappa^4)\lambda + \frac{15}{2}\kappa^4(1+\frac{2}{5}\kappa^2) = 0. \quad (228)$$

A discussion of results concerns the following two items:

1. The approach used avoids expansion into powers of the Knudsen number, and thus we obtain a hydrodynamics valid (at least formally) for moderate Knudsen numbers as an immediate correction to Euler hydrodynamics. This is in a contrast to a usual treatment of a high-order hydrodynamics as "(a well established) Navier-Stokes approximation + high-order terms". Navier-Stokes hydrodynamics is recovered a posteriori, as a limiting case, but not as a necessary intermediate step of computations.

2. Linear hydrodynamics derived is stable for all k, same as the Navier-Stokes hydrodynamics alone. The $(1+\alpha k^2)^{-1}$ "cut-off", as in (225) and (227), was earlier found in a "partial summing" of Enskog series [22, 21].

Thus, we come to the following two conclusions:

1. A preliminary positive answer is given to the question of whether is it possible to construct solutions of the Boltzmann equation valid for the Knudsen number of order unity.

2. Linear hydrodynamics derived can be used as a model for $\varepsilon = 1$ with no danger to get a violation of acoustic spectra at large k.

Example 5: Dynamic correction to moment approximations

Dynamic correction or extension of the list of variables?

Considering the Grad moment ansatz as a suitable first approximation to a closed finite-moment dynamics, the correction is derived from the Boltzmann equation. The correction consists of two parts, local and nonlocal. Locally corrected thirteen-moment equations are demonstrated to contain exact transport coefficients. Equations resulting from the nonlocal correction give a microscopic justification to some phenomenological theories of extended hydrodynamics.

A considerable part of the modern development of nonequilibrium thermodynamics is based on the idea of extension of the list of relevant variables. Various phenomenological and semi-phenomenological theories in this domain are known under the common title of the extended irreversible thermodynamics (EIT) [131]. With this, the question of a microscopic justification of the EIT becomes important. Recall that a justification for some of the versions of the EIT was found witin the well known Grad moment method [113].

Originally, the Grad moment approximation was introduced for the purpose of solving the Boltzmann-like equations of the classical kinetic theory. The Grad method is used in various kinetic problems, e.g., in plasma and in phonon transport. We mention also that Grad equations assist in understanding asymptotic features of gradient expansions, both in linear and nonlinear domains [129, 118, 117, 20, 21].

The essence of the Grad method is to introduce an approximation to the one-particle distribution function f which would depend only on a finite number N of moments, and, subsequently, to use this approximation to derive a closed system of N moment equations from the kinetic equation. The number N (the level at which the moment transport hierarchy is truncated) is not specified in the Grad method. One practical way to choose N is to obtain an estimation of the transport coefficients (viscosity and heat conductivity) sufficiently close to their exact values provided by the Chapman–Enskog method (CE) [43]. In particular, for the thirteen-moment (13M) Grad approximation it is well known that transport coefficients are equal to the first Sonine polynomial approximation to the exact CE values. Accounting for higher moments with $N > 13$ can improve this approximation (good for neutral gases but poor for plasmas [128]).

However, what should be done, starting with the 13M approximation, to come to the exact CE transport coefficients is an open question. It is also well known [116] that the Grad method provides a poorly converging approximation when applied to strongly nonequilibrium problems (such as shock and kinetic layers).

Another question coming from the approximate character of the Grad equations is discussed in frames of the EIT: while the Grad equations are strictly hyperbolic at any level N (i.e., predicting a finite speed of propagation), whether this feature will be preserved in the further corrections.

These two questions are special cases of a more general one, namely, how to derive a closed description with a given number of moments? Such a description is sometimes called mesoscopic [145] since it occupies an intermediate level between the hydrodynamic (macroscopic) and the kinetic (microscopic) levels of description.

Here we aim at deriving the mesoscopic dynamics of thirteen moments [6] in the simplest case when the kinetic description satisfies the linearized Boltzmann equation. Our approach will be based on the two assumptions: (i). The mesoscopic dynamics of thirteen moments exists, and is invariant with respect to the microscopic dynamics, and (ii). The 13M Grad approximation is a suitable first approximation to this mesoscopic dynamics. The assumption (i) is realized as the invariance equation for the (unknown) mesoscopic distribution function. Following the assumption (ii), we solve the invariance equation iteratively, taking the 13M Grad approximation for the input approximation, and consider the first iteration (further we refer to this as to the dynamic correction, to distinguish from constructing another ansatz). We demonstrate that the correction results in the exact CE transport coefficients. We also demonstrate how the dynamic correction modifies the hyperbolicity of the Grad equations. A similar viewpoint on derivation of hydrodynamics was earlier developed in [3] (see previous Examples). We will return to a comparison below.

Invariance equation for 13M parameterization

We denote as n_0, $\boldsymbol{u}_0 = 0$, and p_0 the equilibrium values of the hydrodynamic parameters (n is the number density, $\boldsymbol{u}$ is the average velocity, and $p = nk_BT$ is the pressure). The global Maxwell distribution function is

$$F = n_0(v_T)^{-3}\pi^{-3/2}\exp(-c^2),$$

where $v_T = \sqrt{2k_BT_0m^{-1}}$ is the equilibrium heat velocity, and $\mathbf{c} = \boldsymbol{v}/v_T$ is the peculiar velocity of a particle. The near-equilibrium dynamics of the distribution function, $f = F(1+\varphi)$, is due to the linearized Boltzmann equation:

$$\partial_t\varphi = \hat{J}\varphi \equiv -v_T\mathbf{c}\cdot\nabla\varphi + \hat{L}\varphi,$$
$$\hat{L}\varphi = \int wF(\boldsymbol{v}_1)[\varphi(\boldsymbol{v}_1')+\varphi(\boldsymbol{v}')-\varphi(\boldsymbol{v}_1)-\varphi(\boldsymbol{v})]d\boldsymbol{v}_1'd\boldsymbol{v}'d\boldsymbol{v}_1,$$

where $\hat{L}$ is the linearized collision operator, and w is the probability density of pair encounters.

Let $n = \delta n/n_0$, $\boldsymbol{u} = \delta\boldsymbol{u}/v_T^0$, $p = \delta p/p_0$ ($p = n + T$, $T = \delta T/T_0$), are dimensionless deviations of the hydrodynamic variables, while $\boldsymbol{\sigma} = \delta\boldsymbol{\sigma}/p_0$ and $\mathbf{q} = \delta\mathbf{q}/(p_0v_T^0)$ are dimensionless deviations of the stress tensor $\boldsymbol{\sigma}$, and of the heat flux $\mathbf{q}$. The linearized 13M Grad distribution function is $f_0 = F(\mathbf{c})\,[1+\varphi_0]$, where

$$\varphi_0 = \varphi_1 + \varphi_2, \tag{229}$$
$$\varphi_1 = n + 2\boldsymbol{u}\cdot\mathbf{c} + T\left[c^2 - (3/2)\right],$$
$$\varphi_2 = \boldsymbol{\sigma} : \overline{\mathbf{cc}} + (4/5)\mathbf{q}\cdot\mathbf{c}\left[c^2 - (5/2)\right].$$

The overline denotes a symmetric traceless dyad.

The 13M Grad's equations are derived in two steps: first, the 13M Grad's distribution function (229) is inserted into the Boltzmann equation to give a formal expression, $\partial_t \varphi_0 = \hat{J}\varphi_0$, second, projector P_0 is applied to this expression, where $P_0 = P_1 + P_2$:

$$P_1 = \frac{f_0}{n_0}\left\{X_0 \int X_0 \bullet d\boldsymbol{v} + \boldsymbol{x}\cdot \int \boldsymbol{x} \bullet d\boldsymbol{v} + X_4 \int X_4 \bullet d\boldsymbol{v}\right\}, \tag{230}$$
$$P_2 = \frac{f_0}{n_0}\left\{\mathsf{Y} : \int \mathsf{Y} \bullet d\boldsymbol{v} + \mathbf{Z}\cdot \int \mathbf{Z} \bullet d\boldsymbol{v}\right\}.$$

Here $X_0 = 1$, $\boldsymbol{x} = \sqrt{2}\mathbf{c}$, $X_4 = \sqrt{2/3}\left(c^2 - \frac{3}{2}\right)$, $\mathsf{Y} = \sqrt{2}\overline{\mathbf{cc}}$, and $\mathbf{Z} = \frac{2}{\sqrt{5}}\mathbf{c}\left(c^2 - \frac{5}{2}\right)$. The resulting equation,

$$P_0[F\partial_t \varphi_0] = P_0[F\hat{J}\varphi_0],$$

is a compressed representation for the 13M Grad equations for the macroscopic variables $M_{13} = \{n, \boldsymbol{u}, T, \boldsymbol{\sigma}, \mathbf{q}\}$.

Now we turn to the main purpose of this Example, and derive the dynamic correction to the 13M distribution function (229). The assumption (i) [existence of closed dynamics of thirteen moments] implies the invariance equation for the true mesoscopic distribution function, $\tilde{f}(M_{13}, \mathbf{c}) = f_0[1 + \tilde{\varphi}(M_{13}, \mathbf{c})]$, where we have stressed that this function depends parametrically on the same thirteen macroscopic parameters. The invariance condition for $\tilde{f}(M_{13}, \mathbf{c})$ reads [3]:

$$(1 - \tilde{P})[f_0\hat{J}\tilde{\varphi}] = 0, \tag{231}$$

where $\tilde{P}$ is the projector associated with $\tilde{f}$. Following the assumption (ii) [13M Grad's distribution function (229) is a good initial approximation], the Grad's function f_0, and the projector P_{G}, are chosen as the input data for solving the equation (231) iteratively. The dynamic correction amounts to the first iterate. Let us consider these steps in a more detail.

Substituting φ_{G} (229) and P_{G} (230) instead of φ and P in the equation (231), we get: $(1 - P_{\mathrm{G}})[f_0\hat{J}\varphi_{\mathrm{G}}] \equiv \Delta_{\mathrm{G}} \neq 0$, which demonstrates that (229) is not a solution to the equation (231). Moreover, Δ_{G} splits in two natural pieces: $\Delta_{\mathrm{G}} = \Delta_{\mathrm{G}}^{\mathrm{loc}} + \Delta_{\mathrm{G}}^{\mathrm{nloc}}$, where

$$\begin{aligned} \Delta_{\mathrm{G}}^{\mathrm{loc}} &= (1 - P_2)[f_0\hat{L}\varphi_2], \\ \Delta_{\mathrm{G}}^{\mathrm{nloc}} &= (1 - P_{\mathrm{G}})[-v_T^0 f_0 \mathbf{c}\cdot\nabla\varphi_{\mathrm{G}}]. \end{aligned} \tag{232}$$

Here we have accounted for $P_1[f_0\hat{L}\varphi] = 0$, and $\hat{L}\varphi_1 = 0$. The first piece of Eq. (232), $\Delta_{\mathrm{G}}^{\mathrm{loc}}$, can be termed *local* because it does not account for spatial gradients. Its origin is twofold. In the first place, recall that we are performing our analysis in a non-local-equilibrium state (the 13M approximation is not a zero point of the Boltzmann collision integral, hence $\hat{L}\varphi_{\mathrm{G}} \neq 0$). In the second place, specializing to the linearized case under consideration, functions $\overline{\mathbf{cc}}$ and $\mathbf{c}[c^2 - (5/2)]$, in general, are not the eigenfunctions of the linearized collision integral, and hence $P_2[f_0\hat{L}\varphi_{\mathrm{G}}] \neq f_0\hat{L}\varphi_{\mathrm{G}}$, resulting in $\Delta_{\mathrm{G}}^{\mathrm{loc}} \neq 0$ [8].

[8] Except for Maxwellian molecules (interaction potential $U \sim r^{-4}$) for which $\hat{L}\varphi_{\mathrm{G}} \neq 0$ but $P_2[f_0\hat{L}\varphi_{\mathrm{G}}] = f_0\hat{L}\varphi_{\mathrm{G}}$. Same goes for the relaxation time approximation of the collision integral ($\hat{L} = -\tau^{-1}$).

Using Cartesian coordinates and summation convention, the nonlocal part may be written as:

$$\Delta_{\mathrm{G}}^{\mathrm{nloc}} = -v_T^0 f_0 (\Pi_{1|krs}\partial_k \sigma_{rs} + \Pi_{2|ik}\overline{\partial_k q_i} + \Pi_3 \partial_k q_k) \tag{233}$$

where $\partial_i = \partial/\partial x_i$, and Π are velocity polynomials:

$$\begin{aligned}
\Pi_{1|krs} &= c_k \left[c_r c_s - (1/3)\delta_{rs}c^2\right] - (2/5)\delta_{ks}c_r c^2, \\
\Pi_{2|ik} &= (4/5)\left[c^2 - (7/2)\right]\left[c_i c_k - (1/3)\delta_{ik}c^2\right], \\
\Pi_3 &= (4/5)\left[c^2 - (5/2)\right]\left[c^2 - (3/2)\right] - c^2.
\end{aligned}$$

We seek the dynamic correction of the form:

$$f_{\mathrm{C}} = f_0[1 + \varphi_{\mathrm{G}} + \phi_{\mathrm{C}}].$$

Substituting $\varphi = \varphi_{\mathrm{G}} + \phi_{\mathrm{C}}$, and $P = P_{\mathrm{G}}$, into Eq. (231), we derive an equation for the correction ϕ_{C}:

$$(1-P_2)[f_0 \hat{L}(\varphi_2+\phi_{\mathrm{C}})] = (1-P_{\mathrm{G}})[v_T^0 f_0 \mathbf{c}\cdot\nabla(\varphi_{\mathrm{G}}+\phi_{\mathrm{C}})]. \tag{234}$$

Eq. (234) should be supplied with the additional condition, $P_{\mathrm{G}}[f_0\phi_{\mathrm{C}}] = 0$.

Solution of the invariance equation

Let us apply the usual ordering to solve the Eq. (234), introducing a small parameter ε, multiplying the collision integral $\hat{L}$ with ε^{-1}, and expanding $\phi_C = \sum_n \varepsilon^n \phi_C^{(n)}$. Subject to the additional condition, the resulting sequence of linear integral equations is uniquely soluble. Let us consider the first two orders in ε.

Because $\Delta_{\mathrm{G}}^{\mathrm{loc}} \neq 0$, the leading correction is of the order ε^0, i.e. of the same order as the initial approximation φ_{G}. The function $\phi_{\mathrm{C}}^{(0)}$ is due the following equation:

$$(1 - P_2)[f_0 \hat{L}(\varphi_2 + \phi_{\mathrm{C}}^{(0)})] = 0, \tag{235}$$

subject to the condition, $P_{\mathrm{G}}[f_0\phi_{\mathrm{C}}^{(0)}] = 0$. Eq. (235) has the unique solution: $\varphi_2 + \phi_{\mathrm{C}}^{(0)} = \boldsymbol{\sigma} : \mathsf{Y}_{\mathrm{C}} + \mathbf{q}\cdot\mathbf{Z}_{\mathrm{C}}$, where functions, Y_{C} and $\mathbf{Z}_{\mathrm{C}}$, are solutions to the integral equations:

$$\hat{L}\mathsf{Y}_{\mathrm{C}} = b\mathsf{Y}, \quad \hat{L}\mathbf{Z}_{\mathrm{C}} = a\mathbf{Z}, \tag{236}$$

subject to the conditions, $P_1[f_0\mathsf{Y}_{\mathrm{C}}] = 0$ and $P_1[f_0\mathbf{Z}_{\mathrm{C}}] = 0$. Factors a and b are:

$$a = \pi^{-3/2}\int e^{-c^2}\mathbf{Z}_{\mathrm{C}}\cdot\hat{L}\mathbf{Z}_{\mathrm{C}}d\mathbf{c},$$
$$b = \pi^{-3/2}\int e^{-c^2}\mathsf{Y}_{\mathrm{C}} : \hat{L}\mathsf{Y}_{\mathrm{C}}d\mathbf{c}.$$

Now we are able to notice that the equation (236) coincides with the CE equations [43] for the *exact transport coefficients* (viscosity and temperature conductivity). Emergency of these well known equations in the present context is important and rather unexpected:

when the moment transport equations are closed with the locally corrected function $f_C^{loc} = f_0(1+\varphi_G+\phi_C^{(0)})$*, we come to a closed set of thirteen equations containing the exact CE transport coefficients.*

Let us analyze the next order (ε^1), where $\Delta_{\mathrm{G}}^{\mathrm{nloc}}$ comes into play. To simplify matters, we neglect the difference between the exact and the approximate CE transport coefficients. The correction $\phi_{\mathrm{C}}^{(1)}$ is due to the equation,

$$(1-P_2)[f_0\hat{L}\phi_{\mathrm{C}}^{(1)}] + \Delta_{\mathrm{G}}^{\mathrm{nloc}} = 0, \tag{237}$$

the additional condition is: $P_{\mathrm{G}}[f_0\phi^{(1)}] = 0$. The problem (237) reduces to three integral equations of a familiar form:

$$\hat{L}F_{1|krs} = \Pi_{1|krs}, \quad \hat{L}F_{2|ik} = \Pi_{2|ik}, \quad \hat{L}F_3 = \Pi_3, \tag{238}$$

subject to conditions: $P_1[f_0F_{1|krs}] = 0$, $P_1[f_0F_{2|ik}] = 0$, and $P_1[f_0F_3] = 0$. Integral equations (238) are of the same structure as are the integral equations appearing in the CE method, and the methods to handle them are well developed [43]. In particular, a reasonable and simple approximation is to take $F_{i|\ldots} = -A_i\Pi_{i|\ldots}$. Then

$$\phi_{\mathrm{C}}^{(1)} = -v_T^0(A_1\Pi_{1|krs}\partial_k\sigma_{rs} + A_2\Pi_{2|ik}\overline{\partial_k q_i} + A_3\Pi_3\partial_k q_k), \tag{239}$$

where A_i are the approximate values of the kinetic coefficients, and which are expressed via matrix elements of the linearized collision integral:

$$A_i^{-1} \propto -\int \exp(-c^2)\Pi_{i|\ldots}\hat{L}\Pi_{i|\ldots}d\mathbf{c} > 0. \tag{240}$$

The estimation can be extended to a computational scheme for any given molecular model (e. g., for the Lennard-Jones potential), in the manner of the transport coefficients computations in the CE method.

Corrected 13M equations

To summarize the results of the dynamic correction, we quote first the unclosed equations for the variables $M_{13} = M_{13} = \{n, \boldsymbol{u}, T, \boldsymbol{\sigma}, \mathbf{q}\}$:

$$\begin{aligned}
&(1/v_T^0)\partial_t n + \nabla\cdot\boldsymbol{u} = 0,\\
&(2/v_T^0)\partial_t\boldsymbol{u} + \nabla(T+n) + \nabla\cdot\boldsymbol{\sigma} = 0,\\
&(1/v_T^0)\partial_t T + (2/3)\nabla\cdot\boldsymbol{u} + (2/3)\nabla\cdot\mathbf{q} = 0,\\
&(1/v_T^0)\partial_t\boldsymbol{\sigma} + 2\overline{\nabla\boldsymbol{u}} - (2/3)\nabla\mathbf{q} + \nabla\cdot\mathsf{h} = \mathsf{R},\\
&(2/v_T^0)\partial_t\mathbf{q} - (5/2)\nabla p - (5/2)\nabla\cdot\boldsymbol{\sigma} + \nabla\cdot\mathsf{g} = \mathbf{R}.
\end{aligned} \tag{241}$$

Terms spoiling the closure are: the higher moments of the distribution function,

$$\mathsf{h} = 2\pi^{-3/2}\int e^{-c^2}\varphi\mathbf{ccc}d\mathbf{c},$$

$$\mathsf{g} = 2\pi^{-3/2}\int e^{-c^2}\varphi\mathbf{cc}c^2d\mathbf{c},$$

and the "moments" of the collision integral,

$$\mathsf{R} = \frac{2}{v_T^0}\pi^{-3/2}\int e^{-c^2}\mathbf{c}\mathbf{c}\hat{L}\varphi d\mathbf{c},$$
$$\mathbf{R} = \frac{2}{v_T^0}\pi^{-3/2}\int e^{-c^2}\mathbf{c}c^2\hat{L}\varphi d\mathbf{c}.$$

The 13M Grad's distribution function (229) provides the closing approximation to both the higher moments and the "moments" of collision integral:

$$\begin{aligned}
&\mathsf{R}_{\rm G} = -\mu_0^{-1}\boldsymbol{\sigma},\ \mathbf{R}_{\rm G} = -\lambda_0^{-1}\mathbf{q},\\
&\nabla\cdot\mathsf{h}_{\rm G} = (2/3)\mathsf{I}\nabla\cdot\mathbf{q} + (4/5)\overline{\nabla\mathbf{q}},\\
&\nabla\cdot\mathsf{g}_{\rm G} = (5/2)\nabla(p+T) + (7/2)\nabla\cdot\boldsymbol{\sigma},
\end{aligned} \tag{242}$$

where μ_0 and λ_0 are the first Sonine polynomial approximations to the viscosity and the temperature conductivity coefficients [43], respectively.

The local correction improves the closure of the "moments" of collision integral:

$$\mathsf{R}_{\rm C} = -\mu_{\rm CE}^{-1}\boldsymbol{\sigma}, \quad \mathbf{R}_{\rm C} = -\lambda_{\rm CE}^{-1}\mathbf{q}, \tag{243}$$

where index CE corresponds to exact Chapman–Enskog values of the transport coefficients.

The nonlocal correction adds the following terms to the higher moments:

$$\begin{aligned}
\nabla\cdot\mathsf{g}_{\rm C} &= \nabla\cdot\mathsf{g}_{\rm G} - A_3\nabla\nabla\cdot\mathbf{q} - A_2\nabla\cdot\overline{\nabla\mathbf{q}}, \\
\nabla\cdot\mathsf{h}_{\rm C} &= \nabla\cdot\mathsf{h}_{\rm G} - A_1\nabla\cdot\nabla\boldsymbol{\sigma}
\end{aligned} \tag{244}$$

where A_i are the kinetic coefficients derived above.

In order to illustrate what changes in Grad equations with the nonlocal correction, let us consider a model with two scalar variables, $T(x,t)$ and $q(x,t)$ (a simplified case of the one-dimensional corrected 13M system where one retains only the variables responsible for heat conduction):

$$\partial_t T + \partial_x q = 0, \quad \partial_t q + \partial_x T - a\partial_x^2 q + q = 0. \tag{245}$$

Parameter $a \geq 0$ controls "turning on" the nonlocal correction. Using $\{q(k,\omega), T(k,\omega)\}\exp(\omega t + ikx)$, we come to a dispersion relation for the two roots $\omega_{1,2}(k)$. Without the correction ($a = 0$), there are two domains of k: for $0 \leq k < k_-$, dispersion is diffusion-like ($\mathrm{Re}\omega_{1,2}(k) \leq 0$, $\mathrm{Im}\omega_{1,2}(k) = 0$), while as $k \geq k_-$, dispersion is wave-like ($\omega_1(k) = \omega_2^*(k)$, $\mathrm{Im}\omega_1(k) \neq 0$). For a between 0 and 1, the dispersion modifies in the following way: The wave-like domain becomes bounded, and exists for $k \in]k_-(a), k_+(a)[$, while the diffusion-like domain consists of two pieces, $k < k_-(a)$ and $k > k_+(a)$.

The dispersion relation for $a = 1/2$ is shown in the Fig. 4. As a increases to 1, the boundaries of the wave-like domain, $k_-(a)$ and $k_+(a)$, move towards each other, and collapse at $a = 1$. For $a > 1$, the dispersion relation becomes purely diffusive ($\mathrm{Im}\omega_{1,2} = 0$) for all k.

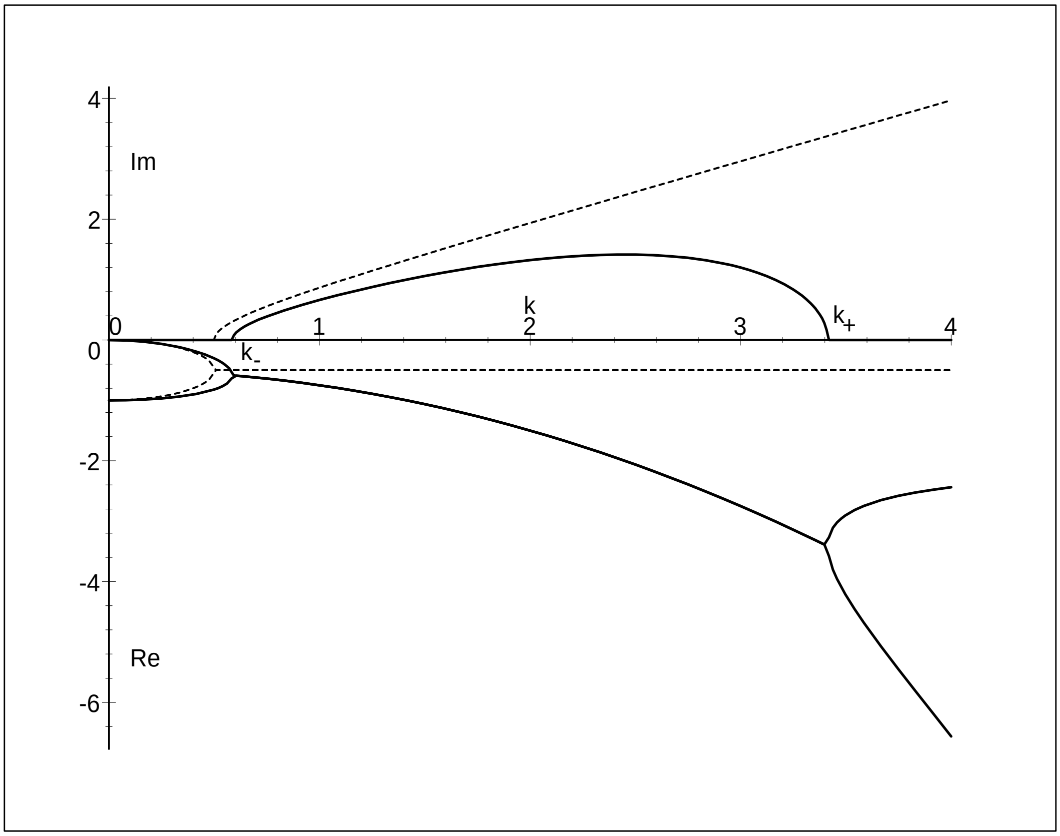


Figure 4: Attenuation $\mathrm{Re}\omega_{1,2}(k)$ (lower pair of curves), frequency $\mathrm{Im}\omega_{1,2}(k)$ (upper pair of curves). Dashed lines - Grad case ($a = 0$), drawn lines - dynamic correction ($a = 0.5$).

Discussion: transport coefficients, destroying of the hyperbolicity, etc.

(i). Considering the 13M Grad ansatz as a suitable approximation to the closed dynamics of thirteen moments, we have found that the first correction leads to exact Chapman-Enskog transport coefficients. Further, the nonlocal part of this correction extends the Grad equations with terms containing spatial gradients of the heat flux and of the stress tensor, destroying the hyperbolic nature of the former. Corresponding kinetic coefficients are explicitly derived for the Boltzmann equation.

(ii). Extension of Grad equations with terms like in (244) was mentioned in many versions of the EIT [146]. These derivations were based on phenomenological and semi-phenomenological argument. In particular, the extension of the heat flux with appealing to nonlocality effects in *dense* fluids. Here we have derived the similar contribution from the *simplest* (i. e. dilute gas) kinetics, in fact, from the assumption about existence of the mesoscopic dynamics. The advantage of using the simplest kinetics is that corresponding kinetic coefficients (240) become a matter of a *computation* for any molecular model. This computational aspect will be discussed elsewhere, since it affects the dilute gas contribution to dense fluids fits. Here we would like to stress a formal support of relevancy of the above analysis: the nonlocal peace of dynamic correction is intermediated by the local correction, *improving* the 13M Grad estimation to the ordinary transport coefficients.

(iii). When the invariance principle is applied to derive hydrodynamics (closed equations for the variables n, $\boldsymbol{u}$ and T) then [3] the local Maxwellian $f_{\rm LM}$ is chosen as the input distribution function for the invariance equation. In the linear domain, $f_{\rm LM}=f_0[1+\varphi_1]$, and the projector is $P_{\rm LM}=P_1$, see eqs. (229) and (230). When the latter expressions are substituted into the invariance equation (231), we obtain $\Delta_{\rm LM}=\Delta_{\rm LM}^{\rm nloc}=-v_T^0 f_0\{2\nabla\boldsymbol{u}:\overline{\mathbf{cc}}+\nabla T\cdot\mathbf{c}[c^2-(5/2)]\}$, while $\Delta_{\rm LM}^{\rm loc}\equiv 0$ because the local Maxwellians are zero points of the Boltzmann collision integral. Consequently, the dynamic correction begins with the order ε, and the analog of the equation (237) reads:

$$\hat{L}\phi_{\rm LM}^{(1)}=v_T^0\{2\nabla\boldsymbol{u}:\overline{\mathbf{cc}}+\nabla T\cdot\mathbf{c}[c^2-(5/2)]\},$$

subject to a condition, $P_1[f_0\phi_{\rm LM}^{(1)}]=0$. The latter is the familiar Chapman-Enskog equation, resulting in the Navier-Stokes correction to the Euler equations [43]. Thus, *the nonlocal dynamic correction is related to the 13M Grad equations entirely in the same way as the Navier-Stokes are related to the Euler equations.* As the final comment to this point, it was recently demonstrated with simple examples [21] that the invariance principle, as applied to derivation of hydrodynamics, is equivalent to the summation of the Chapman-Enskog expansion.

(iv). Let us discuss briefly the further corrections. The first local correction (the functions Y_1 and $\mathbf{Z}_1$ in the Eq. (236)) is not the limiting point of our iterational procedure. When the latter is continued, the subsequent local corrections are found from integral equations, $\hat{L}\mathsf{Y}_{n+1}=b_{n+1}\mathsf{Y}_n$, and $\hat{L}\mathbf{Z}_{n+1}=a_{n+1}\mathbf{Z}_{\ n}$. Thus, we are led to the following two eigenvalue problems: $\hat{L}\mathsf{Y}_\infty=b_\infty\mathsf{Y}_\infty$, and $\hat{L}\mathbf{Z}_\infty=a_\infty\mathbf{Z}_\infty$, where, in accord with general argument [3], a_∞ and b_∞ are the closest to zero eigenvalues among all the eigenvalue problems with the given tensorial structure [142].

(v). Approach of this Example [6] can be extended to derive dynamic corrections to other (non-moment) approximations of interest in the kinetic theory. The above analysis has demonstrated, in particular, the importance of the local correction, generically relevant to an approximation which is not a zero point of the collision integral. Very recently, this approach was successfully applied to improve the nonlinear Grad's 13 moment equations [147].

7 Decomposition of motions, non-uniqueness of selection of fast motions, self-adjoint linearization, Onsager filter and quasi-chemical representation

In section 5 we have used second law of thermodynamics - existence of the entropy - in order to equip the problem of constructing slow invariant manifolds with a geometric structure. The requirement of the entropy growth (universally, for all the reduced models) restricts significantly the form of the projectors (89).

In this section we introduce a different but equally important argument - the micro-reversibility (T-invariance), and its macroscopic consequences, the reciprocity relations. As first discussed by Onsager in 1931, the implication of the micro-reversibility is the self-adjointness of the linear approximation of the system (34) in the equilibrium x^*:

$$\langle (D_x J)_{x^*} z | p \rangle_{x^*} \equiv \langle z | (D_x J)_{x^*} p \rangle_{x^*}. \tag{246}$$

The main idea in the present section is to use the *reciprocity relations* (246) *for the fast motions*. In order to appreciate this idea, we should mention that the decomposition of motions into fast and slow is not unique. Requirement (246) for any equilibrium point of fast motions means the selection (filtration) of the fast motions. We term this *Onsager filter*. Equilibrium points of fast motions are all the points on manifolds of slow motions.

There exist a trivial way to symmetrization, linear operator A is decomposed into symmetric and skew-symmetric parts, $A = \frac{1}{2}(A + A^\dagger) + \frac{1}{2}(A - A^\dagger)$. Here $A^\dagger$ is adjoint to A with respect to a fixed scalar product (entropic scalar product in present context). However, replacement of an operator with its symmetric part can lead to catastrophic (from the physical standpoint) consequences such as, for example, loss of stability. In order to construct a sensible Onsager filter, we shall use the *quasi-chemical representation*.

The formalism of the quasi-chemical representation is one of the most developed means of modelling, it makes it possible to "assemble" complex processes out of elementary processes. There exist various presentations of the quasi-chemical formalism. Our presentation here is a generalization of an approach suggested first by Feinberg [138] (see also [137, 139, 50]).

We shall describe the quasi-chemical formalism for finite-dimensional systems. Infinite-dimensional generalizations are almost obvious in many important cases, and are achieved by a mere replacement of summation by integration. In the Example to this section we consider the Boltzmann collision integral from this standpoint.

Symbol A_i ("quasi-substance") is put into correspondence to each variable x_i. The *elementary reaction* is defined according to the *stoichiometric equation*,

$$\sum_i \alpha_i A_i \rightleftharpoons \sum_i \beta_i A_i, \tag{247}$$

where α_i (*loss stoichiometric coefficients*) and β_i (*gain stoichiometric coefficients*) are real numbers. Apart from the entropy, one specifies a monotonic function of one variable, $\Psi(a)$,

$\Psi'(a) > 0$. In particular, function $\Psi(a) = \exp(\lambda a)$, $\lambda = \text{const}$, is frequently encountered in applications.

Given the elementary reaction (247), one defines the rates of the direct and of the inverse reactions:

$$\begin{aligned} W^+ &= w^* \Psi\left(\sum_i \alpha_i \mu_i\right), \\ W^- &= w^* \Psi\left(\sum_i \beta_i \mu_i\right), \end{aligned} \tag{248}$$

where $\mu_i = \frac{\partial S}{\partial x_i}$, $x^* = \text{const}$, $x^* > 0$. The rate of the elementary reaction is then defined as, $W = W^+ - W^-$.

The equilibrium of the elementary reaction (247) is given by the following equation:

$$W^+ = W^-. \tag{249}$$

Thanks to the strict monotonicity of the function Ψ, equilibrium of the elementary reaction is reached when the arguments of the functions coincide in equation (248), that is, whenever

$$\sum_i (\beta_i - \alpha_i)\mu_i = 0. \tag{250}$$

Vector with the components $\gamma_i = \beta_i - \alpha_i$ is termed the *stoichiometric vector of the reaction.*

Let x^0 be a point of equilibrium of the reaction (247). The linear approximation of the reaction rate has a particularly simple form:

$$W(x^0 + \delta) = -w^* \Psi'(a(x^0)) \langle \gamma | \delta \rangle_{x^0} + o(\delta), \tag{251}$$

where $a(x^0) = \sum_i \alpha_i \mu_i(x^0) = \sum_i \beta_i \mu_i(x^0)$, and $\langle | \rangle_{x^0}$ is the entropic scalar product in the equilibrium. In other words,

$$(D_x W)_{x^0} = -w^* \Psi'(a(x^0)) \langle \gamma |. \tag{252}$$

Let us write down the kinetic equation for one elementary reaction:

$$\frac{dx}{dt} = \gamma W(x). \tag{253}$$

Linearization of this equation in the equilibrium x^0 has the following form:

$$\frac{d\delta}{dt} = -w^* \Psi'(a(x^0)) \gamma \langle \gamma | \delta \rangle_{x^0}. \tag{254}$$

That is, the matrix of the linear approximation has the form,

$$K = -k^* |\gamma\rangle \langle \gamma |, \tag{255}$$

where

$$k^* = w^* \Psi'(a(x^0)) > 0,$$

while the entropic scalar product of bra- and ket vectors is taken in the equilibrium point x^0.

If there are several elementary reactions, then the stoichiometric vectors γ^r and the reaction rates $W_r(x)$ are specified for each reaction, while the kinetic equation is obtained by summing the right hand sides of equation (253) for individual reactions,

$$\frac{dx}{dt} = \sum_r \gamma^r W_r(x). \tag{256}$$

Let us assume that under the inversion of motions, the direct reaction transforms into the inverse reaction. Thus, the T-invariance of the equilibrium means that it is reached in the point of the *detail balance*, where all the elementary reaction come to equilibrium simultaneously:

$$W_r^+(x^*) = W_r^-(x^*). \tag{257}$$

This assumption is nontrivial if vectors γ^r are linearly dependent (for example, if the number of reactions is greater than the number of species minus the number of conservation laws).

In the detail balance case, the linearization of equation (256) about x^* has the following form ($x = x^* + \delta$):

$$\frac{d\delta}{dt} = -\sum_r k_r^* \gamma^r \langle \gamma^r | \delta \rangle_{x^*}, \tag{258}$$

where

$$\begin{aligned} k_r^* &= w_r^* \Psi'_r(a_r^*) > 0, \\ a_r^* &= \sum_i \alpha_i^r \mu_i(x^*) = \sum_i \beta_i^r \mu_i(x^*). \end{aligned}$$

The following matrix of the linear approximation is obviously self-adjoint and stable:

$$K = -\sum_r k_r^* |\gamma^r\rangle\langle\gamma^r|. \tag{259}$$

Note that matrix K is the sum of matrices of rank one.

Let us now extract the self-adjoint part of the form (259) in the *arbitrary* point x. After linearizing the reaction rate about x, we obtain:

$$W(x+\delta) = w^* \left(\Psi'(a(x))\langle\alpha|\delta\rangle_x - \Psi'(b(x))\langle\beta|\delta\rangle_x\right) + o(\delta), \tag{260}$$

where

$$\begin{aligned} a(x) &= \sum_i \alpha_i \mu_i(x), \\ b(x) &= \sum_i \beta_i \mu_i(x). \end{aligned}$$

Let us introduce notation,

$$\begin{aligned} k^{\mathrm{s}}(x) &= \frac{1}{2} w^* \left(\Psi'(a(x)) + \Psi'(b(x))\right) > 0, \\ k^{\mathrm{a}}(x) &= \frac{1}{2} w^* \left(\Psi'(a(x)) - \Psi'(b(x))\right). \end{aligned}$$

In terms of this notation, equation (260) may be rewritten,

$$W(x+\delta) = -k^{\mathrm{s}}(x)\langle\gamma|\delta\rangle_x + k^{\mathrm{a}}(x)\langle\alpha+\beta|\delta\rangle_x + o(\delta). \tag{261}$$

The second term vanishes in the equilibrium ($k^{\mathrm{a}}(x^*) = 0$, thanks to detail balance).

Symmetric linearization (Onsager filter) consists in using only the first term in the linearized vector field (261) when analyzing the fast motion towards the (approximate) slow manifolds, instead of the full expression (260). Matrix $K(x)$ of the linear approximation becomes then the form similar to equation (259):

$$K(x) = -\sum_r k_r^{\mathrm{s}}(x)|\gamma^r\rangle\langle\gamma^r|, \tag{262}$$

where

$$\begin{aligned} k_r^{\mathrm{s}}(x) &= \frac{1}{2} w_r^* \left(\Psi_r'(a(x)) + \Psi_r'(b(x))\right) > 0, \\ a_r(x) &= \sum_i \alpha_i^r \mu_i(x), \\ b_r(x) &= \sum_i \beta_i^r \mu_i(x), \end{aligned}$$

while the entropic scalar product $\langle|\rangle_x$ is taken in the point x. For each index of the elementary reaction r, function $k_r^{\mathrm{s}}(x)$ is positive. Thus, stability of the symmetric matrix (262) is evident.

Symmetric linearization (262) is distinguished also by the fact that it preserves the rank of the elementary processes contributing to the complex mechanism: Same as in the equilibrium, matrix $K(x)$ is the sum of rank one operators corresponding to each individual process. This is not the case of the standard symmetrization.

Using the symmetric operator (262) in the above Newton method with incomplete linearization can be consider as a version of a heuristic strategy of "we act in such a way as if the manifold $F(W)$ were already slow invariant manifold". If this were the case, then, in particular, the fast motions were described by the self-adjoint linear approximation.

Example 6: Quasi-chemical representation and Self-adjoint linearization of the Boltzmann collision operator

A decomposition of motions near thermodynamically nonequilibrium states results in a linear relaxation towards this state. A linear operator of this relaxation is explicitly constructed in the case of the Boltzmann equation.

An entropy-related specification of an equilibrium state is due to the two points of view. From the first, thermodynamic viewpoint, equilibria is a state in which the entropy is maximal. From the second, kinetic viewpoint, a quadratic form of entropy increases in a course of a linear regression towards this state. If an underlying microscopic dynamics is time-reversible, the kinetic viewpoint is realized due to known symmetric properties of a linearized kinetic operator.

In most of near-equilibrium studies, a principle of a decomposition of motions into rapid and slow occupies a distinct place. In some special cases, decomposition of motions is taken into account explicitly, by introducing a small parameter into dynamic equations. More frequently, however, it comes into play implicitly, for example, through an assumption of a rapid decay of memory in projection operator formalism [109]. Even in presence of long-living dynamic effects (mode coupling), a decomposition of motions appears as a final instance to get a closed set of equations for slow variables.

However, for closed systems, there remains a question: whether and to what extend the two aforementioned entropy-related points of view are applicable to non-equilibrium states? Further, if an answer is positive, then how to make explicitly a corresponding specification?

This Example is aimed at answering the questions just mentioned, and it is a straightforward continuation of results [1, 3]. Namely, in [1, 3], it was demonstrated that a principle of a decomposition of motions alone constitutes a necessary and sufficient condition for the thermodynamic specification of a non-equilibrium state (this will be briefly reviewed in the next section). However, in a general situation, one deals with states f other than f_0. A question is, whether these two ideas can be applied to $f \neq f_0$ (at least approximately), and if so, then how to make the presentation explicit.

A positive answer to this question was given partially in frames of the method of invariant manifolds [1, 2, 3]. Objects studied in [1, 2, 3] were manifolds in a space of distribution functions, and the goal was to construct iteratively a manifold that is tangent in all its points to a vector field of a dissipative system (an invariant manifold), beginning with some initial manifold with no such property. It was natural to employ methods of KAM-theory (Newton-type linear iterations to improve the initial manifold). However, an extra idea of a decomposition of motions into rapid and slow near the manifold was strongly necessary to adapt KAM-theory to dissipative systems. A geometrical formulation of this idea [1, 2, 3] results in a definition of a hyperplane of rapid motion, Γ_f , associated with the state f, and orthogonal to the gradient of the entropy in f. In a physical interpretation, Γ_f contains all those states from a neighborhood of f, which come into f in the course of rapid relaxation (as if f were the final state of rapid processes occuring in its neighborhood). Usually, Γ_f contains more states than can come into f in a rapid relaxation because of conservation of some macroscopic quantities (e.g. density, momentum, and energy, as well as, possibly, higher moments of f which practically do not vary in rapid processes). Extra states are eliminated by imposing additional restrictions, cutting out "thinner" linear manifolds, planes of rapid motions P_f, inside Γ_f. Extremal property of f on Γ_f is preserved on P_f as well (cf.[1, 2, 3]).

Thus, decomposition of motions near a manifold results in the thermodynamical viewpoint: states f belonging to the manifold are described as unique points of maximum of entropy on corresponding hyperplanes of rapid motions Γ_f. This formulation defines a slow dynamics on manifolds in agreement with the H-theorem for the Boltzmann equation, or with its analogs for other systems (see [1, 2, 3] for details). As it was shown in [1, 2, 3], decomposition of motions in a neighborhood of f is a criteria (a necessary and sufficient condition) of an existence of the thermodynamic description of f.

Newton iteration gives a correction, $f+\delta f$, to states of a non-invariant manifold, while δf is thought on Γ_f. Equation for δf involves a linearization of the collision integral in state f. Here, if $f \neq f_0$, we come to a problem of how to perform a linearization of collision integral in concordance with the H-theorem (corrections to the manifold of local equilibrium states were studied in a detail in [3]).

In this short communication we show that the aforementioned decomposition of motions results in the kinetic description of states on manifolds of slow motions, and that Onsager's principle can be applied in a natural way to linearize the Boltzmann collision integral.

Due to definition of Γ_f, the state f is the unique point of minimum of the H-function on Γ_f. In the first non-vanishing approximation, we have the following expression for H in the states on Γ_f:

$$H(f+\delta f) \approx H(f) + \frac{1}{2}\langle \delta f | \delta f \rangle_f$$

Here $\langle \cdot | \cdot \rangle_f$ denotes a scalar product generated by the second derivative of H in the state f: $\langle g_1 | g_2 \rangle_f = \int f^{-1} g_1 g_2 d\boldsymbol{v}$.

Decomposition of motions means that quadratic form $\langle \delta f | \delta f \rangle_f$ decays monotonically in the course of the linear relaxation towards the state f. It is natural, therefore, to impose a request that this linear relaxation should obey the Onsager's principle. Namely, the corresponding linear operator should be symmetric (formally self-adjoint) and non-positively definite in scalar product $\langle \cdot | \cdot \rangle_f$, and its kernel should consist of linear combinations of conserved quantities (1, $\boldsymbol{v}$, and v^2). In other words, decomposition of motions should give a picture of linear relaxation in a small neighborhood of f similar to that in a small neighborhood of f_0. Following this idea, we will now decompose the linearized collision integral L_f in two parts: L_f^{SYM} (satisfying the Onsager's principle), and L_f^{NT} (non-thermodynamic part).

In the state f, each direct encounter, $(\boldsymbol{v}, \boldsymbol{v}_1) \to (\boldsymbol{v}', \boldsymbol{v}_1')$, together with the reverse encounter, $(\boldsymbol{v}', \boldsymbol{v}_1') \to (\boldsymbol{v}, \boldsymbol{v}_1)$, contribute a rate, $W(f) - W'(f)$, to the collision integral, where

$$W(f) = w(\boldsymbol{v}', \boldsymbol{v}_1'; \boldsymbol{v}, \boldsymbol{v}_1) \exp\left\{D_f H|_{f=f(\boldsymbol{v})} + D_f H|_{f=f(\boldsymbol{v}_1)}\right\};$$

$$W'(f) = w(\boldsymbol{v}', \boldsymbol{v}_1'; \boldsymbol{v}, \boldsymbol{v}_1) \exp\left\{D_f H|_{f=f(\boldsymbol{v}')} + D_f H|_{f=f(\boldsymbol{v}_1')}\right\};$$

A deviation δf from the state f will change the rates of both the direct and the reverse processes. Resulting deviations of rates are:

$$\delta W = W(f)\left\{D_f^2 H|_{f=f(\boldsymbol{v})} \cdot \delta f(\boldsymbol{v}) + D_f^2 H|_{f=f(\boldsymbol{v}_1)} \cdot \delta f(\boldsymbol{v}_1)\right\};$$

$$\delta W' = W'(f)\left\{D_f^2 H|_{f=f(\boldsymbol{v}')} \cdot \delta f(\boldsymbol{v}') + D_f^2 H|_{f=f(\boldsymbol{v}_1')} \cdot \delta f(\boldsymbol{v}_1')\right\};$$

Symmetrization with respect to direct and reverse encounters will give a term proportional to a balanced rate, $W^{SYM}(f) = \frac{1}{2}(W(f) + W'(f))$, in both of the expressions δW and $\delta W'$. Thus, we come to the decomposition $L_f = L_f^{SYM} + L_f^{NT}$, where

$$L_f^{SYM}|\delta f\rangle = \int w \frac{f' f_1' + f f_1}{2} \left\{\frac{\delta f'}{f'} + \frac{\delta f_1'}{f_1'} - \frac{\delta f_1}{f_1} - \frac{\delta f}{f}\right\} d\boldsymbol{v}_1' d\boldsymbol{v}' d\boldsymbol{v}_1 \tag{263}$$

$$L_f^{NT}(\delta f) = \int w \frac{f' f_1' - f f_1}{2} \left\{\frac{\delta f'}{f'} + \frac{\delta f_1'}{f_1'} + \frac{\delta f_1}{f_1} + \frac{\delta f}{f}\right\} d\boldsymbol{v}_1' d\boldsymbol{v}' d\boldsymbol{v}_1 \tag{264}$$

Operator $L_f^{SYM}|\cdot\rangle$ (263) has the complete set of the aforementioned properties corresponding to the Onsager's principle, namely:

i) $\langle g_1|L_f^{SYM}|g_2\rangle_f = \langle g_2|L_f^{SYM}|g_1\rangle_f$;

ii) $\langle g|L_f^{SYM}|g\rangle_f \le 0$;

iii) $\ker L_f^{SYM} = \mathrm{lin}\{1, \boldsymbol{v}, v^2\}$.

For an unspecified f, non-thermodynamic operator L_f^{NT} (264) satisfies none of these properties. If $f = f_0$, then the part (264) vanishes, while operator $L_{f_0}^{SYM}|\cdot\rangle$ becomes the usual linearized collision integral due to the balance $W(f_0) = W'(f_0)$.

Non-negative definite form $\langle\delta f|\delta f\rangle_f$ decays monotonically due to an equation of linear relaxation, $\partial_t|\delta f\rangle = L_f SYM|\delta f\rangle$, and the unique point of minimum, $\delta f = 0$, of $\langle\delta f|\delta f\rangle_f$ corresponds to the equilibrium point of vector field $L_f^{SYM}|\delta f\rangle$.

Operator L_f^{SYM} describes the state f as the equilibrium state of a linear relaxation. Note that the method of extracting the symmetric part (263) is strongly based on the representation of direct and reverse processes, and it is not a simple procedure like, e.g., $\frac{1}{2}(L_f + L_f^+)$. The latter expression cannot be used as a basis for Onsager's principle since it would violate conditions (ii) and (iii).

Thus, if motions do decompose into a rapid motion towards the manifold and a slow motion along the manifold, then states on this manifold can be described from both the thermodynamical and kinetic points of view. Our consideration results in an explicit construction of operator L_f^{SYM} (263) responsible for the rapid relaxation towards the state f. It can be used, in particular, for obtaining corrections to such approximations as Grad moment approximations and Tamm–Mott-Smith approximation, in frames of the method [1, 2, 6]. The non-thermodynamic part (264) is always present in L_f, when $f \neq f_0$, but if trajectories of an equation $\partial_t \delta f = L_f \delta f$ are close to trajectories of an equation $\partial_t |\delta f\rangle = L_f^{SYM} |\delta f\rangle$, then L_f^{SYM} gives a good approximation to L_f. A conclusion on a closeness of trajectories depends on particular features of f, and normally it can be made on a base of a small parameter. On the other hand, the explicit thermodynamic and kinetic presentation of states on a manifold of slow motions (the extraction of L_f^{SYM} performed above and construction of hyper-planes Γ_f [1, 2, 3]) is based only the very idea of a decomposition of motions, and can be obtained with no consideration of a small parameter. Finally, though we have considered only the Boltzmann equation, the method of symmetrization can be applied to other dissipative systems with the same level of generality as the method [1, 2, 3].

8 Relaxation methods

Relaxation method is an alternative to the Newton iteration method described in section 6: The initial approximation to the invariant manifold F_0 is moved with the film extension, equation (41),

$$\frac{dF_t(y)}{dt} = (1 - P_{t,y})J(F_t(y)) = \Delta_{F(y)},$$

till a fixed point is reached. Advantage of this method is a relative freedom in its implementation, because equation (41) need not be solved exactly, one is interested only in finding fixed points. Therefore, "large stepping" in the direction of the defect, $\Delta_{F(y)}$ is possible, the termination point is defined by the condition that the vector field becomes orthogonal to $\Delta_{F(y)}$. For simplicity, let us consider the procedure of termination in the linear approximation of the vector field. Let $F_0(y)$ be the initial approximation to the invariant manifold, and we seek the first correction,

$$F_1(y) = F_0(y) + \tau_1(y)\Delta_{F_0(y)},$$

where function $\tau(y)$ has a dimension of the time, and is found from the condition that the linearized vector field attached to the points of the new manifold is orthogonal to the initial defect,

$$\langle \Delta_{F_0(y)} | (1 - P_y)[J(F_0(y)) + \tau_1(y)(D_x J)_{F_0(y)}\Delta_{F_0(y)}]\rangle_{F_0(y)} = 0. \tag{265}$$

Explicitly,

$$\tau_1(y) = -\frac{\langle \Delta_{F_0(y)} | \Delta_{F_0(y)} \rangle_{F_0(y)}}{\langle \Delta_{F_0(y)} | (D_x J)_{F_0(y)} | \Delta_{F_0(y)} \rangle_{F_0(y)}}. \tag{266}$$

Further steps $\tau_k(y)$ are found in the same way. It is clear from the latter equations that the step of the relaxation method for the film extension is equivalent to the Galerkin approximation for solving the step of the Newton method with incomplete linearization. Actually, the relaxation method was first introduced in these terms in [9]. The partially similar idea of using the explicit Euler method to approximate the finite-dimensional invariant manifold on the basis of spectral decomposition was proposed earlier in the paper [10].

An advantage of the equation (266) is the explicit form of the size of the steps $\tau_k(y)$. This method was successfully applied to the Fokker-Plank equation [9].

Example 7: Relaxation method for the Fokker-Planck equation

Here we address the problem of closure for the FPE (31) in a general setting. First, we review the maximum entropy principle as a source of suitable quasiequilibrium initial approximations for the closures. We also discuss a version of the maximum entropy principle, valid for a near-equilibrium dynamics, and which results in explicit formulae for arbitrary U and D.

In this Example we consider the FPE of the form (31):

$$\partial_t W(\boldsymbol{x},t) = \partial_x \cdot \{D \cdot [W \partial_x U + \partial_x W]\}\,. \tag{267}$$

Here $W(\boldsymbol{x},t)$ is the probability density over the configuration space $\boldsymbol{x}$, at the time t, while $U(\boldsymbol{x})$ and $D(\boldsymbol{x})$ are the potential and the positively semi-definite ($y \cdot D \cdot y \geq 0$) diffusion matrix.

Quasi-equilibrium approximations for the Fokker-Planck equation

The quasi-equilibrium closures are almost never invariants of the true moment dynamics. For corrections to the quasi-equilibrium closures, we apply the method of invariant manifold [3], which is carried out (subject to certain approximations explained below) to explicit recurrence formulae for one–moment near–equilibrium closures for arbitrary U and D. These formulae give a method for computing the lowest eigenvalue of the problem, and which dominates the near-equilibrium FPE dynamics. Results are tested with model potential, including the FENE-like potentials [86, 87, 88].

Let us denote as M the set of linearly independent moments $\{M_0, M_1, \ldots, M_k\}$, where $M_i[W] = \int m_i(x)W(x)dx$, and where $m_0 = 1$. We assume that there exists a function $W^*(M,x)$ which extremizes the entropy S (32) under the constrains of fixed M. This quasi-equilibrium distribution function may be written

$$W^* = W_{eq} \exp\left[\sum_{i=0}^{k} \Lambda_i m_i(x) - 1\right], \tag{268}$$

where $\Lambda = \{\Lambda_0, \Lambda_1, \ldots, \Lambda_k\}$ are Lagrange multipliers. Closed equations for moments M are derived in two steps. First, the quasi-equilibrium distribution (268) is substituted into the FPE (267) or (33) to give a formal expression: $\partial_t W^* = \hat{M}_{W^*}(\delta S/\delta W)|_{W=W^*}$. Second, introducing a projector Π^*,

$$\Pi^* \bullet = \sum_{i=0}^{k} (\partial W^*/\partial M_i) \int m(x) \bullet dx,$$

and applying Π^* on both sides of the formal expression, we derive closed equations for M in the quasi-equilibrium approximation. Further processing requires an explicit solution to the constrains, $\int W^*(\Lambda,x)m_i(x)dx = M_i$, to get the dependence of Lagrange multipliers Λ on the moments M. Though typically the functions $\Lambda(M)$ are not known explicitly, one general remark about the moment equations is readily available. Specifically, the moment equations in the quasi-equilibrium approximation have the form:

$$\dot{M}_i = \sum_{j=0}^{k} M^*_{ij}(M)(\partial S^*(M)/\partial M_j), \tag{269}$$

where $S^*(M) = S[W^*(M)]$ is the macroscopic entropy, and where M^*_{ij} is an M-dependent $(k+1) \times (k+1)$ matrix:

$$M^*_{ij} = \int W^*(M,x)[\partial_x m_i(x)] \cdot D(x) \cdot [\partial_x m_j(x)]dx.$$

The matrix M^*_{ij} is symmetric, positive semi–definite, and its kernel is the vector δ_{0i}. Thus, *the quasi-equilibrium closure reproduces the GENERIC structure on the macroscopic level*, the vector field of macroscopic equations (269) is a metric transform of the gradient of the macroscopic entropy.

The following version of the quasi-equilibrium closures makes it possible to derive more explicit results in the general case [140, 141, 129, 142]: In many cases, one can split the set of moments M in two parts, $M_I = \{M_0, M_1, \dots, M_l\}$ and $M_{II} = \{M_{l+1}, \dots, M_k\}$, in such a way that the quasi-equilibrium distribution can be constructed explicitly for M_I as $W^*_I(M_I, x)$. The full quasi-equilibrium problem for $M = \{M_I, M_{II}\}$ in the "shifted" formulation reads: extremize the functional $S[W^*_I + \Delta W]$ with respect to ΔW, under the constrains $M_I[W^*_I + \Delta W] = M_I$ and $M_{II}[W^*_I + \Delta W] = M_{II}$. Let us denote as $\Delta M_{II} = M_{II} - M_{II}(M_I)$ deviations of the moments M_{II} from their values in the MEP state W^*_I. For small deviations, the entropy is well approximated with its quadratic part

$$\Delta S = -\int \Delta W \left[1 + \ln \frac{W^*_I}{W_{eq}}\right] dx - \frac{1}{2}\int \frac{\Delta W^2}{W^*_I} dx.$$

Taking into account the fact that $M_I[W^*_I] = M_I$, we come to the following maximizaton problem:

$$\Delta S[\Delta W] \to max, \;\; M_I[\Delta W] = 0, \;\; M_{II}[\Delta W] = \Delta M_{II}. \tag{270}$$

The solution to the problem (270) is always explicitly found from a $(k+1) \times (k+1)$ system of linear algebraic equations for Lagrange multipliers. This method was applied to systems of Boltzmann equations for chemical reacting gases [140, 141], and for an approximate solution to the Boltzmann equation: scattering rates "moments of collision integral" are treated as independent variables, and as an alternative to moments of the distribution function, to describe the rarefied gas near local equilibrium. Triangle version of the entropy maximum principle is used to derive the Grad-like description in terms of a finite number of scattering rates. The equations are compared to the Grad moment system in the heat nonconductive case. Estimations for hard spheres demonstrate, in particular, some 10% excess of the viscosity coefficient resulting from the scattering rate description, as compared to the Grad moment estimation [142].

In the remainder of this section we deal solely with one-moment near-equilibrium closures: $M_I = M_0$, (i. e. $W^*_I = W_{eq}$), and the set M_{II} contains a single moment

$M = \int mW dx$, $m(x) \neq 1$. We shall specify notations for the near–equilibrium FPE, writing the distribution function as $W = W_{eq}(1 + \Psi)$, where the function Ψ satisfies an equation:

$$\partial_t \Psi = W_{eq}^{-1} \hat{J} \Psi, \tag{271}$$

where $\hat{J} = \partial_x \cdot [W_{eq} D \cdot \partial_x]$. The triangle one-moment quasi-equilibrium function reads:

$$W^{(0)} = W_{eq} \left[1 + \Delta M m^{(0)}\right] \tag{272}$$

where

$$m^{(0)} = [\langle mm \rangle - \langle m \rangle^2]^{-1} [m - \langle m \rangle]. \tag{273}$$

Here brackets $\langle \dots \rangle = \int W_{eq} \dots dx$ denote equilibrium averaging. The superscript (0) indicates that the triangle quasi-equilibrium function (272) will be considered as an initial approximation to a procedure which we address below. Projector for the approximation (272) has the form

$$\Pi^{(0)} \bullet = W_{eq} \frac{m^{(0)}}{\langle m^{(0)} m^{(0)} \rangle} \int m^{(0)}(x) \bullet dx. \tag{274}$$

Substituting the function (272) into the FPE (271), and applying the projector (274) on both the sides of the resulting formal expression, we derive an equation for M:

$$\dot{M} = -\lambda_0 \Delta M, \tag{275}$$

where $1/\lambda_0$ is an effective time of relaxation of the moment M to its equilibrium value, in the quasi-equilibrium approximation (272):

$$\lambda_0 = \langle m^{(0)} m^{(0)} \rangle^{-1} \langle \partial_x m^{(0)} \cdot D \cdot \partial_x m^{(0)} \rangle. \tag{276}$$

The invariance equation for the Fokker-Planck equation

Both the quasi-equilibrium and the triangle quasi-equilibrium closures are almost never invariants of the FPE dynamics. That is, the moments M of solutions to the FPE (267) vary in time differently from the solutions to the closed moment equations like (269), and these variations are generally significant even for the near–equilibrium dynamics. Therefore, we ask for corrections to the quasi-equilibrium closures to finish with the invariant closures. This problem falls precisely into the framework of the method of invariant manifold [3], and we shall apply this method to the one–moment triangle quasi-equilibrium closing approximations.

First, the invariant one–moment closure is given by an unknown distribution function $W^{(\infty)} = W_{eq}[1 + \Delta M m^{(\infty)}(x)]$ which satisfyes an equation

$$[1 - \Pi^{(\infty)}] \hat{J} m^{(\infty)} = 0. \tag{277}$$

Here $\Pi^{(\infty)}$ is a projector, associated with an unknown function $m^{(\infty)}$, and which is also yet unknown. Eq. (277) is a formal expression of the invariance principle for a one–moment near–equilibrium closure: considering $W^{(\infty)}$ as a manifold in the space of distribution functions, parameterized with the values of the moment M, we require that the microscopic vector field $\hat{J}m^{(\infty)}$ be equal to its projection, $\Pi^{(\infty)}\hat{J}m^{(\infty)}$, onto the tangent space of the manifold $W^{(\infty)}$.

Now we turn our attention to solving the invariance equation (277) iteratively, beginning with the triangle one–moment quasi-equilibrium approximation $W^{(0)}$ (272). We apply the following iteration process to the Eq. (277):

$$[1-\Pi^{(k)}]\hat{J}m^{(k+1)}=0, \tag{278}$$

where $k=0,1,\ldots$, and where $m^{(k+1)}=m^{(k)}+\mu^{(k+1)}$, and the correction satisfies the condition $\langle\mu^{(k+1)}m^{(k)}\rangle=0$. Projector is updated after each iteration, and it has the form

$$\Pi^{(k+1)}\bullet=W_{eq}\frac{m^{(k+1)}}{\langle m^{(k+1)}m^{(k+1)}\rangle}\int m^{(k+1)}(x)\bullet dx. \tag{279}$$

Applying $\Pi^{(k+1)}$ to the formal expression,

$$W_{eq}m^{(k+1)}\dot{M}=\Delta M[1-\Pi^{(k+1)}]m^{(k+1)},$$

we derive the $(k+1)$th update of the effective time (276):

$$\lambda_{k+1}=\frac{\langle\partial_x m^{(k+1)}\cdot D\cdot\partial_x m^{(k+1)}\rangle}{\langle m^{(k+1)}m^{(k+1)}\rangle}. \tag{280}$$

Specializing to the one-moment near-equilibrium closures, and following a general argument [3], solutions to the invariance equation (277) are eigenfunctions of the operator $\hat{J}$, while the formal limit of the iteration process (278) is the eigenfunction which corresponds to the eigenvalue with the minimal nonzero absolute value.

Diagonal approximation

To obtain more explicit results, we shall now turn to an approximate solution to the problem (278) *at each iteration*. The correction $\mu^{(k+1)}$ satisfyes the condition $\langle m^{(k)}\mu^{(k+1)}\rangle=0$, and can be decomposed as follows: $\mu^{(k+1)}=\alpha_k e^{(k)}+e^{(k)}_{ort}$. Here $e^{(k)}$ is the variance of the kth approximation: $e^{(k)}=W_{eq}^{-1}[1-\Pi^{(k)}]\hat{J}m^{(k)}=\lambda_k m^{(k)}+R^{(k)}$, where

$$R^{(k)}=W_{eq}^{-1}\hat{J}m^{(k)}. \tag{281}$$

The function $e^{(k)}_{ort}$ is orthogonal to both $e^{(k)}$ and $m^{(k)}$ ($\langle e^{(k)}e^{(k)}_{ort}\rangle=0$, and $\langle m^{(k)}e^{(k)}_{ort}\rangle=0$).

Our diagonal approximation (DA) consists in disregarding the part $e^{(k)}_{ort}$. In other words, we seek an improvement of the non–invariance of the kth approximation *along its variance* $e^{(k)}$. Specifically, we consider the following ansatz at the kth iteration:

$$m^{(k+1)}=m^{(k)}+\alpha_k e^{(k)}. \tag{282}$$

Substituting the ansatz (282) into the Eq. (278), and integrating the latter expression with the functon $e^{(k)}$ to evaluate the coefficient α_k:

$$\alpha_k = \frac{A_k - \lambda_k^2}{\lambda_k^3 - 2\lambda_k A_k + B_k}, \tag{283}$$

where parameters A_k and B_k represent the following equilibrium averages:

$$\begin{aligned} A_k &= \langle m^{(k)} m^{(k)} \rangle^{-1} \langle R^{(k)} R^{(k)} \rangle \\ B_k &= \langle m^{(k)} m^{(k)} \rangle^{-1} \langle \partial_x R^{(k)} \cdot D \cdot \partial_x R^{(k)} \rangle. \end{aligned} \tag{284}$$

Finally, putting together Eqs. (280), (281), (282), (283), and (284), we arrive at the following DA recurrence solution, and which is our main result:

$$m^{(k+1)} = m^{(k)} + \alpha_k [\lambda_k m^{(k)} + R^{(k)}], \tag{285}$$

$$\lambda_{k+1} = \frac{\lambda_k - (A_k - \lambda_k^2)\alpha_k}{1 + (A_k - \lambda_k^2)\alpha_k^2}. \tag{286}$$

Notice that the stationary points of the DA process (286) are the true solutions to the invariance equation (277). What *may be* lost within the DA is the convergency to the true limit of the procedure (278), i. e. to the *minimal* eigenvalue.

To test the convergency of the DA process (286) we have considered two potentials U in the FPE (267) with a constant diffusion matrix D. The first test was with the square potential $U = x^2/2$, in the three–dimensional configuration space, since for this potential the detail structure of the spectrum is well known. We have considered two examples of initial one–moment quasi-equilibrium closures with $m^{(0)} = x_1 + 100(x^2 - 3)$ (example 1), and $m^{(0)} = x_1 + 100x^6 x_2$ (example 2), in the Eq. (273). The result of performance of the DA for λ_k is presented in the Table 2, together with the error δ_k which was estimated as the norm of the variance at each iteration: $\delta_k = \langle e^{(k)} e^{(k)} \rangle / \langle m^{(k)} m^{(k)} \rangle$. In both examples, we see a good monotonic convergency to the minimal eigenvalue $\lambda_\infty = 1$, corresponding to the eigenfunction x_1. This convergency is even striking in the example 1, where the initial choice was very close to a different eigenfunction $x^2 - 3$, and which can be seen in the non–monotonic behavior of the variance. Thus, we have an example to trust the DA approximation as converging to the proper object.

For the second test, we have taken a one–dimensional potential $U = -50 \ln(1 - x^2)$, the configuration space is the segment $|x| \leq 1$. Potentials of this type (so-called FENE potential) are used in applications of the FPE to models of polymer solutions ([86, 87, 88]). Results are given in the Table 3 for the two initial functions, $m^{(0)} = x^2 + 10x^4 - \langle x^2 + 10x^4 \rangle$ (example 3), and $m^{(0)} = x^2 + 10x^8 - \langle x^2 + 10x^8 \rangle$ (example 4). Both the examples demonstrate a stabilization of the λ_k at the same value after some ten iterations.

In conclusion, we have developed the principle of invariance to obtain moment closures for the Fokker-Planck equation (267), and have derived explicit results for the one–moment near-equilibrium closures, particularly important to get information about the spectrum of the FP operator.

Table 2: Iterations λ_k and the error δ_k for $U = x^2/2$.

Ex. 1		0	1	4	8	12	16	20
	λ	1.99998	1.99993	1.99575	1.47795	1.00356	1.00001	1.00000
	δ	$0.16 \cdot 10^{-4}$	$0.66 \cdot 10^{-4}$	$0.42 \cdot 10^{-2}$	0.24	$0.35 \cdot 10^{-2}$	$0.13 \cdot 10^{-4}$	$0.54 \cdot 10^{-7}$
Ex. 2		0	1	2	3	4	5	6
	λ	3.399	2.437	1.586	1.088	1.010	1.001	1.0002
	δ	1.99	1.42	0.83	0.16	$0.29 \cdot 10^{-1}$	$0.27 \cdot 10^{-2}$	$0.57 \cdot 10^{-3}$

Table 3: Iterations λ_k for $U = -50 \ln(1 - x^2)$.

		0	1	2	3	4	5	6	7	8
Ex. 3	λ	213.17	212.186	211.914	211.861	211.849	211.845	211.843	211.842	211.841
Ex. 4	λ	216.586	213.135	212.212	211.998	211.929	211.899	211.884	211.876	211.871

9 Method of invariant grids

Elsewhere above in this paper, we considered immersions $F(y)$, and methods for their construction, without addressing the question of how to implement F in a constructive way. In most of the works (of us and of other people on similar problems), analytic forms were needed to represent manifolds (see, however, dual quasiequilibrium integrators [148, 149]). However, in order to construct manifolds of a relatively low dimension, grid-based representations of manifolds become a relevant option. The *Method of invariant grids* (MIG) was suggested recently in [7].

The principal idea of (MIG) is to find a mapping of finite-dimensional grids into the phase space of a dynamic system. That is we construct not just a point approximation of the invariant manifold $F^*(y)$, but an *invariant grid*. When refined, in the limit it is expected to converge, of course, to $F^*(y)$, but it is a separate, independently defined object.

Let's denote $L = R^n$, G is a discrete subset of R^n. A natural choice would be a regular grid, but, this is not crucial from the point of view of the general formalism. For every point $y \in G$, a neighborhood of y is defined: $V_y \subset G$, where V_y is a finite set, and, in particular, $y \in V_y$. On regular grids, V_y includes, as a rule, the nearest neighbors of y. It may also include next to nearest points.

For our purposes, one should define a grid differential operator. For every function, defined on the grid, also all derivatives are defined:

$$\left.\frac{\partial f}{\partial y_i}\right|_{y \in G} = \sum_{z \in V_y} q_i(z, y) f(z), i = 1, \dots n. \tag{287}$$

where $q_i(z, y)$ are some coefficients.

Here we do not specify the choice of the functions $q_i(z, y)$. We just mention in passing that, as a rule, equation (287) is established using some interpolation of f in the neighborhood of y in R^n by some differentiable functions (for example, polynomial). This interpolation is based on the values of f in the points of V_y. For regular grids, $q_i(z, y)$ are functions of the difference $z - y$. For some ys which are close to the edges of the grid, functions are defined only on the part of V_y. In this case, the coefficients in (287) should be modified appropriately in order to provide an approximation using available values of f. Below we will assume this modification is always done. We also assume that the number of points in the neighborhood V_y is always sufficient to make the approximation possible. This assumption restricts the choice of the grids G. Let's call *admissible* all such subsets G, on which one can define differentiation operator in every point.

Let F be a given mapping of some admissible subset $G \subset R^n$ into U. For every $y \in V$ we define tangent vectors:

$$T_y = Lin\{g_i\}_1^n, \tag{288}$$

where vectors $g_i (i = 1, \dots n)$ are partial derivatives (287) of the vector-function F:

$$g_i = \frac{\partial F}{\partial y_i} = \sum_{z \in V_y} q_i(z, y) F(z), \tag{289}$$

or in the coordinate form:

$$(g_i)_j = \frac{\partial F_j}{\partial y_i} = \sum_{z \in V_y} q_i(z, y) F_j(z). \tag{290}$$

Here $(g_i)_j$ is the jth coordinate of the vector (g_i), and $F_j(z)$ is the jth coordinate of the point $F(z)$.

The grid G is *invariant*, if for every node $y \in G$ the vector field $J(F(y))$ belongs to the tangent space T_y (here J is the right hand site of the kinetic equations (34)).

So, the definition of the invariant grid includes:
1) Finite admissible subset $G \subset R^n$;
2) A mapping F of this admissible subset G into U (where U is the phase space for kinetic equations (34));
3) The differentiation formulae (287) with given coefficients $q_i(z, y)$;

The grid invariance equation has a form of inclusion:

$$J(F(y)) \in T_y \text{ for every } y \in G,$$

or a form of equation:

$$(1 - P_y) J(F(y)) = 0 \text{ for every } y \in G,$$

where P_y is the thermodynamic projector (89).

The grid differentiation formulae (287) are needed, in the first place, to establish the tangent space T_y, and the null space of the thermodynamic projector P_y in each node. It is important to realise that locality of construction of thermodynamic projector enables this without a need for a global parametrization.

Basically, in our approach, the grid specifics are in:(a) differentiation formulae, (b) grid construction strategy (the grid can be extended, contracted, refined, etc.) The invariance equations (36), equations of the film dynamics extension (41), the iteration Newton method (124), and the formulae of the relaxation approximation (266) do not change at all. For convenience, let us repeat all these formulae in the grid context.

Let $x = F(y)$ be position of a grid's node y immersed into U. We have set of tangent vectors $g_i(x)$, defined in x (289), (290). Thus, the tangent space T_y is defined by (288). Also, one has entropy function $S(x)$, the linear functional $D_x S|_x$, and the subspace $T_{0y} = T_y \bigcap \ker D_x S|_x$ in T_y. Let $T_{0y} \neq T_y$. In this case we have a vector $\mathbf{e}_y \in T_y$, orthogonal to T_{0y}, $D_x S|_x(\mathbf{e}_y) = 1$. Then, the thermodynamic projector is defined as:

$$P_y \bullet = P_{0y} \bullet + \mathbf{e}_y D_x S|_x \bullet, \tag{291}$$

where P_{0y} is the orthogonal projector on T_{0y} with respect to the entropic scalar product $\langle | \rangle_x$.

If $T_{0y} = T_y$, then the thermodynamic projector is the orthogonal projector on T_y with respect to the entropic scalar product $\langle | \rangle_x$.

For the Newton method with incomplete linearization, the equations for calculating new node position $x' = x + \delta x$ are:

$$\left\{ \begin{array}{l} P_y \delta x = 0 \\ (1 - P_y)(J(x) + DJ(x)\delta x) = 0. \end{array} \right. \tag{292}$$

Here $DJ(x)$ is a matrix of derivatives of J, calculated in x. The self-adjoint linearization may be useful too (see section 8).

Equation (292) is a system of linear algebraic equations. In practice, it is convenient to choose some orthonormal (with respect to the entropic scalar product) basis $\mathbf{b_i}$ in $ker P_y$. Let $r = dim(ker P_y)$. Then $\delta x = \sum_{i=1}^{r} \delta_i \mathbf{b_i}$, and the system looks like

$$\sum_{k=1}^{r} \delta_k \langle \mathbf{b_i} \mid DJ(x) \mathbf{b_k} \rangle_x = -\langle J(x) \mid \mathbf{b_i} \rangle_x, i = 1...r. \tag{293}$$

Here $\langle | \rangle_x$ is the entropic scalar product. This is the system of linear equations for adjusting the node position accordingly to the Newton method with incomplete linearization.

For the relaxation method, one needs to calculate the defect $\Delta_x = (1 - P_y)J(x)$, and the relaxation step

$$\tau(x) = -\frac{\langle \Delta_x | \Delta_x \rangle_x}{\langle \Delta_x | DJ(x) \Delta_x \rangle_x}. \tag{294}$$

Then, new node position x' is calculated as

$$x' = x + \tau(x) \Delta_x. \tag{295}$$

This is the equation for adjusting the node position according to the relaxation method.

9.1 Grid construction strategy

From all reasonable strategies of the invariant grid construction we will consider here the following two: *growing lump* and *invariant flag*.

9.1.1 Growing lump

In this strategy one chooses as initial the equilibrium point y^*. The first approximation is constructed as $F(y^*) = x^*$, and for some initial V_0 ($V_{y^*} \subset V_0$) one has $F(y) = x^* + A(y - y^*)$, where A is an isometric embedding (in the standard Euclidean metrics) of R^n in E.

For this initial grid one makes a fixed number of iterations of one of the methods chosen (Newton's method with incomplete linearization or the relaxation method), and, after that, puts $V_1 = \bigcup_{y \in V_0} V_y$ and extends F from V_0 onto V_1 using linear extrapolation and the process continues. One of the possible variants of this procedure is to extend the grid from V_i to V_{i+1} not after a fixed number of iterations, but when invariance defect Δ_y becomes smaller than a given ϵ (in a given norm, which is entropic, as a rule), for all nodes $y \in V_i$. The lump stops growing when it reaches the boundary and is within a given accuracy $\|\Delta\| < \epsilon$.

9.1.2 Invariant flag

For the invariant flag one uses sufficiently regular grids G, in which many points are situated on the coordinate lines, planes, etc. One considers the standard flag $R^0 \subset R^1 \subset R^2 \subset ... \subset R^n$ (every next space is constructed by adding one more coordinate). It corresponds to a succession of grids $\{y\} \subset G^1 \subset G^2 ... \subset G^n$, where $\{y^*\} = R^0$, and G^i is a grid in R^i.

First, y^* is mapped in x^* and further $F(y^*) = x^*$. Then an invariant grid is constructed on $V^1 \subset G^1$ (up to the boundaries U and within a given accuracy $\|\Delta\| < \epsilon$). After the neighborhoods in G^2 are added to the points V^1, and, using such extensions, the grid $V^2 \subset G^2$ is constructed (up to the boundaries and within a given accuracy) and so on, until $V^n \subset G^n$ will be constructed.

We must underline here that, constructing the k-th grid $V^k \subset G^k$, the important role of the grids of smaller dimension $V^0 \subset ... \subset V^{k-1} \subset V^k$ embedded in it, is preserved. The point $F(y^*) = x^*$ is preserved. For every $y \in V^q$ $(q < k)$ the tangent vectors $g_1, ..., g_q$ are constructed, using the differentiation operators (287) on the whole V^k. Using the tangent space $T_y = Lin\{g_1, .., g_q\}$, the projector P_y is constructed, the iterations are applied and so on. All this is done to obtain a succession of embedded invariant grids, given by the same map F.

9.1.3 Boundaries check and the entropy

We construct grid mapping of F onto the finite set $V \in G$. The technique of checking if the grid still belongs to the phase space U of kinetic system U $(F(V) \subset U)$ is quite straightforward: all the points $y \in V$ are checked to belong to U. If at the next iteration a point $F(y)$ leaves U, then it is returned inside by a homothety transform with the center in x^*. Since the entropy is a concave function, the homothety contraction with the center in x^* increases the entropy monotonously. Another variant is cutting off the points leaving U.

By the way it was constructed, (89), the kernel of the entropic projector is annulled by the entropy differential. Thus, in the first order, steps in the Newton method with incomplete linearization (124) as well as in the relaxation methods (265),(266) do not change the entropy. But, if the steps are quite large, then the increasing of the entropy can become essential and the points are returned on their entropy level by the homothety contraction with the center in the equilibrium point.

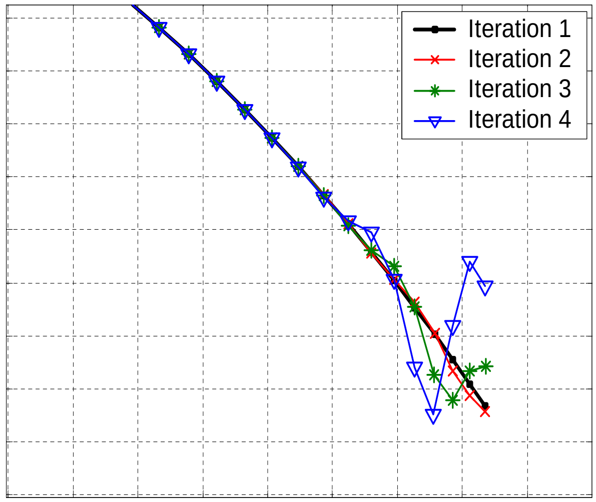


Figure 5: Grid instability. For small grid steps approximations in the calculation of grid derivatives lead to the grid instability effect. On the figure several successive iterations of the algorithm without adaptation of the time step are shown that lead to undesirable "oscillations", which eventually destruct the grid starting from one of it's ends.

9.2 Instability of fine grids

When one reduces the grid step (spacing between the nodes) in order to get a finer grid, then, starting from a definite step, it is possible to face the problem of the Courant instability [150, 151, 152]. Instead of converging, at the every iteration the grid becomes entangled (see Fig. 5).

The way to get rid off this instability is well-known. This is decreasing the time step. Instead of the real time step, we have a shift in the Newtonian direction. Formally, we can assign for one complete step in the Newtonian direction a value $h = 1$. Let us consider now the Newton method with an arbitrary h. For this, let us find $\delta x = \delta F(y)$ from (292), but we will change δx proportionally to h: the new value of $x_{n+1} = F_{n+1}(y)$ will be equal to

$$F_{n+1}(y) = F_n(y) + h_n \delta F_n(y) \tag{296}$$

where the lower index n denotes the step number.

One way to choose the h step value is to make it adaptive, controlling the average value of the invariance defect $\|\Delta_y\|$ at every step. Another way is the convergence control: then $\sum h_n$ plays a role of time.

Elimination of Courant instability for the relaxation method can be made quite analogously. Everywhere the step h is maintained as big as it is possible without convergence problems.

9.3 What space is the most appropriate for the grid construction?

For the kinetics systems there are two distinguished representations of the phase space:

- The densities space (concentrations, energy or probability densities, etc.)
- The spaces of conjugate intensive quantities, potentials (temperature, chemical potentials, etc.)

The density space is convenient for the construction of quasi-chemical representations. Here the balance relations are linear and the restrictions are in the form of linear inequalities (the densities themselves or some linear combinations of them must be positive).

The conjugate variables space is convenient in the sense that the equilibrium conditions, given the linear restrictions on the densities, are in the linear form (with respect to the conjugate variables). In these spaces the quasiequilibrium manifolds exist in the form of linear subspaces and, vise versa, linear balance equations turns out to be equations of the conditional entropy maximum.

The duality we've just described is very well-known and studied in details in many works on thermodynamics and Legendre transformations [155, 156]. This viewpoint of nonequilibrium thermodynamics unifies many well-established mesoscopic dynamical theories, as for example the Boltzmann kinetic theory and the Navier-Stokes-Fourier hydrodynamics [157]. In the previous section, the grids were constructed in the density space. But the procedure of constructing them in the space of the conjugate variables seems to be more consistent. The principal argument for this is the specific role of quasiequilibrium, which exists as a linear manifold. Therefore, linear extrapolation gives a thermodynamically justified quasiequilibrium approximation. Linear approximation of the slow invariant manifold in the neighborhood of the equilibrium in the conjugate variables space already gives the global quasiequilibrium manifold, which corresponds to the motion separation (for slow and fast motions) in the neighborhood of the equilibrium point.

For the mass action law, transition to the conjugate variables is simply the logarithmic transformation of the coordinates.

9.4 Carleman's formulae in the analytical invariant manifolds approximations. First benefit of analyticity: superresolution

When constructing invariant grids, one must define the differential operators (287) for every grid node. For calculating the differential operators in some point y, an interpolation procedure in the neighborhood of y is used. As a rule, it is an interpolation by a low-order polynomial, which is constructed using the function values in the nodes belonging to the neighbourhood of y in G. This approximation (using values in the closest nodes) is natural for smooth functions. But, we are looking for the *analytical* invariant manifold (see discussion in the section: "Film extension: Analyticity instead of the boundary conditions"). Analytical functions have much more "rigid" structure than the smooth ones. One can change a smooth function in the neighborhood of any point in such a way, that outside this neighborhood the function will not change. In general, this is not possible for analytical functions: a kind of "long-range" effect takes place (as is well known) .

The idea is to use this effect and to reconstruct some analytical function f_G using function given on G. There is one important requirement: if these values on G are values (given in the points of G) of some function f which is analytical in the given neighborhood U, then if the G is refined "correctly", one must have $f_G \to f$. The sequence of reconstructed function f_G should should converge to the "proper" function f.

What is the "correct refinement"? For smooth functions for the convergence $f_G \to f$ it is necessary and sufficient that, in the course of refinement, G would approximate the whole U with arbitrary accuracy. For analytical functions it is necessary only that, under the refinement, G would approximate some uniqueness set [9] $A \subset U$. Suppose we have a sequence of grids G, each next is finer than previous, which approximates a set A. For smooth functions, using function values defined on the grids, one can reconstruct the function in A. For analytical functions, if the analyticity area U is known, and A is a uniqueness set in U, then one can reconstruct the function in U. The set U can be essentially bigger than A; because of this such extension was named as *superresolution effects* [158]. There exist constructive formulae for construction of analytical functions f_G for different areas U, uniqueness sets $A \subset U$ and for different ways of discrete approximation of A by a sequence of fined grids G [158]. Here we provide only one Carleman's formula which is the most appropriate for our purposes.

Let area $U = Q_\sigma^n \subset C^n$ be a product of strips $Q_\sigma \subset C$, $Q_\sigma = \{z|\mathrm{Im}z < \sigma\}$. We will construct functions holomorphic in Q_σ^n. This is effectively equivalent to the construction of real analytical functions f in whole R^n with a condition on the convergence radius $r(x)$ of the Taylor series for f as a function of each coordinate: $r(x) \geq \sigma$ in every point $x \in R^n$.

The sequence of fined grids is constructed as follows: let for every $l = 1, ..., n$ a finite sequence of distinct points $N_l \subset D_\sigma$ be defined:

$$N_l = \{x_{lj}|j = 1, 2, 3...\}, x_{lj} \neq x_{li} \;\; for \;\; i \neq j \tag{297}$$

The uniqueness set A, which is approximated by a sequence of fined finite grids, has the form:

$$A = N_1 \times N_2 \times ... \times N_n = \{(x_{1i_1}, x_{2i_2}, .., x_{ni_n})|i_{1,..,n} = 1, 2, 3, ...\} \tag{298}$$

The grid G_m is defined as the product of initial fragments N_l of length m:

$$G_m = \{(x_{1i_1}, x_{2i_2}...x_{ni_n})|1 \leq i_{1,..,n} \leq m\} \tag{299}$$

[9] Let's remind to the reader that $A \subset U$ is called *uniqueness set* in U if for analytical in U functions ψ and φ from $\psi|_A \equiv \varphi|_A$ it follows $\psi = \varphi$.

Let's denote $\lambda = 2\sigma/\pi$ (σ is a half-width of the strip Q_σ). The key role in the construction of the Carleman's formula is played by the functional $\omega_m^\lambda(u,p,l)$ of 3 variables: $u \in U = Q_\sigma^n$, p is an integer, $1 \leq p \leq m$, l is an integer, $1 \leq p \leq n$. Further u will be the coordinate value in the point where the extrapolation is calculated, l will be the coordinate number, and p will be an element of multi-index $\{i_1, ..., i_n\}$ for the point $(x_{1i_1}, x_{2i_2}, ..., x_{ni_n}) \in G$:

$$\omega_m^\lambda(u,p,l) = \frac{(e^{\lambda x_{lp}} + e^{\lambda \bar{x}_{lp}})(e^{\lambda u} - e^{\lambda x_{lp}})}{\lambda(e^{\lambda u} + e^{\lambda \bar{x}_{lp}})(u - x_{lp})e^{\lambda x_{lp}}} \times \prod_{j=1 j\neq p}^{m} \frac{(e^{\lambda x_{lp}} + e^{\lambda \bar{x}_{lj}})(e^{\lambda u} - e^{\lambda x_{lj}})}{(e^{\lambda x_{lp}} - e^{\lambda x_{lj}})(e^{\lambda u} + e^{\lambda \bar{x}_{lj}})} \tag{300}$$

For real-valued x_{pk} formula (300) becomes simpler:

$$\omega_m^\lambda(u,p,l) = 2\frac{e^{\lambda u} - e^{\lambda x_{lp}}}{\lambda(e^{\lambda u} + e^{\lambda x_{lp}})(u - x_{lp})} \times \prod_{j=1 j\neq p}^{m} \frac{(e^{\lambda x_{lp}} + e^{\lambda x_{lj}})(e^{\lambda u} - e^{\lambda x_{lj}})}{(e^{\lambda x_{lp}} - e^{\lambda x_{lj}})(e^{\lambda u} + e^{\lambda x_{lj}})} \tag{301}$$

The Carleman's formula for extrapolation from G_M on $U = Q_\sigma^n$ ($\sigma = \pi\lambda/2$) has the form ($z = (z_1, ..., z_n)$):

$$f_m(z) = \sum_{k_1,...,k_n=1}^{m} f(x_k) \prod_{j=1}^{n} \omega_m^\lambda(z_j, k_j, j), \tag{302}$$

where $k = k_1, .., k_n$, $x_k = (x_{1k_1}, x_{2k_2}, ..., x_{nk_n})$.

There exists a theorem [158]:

If $f \in H^2(Q_\sigma^n)$, then $f(z) = lim_{m\to\infty} f_m(z)$, where $H^2(Q_\sigma^n)$ is the Hardy class of holomorphic in Q_σ^n functions.

It is useful to present the asymptotics of (302) for big $|\mathrm{Re} z_j|$. For this we will consider the asymptotics of (302) for big $|\mathrm{Re} u|$:

$$|\omega_m^\lambda(u,p,l)| = \left| \frac{2}{\lambda u} \prod_{j=1 j\neq p}^{m} \frac{e^{\lambda x_{lp}} + e^{\lambda x_{lj}}}{e^{\lambda x_{lp}} - e^{\lambda x_{lj}}} \right| + o(|\mathrm{Re} u|^{-1}). \tag{303}$$

From the formula (302) one can see that for the finite m and $|\mathrm{Re} z_j| \to \infty$ function $|f_m(z)|$ behaves like $const \cdot \prod_j |z_j|^{-1}$.

This property (zero asymptotics) must be taken into account when using the formula (302). When constructing invariant manifolds $F(W)$, it is natural to use (302) not for the immersion $F(y)$, but for the deviation of $F(y)$ from some analytical ansatz $F_0(y)$ [159, 160].

The analytical ansatz $F_0(y)$ can be obtained using Taylor series, just as in the Lyapunov auxiliary theorem [98] (also see above in the sections about the film extensions). Another variant is using Taylor series for the construction of Pade-approximations.

It is natural to use approximations (302) in dual variables as well, since there exists for them (as the examples demonstrate) a simple and very effective linear ansatz for the invariant manifold. This is the slow invariant subspace E_{slow} of the operator of linearized system (34) in dual variables in the equilibrium point. This invariant subspace corresponds to the the set of "slow" eigenvalues (with small $|\mathrm{Re}\lambda|$, $\mathrm{Re}\lambda < 0$). In the initial space (of concentrations or densities) this invariant subspace is the quasiequilibrium manifold. It consist of the maximal entropy points on the affine manifolds of the $x + E_{\mathrm{fast}}$ form, where E_{fast} is the "fast" invariant subspace of the operator of linearized system (34) in the initial variables in the equilibrium point. It corresponds to the "fast" eigenvalues (big $|\mathrm{Re}\lambda|$, $\mathrm{Re}\lambda < 0$).

In the problem of invariant grids constructing we can use the Carleman's formulae in two moments: first, for the definition grid differential operators (287), second, for the analitical continuation the manifold from the grid.

Example 8: Two-step catalytic reaction

Let us consider a two-step four-component reaction with one catalyst A_2:

$$A_1 + A_2 \leftrightarrow A_3 \leftrightarrow A_2 + A_4 \tag{304}$$

We assume the Lyapunov function of the form $S = -G = -\sum_{i=1}^{4} c_i[ln(c_i/c_i^{eq}) - 1]$. The kinetic equation for the four-component vector of concentrations, $\mathbf{c} = (c_1, c_2, c_3, c_4)$, has the form

$$\dot{\mathbf{c}} = \gamma_1 W_1 + \gamma_2 W_2. \tag{305}$$

Here $\gamma_{1,2}$ are stoichiometric vectors,

$$\gamma_1 = (-1, -1, 1, 0),\ \gamma_2 = (0, 1, -1, 1), \tag{306}$$

while functions $W_{1,2}$ are reaction rates:

$$W_1 = k_1^+ c_1 c_2 - k_1^- c_3,\ W_2 = k_2^+ c_3 - k_2^- c_2 c_4. \tag{307}$$

Here $k_{1,2}^{\pm}$ are reaction rate constants. The system under consideration has two conservation laws,

$$c_1 + c_3 + c_4 = B_1,\ c_2 + c_3 = B_2, \tag{308}$$

or $\langle \mathbf{b_{1,2}}, \mathbf{c} \rangle = B_{1,2}$, where $\mathbf{b_1} = (1, 0, 1, 1)$ and $\mathbf{b_1} = (0, 1, 1, 0)$. The nonlinear system (304) is effectively two-dimensional, and we consider a one-dimensional reduced description. For our example, we chose the following set of parameters:

$$\begin{array}{l} k_1^+ = 0.3,\ k_1^- = 0.15,\ k_2^+ = 0.8,\ k_2^- = 2.0; \\ c_1^{eq} = 0.5,\ c_2^{eq} = 0.1, c_3^{eq} = 0.1,\ c_4^{eq} = 0.4; \\ B_1 = 1.0,\ B_2 = 0.2 \end{array} \tag{309}$$

In Fig. 6 one-dimensional invariant grid is shown in the (c_1,c_4,c_3) coordinates. The grid was constructed by growing the grid, as described above. We used Newtonian iterations to adjust the nodes. The grid was grown up to the boundaries of the phase space.

The grid derivatives for calculating tangent vectors g were taken as simple as $g(x_i) = (x_{i+1} - x_{i-1})/||x_{i+1} - x_{i-1}||$ for the internal nodes and $g(x_1) = (x_1 - x_2)/||x_1 - x_2||$, $g(x_n) = (x_n - x_{n-1})/||x_n - x_{n-1}||$ for the grid's boundaries. Here x_i denotes the vector of the ith node position, n is the number of nodes in the grid.

Close to the phase space boundaries we had to apply an adaptive algorithm for choosing the time step h: if, after the next growing step and applying $N = 20$ complete Newtonian steps, the grid did not converged, then we choose a new $h_{n+1} = h_n/2$ and recalculate the grid. The final value for h was $h \approx 0.001$.

The nodes positions are parametrized with entropic distance to the equilibrium point measured in the quadratic metrics given by $\mathbf{H_c} = -||\partial^2 S(\mathbf{c})/\partial c_i \partial c_j||$ in the equilibrium c^{eq}. It means that every node is on a sphere in this quadratic metrics with a given radius, which increases linearly. On this figure the step of the increase is chosen to be 0.05. Thus, the first node is on the distance 0.05 from the equilibrium, the second is on the distance 0.10 and so on. Fig. 7 shows several basic values which facilitate understanding of the object (invariant grid) extracted. The sign on the x-axis of the graphs at Fig. 7 is meaningless, since the distance is always positive, but in this situation it denotes two possible directions from the equilibrium point.

Fig. 7a,b effectively represents the slow one-dimensional component of the dynamics of the system. Given any initial condition, the system quickly finds the corresponding point on the manifold and starting from this point the dynamics is given by a part of the graph on the Fig. 7a,b.

One of the useful values is shown on the Fig. 7c. It is the relation between the relaxation times "toward" and "along" the grid (λ_2/λ_1, where λ_1,λ_2 are the smallest and the second smallest by absolute value non-zero eigenvalue of the system, symmetrically linearized in the point of the grid node). It shows that the system is very stiff close to the equilibrium point, and less stiff (by one order of magnitude) on the borders. This leads to the conclusion that the reduced model is more adequate in the neighborhood of the equilibrium where fast and slow motions are separated by two orders of magnitude. On the very end of the grid which corresponds to the positive absciss values, our one-dimensional consideration faces with definite problems (slow manifold is not well-defined).

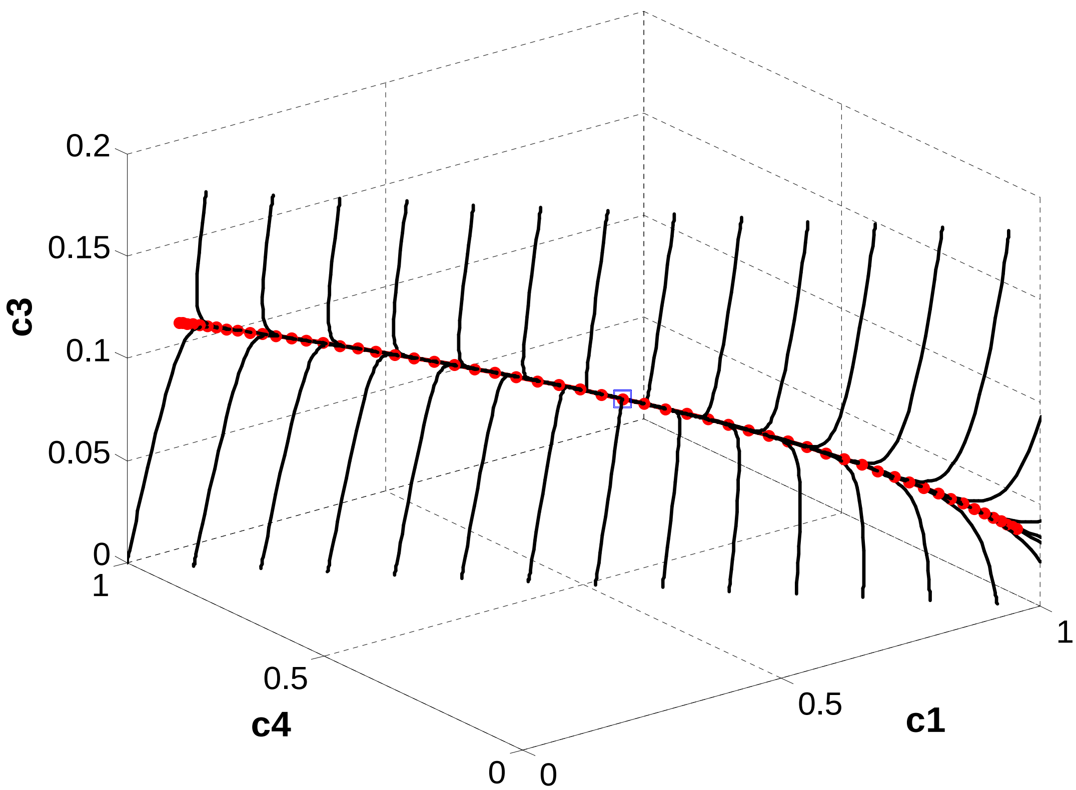
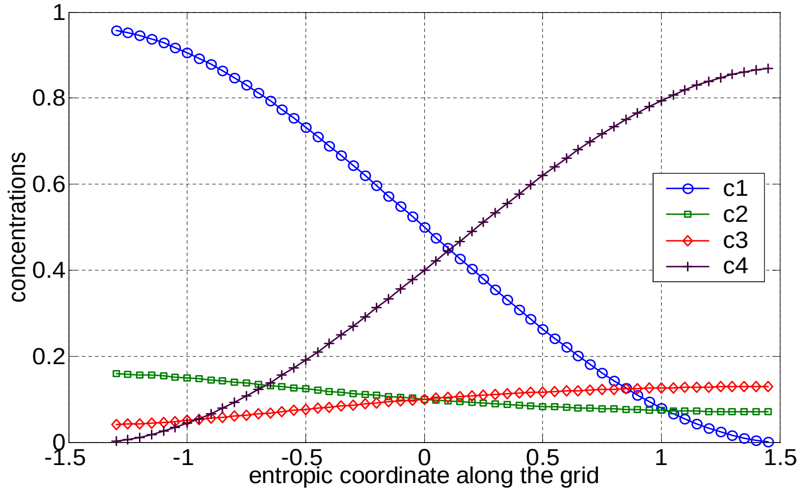
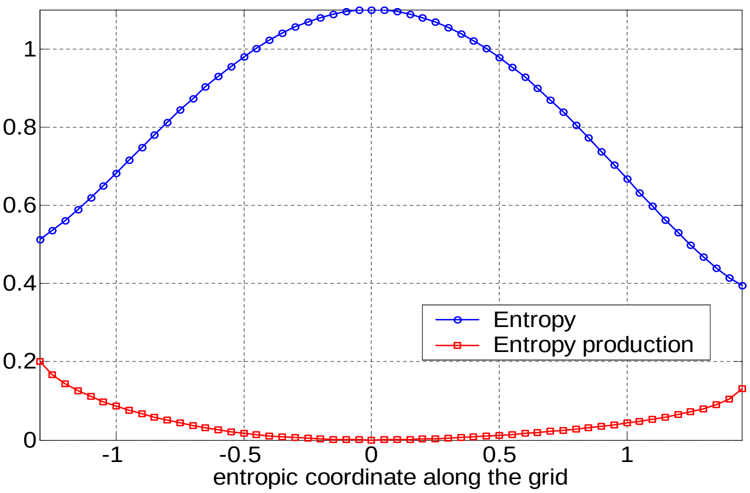


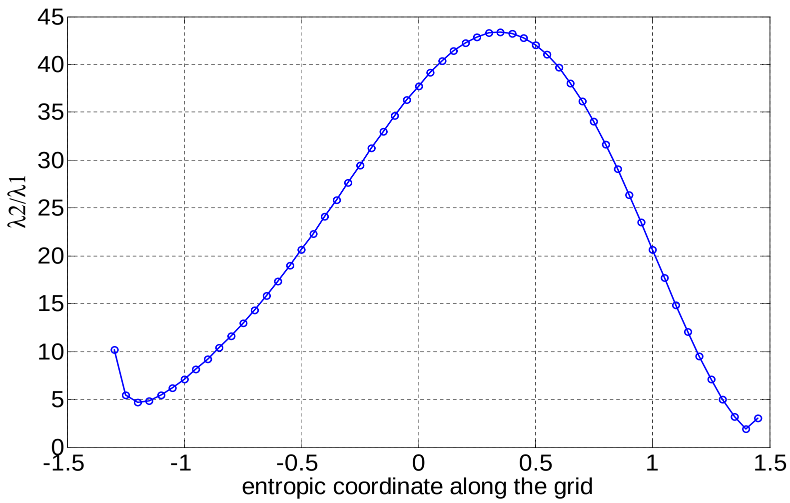
Figure 6: One-dimensional invariant grid (circles) for two-dimensional chemical system. Projection into the 3d-space of c_1, c_4, c_3 concentrations. The trajectories of the system in the phase space are shown by lines. The equilibrium point is marked by square. The system quickly reaches the grid and further moves along it.



a)



b)



c)

Figure 7: One-dimensional invariant grid for two-dimensional chemical system. a) Values of the concentrations along the grid. b) Values of the entropy and the entropy production (-dG/dt) along the grid. c) Relation of the relaxation times "toward" and "along" the manifold. The nodes positions are parametrized with entropic distance measured in the quadratic metrics given by $\mathbf{H_c} = -||\partial^2 S(\mathbf{c})/\partial c_i \partial c_j||$ in the equilibrium c^{eq}. Zero corresponds to the equilibrium.

Example 9: Model hydrogen burning reaction

In this section we consider a more interesting illustration, where the phase space is 6-dimensional, and the system is 4-dimensional. We construct an invariant flag which consists of 1- and 2-dimensional invariant manifolds.

We consider chemical system with six species called (provisionally) H_2 (hydrogen), O_2 (oxygen), H_2O (water), H, O, OH (radicals). We assume the Lyapunov function of the form $S = -G = -\sum_{i=1}^{6} c_i[ln(c_i/c_i^{eq}) - 1]$. The subset of the hydrogen burning reaction and corresponding (direct) rate constants have been taken as:

$$
\begin{array}{ll}
1.\ H_2 \leftrightarrow 2H & k_1^+ = 2 \\
2.\ O_2 \leftrightarrow 2O & k_2^+ = 1 \\
3.\ H_2O \leftrightarrow H + OH & k_3^+ = 1 \\
4.\ H_2 + O \leftrightarrow H + OH & k_4^+ = 10^3 \\
5.\ O_2 + H \leftrightarrow O + OH & k_5^+ = 10^3 \\
6.\ H_2 + O \leftrightarrow H_2O & k_6^+ = 10^2
\end{array}
\tag{310}
$$

The conservation laws are:

$$
\begin{array}{l}
2c_{H_2} + 2c_{H_2O} + c_H + c_{OH} = b_H \\
2c_{O_2} + c_{H2O} + c_O + c_{OH} = b_O
\end{array}
\tag{311}
$$

For parameter values we took $b_H = 2$, $b_O = 1$, and the equilibrium point:

$$
c_{H_2}^{eq} = 0.27 \quad c_{O_2}^{eq} = 0.135 \quad c_{H_2O}^{eq} = 0.7 \quad c_H^{eq} = 0.05 \quad c_O^{eq} = 0.02 \quad c_{OH}^{eq} = 0.01 \tag{312}
$$

Other rate constants $k_i^-, i = 1..6$ were calculated from $\mathbf{c^{eq}}$ value and k_i^+. For this system the stoichiometric vectors are:

$$
\begin{array}{ll}
\gamma_1 = (-1, 0, 0, 2, 0, 0) & \gamma_2 = (0, -1, 0, 0, 2, 0) \\
\gamma_3 = (0, 0, -1, 1, 0, 1) & \gamma_4 = (-1, 0, 0, 1, -1, 1) \\
\gamma_5 = (0, -1, 0, -1, 1, 1) & \gamma_6 = (-1, 0, 1, 0, -1, 0)
\end{array}
\tag{313}
$$

We stress here once again that the system under consideration is fictional in that sense that the subset of equations corresponds to the simplified picture of this physical-chemical process and the constants do not correspond to any measured ones, but reflect only basic orders of magnitudes of the real-world system. In this sense we consider here a qualitative model system, which allows us to illustrate the invariant grids method without excessive complication. Nevertheless, modeling of real systems differs only in the number of species and equations. This leads, of course, to computationally harder problems, but not the crucial ones, and the efforts on the modeling of real-world systems are on the way.

Fig. 8a presents a one-dimensional invariant grid constructed for the system. Fig. 8b shows the picture of reduced dynamics along the manifold (for the explanation of the meaning of the x-coordinate, see the previous subsection). On Fig. 8c the three smallest by absolute value non-zero eigen values of the symmetrically linearized system A^{sym} have been shown. One can see that the two smallest values "exchange" on one of the grid end. It means that one-dimensional "slow" manifold has definite problems in this region, it is just not defined there. In practice, it means that one has to use at least two-dimensional grids there.

Fig. 9a gives a view onto the two-dimensional invariant grid, constructed for the system, using the "invariant flag" strategy. The grid was grown starting from the 1D-grid constructed at the previous step. At the first iteration for every node of the initial grid, two nodes (and two edges) were added. The direction of the step was chosen as the direction of the eigenvector of the matrix A^{sym} (in the point of the node), corresponding to the second "slowest" direction. The value of the step was chosen to be $\epsilon = 0.05$ in terms of entropic distance. After several Newtonian iterations done until convergence, new nodes were added in the direction "ortogonal" to the 1D-grid. This time it is done by linear extrapolation of the grid on the same step $\epsilon = 0.05$. When some new nodes have one or several negative coordinates (the grid reaches the boundaries) they were cut off. If a new node has only one edge, connecting it to the grid, it was excluded (since it does not allow calculating 2D-tangent space for this node). The process continues until the expansion is possible (after this, every new node has to be cut off).

Strategy of calculating tangent vectors for this regular rectangular 2D-grid was chosen to be quite simple. The grid consists of *rows*, which are co-oriented by construction to the initial 1D-grid, and *columns* that consist of the adjacent nodes in the neighboring rows. The direction of "columns" corresponds to the second slowest direction along the grid. Then, every row and column is considered as 1D-grid, and the corresponding tangent vectors are calculated as it was described before:

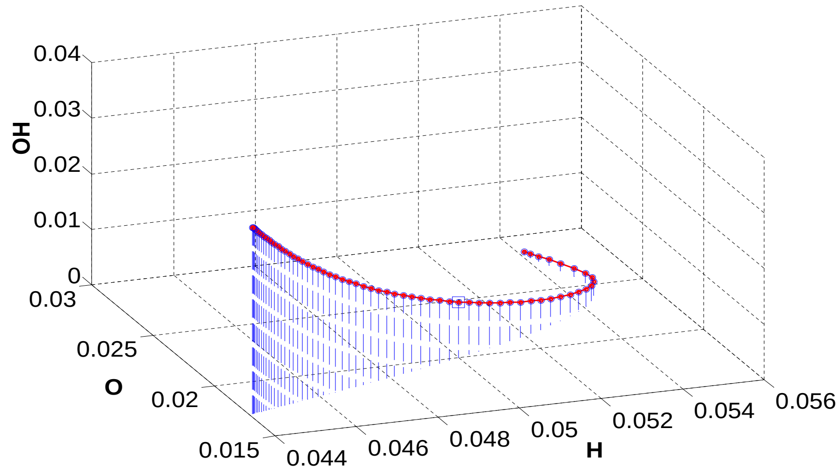
$$g_{row}(x_{k,i}) = (x_{k,i+1} - x_{k,i-1})/\|x_{k,i+1} - x_{k,i-1}\|$$

for the internal nodes and

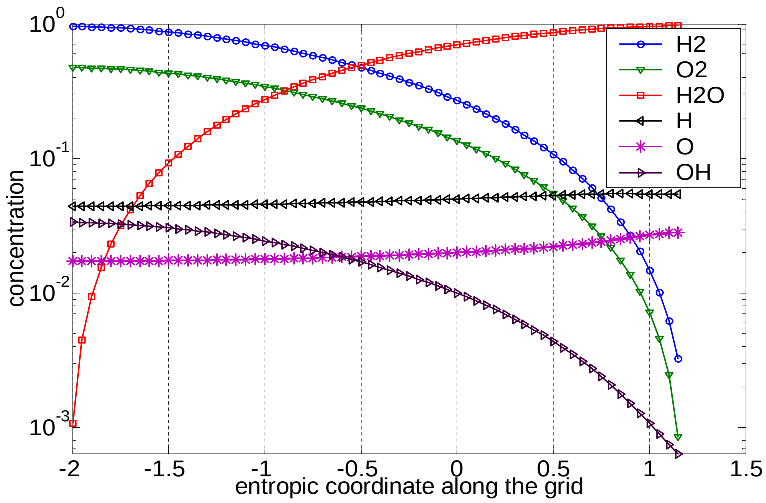
$$g_{row}(x_{k,1}) = (x_{k,1} - x_{k,2})/\|x_{k,1} - x_{k,2}\|, g_{row}(x_{k,n_k}) = (x_{k,n_k} - x_{k,n_k-1})/\|x_{k,n_k} - x_{k,n_k-1}\|$$

for the nodes which are close to the grid's edges. Here $x_{k,i}$ denotes the vector of the node in the kth row, ith column; n_k is the number of nodes in the kth row. Second tangent vector $g_{col}(x_{k,i})$ is calculated completely analogously. In practice, it is convenient to orthogonalize $g_{row}(x_{k,i})$ and $g_{col}(x_{k,i})$.

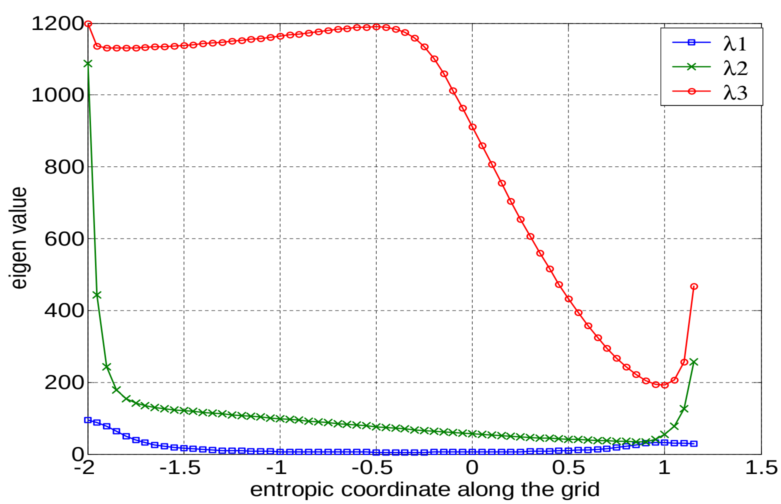
Since the phase space is four-dimensional, it is impossible to visualize the grid in one of the coordinate 3D-views, as it was done in the previous subsection. To facilitate visualization one can utilize traditional methods of multi-dimensional data visualization. Here we make use of the principal components analysis (see, for example, [154]), which constructs a three-dimensional linear subspace with maximal dispersion of the othogonally projected data (grid nodes in our case). In other words, method of principal components constructs in multi-dimensional space such a three-dimensional box inside which the grid can be placed maximally tightly (in the mean square distance meaning). After projection of the grid nodes into this space, we get more or less adequate representation of the two-dimensional grid embedded into the six-dimensional concentrations space (Fig. 9b). The



a)

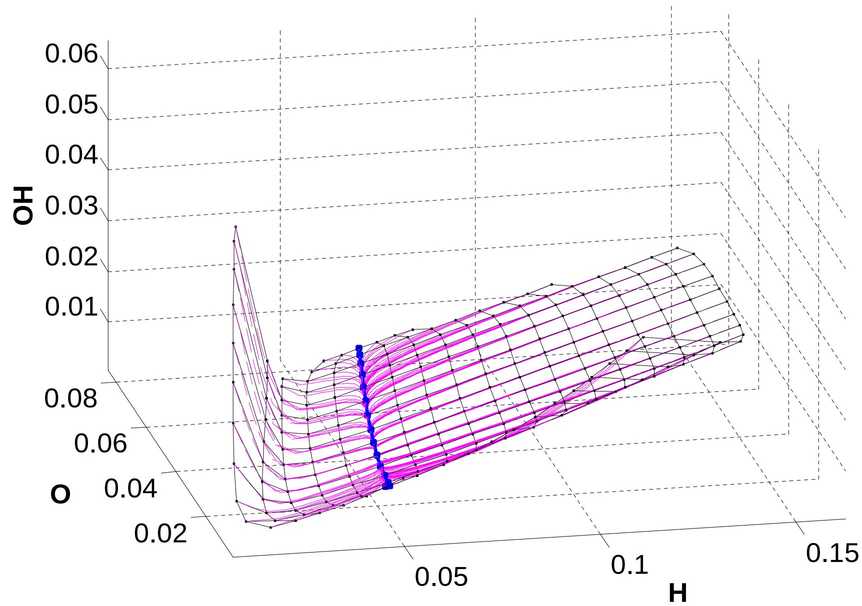


b)

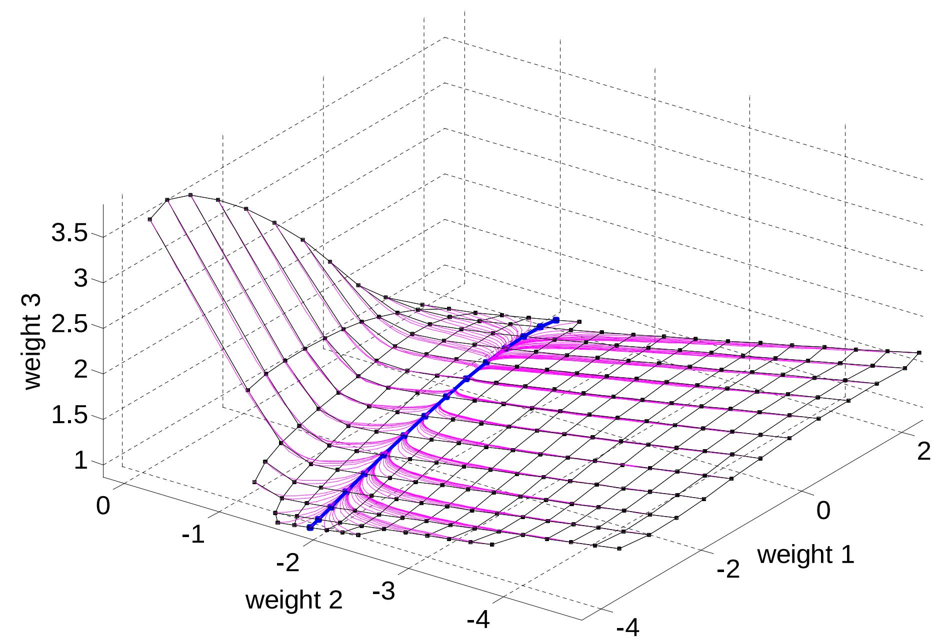


c)

Figure 8: One-dimensional invariant grid for model hydrogen burning system. a) Projection into the 3d-space of c_H, c_O, c_{OH} concentrations. b) Concentration values along the grid. c) three smallest by absolute value non-zero eigen values of the symmetrically linearized system.



a)



b)

Figure 9: Two-dimensional invariant grid for the model hydrogen burning system. a) Projection into the 3d-space of c_H, c_O, c_{OH} concentrations. b) Projection into the principal 3D-subspace. Trajectories of the system are shown coming out from the every grid node. Bold line denotes the one-dimensional invariant grid, starting from which the 2D-grid was constructed.

disadvantage of the approach is that the axes now do not have explicit meaning, being some linear combinations of the concentrations.

One attractive feature of two-dimensional grids is the possibility to use them as a screen, on which one can display different functions $f(\mathbf{c})$ defined in the concentrations space. This technology was exploited widely in the non-linear data analysis by the elastic maps method [153]. The idea is to "unfold" the grid on a plane (to present it in the two-dimensional space, where the nodes form a regular lattice). In other words, we are going to work in the internal coordinates of the grid. In our case, the first internal coordinate (let's call it s_1) corresponds to the direction, co-oriented with the one-dimensional invariant grid, the second one (let's call it s_2) corresponds to the second slow direction. By how it was constructed, $s_2 = 0$ line corresponds to the one-dimensional invariant grid. Units of s_1 and s_2 are entropic distances in our case.

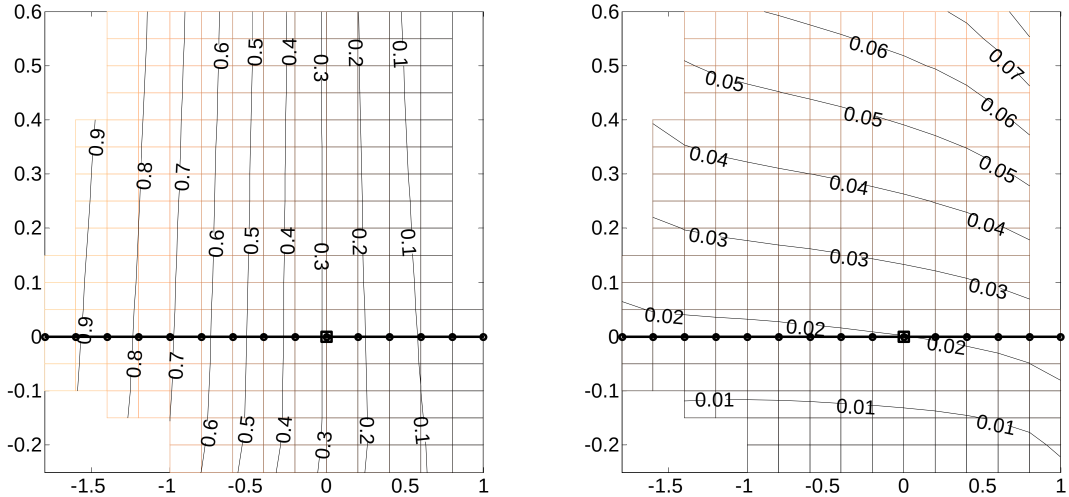
Every grid node has two internal coordinates (s_1, s_2) and, simultaneously, corresponds to a vector in the concentration space. This allows us to map any function $f(\mathbf{c})$ from the multi-dimensional concentration space to the two-dimensional space of the grid. This mapping is defined in a finite number of points (grid nodes), and can be interpolated (linearly, in the simplest case) in between them. Using coloring and isolines one can visualize the values of the function in the neighborhood of the invariant manifold. This is meaningful, since, by the definition, the system spends most of the time in the vicinity of the invariant manifold, thus, one can visualize the behaviour of the system. As a result of applying the technology, one obtains a set of color illustrations (a stack of information layers), put onto the grid as a map. This allows applying all the methods, working with stack of information layers, like geographical information systems (GIS) methods, which are very well developed.

In short words, the technique is a useful tool for exploration of dynamical systems. It allows to see simultaneously many different scenarios of the system behaviour, together with different system's characteristics.

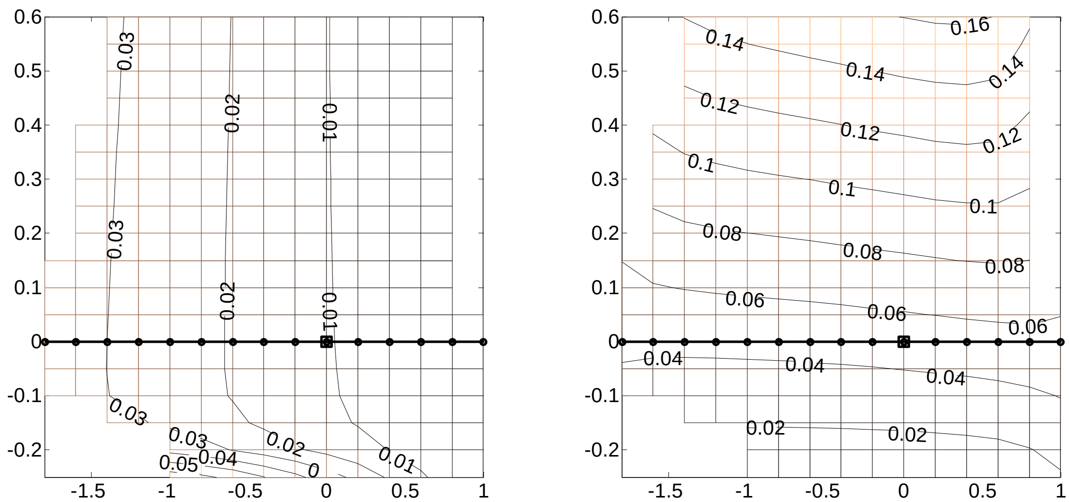
The simplest functions to visualize are the coordinates: $c_i(\mathbf{c}) = c_i$. On Fig. 10 we displayed four colorings, corresponding to the four arbitrarily chosen concentrations functions (of H_2, O, H and OH; Fig. 10a-d). The qualitative conclusions that can be made from the graphs are that, for example, the concentration of H_2 practically does not change during the first fast motion (towards the 1D-grid) and then, gradually changes to the equilibrium value (the H_2 coordinate is "slow"). The O coordinate is the opposite case, it is "fast" coordinate which changes quickly (on the first stage of motion) to the almost equilibrium value, and then it almost does not change. Basically, the slope angles of the coordinate isolines give some presentation of how "slow" a given concentration is. Fig. 10c shows interesting behaviour of the OH concentration. Close to the 1D grid it behaves like "slow coordinate", but there is a region on the map where it has clear "fast" behaviour (middle bottom of the graph).

The next two functions which one can want to visualize are the entropy S and the entropy production $\sigma(\mathbf{c}) = -dG/dt(\mathbf{c}) = \sum_i \ln(c_i/c_i^{eq})\dot{c}_i$. They are shown on Fig. 11a,b.

Finally, we visualize the relation between the relaxation times of the fast motion towards the 2D-grid and along it. This is given on the Fig. 11c. This picture allows to make a conclusion that two-dimensional consideration can be appropriate for the system (especially in the "high H_2, high O" region), since the relaxation times "towards" and "along" the grid are definitely separated. One can compare this to the Fig. 11d, where the relation between relaxation times towards and along the 1D-grid is shown.

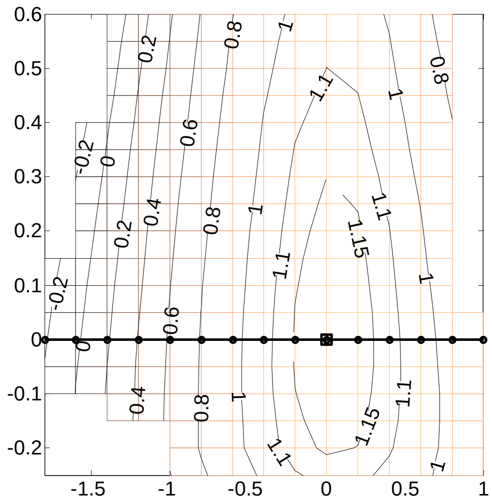


a) Concentration H_2 b) Concentration O

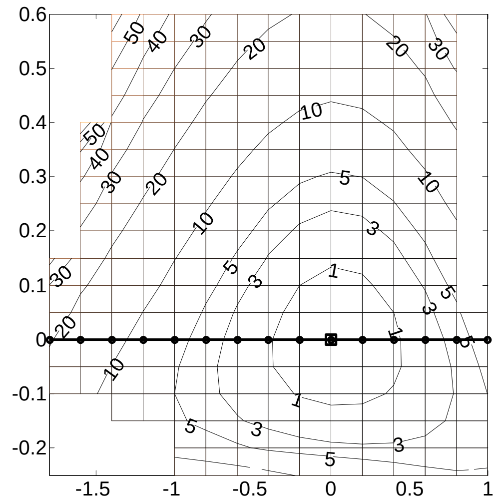


c) Concentration OH d) Concentration H

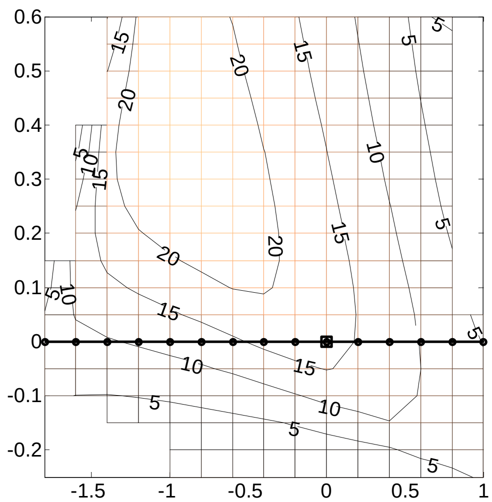
Figure 10: Two-dimensional invariant grid as a screen for visualizing different functions defined in the concentrations space. The coordinate axes are entropic distances (see the text for the explanations) along the first and the second slowest directions on the grid. The corresponding 1D invariant grid is denoted by bold line, the equilibrium is denoted by square.



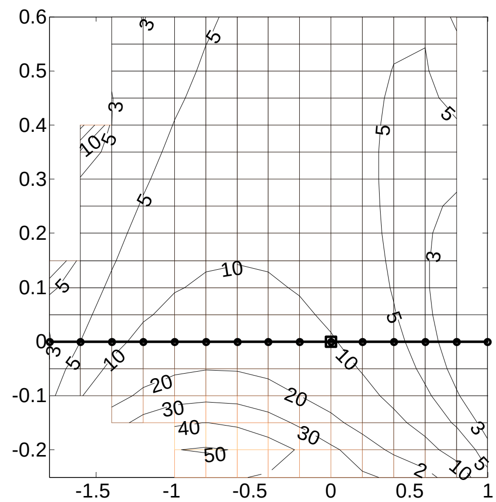
a) Entropy



b) Entropy Production



c) λ_3/λ_2 relation



d) λ_2/λ_1 relation

Figure 11: Two-dimensional invariant grid as a screen for visualizing different functions defined in the concentrations space. The coordinate axes are entropic distances (see the text for the explanations) along the first and the second slowest directions on the grid. The corresponding 1D invariant grid is denoted by bold line, the equilibrium is denoted by square.

10 Method of natural projector

Ehrenfest suggested in 1911 a model of dynamics with a coarse-graining of the original conservative system in order to introduce irreversibility [163]. The idea of Ehrenfest 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 it 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 formally most general construction extending the Ehrenfest idea is given below. Let us stay with notation of section 3, and let a submanifold $F(W)$ be defined in the phase space U. Furthermore, we assume a map (a projection) is defined, $\Pi : U \to W$, with the properties:

$$\Pi \circ F = 1, \;\; \Pi(F(y)) = y. \tag{314}$$

In addition, one requires some mild properties of regularity, in particular, surjectivity of the differential, $D_x\Pi : E \to L$, 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,

$$\frac{dy}{dt} = \Psi(y), \tag{315}$$

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

$$\Pi(T_\tau F(y)) = \Theta_\tau y, \tag{316}$$

where T_τ is the shift operator for the system (34), and Θ_τ is the (yet unknown!) shift operator for the system in question (315).

Equation (316) means that one projects not the vector fields but segments of trajectories. 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 (34): 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 (41). 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 $\tau \to \infty$:

$$\Psi_\infty(y) = D_x\Pi|_{x=F_\infty(y)} J(F_\infty(y)). \tag{317}$$

For stiff dynamic systems, the limit (317) is qualitatively almost obvious: After some relaxation time τ_0 (for $t > t_0$), 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 (315) and (316)) is defined by the vector field attached to F_∞ with any predefined accuracy. Rigorous proofs requires existence and uniqueness theorems, as well as homogeneous continuous dependence of solutions on 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 expansion[10] in powers of τ. Various other approximation schemes like Pade approximation are possible too.

[10]In the well known work of Lewis [164], this expansion was executed incorrectly (terms of different orders were matched on the left and on the right hand sides of equation (316). This created an obstacle in a development of the method. See more detailed discussion in the section Example 10.

Example 10: 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, $S \to \max$, where S in 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 our method.

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 Boltzmann collision integral.

(iii) The most significant advantage of this formalization 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 [13, 14, 18] to derivations of macroscopic equations in various cases, with and without mean field interaction potentials, for various choices of macroscopic variables, 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, for the sake of completeness, we describe briefly the formalization of Ehrenfest's approach [13, 14]. 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. In section 3, we begin the discussion of applications. 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 system of 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 post-Navier-Stokes equations as derived from the Boltzmann kinetic equation by the Chapman-Enskog method (Burnett and super-Burnett hydrodynamics) suffer from unphysical instability already in the linear approximation [45]. We demonstrate it by the explicit computation that the linearized higher-order hydrodynamic equations derived within our method are free from this drawback.

General construction

Let us consider a microscopic dynamics given by an equation,

$$\dot{f} = J(f), \tag{318}$$

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 [108, 107]:

$$S(f) \to \max,\ \ \mu(f) = M, \tag{319}$$

where S is the entropy functional, which is assumed to be strictly concave, and M is the set of the macroscopic variables $\{M\}$, and μ is the set of the corresponding operators. If the solution to the problem (319) exists, it is unique thanks to the concavity of the entropy functionals. Solution to equation (319) 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, $\mu(f) = \int \{1, \boldsymbol{v}, v^2\} f d\boldsymbol{v}$, with $\boldsymbol{v}$ the particle's velocity; the corresponding $f^*(M)$ is called the local Maxwell distribution function.

If the microscopic dynamics is given by equation (318), then the quasiequilibrium dynamics of the variables M reads:

$$\dot{M}_k = \mu_k(J(f^*(M)) = \phi_k^*. \tag{320}$$

The quasiequilibrium approximation has important property, it conserves the type of the dynamics: If the entropy monotonically increases (or not decreases) due to equation (318), then the same is true for the quasiequilibrium entropy, $S^*(M) = S(f^*(M))$, due to the quasiequilibrium dynamics (320). That is, if

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

then

$$\dot{S}^* = \sum_k \frac{\partial S^*}{\partial M_k}\dot{M}_k = \sum_k \frac{\partial S^*}{\partial M_k}\mu_k(J(f^*(M))) \geq 0. \tag{321}$$

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 (318) then $S^*(M)$ is the integral of motion for the quasiequilibrium equation (320). 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 (318) is the (reversible) Liouville equation, then (320) is the Vlasov equation which is reversible, too. On the other hand, if the entropy was monotonically increasing on solutions to equation (318), then the quasiequilibrium entropy also increases monotonically on solutions to the quasiequilibrium dynamic equations (320). For instance, if equation (318) 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 (319) exists), then (320) 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).

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's in their seminal work [163]: 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.

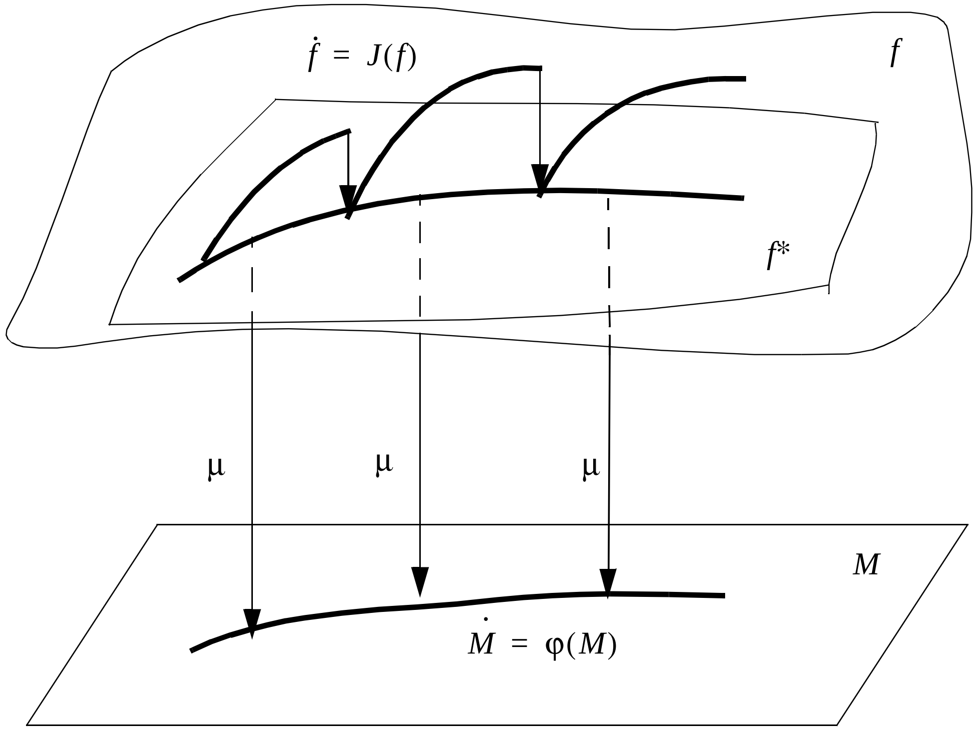


Figure 12: Coarse-graining scheme. f is the space of microscopic variables, M is the space of the macroscopic variables, f^* is the quasiequilibrium manifold, μ is the mapping from the microscopic to the macroscopic space.

From the perspective of 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 (318) 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. 12.

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

$$S(f_i^*) \leq S(f_{i+1}^*), \tag{322}$$

the equality occurs if and only if the quasiequilibrium is the invariant manifold of the dynamic system (318). Whenever the quasiequilibrium is *not* the solution to equation (318), the strict inequality in (322) demonstrates the entropy increase.

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 keeping the 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 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 the Ref. [13, 14] is based on using an expansion of both the microscopic and the macroscopic trajectories. Here we present this construction to the third order accuracy, in a general form, whereas only the second-order accurate construction has been discussed in [13, 14].

Let us write down the solution to the microscopic equation (318), and approximate this solution by the polynomial of third oder in τ. Introducing notation, $J^* = J(f^*(M(t)))$, we write,

$$f(t+\tau) = f^* + \tau J^* + \frac{\tau^2}{2}\frac{\partial J^*}{\partial f}J^* + \frac{\tau^3}{3!}\left(\frac{\partial J^*}{\partial f}\frac{\partial J^*}{\partial f}J^* + \frac{\partial^2 J^*}{\partial f^2}J^*J^*\right) + o(\tau^3). \qquad (323)$$

Evaluation of the macroscopic variables on the function (323) gives

$$\begin{aligned} M_k(t+\tau) &= M_k + \tau\phi_k^* + \frac{\tau^2}{2}\mu_k\left(\frac{\partial J^*}{\partial f}J^*\right) \\ &+ \frac{\tau^3}{3!}\left\{\mu_k\left(\frac{\partial J^*}{\partial f}\frac{\partial J^*}{\partial f}J^*\right) + \mu_k\left(\frac{\partial^2 J^*}{\partial f^2}J^*J^*\right)\right\} + o(\tau^3), \end{aligned} \qquad (324)$$

where $\phi_k^* = \mu_k(J^*)$ is the quasiequilibrium macroscopic vector field (the right hand side of equation (320)), 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 (320) with the right-hand side not yet defined, give the following third-order result:

$$\begin{aligned} M_k(t+\tau) &= M_k + \tau\phi_k + \frac{\tau^2}{2}\sum_j \frac{\partial \phi_k}{\partial M_j}\phi_j \\ &+ \frac{\tau^3}{3!}\sum_{ij}\left(\frac{\partial^2\phi_k}{\partial M_i M_j}\phi_i\phi_j + \frac{\partial \phi_k}{\partial M_i}\frac{\partial \phi_i}{\partial M_j}\phi_j\right) + o(\tau^3). \end{aligned} \qquad (325)$$

Expanding functions ϕ_k into the series $\phi_k = R_k^{(0)} + \tau R_k^{(1)} + \tau^2 R_k^{(2)} + ...$, ($R_k^{(0)} = \phi^*$), and requiring that the microscopic and the macroscopic dynamics coincide to the order of τ^3, we obtain the sequence of corrections for 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:

$$R_k^{(1)} = \frac{1}{2}\left\{\mu_k\left(\frac{\partial J^*}{\partial f}J^*\right) - \sum_j \frac{\partial \phi_k^*}{\partial M_j}\phi_j^*\right\}. \qquad (326)$$

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

$$
\begin{aligned}
R_k^{(2)} &= \frac{1}{3!}\left\{\mu_k\left(\frac{\partial J^*}{\partial f}\frac{\partial J^*}{\partial f}J^*\right)+\mu_k\left(\frac{\partial^2 J^*}{\partial f^2}J^*J^*\right)\right\}-\frac{1}{3!}\sum_{ij}\left(\frac{\partial \phi_k^*}{\partial M_i}\frac{\partial \phi_i^*}{\partial M_j}\phi_j^*\right)\\
&- \frac{1}{3!}\sum_{ij}\left(\frac{\partial^2 \phi_k^*}{\partial M_i \partial M_j}\phi_i^*\phi_j^*\right)-\frac{1}{2}\sum_j\left(\frac{\partial \phi_k^*}{\partial M_j}R_j^{(1)}+\frac{\partial R_j^{(1)}}{\partial M_j}\phi_j^*\right),
\end{aligned}
\tag{327}
$$

Further corrections are found by the same token. Equations (326)–(327) give explicit closed expressions for corrections to the quasiequilibrium dynamics to the order of accuracy specified above. They are used below in various specific examples.

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 (322) 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,

$$
P^* g = \sum_k \frac{\partial f^*}{\partial M_k}\mu_k(g). \tag{328}
$$

It has been demonstrated in [14] that the entropy production,

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

equals

$$
\dot{S}^*_{(1)} = -\frac{\tau}{2}(1-P^*)J^* \left.\frac{\partial^2 S^*}{\partial f \partial f}\right|_{f^*}(1-P^*)J^*. \tag{329}
$$

Equation (329) is nonnegative definite due to concavity of the entropy. Entropy production (329) 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 (329) is proportional to τ. Note also that projection operator does not appear in our consideration a priory, rather, it is the result of exploring the coarse-graining condition in the previous section.

Though equation (329) looks very natural, its existence is rather subtle. Indeed, equation (329) 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 quasiequilibrium vector field). Each of these expressions separately gives a positive contribution to the entropy production, and equation (329) 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 nth 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 (329), $\delta S \sim \tau^2$ 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 (329) 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.

Relation to the work of Lewis

Among various realizations of the coarse-graining procedures, the work of Lewis [164] 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,

$$M_k(t+\tau) = \mu_k\left(T_\tau f^*(M(t))\right), \tag{330}$$

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 (330), in terms of the coarse-graining time τ. In the work of Lewis [164], it was suggested, as a general way to exploring the condition (330), to write the first-order equation for M in the form of the differential pursuit,

$$M_k(t) + \tau \frac{dM_k(t)}{dt} \approx \mu_k\left(T_\tau f^*(M(t))\right). \tag{331}$$

In other words, in the work of Lewis [164], the expansion to the first order was considered on the left (macroscopic) side of equation (330), 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 Ref. [13, 14] for details). Namely, the expansion to the second order of the right hand side of Lewis' equation ([164]) 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 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, see next section) 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 [164], that the exploration of the condition (330) 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 (330) 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 (330),

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

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 (330), the Boltzmann equation is derived (see also a recent elegant renormalization-group argument for this derivation [33]).

We stress that our approach of matched expansion for exploring the coarse-graining condition (330) 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 (330) 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 future work.

Equations of hydrodynamics for simple fluid

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 section, the microscopic dynamics is given by the Liouville equation, similar to the previous case.

However, we take another set of macroscopic variables: density, average velocity, and average temperature of the fluid. Under this condition the solution to the problem (319) 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 (so-called Burnett approximation), are subject to various difficulties, in particular, they exhibit an instability of sound waves at sufficiently short wave length (see, e. g. [21] for a recent review). Here we demonstrate how model hydrodynamic equations, including post-Navier-Stokes approximations, can be derived on the basis of coarse-graining idea, and investigate the linear stability of the obtained equations. We will find that the resulting equations are stable.

Two points need a clarification before we proceed further [14]. First, below we consider the simplest Liouville equation for the one-particle distribution, describing a free moving particle 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 [71]). 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 linearly unstable).

Derivation of the Navier-Stokes equations

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

$$\frac{\partial f}{\partial t} = -v_i \frac{\partial f}{\partial r_i}, \tag{332}$$

where $f = f(\boldsymbol{r}, \boldsymbol{v}, t)$ 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 $S = -k_{\rm B} \int f \ln f d\boldsymbol{v} d\boldsymbol{r}$.

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

$$\begin{aligned} &M_0 = n, \quad M_i = n u_i, \quad M_4 = \frac{3 n k_B T}{m} + n u^2, \\ &n = M_0, \quad u_i = M_0^{-1} M_i, \quad T = \frac{m}{3 k_B M_0}(M_4 - M_0^{-1} M_i M_i). \end{aligned} \tag{333}$$

The quasiequilibrium distribution function (local Maxwellian) reads:

$$f_0 = n \left(\frac{m}{2\pi k_B T} \right)^{3/2} \exp \left(\frac{-m(v-u)^2}{2k_B T} \right). \tag{334}$$

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

Based on the microscopic dynamics (332), the set of macroscopic variables (333), and the quasiequilibrium (334), 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),

$$\frac{\partial n}{\partial t} = -\frac{\partial n u_i}{\partial r_i}, \tag{335}$$

should be excluded out of the further corrections. This rule should be applied generally: If a part of the chosen macroscopic variables (momentum flux $n\boldsymbol{u}$ 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 $\mu_k = \int v_k \cdot d\boldsymbol{v}$ on both the sides of the equation (332). We have:

$$\frac{\partial n u_k}{\partial t} = -\frac{\partial}{\partial r_k} \frac{n k_B T}{m} - \frac{\partial n u_k u_j}{\partial r_j}.$$

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

$$\begin{aligned} \frac{\partial n}{\partial t} &= -\frac{\partial n u_i}{\partial r_i}, \\ \frac{\partial n u_k}{\partial t} &= -\frac{\partial}{\partial r_k} \frac{n k_B T}{m} - \frac{\partial n u_k u_j}{\partial r_j}, \\ \frac{\partial \varepsilon}{\partial t} &= -\frac{\partial}{\partial r_i} \left(\frac{5 k_B T}{m} n u_i + u^2 n u_i \right). \end{aligned} \tag{336}$$

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:

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

where ϕ_j are the corresponding right hand sides of the Euler equations (336). In order to take derivatives with respect to macroscopic moments $\{M_0, M_i, M_4\}$, we need to rewrite equations (336) in terms of these variables instead of $\{n, u_i, T\}$. After some computation, we obtain:

$$R_{nu_k} = \frac{1}{2} \frac{\partial}{\partial r_j} \left(\frac{n k_B T}{m} \left[\frac{\partial u_k}{\partial r_j} + \frac{\partial u_j}{\partial r_k} - \frac{2}{3} \frac{\partial u_n}{\partial r_n} \delta_{kj} \right] \right). \tag{337}$$

For the energy we obtain:

$$R_\varepsilon = \frac{1}{2}\left(\int v^2 v_i v_j \frac{\partial^2 f_0}{\partial r_i \partial r_j} d\boldsymbol{v} - \sum_j \frac{\partial \phi_\varepsilon}{\partial M_j}\phi_j\right) = \frac{5}{2}\frac{\partial}{\partial r_i}\left(\frac{n k_B^2 T}{m^2}\frac{\partial T}{\partial r_i}\right). \tag{338}$$

Thus, we get the system of the Navier-Stokes equation in the following form:

$$\begin{aligned}
\frac{\partial n}{\partial t} &= -\frac{\partial n u_i}{\partial r_i}, \\
\frac{\partial n u_k}{\partial t} &= -\frac{\partial}{\partial r_k}\frac{n k_B T}{m} - \frac{\partial n u_k u_j}{\partial r_j} + \\
&\quad \frac{\tau}{2}\frac{\partial}{\partial r_j}\frac{n k_B T}{m}\left(\frac{\partial u_k}{\partial r_j} + \frac{\partial u_j}{\partial r_k} - \frac{2}{3}\frac{\partial u_n}{\partial r_n}\delta_{kj}\right), \\
\frac{\partial \varepsilon}{\partial t} &= -\frac{\partial}{\partial r_i}\left(\frac{5 k_B T}{m} n u_i + u^2 n u_i\right) + \tau \frac{5}{2}\frac{\partial}{\partial r_i}\left(\frac{n k_B^2 T}{m^2}\frac{\partial T}{\partial r_i}\right).
\end{aligned} \tag{339}$$

We see that 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 [71] in the first approximation of the Chapman-Enskog method [43] (also, in particular, no bulk viscosity) .

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 will compare qualitatively the result with the Burnett approximation. The comparison concerns stability of the hydrodynamic modes near global equilibrium, which is violated for 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:

$$\begin{aligned}
f &= n_0 \left(\frac{m}{2\pi k_B T_0}\right)^{3/2} \left(\frac{n}{n_0} + \frac{m v_n}{k_B T_0} u_n + \left(\frac{m v^2}{2 k_B T_0} - \frac{3}{2}\right)\frac{T}{T_0}\right) e^{\frac{-m v^2}{2 k_B T_0}} = \\
&= \left\{(M_0 + 2 M_i c_i + \left(\frac{2}{3}M_4 - M_0\right)\left(c^2 - \frac{3}{2}\right)\right\} e^{-c^2},
\end{aligned} \tag{340}$$

where we have introduced dimensionless variables: $c_i = v_i/v_T$, $v_T = \sqrt{2 k_B T_0/m}$ is the thermal velocity, $M_0 = \delta n/n_0$, $M_i = \delta u_i/v_T$, $M_4 = (3/2)(\delta n/n_0 + \delta T/T_0)$. 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:

$$\begin{aligned}
\frac{\partial M_0}{\partial t} &= -\frac{\partial M_i}{\partial r_i}, \\
\frac{\partial M_k}{\partial t} &= -\frac{1}{3}\frac{\partial M_4}{\partial r_k} + \frac{\tau}{4}\frac{\partial}{\partial r_j}\left(\frac{\partial M_k}{\partial r_j} + \frac{\partial M_j}{\partial r_k} - \frac{2}{3}\frac{\partial M_n}{\partial r_n}\delta_{kj}\right), \\
\frac{\partial M_4}{\partial t} &= -\frac{5}{2}\frac{\partial M_i}{\partial r_i} + \tau \frac{5}{2}\frac{\partial^2 M_4}{\partial r_i \partial r_i}.
\end{aligned} \tag{341}$$

Let us first compute the post-Navier-Stokes correction to the velocity equation. In accordance with the equation (327), the first part of this term under linear approximation is:

$$
\begin{aligned}
& \frac{1}{3!}\mu_k\left(\frac{\partial J^*}{\partial f}\frac{\partial J^*}{\partial f}J^*\right)-\frac{1}{3!}\sum_{ij}\left(\frac{\partial \phi_k^*}{\partial M_i}\frac{\partial \phi_i^*}{\partial M_j}\phi_j^*\right)= \\
= & -\frac{1}{6}\int c_k\frac{\partial^3}{\partial r_i\partial r_j\partial r_n}c_ic_jc_n\left\{(M_0+2M_ic_i+\left(\frac{2}{3}M_4-M_0\right)\left(c^2-\frac{3}{2}\right)\right\}e^{-c^2}d^3c \\
+ & \frac{5}{108}\frac{\partial}{\partial r_i}\frac{\partial^2 M_4}{\partial r_s\partial r_s}=\frac{1}{6}\frac{\partial}{\partial r_k}\left(\frac{3}{4}\frac{\partial^2 M_0}{\partial r_s\partial r_s}-\frac{\partial^2 M_4}{\partial r_s\partial r_s}\right)+\frac{5}{108}\frac{\partial}{\partial r_k}\frac{\partial^2 M_4}{\partial r_s\partial r_s} \\
= & \frac{1}{8}\frac{\partial}{\partial r_k}\frac{\partial^2 M_0}{\partial r_s\partial r_s}-\frac{13}{108}\frac{\partial}{\partial r_k}\frac{\partial^2 M_4}{\partial r_s\partial r_s}.
\end{aligned} \tag{342}
$$

The part of equation (327) proportional to the first-order correction is:

$$
-\frac{1}{2}\sum_j\left(\frac{\partial \phi_k^*}{\partial M_j}R_j^{(1)}+\frac{\partial R_k^{(1)}}{\partial M_j}\phi_j^*\right)=\frac{5}{6}\frac{\partial}{\partial r_k}\frac{\partial^2 M_4}{\partial r_s\partial r_s}+\frac{1}{9}\frac{\partial}{\partial r_k}\frac{\partial^2 M_4}{\partial r_s\partial r_s}. \tag{343}
$$

Combining together terms (342), and (343), 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:

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

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:

$$
R_{M_4}^{(2)}=\frac{59}{9}\left(\frac{\partial^2}{\partial r_s\partial r_s}\frac{\partial M_i}{\partial r_i}\right). \tag{344}
$$

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

$$
\begin{aligned}
\frac{\partial M_0}{\partial t} &= -\frac{\partial M_i}{\partial r_i}, \\
\frac{\partial M_k}{\partial t} &= -\frac{1}{3}\frac{\partial M_4}{\partial r_k}+\frac{\tau}{4}\frac{\partial}{\partial r_j}\left(\frac{\partial M_k}{\partial r_j}+\frac{\partial M_j}{\partial r_k}-\frac{2}{3}\frac{\partial M_n}{\partial r_n}\delta_{kj}\right)+ \\
& \quad \tau^2\left\{\frac{1}{8}\frac{\partial}{\partial r_k}\frac{\partial^2 M_0}{\partial r_s\partial r_s}+\frac{89}{108}\frac{\partial}{\partial r_k}\frac{\partial^2 M_4}{\partial r_s\partial r_s}\right\}, \\
\frac{\partial M_4}{\partial t} &= -\frac{5}{2}\frac{\partial M_i}{\partial r_i}+\tau\frac{5}{2}\frac{\partial^2 M_4}{\partial r_i\partial r_i}+\tau^2\frac{59}{9}\left(\frac{\partial^2}{\partial r_s\partial r_s}\frac{\partial M_i}{\partial r_i}\right).
\end{aligned} \tag{345}
$$

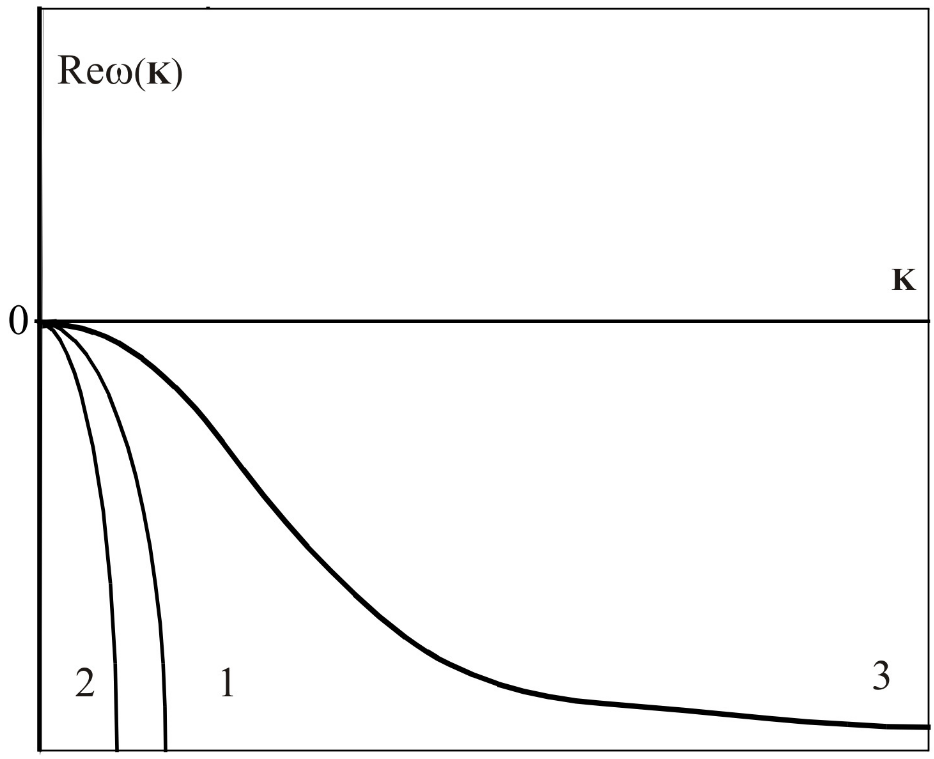


Figure 13: Attenuation rates of various modes of the post-Navier-Stokes equations as functions of the wave vector. Attenuation rate of the twice degenerated shear mode is curve 1. Attenuation rate of the two sound modes is curve 2. Attenuation rate of the diffusion mode is curve 3.

Now we are in a position to investigate the dispersion relation of this system. Substituting $M_i = \tilde{M}_i \exp(\omega t + i(\boldsymbol{k}, \boldsymbol{r}))$ $(i = 0,\, k,\, 4)$ into equation (345), we reduce the problem to finding the spectrum of the matrix:

$$\begin{pmatrix} 0 & -ik_x & -ik_y & -ik_z & 0 \\ -ik_x\frac{k^2}{8} & -\frac{1}{4}k^2 - \frac{1}{12}k_x^2 & -\frac{k_xk_y}{12} & -\frac{k_xk_z}{12} & -ik_x\left(\frac{1}{3}+\frac{89k^2}{108}\right) \\ -ik_y\frac{k^2}{8} & -\frac{k_xk_y}{12} & -\frac{1}{4}k^2 - \frac{1}{12}k_y^2 & -\frac{k_yk_z}{12} & -ik_y\left(\frac{1}{3}+\frac{89k^2}{108}\right) \\ -ik_z\frac{k^2}{8} & -\frac{k_xk_z}{12} & -\frac{k_yk_z}{12} & -\frac{1}{4}k^2 - \frac{1}{12}k_z^2 & -ik_z\left(\frac{1}{3}+\frac{89k^2}{108}\right) \\ 0 & -ik_x\left(\frac{5}{2}+\frac{59k^2}{9}\right) & -ik_y\left(\frac{5}{2}+\frac{59k^2}{9}\right) & -ik_z\left(\frac{5}{2}+\frac{59k^2}{9}\right) & -\frac{5}{2}k^2 \end{pmatrix}$$

This matrix has five eigenvalues. The real parts of these eigenvalues responsible for the decay rate of the corresponding modes are shown in Fig.13 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 becomes positive after some value of the wave vector [45, 21] 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 linearly stable post-Navier-Stokes correction strongly indicates that it might be more suited to establishing models of highly nonequilibrium hydrodynamics.

Example 11: Natural projector for the Mc Kean model

In this section the fluctuation-dissipation formula recently derived by the method of natural projector [15] is illustrated by the explicit computation for McKean's kinetic model [165]. It is demonstrated that the result is identical, on the one hand, to the sum of the Chapman-Enskog expansion, and, on the other hand, to the exact solution of the invariance equation. The equality between all the three results holds up to the crossover from the hydrodynamic to the kinetic domain.

General scheme

Let us consider a microscopic dynamics (34) given by an equation for the distribution function $f(x,t)$ over a configuration space x:

$$\partial_t f = J(f), \tag{346}$$

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

$$\boldsymbol{m}(f(\boldsymbol{M})) = \boldsymbol{M}. \tag{347}$$

The choice of the relevant distribution functions is the point of central importance which we discuss later on but for the time being we need only specification (347).

The starting point has been the following observation [13, 14]: Given a finite time interval τ, it is possible to reconstruct uniquely the macroscopic dynamics from a single condition. For the sake of completeness, we shall formulate this condition here. Let us denote as $\boldsymbol{M}(t)$ the initial condition at the time t to the *yet unknown* equations of the macroscopic motion, and let us take $f(\boldsymbol{M}(t), x)$ for the initial condition of the microscopic equation (346) at the time t. Then the condition for the reconstruction of the macroscopic dynamics reads as follows: For every initial condition $\{\boldsymbol{M}(t), t\}$, solutions to the macroscopic dynamic equations at the time $t+\tau$ are equal to the values of the macroscopic variables on the solution to equation (346) with the initial condition $\{f(\boldsymbol{M}(t), x), t\}$:

$$\boldsymbol{M}(t+\tau) = \boldsymbol{m}\left(T_\tau f(\boldsymbol{M}(t))\right), \tag{348}$$

where T_τ is the formal solution operator of the microscopic equation (346). The right hand side of equation (348) represents an operation on trajectories of the microscopic equation (346), introduced in a particular form by Ehrenfest's [163] (the coarse-graining): The solution at the time $t+\tau$ is replaced by the state on the manifold $f(\boldsymbol{M}, x)$. Notice that the coarse-graining time τ in equation (348) 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 [13, 14]: Seeking the macroscopic equations in the form,

$$\partial_t \boldsymbol{M} = \boldsymbol{R}(\boldsymbol{M}, \tau), \tag{349}$$

we proceed with Taylor expansion of the unknown functions $\boldsymbol{R}$ in terms of powers τ^n, where $n = 0, 1, \ldots$, and require that each approximation, $\boldsymbol{R}^{(n)}$, of the order n, is such that resulting macroscopic solutions satisfy the condition (349) to the order τ^{n+1}. This process of successive approximation is solvable. Thus, the unknown macroscopic equation (349) can be reconstructed to any given accuracy.

Coming back to the problem of choosing the distribution function $f(\boldsymbol{M}, x)$, we recall that many physically relevant cases of the microscopic dynamics (346) are characterized by existence of a concave functional $S(f)$ (the entropy functional; discussions of S can be found in [105, 106, 107]). Traditionally, two cases are distinguished, the conservative [$dS/dt \equiv 0$ due to equation (346)], and the dissipative [$dS/dt \geq 0$ due to equation (346), where equality sign corresponds to the stationary solution]. The approach (348) and (349) is applicable to both these situations. In both of these cases, among the possible sets of distribution functions $f(\boldsymbol{M}, x)$, the distinguished role is played by the well known quasiequilibrium approximations, $f^*(\boldsymbol{M}, x)$, which are maximizers of the functional $S(f)$ for fixed $\boldsymbol{M}$. We recall that, due to convexity of the functional S, if such maximizer exist then it is unique. The special role of the quasiequilibrium approximations is due to the well known fact that they preserve the type of dynamics: If $dS/dt \geq 0$ due to equation (346), then $dS^*/dt \geq 0$ due to the quasiequilibrium dynamics, where $S^*(\boldsymbol{M}) = S(f^*(\boldsymbol{M}))$ is the quasiequilibrium entropy, and where the quasiequilibrium dynamics coincides with the zeroth order in the above construction, $\boldsymbol{R}^{(0)} = \boldsymbol{m}(J(f^*(\boldsymbol{M}))$. We notice it in passing that, since the well known work of Jaynes [108], the usefulness of quasiequilibrium approximations is well understood in various versions of projection operator formalism for the conservative case [77, 109, 110, 111], as well as for the dissipative dynamics [107, 1, 3, 2]. Relatively less studied remains the case of open or externally driven systems, where invariant quasiequilibrium manifolds may become unstable [66]. The use of the quasiequilibrium approximations for the above construction has been stressed in [13, 14, 17]. In particular, the strict increase in the quasiequilibrium entropy has been demonstrated for the first and higher order approximations[14]. Examples have been provided [14], focusing on the conservative case, and demonstrating that several well known dissipative macroscopic equations, such as the Navier-Stokes equation and the diffusion equation for the one-body distribution function, are derived as the lowest order approximations of this construction.

The advantage of the approach [13, 14] 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. Going away from the limitations imposed by the finite coarse graining time [13, 14] can be recognized as the major problem of a consistent formulation of the nonequilibrium statistical thermodynamics. Intuitively, this requires taking the limit $\tau \to \infty$, allowing for all the relevant correlations to be developed by the microscopic dynamics, rather than to be cut off at the finite τ. Indeed, in the case of the dissipative dynamics, in particular, for the linearized Boltzmann equation, one typically expects an initial layer [69] which is completely cut off in the short-memory approximation, whereas those effects can be made small by taking τ large enough. A way of doing this in the general nonlinear setting for entropy-conserving systems still requires further work at the time of this writing.

Natural projector for linear systems

However, there is one important exception when the '$\tau \to \infty$ problem' is readily solved [14, 15]. This is the case where equation (346) is linear,

$$\partial_t f = Lf, \tag{350}$$

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

$$\partial_t \boldsymbol{M} = \boldsymbol{R}\boldsymbol{M}, \tag{351}$$

where the linear operator $\boldsymbol{R}$ is determined by the coarse-graining condition (348) in the limit $\tau \to \infty$:

$$\boldsymbol{R} = \lim_{\tau\to\infty} \frac{1}{\tau} \ln\left[\boldsymbol{m}\left(e^{\tau L} f^{\mathrm{eq}} \boldsymbol{m}^{\dagger}\right)\right]. \tag{352}$$

Formula (352) has been already briefly mentioned in [14], and its relation to the Green-Kubo formula has been demonstrated in [15]. In our case, the Green-Kubo formula reads:

$$\boldsymbol{R}_{\mathrm{GK}} = \int_0^{\infty} \langle \dot{\boldsymbol{m}}(0)\dot{\boldsymbol{m}}(t)\rangle, \tag{353}$$

where angular brackets denote equilibrium averaging, and where $\dot{\boldsymbol{m}} = L^{\dagger}\boldsymbol{m}$. The difference between the formulae (352) and (353) stems from the fact that condition (348) does not use an a priori hypothesis of the separation of the macroscopic and the microscopic time scales. For the classical N-particle dynamics, equation (352) is a complicated expression, involving a logarithm of non-commuting operators. It is therefore very desirable to gain its understanding in simple model situations.

Explicit example of the the fluctuation-dissipation formula

In this section we want to give explicit example of the formula (352). 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 [165] 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 (352) is underpinned by the entropy growth in both the rapid and the slow parts of the dynamics. This physical idea underlies generically the extraction of the slow (hydrodynamic) component of motion through the concept of normal solutions to kinetic equations, as pioneered by Hilbert [44], and has been discussed by many authors, e. g. . [69, 112, 113]. Case studies for linear kinetic equation help clarifying the concept of this extraction [114, 115, 165].

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 (352). Specifically, we compare the result with the exact sum of the Chapman-Enskog expansion [43], and with the exact solution in the framework of the method of invariant manifold [1, 3, 2]. 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 $\boldsymbol{f}(r,t) = (f_+(r,t), f_-(r,t))^\dagger$:

$$\begin{aligned} \partial_t f_+ &= -\partial_r f_+ + \epsilon^{-1}\left(\frac{f_+ + f_-}{2} - f_+\right), \\ \partial_t f_- &= \partial_r f_- + \epsilon^{-1}\left(\frac{f_+ + f_-}{2} - f_-\right). \end{aligned} \tag{354}$$

Equation (354) 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, $(\boldsymbol{x}, \boldsymbol{y})$, for the standard scalar product of the two-dimensional vectors, we introduce the fields, $n(r,t) = (\boldsymbol{n}, \boldsymbol{f})$ [the local particle's density, where $\boldsymbol{n} = (1,1)$], and $j(r,t) = (\boldsymbol{j}, \boldsymbol{f})$ [the local momentum density, where $\boldsymbol{j} = (1,-1)$]. Equation (354) can be equivalently written in terms of the moments,

$$\begin{aligned} \partial_t n &= -\partial_r j, \\ \partial_t j &= -\partial_r n - \epsilon^{-1} j. \end{aligned} \tag{355}$$

The local equilibrium,

$$\boldsymbol{f}^*(n) = \frac{n}{2}\boldsymbol{n}, \tag{356}$$

is the conditional maximum of the entropy,

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

under the constraint which fixes the density, $(\boldsymbol{n}, \boldsymbol{f}^*) = n$. The quasiequilibrium manifold (356) is linear in our example, as well as is the kinetic equation.

The problem of reducing the description for the model (354) 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 (352), and other methods, extend this result.

Because of the linearity of the equation (354), and of the local equilibrium, it is natural to use the Fourier transform, $h_k = \int \exp(ikr)h(r)dr$. Equation (354) is then written,

$$\partial_t \boldsymbol{f}_k = \boldsymbol{L}_k \boldsymbol{f}_k, \tag{357}$$

where

$$\boldsymbol{L}_k = \begin{pmatrix} -ik - \frac{1}{2\epsilon} & \frac{1}{2\epsilon} \\ \frac{1}{2\epsilon} & ik - \frac{1}{2\epsilon} \end{pmatrix}. \tag{358}$$

Derivation of the formula (352) in our example goes as follows: We seek the macroscopic dynamics of the form,

$$\partial_t n_k = R_k n_k, \tag{359}$$

where the function R_k is yet unknown. In the left-hand side of equation (348) we have:

$$n_k(t+\tau) = e^{\tau R_k} n_k(t). \tag{360}$$

In the right-hand side of equation (348) we have:

$$\left(\boldsymbol{n}, e^{\tau \boldsymbol{L}_k} \boldsymbol{f}^*(n_k(t))\right) = \frac{1}{2}\left(\boldsymbol{n}, e^{\tau \boldsymbol{L}_k} \boldsymbol{n}\right) n_k(t). \tag{361}$$

After equating the expressions (360) and (361), we require that the resulting equality holds in the limit $\tau \to \infty$ independently of the initial data $n_k(t)$. Thus, we arrive at the formula (352):

$$R_k = \lim_{\tau\to\infty} \frac{1}{\tau} \ln\left[\left(\boldsymbol{n}, e^{\tau \boldsymbol{L}_k} \boldsymbol{n}\right)\right]. \tag{362}$$

Equation (362) defines the macroscopic dynamics (359) within the present approach. Explicit evaluation of the expression (362) is straightforward in the present model. Indeed, operator $\boldsymbol{L}_k$ has two eigenvalues, $\Lambda_k^{\pm}$, where

$$\Lambda_k^{\pm} = -\frac{1}{2\epsilon} \pm \sqrt{\frac{1}{4\epsilon^2} - k^2} \tag{363}$$

Let us denote as $\boldsymbol{e}_k^{\pm}$ two (arbitrary) eigenvectors of the matrix $\boldsymbol{L}_k$, corresponding to the eigenvalues $\Lambda_k^{\pm}$. Vector $\boldsymbol{n}$ has a representation, $\boldsymbol{n} = \alpha_k^+ \boldsymbol{e}_k^+ + \alpha_k^- \boldsymbol{e}_k^-$, where $\alpha_k^{\pm}$ are complex-valued coefficients. With this, we obtain in equation (362),

$$R_k = \lim_{\tau\to\infty} \frac{1}{\tau} \ln\left[\alpha_k^+ (\boldsymbol{n}, \boldsymbol{e}_k^+) e^{\tau \Lambda_k^+} + \alpha_k^- (\boldsymbol{n}, \boldsymbol{e}_k^-) e^{\tau \Lambda_k^-}\right]. \tag{364}$$

For $k \le k_{\rm c}$, where $k_{\rm c}^2 = 4\epsilon$, we have $\Lambda_k^+ > \Lambda_k^-$. Therefore,

$$R_k = \Lambda_k^+, \text{ for } k < k_{\rm c}. \tag{365}$$

As was expected, formula (352) in our case results in the exact hydrodynamic branch of the spectrum of the kinetic equation (354). The standard diffusion approximation is recovered from equation (365) as the first non-vanishing approximation in terms of the $(k/k_{\rm c})^2$.

At $k = k_{\rm c}$, the crossover from the extended hydrodynamic to the kinetic regime takes place, and $\mathrm{Re}\Lambda_k^+ = \mathrm{Re}\Lambda_k^-$. However, we may still extend the function R_k for $k \ge k_{\rm c}$ on the basis of the formula (362):

$$R_k = \mathrm{Re}\ \Lambda_k^+ \text{ for } k \ge k_{\rm c} \tag{366}$$

Notice that the function R_k as given by equations (365) and (366) is continuous but non-analytic at the crossover.

Comparison with the Chapman-Enskog method and solution of invariance equation

Let us now compare this result with the Chapman-Enskog method. Since the exact Chapman-Enskog solution for the systems like equation (356) has been recently discussed in detail elsewhere [20, 21, 117, 118, 119, 120], we shall be brief here. Following the Chapman-Enskog method, we seek the momentum variable j in terms of an expansion,

$$j^{\rm CE} = \sum_{n=0}^{\infty} \epsilon^{n+1} j^{(n)} \tag{367}$$

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

$$j^{(n)} = -\sum_{m=0}^{n-1} \partial_t^{(m)} j^{(n-1-m)}, \tag{368}$$

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

$$\partial_t^{(m)} n = -\partial_r j^{(m)}. \tag{369}$$

The recurrence equations (367), (368), and (369), become well defined as soon as the aforementioned zero-order approximation $j^{(0)}$ is specified,

$$j^{(0)} = -\partial_r n. \tag{370}$$

From equations (368), (369), and (370), it follows that the Chapman-Enskog coefficients $j^{(n)}$ have the following structure:

$$j^{(n)} = b_n \partial_r^{2n+1} n, \tag{371}$$

where coefficients b_n are found from the recurrence equation,

$$b_n = \sum_{m=0}^{n-1} b_{n-1-m} b_m,\ b_0 = -1. \tag{372}$$

Notice that coefficients (372) are real-valued, by the sense of the Chapman-Enskog procedure. The Fourier image of the Chapman-Enskog solution for the momentum variable has the form,

$$j_k^{\mathrm{CE}} = ikB_k^{\mathrm{CE}} n_k, \tag{373}$$

where

$$B_k^{\mathrm{CE}} = \sum_{n=0}^{\infty} b_n (-\epsilon k^2)^n. \tag{374}$$

Equation for the function B (374) is easily found upon multiplying equation (372) by $(-k^2)^n$, and summing in n from zero to infinity:

$$\epsilon k^2 B_k^2 + B_k + 1 = 0. \tag{375}$$

Solution to the latter equation which respects condition (370), and which constitutes the exact Chapman-Enskog solution (374) is:

$$B_k^{\mathrm{CE}} = \begin{cases} k^{-2}\Lambda_k^+, & k < k_{\mathrm{c}} \\ \text{none}, & k \geq k_{\mathrm{c}} \end{cases} \tag{376}$$

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

$$\partial_t n_k = -ikj_k^{\mathrm{CE}} = R_k^{\mathrm{CE}} n_k, \tag{377}$$

where

$$R_k^{\mathrm{CE}} = \begin{cases} \Lambda_k^+, & k < k_{\mathrm{c}} \\ \text{none}, & k \geq k_{\mathrm{c}} \end{cases} \tag{378}$$

The Chapman-Enskog solution does not extends beyond the crossover at k_{c}. This happens because the full Chapman-Enskog solution appears as a continuation the diffusion approximation, whereas formula (362) is not based on such an extension a priori.

Finally, let us discuss briefly the comparison with the solution within the method of invariant manifold [1, 3, 2]. Specifically, the momentum variable $j_k^{\mathrm{inv}} = ikB_k^{\mathrm{inv}} n_k$ is required to be invariant of both the microscopic and the macroscopic dynamics, that is, the time derivative of j_k^{inv} due to the macroscopic subsystem,

$$\frac{\partial j_k^{\mathrm{inv}}}{\partial n_k} \partial_t n_k = ikB_k^{\mathrm{inv}}(-ik)[ikB_k^{\mathrm{inv}}], \tag{379}$$

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

$$\partial_t j_k^{\rm inv} = -ikn_k - \epsilon^{-1} ikB_k^{\rm inv} n_k, \tag{380}$$

and that the equality between the equations (379) and (380) should hold independently of the specific value of the macroscopic variable n_k. This amounts to a condition for the unknown function $B_k^{\rm inv}$, which is essentially the same as equation (375), 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 (378).

In conclusion, in this Example we have given the explicit illustration for the formula (352). The example considered above demonstrates that the formula (352) 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 (352) demonstrates a non-analytic extension. The example considered adds to the confidence of the correctness of the approach suggested in [13, 14, 15, 16].

11 Slow invariant manifold for a closed system has been found. What next?

Suppose that the slow invariant manifold is found for a dissipative system. **What for have we constructed it?**

First of all, for solving the Cauchy problem, to separate motions. This means that the Cauchy problem is divided in the following two subproblems:

- Reconstruct the "fast" motion from the initial conditions to the slow invariant manifold (*the initial layer problem*).
- Solve the Cauchy problem for the "slow" motions on the manifold.

Thus, solving the Cauchy problem becomes easier (and in some complicated cases it just becomes possible).

Let us stress here that for any sufficiently reliable solution of the Cauchy problem one must solve not only the reduced Cauchy problem for slow motion, but the initial layer problem for fast motions as well.

In solving the latter problem it was found to be surprisingly effective using piece-wise linear approximations with smoothing or even without it [11, 12]. This method was used for the Boltzman equation, for chemical kinetics equations, and for the Pauli equation.

There exists a different way to model the initial layer in the kinetics problems: it is an introduction of model equations. For example, the BGK-equation is the simplest model equation for the Boltzman equation. It describes relaxation into a small neighborhood of the local Maxwell distribution. There are many types and hierarchies of the model equations [71, 69, 72, 7, 166]. The principal idea of any model equation is to substitute of the fast processes by a simple relaxation term. As a rule, it has a form $dx/dt = \ldots - (x - x_{sl}(x))/\tau$, where $x_{sl}(x)$ is a point of the approximate slow manifold. Such form is used in the BGK-equation, or in the quasi-equilibrium models [72]. Also it can have a gradient form, like in the gradient models [166, 7]. Such simplicity not only allows to study fast motions separately but also to zoom in the details of the interaction of fast and slow motions in the vicinity of the slow manifold.

What concerns solving the Cauchy problem for the "slow" motions, this is the basic problem of the hydrodynamics, gas dynamics (if the initial systems describes kinetics of gas or fluid), etc. Here invariant manifold methods provide equations for further analysis. However, even a preliminary consideration of the practical aspects of these studies shows definite inconsistency. Obtained equations are exploited not only for "closed" systems. The initial equations (34) describe a dissipative system that approaches the equilibrium. The equations of slow motion describe dissipative system too. Then these equations are supplied with *different forces and flows* and after that describe systems with more or less complicated dynamics.

Because of this, there are other answers for our question *what for have we constructed the invariant manifold*:

First of all, to construct models of open system dynamics in the neighborhood of the manifold.

Different approaches for this modeling are described in the following subsections.

11.1 Slow dynamics for open systems. Zero-order approximation and the thermodynamic projector

Let the initial dissipative system (34) be "spoiled" by additional term ("external field" $J_{ex}(x,t)$):

$$\frac{dx}{dt} = J(x) + J_{ex}(x,t), x \subset U \tag{381}$$

For this new system the entropy does not increase everywhere. In the new system (381) different dynamic effects are possible: non-uniqueness of stationary states, auto-oscillations, etc. The "inertial manifold" effect is well-known: solutions of (381) approach some comparably low-dimensional manifold on which all the non-trivial dynamics takes place [181, 182, 183]. This "inertial manifold" can have finite dimension even for infinite-dimensional systems, for example, for the "reaction+diffusion" systems [185].

In the theory of nonlinear control of partial differential equation systems a strategy based on approximate inertial manifolds [186] is proposed to facilitate the construction of finite-dimensional ODE systems, whose solutions can be arbitrarily close to the ones of the infinite dimensional system [187].

It is natural to expect that the inertial manifold of the system (381) is located somewhere close to the slow manifold of the initial dissipative system (34). This hypothesis has the following basis. Suppose that the vector field $J_{ex}(x,t)$ is sufficiently small. Let's introduce, for example, a small parameter $\varepsilon > 0$ and consider $\varepsilon J_{ex}(x,t)$ instead of $J_{ex}(x,t)$. Let's suppose that for the system (34) separation of motions into "slow" and "fast" takes place. In this case, there exists such interval $\varepsilon > 0$ that $\varepsilon J_{ex}(x,t)$ is comparable to J only in a small neighborhood of the given slow motion manifold for the system (34). Outside this neighborhood, $\varepsilon J_{ex}(x,t)$ is negligibly small in comparison with J and only negligibly influences the motion (for correctness of this statement it is important that the system (34) is dissipative and every solution comes in finite time to a small neighborhood of the given slow manifold).

Exactly such conception of the system (381) dynamics allows to exploit slow invariant manifolds constructed for the dissipative system (34) as an ansatz and zero-order approximation in construction of the inertial manifold of the open system (381). In the zero-order approximation, the right part of the equation (381) is simply projected onto the tangent space of the slow manifold.

The choice of the projector is determined by the motion separation which was described above: fast motion is taken from the dissipative system (34). A projector which is suitable for all dissipative systems with given entropy function is unique. It is constructed in the following way (detailed consideration of this is given above in the sections "Entropic projector without a priori parametrization"). Let a point $x \in U$ be defined and some vector space T, on which one needs to construct a projection (T is the tangent space to the slow manifold in the point x). We introduce the entropic scalar product $\langle | \rangle_x$:

$$\langle a \mid b \rangle_x = -(a, D_x^2 S(b)). \tag{382}$$

Let us consider T_0 that is a subspace of T and which is annulled by the differential S in the point x.

$$T_0 = \{a \in T | D_x S(a) = 0\} \tag{383}$$

Suppose[11] that $T_0 \neq T$. Let $e_g \in T$, $e_g \perp T_0$ with respect to the entropic scalar product $\langle | \rangle_x$, and $D_x S(e_g) = 1$. These conditions define vector e_g uniquely.

The projector onto T is defined by the formula

$$P(J) = P_0(J) + e_g D_x S(J) \tag{384}$$

where P_0 is the orthogonal projector with respect to the entropic scalar product $\langle | \rangle_x$. For example, if T a finite-dimensional space, then the projector (384) is constructed in the following way. Let $e_1, .., e_n$ be a basis in T, and for definiteness, $D_x S(e_1) \neq 0$.

1) Let's construct a system of vectors

$$b_i = e_{i+1} - \lambda_i e_1, (i = 1, .., n-1), \tag{385}$$

where $\lambda_i = D_x S(e_{i+1})/D_x S(e_1)$, and hence $D_x S(b_i) = 0$. Thus, $\{b_i\}_1^{n-1}$ is a basis in T_0.

2) Let's orthogonalize $\{b_i\}_1^{n-1}$ with respect to the entropic scalar product $\langle | \rangle_x$ (34). We've got an orthonormal with respect to $\langle | \rangle_x$ basis $\{g_i\}_1^{n-1}$ in T_0.

3) We find $e_g \in T$ from the conditions:

$$\langle e_g \mid g_i \rangle_x = 0, (i = 1, .., n-1), D_x S(e_g) = 1. \tag{386}$$

and, finally we get

$$P(J) = \sum_{i=1}^{n-1} g_i \langle g_i \mid J \rangle_x + e_g D_x S(J) \tag{387}$$

If $D_x S(T) = 0$, then the projector P is simply the orthogonal projector with respect to the $\langle | \rangle_x$ scalar product. This is possible if x is the global maximum of entropy point (equilibrium). Then

$$P(J) = \sum_{i=1}^{n} g_i \langle g_i | J \rangle_x, \langle g_i | g_j \rangle = \delta_{ij}. \tag{388}$$

[11] If $T_0 = T$, then the thermodynamic projector is the orthogonal projector on T with respect to the entropic scalar product $\langle | \rangle_x$.

Remark. In applications, the equation (34) often has additional linear balance constraints. Solving the closed dissipative system (34) we simply choose balance values and consider the dynamics of (34) on the corresponding affine balance subspace.

For the driven system (381) the balances can be violated. Because of this, for the open system (381) the natural balance subspace includes the balance subspace of (34) with different balance values. For every set of balance values there is a corresponding equilibrium. Slow invariant manifold of the dissipative systems that is applied to the description of the driven systems (381) is usually the union of slow manifolds for all possible balance values. The equilibrium of the dissipative closed system corresponds to the entropy maximum *given the balance values fixed.* In the unified phase space of the driven system (381) the entropy gradient in the equilibrium points of the system (34) does not necessarily equal to zero.

In particular, for the Boltzmann entropy in the local finite-dimensional case one gets

$$
\begin{aligned}
&S = -\int f(v)(ln(f(v)) - 1)dv, \\
&D_f S(J) = -\int J(v) \ln f(v) dv, \\
&\langle \psi \mid \varphi \rangle_f = -(\psi, D_f^2 S(\varphi)) = \int \frac{\psi(v)\varphi(v)}{f(v)} dv \\
&P(J) = \sum_{i=1}^{n-1} g_i(v) \int \frac{g_i(v)J(v)}{f(v)} dv - e_g(v) \int J(v) \ln f(v) dv,
\end{aligned}
\tag{389}
$$

where $g_i(v)$ and $e_g(v)$ are constructed accordingly to the scheme described above,

$$\int \frac{g_i(v)g_j(v)}{f(v)} dv = \delta_{ij}, \tag{390}$$

$$\int g_i(v) \ln f(v) dv = 0, \tag{391}$$

$$\int g_i(v) e_g(v) dv = 0, \tag{392}$$

$$\int e_g(v) \ln f(v) dv = 1. \tag{393}$$

If for all $g \in T$ we have $\int g(v) \ln f(v) dv = 0$, then the projector P is defined as the orthogonal projector with respect to the $\langle | \rangle_f$ scalar product.

11.2 Slow dynamics of the open system. First-order approximation

Thermodynamic projector (384) defines the "slow and fast motions" duality: if T is the tangent space of the slow motion manifold then $T = ImP$, and $\ker P$ is the fast motions plane. Let us denote by P_x the projector for a point x of a given slow manifold.

The vector field $J_{ex}(x,t)$ can be decomposed in two components:

$$J_{ex}(x,t) = P_x J_{ex}(x,t) + (1 - P_x) J_{ex}(x,t). \tag{394}$$

Let's denote $J_{ex\,s} = P_x J_{ex}$, $J_{ex\,f} = (1 - P_x) J_{ex}$. The slow component $J_{ex\,s}$ gives a correction to the motion along the slow manifold. This is a zero-order approximation. The "fast" component shifts the slow manifold in the fast motions plane. This shift changes $P_x J_{ex}$ correspondingly. Consideration of this effect gives a first-order approximation. To find it, let us rewrite the invariance equation taking J_{ex} into account:

$$\begin{cases} (1 - P_x)(J(x + \delta x) + \varepsilon J_{ex}(x,t)) = 0 \\ P_x \delta x = 0 \end{cases} \tag{395}$$

The first iteration of the Newtonian method subject to incomplete linearization gives:

$$\begin{cases} (1 - P_x)(D_x J(\delta x) + \varepsilon J_{ex}(x,t)) = 0 \\ P_x \delta x = 0. \end{cases} \tag{396}$$

$$(1 - P_x) D_x J (1 - P_x) J(\delta x) = -\varepsilon J_{ex}(x,t). \tag{397}$$

We've got a linear equation in the space $\ker P$. The operator $(1 - P) D_x J (1 - P)$ is defined in this space.

Utilization of self-adjoint linearization instead of traditional linearization (i.e., of $D_x J$ operator) (see "Decomposition of motions, non-uniqueness of selection..." section) considerably simplifies solving and studying the equation (397). It is necessary to take into account here that the projector P is a sum of the orthogonal projector with respect to the $\langle | \rangle_x$ scalar product and a projector of rank 1.

Suppose that the first-order approximation equation (397) has been solved and the following dependence has been found:

$$\delta_1 x(x, \varepsilon J_{ex\,f}) = -[(1 - P_x) D_x J (1 - P_x)]^{-1} \varepsilon J_{ex\,f}, \tag{398}$$

where $D_x J$ is either the differential of J or symmetrized differential of J (262) depending on the context.

Let x be a point on the initial slow manifold. In the point $x + \delta x(x, \varepsilon J_{ex\,f})$ the right-hand side of the equation (381) in the first-order approximation is given by

$$J(x) + \varepsilon J_{ex}(x,t) + D_x J(\delta x(x, \varepsilon J_{ex\,f})). \tag{399}$$

In concordance with the first-order approximation of (399) the motion of a point projection onto the manifold is given by the following equation

$$\frac{dx}{dt} = P_x(J(x) + \varepsilon J_{ex}(x,t) + D_x J(\delta x(x, \varepsilon J_{ex\,f}(x,t)))). \tag{400}$$

In the equation (400) the field $J(x)$ enters in the combination $P_x J(x)$. For the invariant slow manifold $P_x J(x) = J(x)$, but actually we always deal with an approximately invariant manifolds, hence, it is necessarily to use $P_x J$ instead of J in (400).

Remark. The "projection of a point onto the manifold" notion needs to be defined. For every point x of the slow invariant manifold M there are defined both the thermodynamic projector P_x (384) and the fast motions plane $\ker P_x$. Let us define a projector Π of some neighborhood of M onto M in the following way:

$$\Pi(z) = x, \quad \text{if } P_x(z - x) = 0. \tag{401}$$

Qualitatively it means that z, after all fast motions took place, comes into a small neighborhood of x. The operation (384) is defined uniquely in some small neighborhood of the manifold M.

Derivation of slow motions equations requires not only assumption that εJ_{ex} is small but it must be slow as well: $\frac{d}{dt}(\varepsilon J_{ex})$ must be small too.

One can get the next approximations for slow motions of the system (381), taking into account the time derivatives of J_{ex}. This is an alternative to the usage of the projection operators methods [109]. This is considered in more details in the following Example 12 for a particularly interesting driven system of dilute polymeric solutions. A short scheme description is given in the following subsection.

11.3 Beyond the first-order approximation: higher dynamical corrections, stability loss and invariant manifold explosion

Let us pose formally the invariance problem for the driven system (381) in the neighborhood of the slow manifold M of the initial system.

Let for a given neighborhood of M an operator Π (401) be defined. One needs to define the function $\delta x(x,...) = \delta x(x, J_{ex}, \dot{J}_{ex}, \ddot{J}_{ex}, ...)$, $x \in M$, with the following properties:

$$\begin{aligned}
&P_x(\delta x(x,...)) = 0, \\
&J(x + \delta x(x,...)) + J_{ex}(x + \delta x(x,...), t) = \\
&\dot{x}_{sl} + D_x \delta x(x,...) \dot{x}_{sl} + \sum_{n=0}^{\infty} D_{J_{ex}^{(n)}} \delta x(x,...) J_{ex}^{(n+1)},
\end{aligned} \tag{402}$$

where $\dot{x}_{sl} = P_x(J(x + \delta x(x,...)) + J_{ex}(x + \delta x(x,...), t))$, $J_{ex}^{(n)} = \frac{d^n J_{ex}}{dt^n}$. One can rewrite the equations (402) in the following form:

$$\begin{aligned}
&(1 - P_x - D_x \delta x(x,...))(J(x + \delta x(x,...)) + J_{ex}(x + \delta x(x,...), t)) = \\
&\sum_{n=0}^{\infty} D_{J_{ex}^{(n)}} \delta x(x,...) J_{ex}^{(n+1)}.
\end{aligned} \tag{403}$$

For solving the equation (403) one can use an iterative method, taking into account smallness consideration. The series in the right hand part of the equation (403) can be rewritten as

$$\sum_{n=0}^{k-1} \varepsilon^{n+1} D_{J_{ex}^{(n)}} \delta x(x, ...) J_{ex}^{(n+1)} \tag{404}$$

at the kth iteration, considering the series members only of order less than k. The first iteration equation has been solved in the previous subsection. For the second iteration one gets the following equation:

$$\begin{aligned}
&(1 - P_x - D_x \delta_1 x(x, J_{ex}))(J(x + \delta_1 x(x, J_{ex})) + \\
&D_z J(z)|_{z=x+\delta_1 x(x,J_{ex})} \cdot (\delta_2 x - \delta_1 x(x, J_{ex})) + J_{ex}) = \\
&D_{J_{ex}} \delta_1 x(x, J_{ex}) \dot{J}_{ex}.
\end{aligned} \tag{405}$$

This is a linear equation with respect to $\delta_2 x$. The solution $\delta_2 x(x, J_{ex}, \dot{J}_{ex})$ depends linearly on $\dot{J}_{ex}$, but non-linearly on J_{ex}. Let us remind that the first iteration equation solution depends linearly on J_{ex}.

In all these iteration equations the field J_{ex} and it's derivatives are included in the formulas as if they would be functions of time t only. Indeed, for any solution $x(t)$ of the equations (381) $J_{ex}(x, t)$ can be substituted for $J_{ex}(x(t), t)$. The function $x(t)$ will be a solution of the system (381) in which $J_{ex}(x, t)$ is substituted for $J_{ex}(t)$ in this way.

However, in order to obtain the macroscopic equations (400) one must return to $J_{ex}(x, t)$. For the first iteration such return is quite simple as one can see from (399). There $J_{ex}(x, t)$ is calculated in points of the initial slow manifold. For general case, suppose that $\delta x = \delta x(x, J_{ex}, \dot{J}_{ex}, .., J_{ex}^{(k)})$ has been found. The motion equations for x (400) have the following form:

$$\frac{dx}{dt} = P_x(J(x + \delta x) + J_{ex}(x + \delta x, t)). \tag{406}$$

In these equations the shift δx must be a function of x and t (or a function of x, t, α, where α are external fields, see example 12, but from the point of view of this consideration dependence on the external fields is not essential). One calculates the shift $\delta x(x, t)$ using the following equation:

$$J_{ex} = J_{ex}(x + \delta x(x, J_{ex}, \dot{J}_{ex}, ..., J_{ex}^{(k)}), t). \tag{407}$$

It can be solved, for example, by the iterative method, taking $J_{ex0} = J_{ex}(x, t)$:

$$J_{ex(n+1)} = J_{ex}(x + \delta x(x, J_{ex(n)}, \dot{J}_{ex(n)}, ..., J_{ex(n)}^{(k)}), t). \tag{408}$$

We hope that using J_{ex} in the equations (407) and (408) both as a variable and as a symbol of unknown function $J_{ex}(x, t)$ will not lead to misunderstanding.

In all the constructions introduced above it was supposed that δx is sufficiently small and the driven system (381) will not deviate too far from the slow invariant manifold of the initial system. However, a stability loss is possible: solutions of the equation (381) can deviate arbitrarily far given some perturbations level. The invariant manifold can loose it's stability. Qualitatively this effect of *invariant manifold explosion* can be represented as follows.

Suppose that J_{ex} includes the parameter ε: one has εJ_{ex} in the equation (381). When ε is small, system motions are located in a small neighborhood of the initial manifold. This neighborhood grows monotonously and continuously with increase of ε, but after some ε_0 a sudden change happens ("explosion") and the neighborhood, in which the motion takes place, is essentially wider at $\varepsilon > \varepsilon_0$ than at $\varepsilon < \varepsilon_0$. The stability loss is not necessarily connected with the invariance loss. In the example 13 it is shown how the invariant manifold (which is at the same time the quasi-equlibrium manifold in the example) can loose it's stability. This "explosion" of the invariant manifold leads to essential physical consequences (see example 13).

11.4 Lyapunov norms, finite-dimensional asymptotic and volume contraction

In a general case, it is impossible to prove the existence of a global Lyapunov function on the base of local data. We can only verify or falsify the hypothesis about a given function, is it a global Lyapunov function, or is it not. On the other hand, there exists a more strictly stability property which can be verified or falsified (in principle) on the base of local data analysis. This is a Lyapunov norm existence.

A norm $\| \bullet \|$ is the Lyapunov norm for the system (381), if for any two solutions $x^{(1)}(t)$, $x^{(2)}(t)$, $t \geq 0$ the function $\|x^{(1)}(t) - x^{(2)}(t)\|$ is non increasing in time.

Linear operator A is dissipative with respect to a norm $\| \bullet \|$, if $\exp(At)$ $(t \geq 0)$ is a semigroup of contractions: $\| \exp(At)x\| \leq \|x\|$ for any x and $t \geq 0$. The family of linear operators $\{A_\alpha\}_{\alpha \in K}$ is simultaneously dissipative, if all operators A_α are dissipative with respect to some norm $\| \bullet \|$ (it should be stressed that there exists one norm for all A_α, $\alpha \in K$). The mathematical theory of simultaneously dissipative operators for finite-dimensional spaces was developed in [167, 168, 169, 170, 171].

Let the system (381) be defined in a convex set $U \subset E$, and A_x be a Jacoby operator in the point x: $A_x = D_x(J(x) + J_{ex}(x))$. This system has a Lyapunov norm, if the family of operators $\{A_x\}_{x \in U}$ is simultaneously dissipative. If one can choose such $\varepsilon > 0$ that for all A_x, $t > 0$, any vector z, and this Lyapunov norm $\| \exp(A_x t)z\| \leq \exp(-\varepsilon t)\|z\|$, then for any two solutions $x^{(1)}(t)$, $x^{(2)}(t)$, $t \geq 0$ of equations (381) $\|x^{(1)}(t) - x^{(2)}(t)\| \leq \exp(-\varepsilon t)\|x^{(1)}(0) - x^{(2)}(0)\|$.

The simplest class of nonlinear kinetic (open) systems with Lyapunov norms was described in the paper [172]. These are reaction systems without interactions of various substances. The stoihiometric equation of each elementary reaction has a form

$$\alpha_{ri} A_i \to \sum_j \beta_{rj} A_j, \tag{409}$$

where r is an reaction number, α_{ri}, β_{rj} are nonnegative stoihiometric numbers (usually they are integer), A_i are symbols of substances.

In the right hand part of equation (409) there is one initial reagent, though $\alpha_{ri} > 1$ is possible (there may be several copies of A_i, for example $3A \to 2B + C$).

Kinetic equations for reaction system (409) have a Lyapunov norm [172]. This is l^1 norm with weights: $\|x\| = \sum_i w_i |x_i|$, $w_i > 0$. There exists no quadratic Lyapunov norm for reaction systems without interaction of various substances.

Existence of Lyapunov norm is very strong restriction on nonlinear system, and such systems are not wide spread in applications. But if we go from distance contraction to contraction of k-dimensional volumes ($k = 2, 3, \ldots$) [178], the situation changes. There exist many kinetic systems with monotonous contraction of k-dimensional volumes for sufficiently big k (see, for example, [181, 182, 183, 185]). Let $x(t)$, $t \geq 0$ be a solution of equation (381). Let us write a first approximation equations for small deviations from $x(t)$:

$$\frac{d\Delta x}{dt} = A_{x(t)} \Delta x. \tag{410}$$

This is linear system with coefficients depending on t. Let us study how the system (410) changes k-dimensional volumes. A k-dimensional parallelepiped with edges $x^{(1)}, x^{(2)}, \ldots x^{(k)}$ is an element of the kth exterior power:

$$x^{(1)} \wedge x^{(2)} \wedge \ldots \wedge x^{(k)} \in \underbrace{E \wedge E \wedge \ldots \wedge E}_{k}$$

(this is an antisymmetric tensor). A norm in the kth exterior power of the space E is a measure of k-dimensional volumes (one of the possible measures). Dynamics of parallelepipeds induced by the system (410) can be described by equations

$$\begin{aligned}
&\frac{d}{dt}(\Delta x^{(1)} \wedge \Delta x^{(2)} \wedge \ldots \wedge \Delta x^{(k)}) = \\
&(A_{x(t)} \Delta x^{(1)}) \wedge \Delta x^{(2)} \wedge \ldots \wedge \Delta x^{(k)} + \Delta x^{(1)} \wedge (A_{x(t)} \Delta x^{(2)}) \wedge \ldots \wedge \Delta x^{(k)} + \ldots \\
&+ \Delta x^{(1)} \wedge \Delta x^{(2)} \wedge \ldots \wedge (A_{x(t)} \Delta x^{(k)}) = A_{x(t)}^{D\wedge k}(\Delta x^{(1)} \wedge \Delta x^{(2)} \wedge \ldots \wedge \Delta x^{(k)}).
\end{aligned} \tag{411}$$

Here $A_{x(t)}^{D\wedge k}$ are operators of induced action of $A_{x(t)}$ on the kth exterior power of E. Again decreasing of $\|\Delta x^{(1)} \wedge \Delta x^{(2)} \wedge \ldots \wedge \Delta x^{(k)}\|$ in time is equivalent to dissipativity of all operators $A_{x(t)}^{D\wedge k}$, $t \geq 0$ in the norm $\| \bullet \|$. Existence of such norm for all $A_x^{D\wedge k}$ $(x \in U)$ is equivalent to decreasing of volumes of all parallelepipeds due to first approximation system (410) for any solution $x(t)$ of equations (381). If one can choose such $\varepsilon > 0$ that for all A_x $(x \in U)$, any vector $z \in E \wedge E \wedge \ldots \wedge E$, and this norm $\| \exp(A_x^{D\wedge k} t) z \| \leq \exp(-\varepsilon t) \|z\|$, then the volumes of parallelepipeds decrease exponentially as $\exp(-\varepsilon t)$.

For such systems we can estimate the Hausdorff dimension of the attractor (under some additional technical conditions): *it can not exceed k*. It is necessary to stress here that this estimation of the Hausdorff dimension does not solve the problem of construction the invariant manifold containing this attractor and one needs special technic and additional restriction on the system to obtain this manifold (see [182, 189, 186, 190]).

The simplest conditions of simultaneous dissipativity for the family of operators $\{A_x\}$ can be created on a following way: let us take a norm $\| \bullet \|$. If all operators A_x are dissipative with respect to this norm, then the family A_x is (evidently) simultaneously dissipative in this norm. So, we can verify or falsify a hypothesis about simultaneous dissipativity for a given norm. Simplest examples give us quadratic and l^1 norms.

For quadratic norm associated with a scalar product $\langle | \rangle$ dissipativity of operator A is equivalent to nonpositivity of all points of spectrum $A+A^+$, where A^+ is the ajoined to A operator with respect to scalar product $\langle | \rangle$.

For l^1 norm with weights $\|x\| = \sum_i w_i |x_i|$, $w_i > 0$. The condition of operator A dissipativity for this norm is the weighted diagonal predominance for columns of the A matrix $A = (a_{ij})$:

$$a_{ii} < 0,\ w_i|a_{ii}| \geq \sum_{j,\, j\neq i} w_j|a_{ji}|.$$

For exponential contraction it is necessary and sufficient a gap existence in the dissipativity inequalities:
for quadratic norm $\sigma(A+A^+) < \varepsilon < 0$, where $\sigma(A+A^+)$ is the spectrum of $A+A^+$;
for l^1 norm with weights $a_{ii} < 0$, $w_i|a_{ii}| \geq \sum_{j,\, j\neq i} w_j|a_{ji}| + \varepsilon$, $\varepsilon > 0$.

The sufficient conditions of simultaneous dissipativity can have another form (not only the form of dissipativity checking with respect to given norm) [168, 169, 170, 171], but the problem of necessary and sufficient conditions in general case is open.

The dissipativity conditions for operators $A_x^{D\wedge k}$ of induced action of A_x on the kth exterior power of E have the similar form, for example, if we know the spectrum of $A+A^+$, then it is easy to find the spectrum of $A_{x(t)}^{D\wedge k} + (A_{x(t)}^{D\wedge k})^+$: each eigenvalue of this operator is a sum of k distinct eigenvalues of $A+A^+$; the $A_{x(t)}^{D\wedge k} + (A_{x(t)}^{D\wedge k})^+$ spectrum is a closure of set of sums of k distinct points $A+A^+$ spectrum.

A basis the kth exterior power of E can be constructed from the basis $\{e_i\}$ of E: it is

$$\{e_{i_1 i_2 \ldots i_k}\} = \{e_{i_1} \wedge e_{i_2} \wedge \ldots \wedge e_{i_k}\},\ i_1 < i_2 < \ldots < i_k.$$

For l^1 norm with weights in the kth exterior power of E the set of weights is $\{w_{i_1 i_2 \ldots i_k} > 0,\ i_1 < i_2 < \ldots < i_k\}$. The norm of a vector z is

$$\|z\| = \sum_{i_1 < i_2 < \ldots < i_k} w_{i_1 i_2 \ldots i_k} |z_{i_1 i_2 \ldots i_k}|.$$

The dissipativity conditions for operators $A^{D\wedge k}$ of induced action of A in l^1 norm with weights have the form:

$$\begin{aligned}
&a_{i_1 i_1} + a_{i_2 i_2} + \ldots + a_{i_k i_k} < 0,\\
&w_{i_1 i_2 \ldots i_k} |a_{i_1 i_1} + a_{i_2 i_2} + \ldots + a_{i_k i_k}| \geq \sum_{l=1}^{k} \sum_{j,\, j \neq i_1, i_2, \ldots i_k} w_{i_1 i_2 \ldots i_k}^{l,j} |a_{j i_l}|\\
&\text{for any } i_1 < i_2 < \ldots < i_k,
\end{aligned} \tag{412}$$

where $w_{i_1 i_2 \ldots i_k}^{l,j} = w_I$, multiindex I consists of indexes $i_p\,(p \neq l)$, and j.

For infinite dimensional systems the problem of volume contraction and Lyapunov norms for exterior powers of E consists of three parts: geometrical part concerning the choice of norm for simultaneous dissipativity of operator families, topological part concerning topological nonequivalence of constructed norms, and estimation of the bounded set containing compact attractor.

The difficult problem may concern the appropriate apriori estimations of the bounded convex positively invariant set $V \subset U$ where the compact attractor is situated. It may be crucial to solve the problem of simultaneous dissipativity for the most narrow family of operators $\{A_x,\ x \in V\}$ (and their induced action on the kth exterior power of E).

The estimation of attractor dimension based on Lyapunov norms in the exterior powers is rather rough. This is a local estimation. More exact estimations are based on global Lyapunov exponents (Lyapunov or Kaplan-Yorke dimension [175, 176]. There are many different measures of dimension [174, 177], and many efforts are applied to create good estimations for different dimensions [188]. Estimations of attractor dimension was given for different systems: from Navier-Stokes hydrodynamic [180] to climate dynamics [179]. The introduction and review of many results is given in the book [182]. But local estimations remain the main tools for estimation of attractors dimension, because global estimations for complex systems are much more complicated and often unattainable because computation complexity.

Example 12: The universal limit in dynamics of dilute polymeric solutions

The method of invariant manifold is developed for a derivation of reduced description in kinetic equations of dilute polymeric solutions. It is demonstrated that this reduced description becomes universal in the limit of small Deborah and Weissenberg numbers, and it is represented by the (revised) Oldroyd 8 constants constitutive equation for the polymeric stress tensor. Coefficients of this constitutive equation are expressed in terms of the microscopic parameters. A systematic procedure of corrections to the revised Oldroyd 8 constants equations is developed. Results are tested with simple flows.

Kinetic equations arising in the theory of polymer dynamics constitute a wide class of microscopic models of complex fluids. Same as in any branch of kinetic theory, the problem of reduced description becomes actual as soon as the kinetic equation is established. However, in spite of an enormous amount of work in the field of polymer dynamics [86, 87, 194, 88, 204], this problem remains less studied as compared to other classical kinetic equations.

It is the purpose of this section to suggest a systematic approach to the problem of reduced description for kinetic models of polymeric fluids. First, we would like to specify our motivation by comparing the problem of the reduced description for that case with a similar problem in the familiar case of the rarefied gas obeying the classical Boltzmann kinetic equation [69, 43].

The problem of reduced description begins with establishing a set of slow variables. For the Boltzmann equation, this set is represented by five hydrodynamic fields (density, momentum and energy) which are low–order moments of the distribution function, and which are conserved quantities of the dissipation process due to particle's collisions. The reduced description is a closed system of equations for these fields. One starts with the manifold of local equilibrium distribution functions (local Maxwellians), and finds a correction by the Chapman–Enskog method [43]. The resulting reduced description (the Navier–Stokes hydrodynamic equations) is universal in the sense that the form of equations does not depend on details of particle's interaction whereas the latter shows up explicitly only in the transport coefficients (viscosity, temperature conductivity, etc.).

Coming back to the complex fluids, we shall consider the simplest case of dilute polymer solutions represented by dumbbell models studied below. Two obstacles preclude an application of the traditional techniques. First, the question which variables should be regarded as slow is at least less evident because the dissipative dynamics in the dumbbell models has no nontrivial conservation laws compared to the Boltzmann case. Consequently, a priori, there are no distinguished manifolds of distribution functions like the local equilibria which can be regarded as a starting point. Second, while the Boltzmann kinetic equation provides a self–contained description, the dumbbell kinetic equations are coupled to the hydrodynamic equations. This coupling manifests itself as an external flux in the kinetic equation.

The well known distinguished macroscopic variable associated with the dumbbell kinetic equations is the polymeric stress tensor [86, 204]. This variable is not the conserved quantity but nevertheless it should be treated as a relevant slow variable because it actually contributes to the macroscopic (hydrodynamic) equations. Equations for the stress tensor are known as the constitutive equations, and the problem of reduced description for the dumbbell models consists in deriving such equations from the kinetic equation.

Our approach is based on the method of invariant manifold [3], modified for systems coupled with external fields. This method suggests constructing invariant sets (or manifolds) of distribution functions that represent the asymptotic states of slow evolution of the kinetic system. In the case of dumbbell models, the reduced description is produced by equations which constitute stress–strain relations, and two physical requirements are met by our approach: The first is the principle of *frame–indifference* with respect to any time–dependent reference frame. This principle requires that the resulting equations for the stresses contain only frame–indifferent quantities. For example, the frame–dependent vorticity tensor should not show up in these equations unless being presented in frame–indifferent combinations with another tensors. The second principle is the *thermodynamic stability*: In the absence of the flow, the constitutive model should be purely dissipative, in other words, it should describe the relaxation of stresses to their equilibrium values.

The physical picture addressed below takes into account two assumptions: (i) In the absence of the flow, deviations from the equilibrium are small. Then the invariant manifold is represented by eigenvectors corresponding to the slowest relaxation modes. (ii). When the external flow is taken into account, it is assumed to cause a small deformation of the invariant manifolds of the purely dissipative dynamics. Two characteristic parameters are necessary to describe this deformation. The first is the characteristic time variation of the external field. The second is the characteristic intensity of the external field. For dumbbell models, the first parameter is associated with the conventional Deborah number while the second one is usually called the Weissenberg number. An iteration approach which involves these parameters is developed.

Two main results of the analysis are as follows: First, the lowest–order constitutive equations with respect to the characteristic parameters mentioned above has the form of the revised phenomenological *Oldroyd 8 constants model*. This result is interpreted as the macroscopic limit of the microscopic dumbbell dynamics whenever the rate of the strain is low, and the Deborah number is small. This limit is valid generically, in the absence or in the presence of the hydrodynamic interaction, and for the arbitrary nonlinear elastic force. The phenomenological constants of the Oldroyd model are expressed in a closed form in terms of the microscopic parameters of the model. The universality of this limit is similar to that of the Navier–Stokes equations which are the macroscopic limit of the Boltzmann equation at small Knudsen numbers for arbitrary hard–core molecular interactions. The test calculation for the nonlinear FENE force demonstrates a good quantitative agreement of the constitutive equations with solutions to the microscopic kinetic equation within the domain of their validity.

The second result is a regular procedure of finding corrections to the zero–order model. These corrections extend the model into the domain of higher rates of the strain, and to flows which alternate faster in time. Same as in the zero–order approximation, the higher–order corrections are linear in the stresses, while their dependence on the gradients of the flow velocity and its time derivatives becomes highly nonlinear. These corrections have a similar meaning as the higher–order (Burnett) corrections in the Chapman–Enskog method though, again, the actual form of equations is different.

The section is organized as follows: For the sake of completeness, we present the nonlinear dumbbell kinetic models in the next subsection, "The problem of reduced description in polymer dynamics". In the section, "The method of invariant manifold for weakly driven systems", we describe in details our approach to the derivation of macroscopic equations for an abstract kinetic equation coupled to external fields. This derivation is applied to the dumbbell models in the section, "Constitutive equations". The zero–order constitutive equation is derived and discussed in detail in this section, as well as the structure of the first correction. Tests of the zero–order constitutive equation for simple flow problems are given in the section, "Tests on the FENE dumbbell model".

The problem of reduced description in polymer dynamics

Elastic dumbbell models. The elastic dumbbell model is the simplest microscopic model of polymer solutions [86]. The dumbbell model reflects the two features of real–world macromolecules to be orientable and stretchable by a flowing solvent. The polymeric solution is represented by a set of identical elastic dumbbells placed in an isothermal incompressible liquid. Let $\boldsymbol{Q}$ be the connector vector between the beads of a dumbbell, and $\Psi(\boldsymbol{x}, \boldsymbol{Q}, t)$ be the configuration distribution function which depends on the location in the space $\boldsymbol{x}$ at time t. We assume that dumbbells are distributed uniformly, and consider the normalization, $\int \Psi(\boldsymbol{x}, \boldsymbol{Q}, t) \mathrm{d}\boldsymbol{Q} = 1$. The Brownian motion of beads in the physical space causes a diffusion in the phase space described by the Fokker–Planck equation (FPE) [86]:

$$\frac{D\Psi}{Dt} = -\frac{\partial}{\partial \boldsymbol{Q}} \cdot \boldsymbol{k} \cdot \boldsymbol{Q}\Psi + \frac{2k_{\mathrm{B}}T}{\xi} \frac{\partial}{\partial \boldsymbol{Q}} \cdot \boldsymbol{D} \cdot \left(\frac{\partial}{\partial \boldsymbol{Q}} \Psi + \frac{\boldsymbol{F}}{k_{\mathrm{B}}T} \Psi \right). \tag{413}$$

Here $D/Dt = \partial/\partial t + \boldsymbol{v} \cdot \nabla$ is the material derivative, ∇ is the spatial gradient, $\boldsymbol{k}(\boldsymbol{x}, t) = (\nabla \boldsymbol{v})^{\dagger}$ is the gradient of the velocity of the solvent $\boldsymbol{v}$, $\dagger$ denotes transposition of tensors, $\boldsymbol{D}$ is the dimensionless diffusion matrix, k_{B} is the Boltzmann constant, T is the temperature, ξ is the dimensional coefficient characterizing a friction exerted by beads moving through solvent media (friction coefficient [86, 87]), and $\boldsymbol{F} = -\nabla\phi$ is the elastic spring force defined by the potential well ϕ. We consider forces of the form $\boldsymbol{F} = Hf(Q^2)\boldsymbol{Q}$, where $f(Q^2)$ is a dimensionless function of the variable $Q^2 = \boldsymbol{Q} \cdot \boldsymbol{Q}$, and H is the dimensional constant. Incompressibility of solvent implies $\sum_i k_{ii} = 0$.

Let us introduce a time dimensional constant

$$\lambda_{\mathrm{r}} = \frac{\xi}{4H},$$

which coincides with a characteristic relaxation time of dumbbell configuration in the case when the force $\boldsymbol{F}$ is linear: $f(Q^2) = 1$. It proves convenient to rewrite the FPE (413) in the dimensionless form:

$$\frac{D\Psi}{D\widehat{t}} = -\frac{\partial}{\partial \widehat{\mathbf{Q}}} \cdot \widehat{\mathbf{k}} \cdot \widehat{\mathbf{Q}}\Psi + \frac{\partial}{\partial \widehat{\mathbf{Q}}} \cdot \boldsymbol{D} \cdot \left(\frac{\partial}{\partial \widehat{\mathbf{Q}}}\Psi + \widehat{\mathbf{F}}\Psi\right). \tag{414}$$

Various dimensionless quantities used are: $\widehat{\mathbf{Q}} = (H/k_{\mathrm{B}}T)^{1/2}\boldsymbol{Q}$, $D/D\widehat{t} = \partial/\partial\widehat{t} + \boldsymbol{v}\cdot\overline{\nabla}$, $\widehat{t} = t/\lambda_{\mathrm{r}}$ is the dimensionless time, $\overline{\nabla} = \nabla\lambda_{\mathrm{r}}$ is the reduced space gradient and $\widehat{\mathbf{k}} = \boldsymbol{k}\lambda_{\mathrm{r}} = (\overline{\nabla}\boldsymbol{v})^{\dagger}$ is the dimensionless tensor of the gradients of the velocity. In the sequel, only dimensionless quantities $\widehat{\mathbf{Q}}$ and $\widehat{\mathbf{F}}$ are used, and we keep notations $\boldsymbol{Q}$ and $\boldsymbol{F}$ for them for the sake of simplicity.

The quantity of interest is the stress tensor introduced by Kramers [86]:

$$\boldsymbol{\tau} = -\nu_{\mathrm{s}}\dot{\boldsymbol{\gamma}} + nk_{\mathrm{B}}T(\mathbf{1} - \langle \boldsymbol{F}\boldsymbol{Q}\rangle), \tag{415}$$

where ν_{s} is the viscosity of the solvent, $\dot{\boldsymbol{\gamma}} = \boldsymbol{k} + \boldsymbol{k}^{\dagger}$ is the rate–of–strain tensor, n is the concentration of polymer molecules, and the angle brackets stand for the averaging with the distribution function Ψ: $\langle \bullet \rangle \equiv \int \bullet \Psi(\boldsymbol{Q})\mathrm{d}\boldsymbol{Q}$. The tensor

$$\boldsymbol{\tau}_{\mathrm{p}} = nk_{\mathrm{B}}T(\mathbf{1} - \langle \boldsymbol{F}\boldsymbol{Q}\rangle) \tag{416}$$

gives a contribution to stresses caused by the presence of polymer molecules.

The stress tensor is required in order to write down a closed system of hydrodynamic equations:

$$\frac{D\boldsymbol{v}}{Dt} = -\rho^{-1}\nabla p - \nabla\cdot\boldsymbol{\tau}[\Psi]. \tag{417}$$

Here p is the pressure, and $\rho = \rho_{\mathrm{s}} + \rho_{\mathrm{p}}$ is the mass density of the solution where ρ_{s} is the solvent, and ρ_{p} is the polymeric contributions.

Several models of the elastic force are known in the literature. The Hookean law is relevant to small perturbations of the equilibrium configuration of the macromolecule:

$$\boldsymbol{F} = \boldsymbol{Q}. \tag{418}$$

In that case, the differential equation for $\boldsymbol{\tau}$ is easily derived from the kinetic equation, and is the well known *Oldroyd–B* constitutive model [86].

The second model, the FENE force law [195], was derived as an approximation to the inverse Langevin force law [86] for a more realistic description of the elongation of a polymeric molecule in a solvent:

$$\boldsymbol{F} = \frac{\boldsymbol{Q}}{1 - \boldsymbol{Q}^2/\boldsymbol{Q}_0^2}. \tag{419}$$

This force law takes into account the nonlinear stiffness and the finite extendibility of dumbbells, where $\boldsymbol{Q}_0$ is the maximal extendibility.

The features of the diffusion matrix are important for both the microscopic and the macroscopic behavior. The isotropic diffusion is represented by the simplest diffusion matrix

$$\boldsymbol{D}_{\mathrm{I}} = \frac{1}{2}\mathbf{1}. \tag{420}$$

Here $\mathbf{1}$ is the unit matrix. When the hydrodynamic interaction between the beads is taken into account, this results in an anisotropic contribution to the diffusion matrix (420). The original form of this contribution is the Oseen–Burgers tensor $\boldsymbol{D}_{\mathrm{H}}$ [196, 197]:

$$\boldsymbol{D} = \boldsymbol{D}_{\mathrm{I}} - \kappa \boldsymbol{D}_{\mathrm{H}}, \qquad \boldsymbol{D}_{\mathrm{H}} = \frac{1}{Q}\left(\mathbf{1} + \frac{\boldsymbol{QQ}}{Q^2}\right), \tag{421}$$

where

$$\kappa = \left(\frac{H}{k_{\mathrm{B}}T}\right)^{1/2} \frac{\xi}{16\pi\nu_{\mathrm{s}}}.$$

Several modifications of the Oseen–Burgers tensor can be found in the literature (the *Rotne-Prager-Yamakawa* tensor [198, 199]), but here we consider only the classical version.

Properties of the Fokker–Planck operator. Let us review some of the properties of the Fokker–Planck operator J in the right hand side of the Eq. (414) relevant to what will follow. This operator can be written as $J = J_{\mathrm{d}} + J_{\mathrm{h}}$, and it represents two processes.

The first term, J_{d}, is the dissipative part,

$$J_{\mathrm{d}} = \frac{\partial}{\partial \boldsymbol{Q}} \cdot \boldsymbol{D} \cdot \left(\frac{\partial}{\partial \boldsymbol{Q}} + \boldsymbol{F}\right). \tag{422}$$

This part is responsible for the diffusion and friction which affect internal configurations of dumbbells, and it drives the system to the unique equilibrium state,

$$\Psi_{\mathrm{eq}} = c^{-1}\exp(-\phi(Q^2)),$$

where $c = \int \exp(-\phi)\mathrm{d}\boldsymbol{Q}$ is the normalization constant.

The second part, J_{h}, describes the hydrodynamic drag of the beads in the flowing solvent:

$$J_{\mathrm{h}} = -\frac{\partial}{\partial \boldsymbol{Q}} \cdot \widehat{\mathbf{k}} \cdot \boldsymbol{Q}. \tag{423}$$

The dissipative nature of the operator J_{d} is reflected by its spectrum. We assume that this spectrum consists of real–valued nonpositive eigenvalues, and that the zero eigenvalue is not degenerated. In the sequel, the following scalar product will be useful:

$$\langle g, h\rangle_{\mathrm{s}} = \int \Psi_{\mathrm{eq}}^{-1} g h \mathrm{d}\boldsymbol{Q}.$$

The operator J_{d} is symmetric and nonpositive definite in this scalar product:

$$\langle J_{\mathrm{d}} g, h\rangle_{\mathrm{s}} = \langle g, J_{\mathrm{d}} h\rangle_{\mathrm{s}}, \quad \text{and} \quad \langle J_{\mathrm{d}} g, g\rangle_{\mathrm{s}} \le 0. \tag{424}$$

Since $\langle J_{\mathrm{d}} g, g\rangle_{\mathrm{s}} = -\int \Psi_{\mathrm{eq}}^{-1}(\partial g/\partial \boldsymbol{Q}) \cdot \Psi_{\mathrm{eq}} \boldsymbol{D} \cdot (\partial g/\partial \boldsymbol{Q})\mathrm{d}\boldsymbol{Q}$, the above inequality is valid if the diffusion matrix $\boldsymbol{D}$ is positive semidefinite. This happens if $\boldsymbol{D} = \boldsymbol{D}_{\mathrm{I}}$ (420) but is not generally valid in the presence of the hydrodynamic interaction (421). Let us split the operator J_{d} in accord with the splitting of the diffusion matrix $\boldsymbol{D}$: $J_{\mathrm{d}} = J_{\mathrm{d}}^{\mathrm{I}} - \kappa J_{\mathrm{d}}^{\mathrm{H}}$, where $J_{\mathrm{d}}^{\mathrm{I,H}} = \partial/\partial \boldsymbol{Q} \cdot \boldsymbol{D}_{\mathrm{I,H}} \cdot (\partial/\partial \boldsymbol{Q} + \boldsymbol{F})$. Both the operators $J_{\mathrm{d}}^{\mathrm{I}}$ and $J_{\mathrm{d}}^{\mathrm{H}}$ have nondegenerated eigenvalue 0 which corresponds to their common eigenfunction $\Psi_{\rm eq}$: $J_{\rm d}^{\rm I,H}\Psi_{\rm eq}=0$, while the rest of the spectrum of both operators belongs to the nonpositive real semi–axis. Then the spectrum of the operator $J_{\rm d}=J_{\rm d}^{\rm I}-\kappa J_{\rm d}^{\rm H}$ remains nonpositive for sufficiently small values of the parameter κ. The spectral properties of both operators $J_{\rm d}^{\rm I,H}$ depend only on the choice of spring force $\boldsymbol{F}$. Thus, in the sequel we assume that the hydrodynamic interaction parameter κ is sufficiently small so that the *thermodynamic stability* property (424) holds.

We note that the scalar product $\langle\bullet,\bullet\rangle_{\rm s}$ coincides with the second differential $D^2S|_{\Psi_{\rm eq}}$ of an entropy functional $S[\Psi]$: $\langle\bullet,\bullet\rangle_{\rm s}=-D^2S|_{\Psi_{\rm eq}}[\bullet,\bullet]$, where the entropy has the form:

$$S[\Psi]=-\int\Psi\ln\left(\frac{\Psi}{\Psi_{\rm eq}}\right){\rm d}\boldsymbol{Q}=-\left\langle\ln\left(\frac{\Psi}{\Psi_{\rm eq}}\right)\right\rangle. \tag{425}$$

The entropy S grows in the course of dissipation:

$$DS[J_{\rm d}\Psi]\geq 0.$$

This inequality similar to inequality (424) is satisfied for sufficiently small κ. Symmetry and nonpositiveness of operator $J_{\rm d}$ in the scalar product defined by the second differential of the entropy is a common property of linear dissipative systems.

Statement of the problem. Given the kinetic equation (413), we aim at deriving differential equations for the stress tensor $\boldsymbol{\tau}$ (415). The latter includes the moments $\langle\boldsymbol{F}\boldsymbol{Q}\rangle=\int\boldsymbol{F}\boldsymbol{Q}\Psi{\rm d}\boldsymbol{Q}$.

In general, when the diffusion matrix is non–isotropic and/or the spring force is non-linear, closed equations for these moments are not available, and approximations are required. With this, any derivation should be consistent with the three requirements:

(i). *Dissipativity or thermodynamic stability:* The macroscopic dynamics should be dissipative in the absence of the flow.

(ii). *Slowness*: The macroscopic equations should represent slow degrees of freedom of the kinetic equation.

(iii). *Material frame indifference*: The form of equations for the stresses should be invariant with respect to the Eucluidian, time dependent transformations of the reference frame [86, 200].

While these three requirements should be met by any approximate derivation, the validity of our approach will be restricted by two additional assumptions:

(a). Let us denote θ_1 the inertial time of the flow, which we define via characteristic value of the gradient of the flow velocity: $\theta_1=|\nabla\boldsymbol{v}|^{-1}$, and θ_2 the characteristic time of the variation of the flow velocity. We assume that the characteristic relaxation time of the molecular configuration $\theta_{\rm r}$ is small as compared to both the characteristic times θ_1 and θ_2:

$$\theta_{\rm r}\ll\theta_1 \text{ and } \theta_{\rm r}\ll\theta_2. \tag{426}$$

(b). In the absence of the flow, the initial deviation of the distribution function from the equilibrium is small so that the linear approximation is valid.

While the assumption (b) is merely of a technical nature, and it is intended to simplify the treatment of the dissipative part of the Fokker–Planck operator (422) for elastic forces of a complicated form, the assumption (a) is crucial for taking into account the flow in an adequate way. We have assumed that the two parameters characterizing the composed system 'relaxing polymer configuration + flowing solvent' should be small: These two parameters are:

$$\varepsilon_1 = \theta_{\mathrm{r}}/\theta_1, \quad \varepsilon_2 = \theta_{\mathrm{r}}/\theta_2. \tag{427}$$

The characteristic relaxation time of the polymeric configuration is defined via the coefficient λ_{r}: $\theta_{\mathrm{r}} = c\lambda_{\mathrm{r}}$, where c is some positive dimensionless constant which is estimated by the absolute value of the lowest nonzero eigenvalue of the operator J_{d}. The first parameter ε_1 is usually termed the *Weissenberg number* while the second one ε_2 is the *Deborah number* (cf. Ref. [201], sec. 7–2).

The method of invariant manifold for weakly driven systems

The Newton iteration scheme. In this section we introduce an extension of the method of invariant manifold [3] onto systems coupled with external fields. We consider a class of dynamic systems of the form

$$\frac{\mathrm{d}\Psi}{\mathrm{d}t} = J_{\mathrm{d}}\Psi + J_{\mathrm{ex}}(\alpha)\Psi, \tag{428}$$

where J_{d} is a linear operator representing the dissipative part of the dynamic vector field, while $J_{\mathrm{ex}}(\alpha)$ is a linear operator which represents an external flux and depends on a set of external fields $\alpha = \{\alpha_1, \dots, \alpha_k\}$. Parameters α are either known functions of the time, $\alpha = \alpha(t)$, or they obey a set of equations,

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = \Phi(\Psi, \alpha). \tag{429}$$

Without any restriction, parameters α are adjusted in such a way that $J_{\mathrm{ex}}(\alpha = 0) \equiv 0$. Kinetic equation (414) has the form (428), and general results of this section will be applied to the dumbbell models below in a straightforward way.

We assume that the vector field $J_{\mathrm{d}}\Psi$ has the same dissipative properties as the Fokker–Planck operator (422). Namely there exists the globally convex entropy function S which obeys: $DS[J_{\mathrm{d}}\Psi] \geq 0$, and the operator J_{d} is symmetric and nonpositive in the scalar product $\langle \bullet, \bullet \rangle_{\mathrm{s}}$ defined by the second differential of the entropy: $\langle g, h \rangle_{\mathrm{s}} = -D^2S[g,h]$. Thus, the vector field $J_{\mathrm{d}}\Psi$ drives the system irreversibly to the unique equilibrium state Ψ_{eq}.

We consider a set of n real–valued functionals, $M_i^*[\Psi]$ (macroscopic variables), in the phase space $\mathcal{F}$ of the system (428). A macroscopic description is obtained once we have derived a closed set of equations for the variables M_i^*.

Our approach is based on constructing a relevant invariant manifold in phase space $\mathcal{F}$. This manifold is thought as a finite–parametric set of solutions $\Psi(M)$ to Eqs. (428) which depends on time implicitly via the n variables $M_i[\Psi]$. The latter may differ from the macroscopic variables M_i^*. For systems with external fluxes (428), we assume that the invariant manifold depends also on the parameters α, and on their time derivatives taken to arbitrary order: $\Psi(M, \mathcal{A})$, where $\mathcal{A} = \{\alpha, \alpha^{(1)}, \ldots\}$ is the set of time derivatives $\alpha^{(k)} = \mathrm{d}^k\alpha/\mathrm{d}t^k$. It is convenient to consider time derivatives of α as independent parameters. This assumption is important because then we do not need an explicit form of the Eqs. (429) in the course of construction of the invariant manifold.

By a definition, the dynamic invariance postulates the equality of the "macroscopic" and the "microscopic" time derivatives:

$$J\Psi(M, \mathcal{A}) = \sum_{i=1}^{n} \frac{\partial \Psi(M, \mathcal{A})}{\partial M_i} \frac{\mathrm{d}M_i}{\mathrm{d}t} + \sum_{n=0}^{\infty} \sum_{j=1}^{k} \frac{\partial \Psi(M, \mathcal{A})}{\partial \alpha_j^{(n)}} \alpha_j^{(n+1)}, \tag{430}$$

where $J = J_{\mathrm{d}} + J_{\mathrm{ex}}(\alpha)$. The time derivatives of the macroscopic variables, $\mathrm{d}M_i/\mathrm{d}t$, are calculated as follows:

$$\frac{\mathrm{d}M_i}{\mathrm{d}t} = DM_i[J\Psi(M, \mathcal{A})], \tag{431}$$

where DM_i stands for differentials of the functionals M_i.

Let us introduce the projector operator associated with the parameterization of the manifold $\Psi(M, \mathcal{A})$ by the values of the functionals $M_i[\Psi]$.:

$$P_M = \sum_{i=1}^{n} \frac{\partial \Psi(M, \mathcal{A})}{\partial M_i} DM_i[\bullet] \tag{432}$$

It projects vector fields from the phase space $\mathcal{F}$ onto tangent bundle $T\Psi(M, \mathcal{A})$ of the manifold $\Psi(M, \mathcal{A})$. Then Eq. (430) is rewritten as the *invariance equation*:

$$(1 - P_M)J\Psi(M, \mathcal{A}) = \sum_{n=0}^{\infty} \sum_{j=1}^{k} \frac{\partial \Psi}{\partial \alpha_j^{(n)}} \alpha_j^{(n+1)}, \tag{433}$$

which has the invariant manifolds as its solutions.

Furthermore, we assume the following: (i). The external flux $J_{\mathrm{ex}}(\alpha)\Psi$ is small in comparison to the dissipative part $J_{\mathrm{d}}\Psi$, i.e. with respect to some norm we require: $|J_{\mathrm{ex}}(\alpha)\Psi| \ll |J_{\mathrm{d}}\Psi|$. This allows us to introduce a small parameter ε_1, and to replace the operator J_{ex} with $\varepsilon_1 J_{\mathrm{ex}}$ in the Eq. (428). Parameter ε_1 is proportional to the characteristic value of the external variables α. (ii). The characteristic time θ_α of the variation of the external fields α is large in comparison to the characteristic relaxation time θ_{r}, and the second small parameter is $\varepsilon_2 = \theta_{\mathrm{r}}/\theta_\alpha \ll 1$. The parameter ε_2 does not enter the vector field J explicitly but it shows up in the invariance equation. Indeed, with a substitution, $\alpha^{(i)} \to \varepsilon_2^i \alpha^{(i)}$, the invariance equation (430) is rewritten in a form which incorporates both the parameters ε_1 and ε_2:

$$(1 - P_M)\{J_{\mathrm{d}} + \varepsilon_1 J_{\mathrm{ex}}\}\Psi = \varepsilon_2 \sum_{i} \sum_{j=1}^{k} \frac{\partial \Psi}{\partial \alpha_j^{(i)}} \alpha_j^{(i+1)} \tag{434}$$

We develop a modified Newton scheme for solution of this equation. Let us assume that we have some initial approximation to desired manifold $\Psi_{(0)}$. We seek the correction of the form $\Psi_{(1)} = \Psi_{(0)} + \Psi_1$. Substituting this expression into Eq. (434), we derive:

$$(1 - P_M^{(0)})\{J_{\rm d} + \varepsilon_1 J_{\rm ex}\}\Psi_1 - \varepsilon_2 \sum_i \sum_{j=1}^{k} \frac{\partial \Psi_1}{\partial \alpha_j^{(i)}} \alpha_j^{(i+1)} =$$
$$-(1 - P_M^{(0)}) J \Psi_{(0)} + \varepsilon_2 \sum_i \sum_{j=1}^{k} \frac{\partial \Psi_{(0)}}{\partial \alpha_j^{(i)}} \alpha_j^{(i+1)}. \quad (435)$$

Here $P_M^{(0)}$ is a projector onto tangent bundle of the manifold $\Psi_{(0)}$. Further, we neglect two terms in the left hand side of this equation, which are multiplied by parameters ε_1 and ε_2, regarding them small in comparison to the first term. In the result we arrive at the equation,

$$(1 - P_M^{(0)}) J_{\rm d} \Psi_1 = -(1 - P_M^{(0)}) J \Psi_{(0)} + \varepsilon_2 \sum_i \sum_{j=1}^{k} \frac{\partial \Psi_{(0)}}{\partial \alpha_j^{(i)}} \alpha_j^{(i+1)}. \quad (436)$$

For $(n+1)$-th iteration we obtain:

$$(1 - P_M^{(n)}) J_{\rm d} \Psi_{n+1} = -(1 - P_M^{(0)}) J \Psi_{(n)} + \varepsilon_2 \sum_i \sum_{j=1}^{k} \frac{\partial \Psi_{(n)}}{\partial \alpha_j^{(i)}} \alpha_j^{(i+1)}, \quad (437)$$

where $\Psi_{(n)} = \sum_{i=0}^{n} \Psi_i$ is the approximation of n-th order and $P_M^{(n)}$ is the projector onto its tangent bundle.

It should be noted that deriving equations (436) and (437) we have not varied the projector P_M with respect to yet unknown term Ψ_{n+1}, i.e. we have kept $P_M = P_M^{(n)}$ and have neglected the contribution from the term Ψ_{n+1}. The motivation for this action comes from the original paper [3], where it was shown that such modification generates iteration schemes properly converging to slow invariant manifold.

In order to gain the solvability of Eq. (437) an additional condition is required:

$$P_M^{(n)} \Psi_{n+1} = 0. \quad (438)$$

This condition is sufficient to provide the existence of the solution to linear system (437), while the additional restriction onto the choice of the projector is required in order to guarantee the uniqueness of the solution. This condition is

$$\ker[(1 - P_M^{(n)}) J_{\rm d}] \cap \ker P_M^{(n)} = \mathbf{0}. \quad (439)$$

Here ker denotes a null space of the corresponding operator. How this condition can be met is discussed in the next subsection.

It is natural to begin the iteration procedure (437) starting from the invariant manifold of the non–driven system. In other words, we choose the initial approximation $\Psi_{(0)}$ as the solution of the invariance equation (434) corresponding to $\varepsilon_1 = 0$ and $\varepsilon_2 = 0$:

$$(1 - P_M^{(0)}) J_{\rm d} \Psi_{(0)} = 0. \quad (440)$$

We shall return to the question how to construct solutions to this equation in the subsection "Linear zero-order equations".

The above recurrent equations (437), (438) are simplified Newton method for the solution of invariance equation (434), which involves the small parameters. A similar procedure for Grad equations of the Boltzmann kinetic theory was used recently in the Ref. [6]. When these parameters are not small, one should proceed directly with equations (435).

Above, we have focused our attention on how to organize the iterations to construct invariant manifolds of weakly driven systems. The only question we have not yet answered is how to choose projectors in iterative equations in a consistent way. In the next subsection we discuss the problem of derivation of the reduced dynamics and its relation to the problem of the choice of projector.

Projector and reduced dynamics. Below we suggest the projector which is equally applicable for constructing invariant manifolds by the iteration method (437), (438) and for generating macroscopic equations based on given manifold.

Let us discuss the problem of constructing closed equations for macroparameters. Having some approximation to the invariant manifold, we nevertheless deal with a non-invariant manifold and we face the problem how to construct the dynamics on it. If the $n-$dimensional manifold $\widetilde{\Psi}$ is found the macroscopic dynamics is induced by any projector P onto the tangent bundle of $\widetilde{\Psi}$ as follows [3]:

$$\frac{\mathrm{d}M_i^*}{\mathrm{d}t} = DM_i^*|_{\tilde{\Psi}}\left[PJ\widetilde{\Psi}\right]. \tag{441}$$

To specify the projector we involve the two above mentioned principles: dissipativity and slowness. The dissipativity is required to have the unique and stable equilibrium solution for macroscopic equations, when the external fields are absent ($\alpha = 0$). The slowness condition requires the *induced* vector field $PJ\Psi$ to match the slow modes of the original vector field $J\Psi$.

Let us consider the parameterization of the manifold $\widetilde{\Psi}(M)$ by the parameters $M_i[\Psi]$. This parameterization generates associated projector $P = P_M$ by the Eq. (432). This leads us to look for the admissible parameterization of this manifold, where by admissibility we understand the concordance with the dissipativity and the slowness requirements. We solve the problem of the admissible parameterization in the following way. Let us define the functionals M_i $i = 1, \ldots, n$ by the set of the lowest eigenvectors φ_i of the operator J_{d}:

$$M_i[\widetilde{\Psi}] = \langle\varphi_i, \widetilde{\Psi}\rangle_{\mathrm{s}},$$

where $J_{\mathrm{d}}\varphi_i = \lambda_i\varphi_i$. The lowest eigenvectors $\varphi_1, \ldots, \varphi_n$ are taken as a join of basises in the eigenspaces of the eigenvalues with smallest absolute values: $0 < |\lambda_1| \leq |\lambda_2| \leq \ldots \leq |\lambda_n|$. For simplicity we shall work with the orthonormal set of eigenvectors: $\langle\varphi_i, \varphi_j\rangle_{\mathrm{s}} = \delta_{ij}$ with δ_{ij} the Kronecker symbol. Since the function Ψ_{eq} is the eigenvector of the zero eigenvalue we have: $M_i[\Psi_{\mathrm{eq}}] = \langle\varphi_i, \Psi_{\mathrm{eq}}\rangle_{\mathrm{s}} = 0$.

Then the associated projector P_M, written as:

$$P_M = \sum_{i=1}^{n} \frac{\partial \widetilde{\Psi}}{\partial M_i} \langle \varphi_i, \bullet \rangle_{\mathrm{s}}, \tag{442}$$

will generate the equations in terms of the parameters M_i as follows:

$$\mathrm{d}M_i/\mathrm{d}t = \langle \varphi_i P_M J \widetilde{\Psi} \rangle_{\mathrm{s}} = \langle \varphi_i J \widetilde{\Psi} \rangle_{\mathrm{s}}.$$

Their explicit form is

$$\frac{\mathrm{d}M_i}{\mathrm{d}t} = \lambda_i M_i + \langle J^{+}_{\mathrm{ex}}(\alpha) g_i, \widetilde{\Psi}(M) \rangle_{\mathrm{s}}, \tag{443}$$

where the J^{+}_{ex} is the adjoint to operator J_{ex} with respect to the scalar product $\langle \bullet, \bullet \rangle_{\mathrm{s}}$.

Apparently, in the absence of forcing ($\alpha \equiv 0$) the macroscopic equations $\mathrm{d}M_i/\mathrm{d}t = \lambda_i M_i$ are thermodynamically stable. They represent the dynamics of slowest eigenmodes of equations $\mathrm{d}\Psi/\mathrm{d}t = J_{\mathrm{d}}\Psi$. Thus, the projector (442) complies with the above stated requirements of dissipativity and slowness in the absence external flux.

To rewrite the macroscopic equations (443) in terms of the required set of macroparameters, $M_i^*[\Psi] = \langle m_i^*, \Psi \rangle_{\mathrm{s}}$, we use the formula (441) which is equivalent to the change of variables $\{M\} \to \{M^*(M)\}$, $M_i^* = \langle m_i^*, \widetilde{\Psi}(M) \rangle_{\mathrm{s}}$ in the equations (443). Indeed, this is seen from the relation:

$$DM_i^*|_{\tilde{\Psi}} \left[P_M J \widetilde{\Psi} \right] = \sum_j \frac{\partial M_i^*}{\partial M_j} DM_j|_{\tilde{\Psi}} [J \widetilde{\Psi}].$$

We have constructed the dynamics with the help of the projector P_M associated with the lowest eigenvectors of the operator J_{d}. It is directly verified that such projector (442) fulfills the condition (438) for arbitrary manifold $\Psi_{(n)} = \widetilde{\Psi}$. For this reason it is natural to use the projector (442) for both procedures, constructing the invariant manifold, and deriving the macroscopic equations.

We have to note that the above described approach to defining the dynamics via the projector is different from the concept of "thermodynamic parameterization" proposed in the Refs. [3, 2]. The latter was applicable for arbitrary dissipative systems including nonlinear ones, whereas the present derivations are applied solely for linear systems.

Linear zero-order equations. In this section we focus our attention on the solution of the zero–order invariance equation (440). We seek the *linear* invariant manifold of the form

$$\Psi_{(0)}(a) = \Psi_{\mathrm{eq}} + \sum_{i=1}^{n} a_i m_i, \tag{444}$$

where a_i are coordinates on this manifold. This manifold can be considered as an expansion of the relevant slow manifold near the equilibrium state. This limits the domain of validity of the manifolds (444) because they are not generally positively definite. This remark indicates that nonlinear invariant manifolds should be considered for large deviations from the equilibrium but this goes beyond the scope of this Example.

The linear $n-$dimensional manifold representing the slow motion for the linear dissipative system (428) is associated with n slowest eigenmodes. This manifold should be built up as the linear hull of the eigenvectors φ_i of the operator J_d, corresponding to the lower part of its spectrum. Thus we choose $m_i = \varphi_i$.

Dynamic equations for the macroscopic variables M^* are derived in two steps. First, following the subsection, "Projector and reduced dynamics", we parameterize the linear manifold $\Psi_{(0)}$ with the values of the moments $M_i[\Psi] = \langle \varphi_i, \Psi \rangle_\mathrm{s}$. We obtain that the parameterization of the manifold (444) is given by $a_i = M_i$, or:

$$\Psi_{(0)}(M) = \Psi_\mathrm{eq} + \sum_{i=1}^{n} M_i \varphi_i,$$

Then the reduced dynamics in terms of variables M_i reads:

$$\frac{\mathrm{d}M_i}{\mathrm{d}t} = \lambda_i M_i + \sum_j \langle J_\mathrm{ex}^+ \varphi_i, \varphi_j \rangle_\mathrm{s} M_j + \langle J_\mathrm{ex}^+ \varphi_i, \Psi_\mathrm{eq} \rangle_\mathrm{s}, \tag{445}$$

where $\lambda_i = \langle \varphi_i, J_\mathrm{d} \varphi_i \rangle_\mathrm{s}$ are eigenvalues which correspond to eigenfunctions φ_i.

Second, we switch from the variables M_i to the variables $M_i^*(M) = \langle m_i^*, \Psi_{(0)}(M) \rangle_\mathrm{s}$ in the Eq. (445). Resulting equations for the variables M^* are also linear:

$$\begin{aligned}\frac{\mathrm{d}M_i^*}{\mathrm{d}t} = \sum_{jkl} (B^{-1})_{ij} \Lambda_{jk} B_{kl} \Delta M_l^* &+ \sum_{jk} (B^{-1})_{ij} \langle J_\mathrm{ex}^+ \varphi_j, \varphi_k \rangle_\mathrm{s} \Delta M_k^* \\ &+ \sum_j (B^{-1})_{ij} \langle J_\mathrm{ex}^+ \varphi_j, \Psi_\mathrm{eq} \rangle_\mathrm{s}.\end{aligned} \tag{446}$$

Here $\Delta M_i^* = M_i^* - M_{\mathrm{eq}|i}^*$ is the deviation of the variable M_i^* from its equilibrium value $M_{\mathrm{eq}|i}^*$, and $B_{ij} = \langle m_i^*, \varphi_j \rangle$ and $\Lambda_{ij} = \lambda_i \delta_{ij}$.

Constitutive equations

Iteration scheme. In this section we apply the above developed formalism to the elastic dumbbell model (414). External field variables α are the components of the tensor $\widehat{\mathbf{k}}$.

Since we aim at constructing a closed description for the stress tensor $\boldsymbol{\tau}$ (415) with the six independent components, the relevant manifold in our problem should be six–dimensional. Moreover, we allow a dependence of the manifold on the material derivatives of the tensor $\widehat{\mathbf{k}}$: $\widehat{\mathbf{k}}^{(i)} = D^i \boldsymbol{k}/Dt^i$. Let $\Psi^*(M, \mathcal{K})$ $\mathcal{K} = \{\widehat{\mathbf{k}}, \widehat{\mathbf{k}}^{(1)}, \dots\}$ be the desired manifold parameterized by the six variables M_i $i = 1, \dots, 6$ and the independent components (maximum eight for each $\widehat{\mathbf{k}}^{(l)}$) of the tensors $\widehat{\mathbf{k}}^{(l)}$. Small parameters ε_1 and ε_2, introduced in the section: "The problem of reduced description in polymer dynamics", are established by Eq. (427). Then we define the invariance equation:

$$(1 - P_M)(J_\mathrm{d} + \varepsilon_1 J_\mathrm{h})\Psi = \varepsilon_2 \sum_{i=0}^{\infty} \sum_{lm} \frac{\partial \Psi}{\partial \widehat{k}_{lm}^{(i)}} \widehat{k}_{lm}^{(i+1)}, \tag{447}$$

where $P_M = (\partial\Psi/\partial M_i) DM_i[\bullet]$ is the projector associated with chosen parameterization and summation indexes l, m run only eight independent components of tensor $\widehat{\mathbf{k}}$.

Following the further procedure we straightforwardly obtain the recurrent equations:

$$(1 - P_M^{(n)}) J_{\rm d} \Psi_{n+1} = -(1 - P_M^{(n)})[J_{\rm d} + \varepsilon_1 J_{\rm h}]\Psi_{(n)} + \varepsilon_2 \sum_i \sum_{lm} \frac{\partial \Psi_{(n)}}{\partial \widehat{k}_{lm}^{(i)}} \widehat{k}_{lm}^{(i+1)}, \quad (448)$$

$$P_M^{(n)} \Psi_{n+1} = 0, \quad (449)$$

where Ψ_{n+1} is the correction to the manifold $\Psi_{(n)} = \sum_{i=0}^{n} \Psi_i$.

The zero-order manifold is found as the relevant solution to equation:

$$(1 - P_M^{(0)}) J_{\rm d} \Psi_{(0)} = 0 \quad (450)$$

We construct zero-order manifold $\Psi_{(0)}$ in the subsection, "Zero-order constitutive equation".

The dynamics in general form. Let us assume that some approximation to invariant manifold $\widetilde{\Psi}(a, \mathcal{K})$ is found (here $a = \{a_1, \ldots, a_6\}$ are some coordinates on this manifold). The next step is constructing the macroscopic dynamic equations.

In order to comply with dissipativity and slowness by means of the recipe from the previous section we need to find six lowest eigenvectors of the operator $J_{\rm d}$. We shall always assume in a sequel that the hydrodynamic interaction parameter κ is small enough that the dissipativity of $J_{\rm d}$ (424) is not violated.

Let us consider two classes of functions: $\mathcal{C}_1 = \{w_0(Q^2)\}$ and $\mathcal{C}_2 = \{w_1(Q^2) \ \overset{\circ}{\mathbf{Q}\mathbf{Q}}\}$, where $w_{0,1}$ are functions of Q^2 and the notation $\circ$ indicates traceless parts of tensor or matrix, e.g. for the dyad $\boldsymbol{QQ}$: $(\overset{\circ}{\mathbf{Q}\mathbf{Q}})_{ij} = Q_i Q_j - \frac{1}{3}\delta_{ij} Q^2$. Since the sets $\mathcal{C}_1$ and $\mathcal{C}_2$ are invariant with respect to operator $J_{\rm d}$, i.e. $J_{\rm d}\mathcal{C}_1 \subset \mathcal{C}_1$ and $J_{\rm d}\mathcal{C}_2 \subset \mathcal{C}_2$, and densities $\boldsymbol{FQ} = f \ \overset{\circ}{\mathbf{Q}\mathbf{Q}} + (1/3)\mathbf{1} f Q^2$ of the moments comprising the stress tensor $\boldsymbol{\tau}_p$ (416) belong to the space $\mathcal{C}_1 + \mathcal{C}_2$, we shall seek the desired eigenvectors in the classes $\mathcal{C}_1$ and $\mathcal{C}_2$. Namely, we intend to find one lowest isotropic eigenvector $\Psi_{\rm eq} m_0(Q^2)$ of eigenvalue $-\lambda_0$ ($\lambda_0 > 0$) and five nonisotropic eigenvectors $m_{ij} = \Psi_{\rm eq} m_1(Q^2)(\overset{\circ}{\mathbf{Q}\mathbf{Q}})_{ij}$ of another eigenvalue $-\lambda_1$ ($\lambda_1 > 0$). The method of derivation and analytic evaluation of these eigenvalues are discussed in the Appendix A. For a while we assume that these eigenvectors are known.

In the next step we parameterize given manifold $\widetilde{\Psi}$ by the values of the functionals:

$$M_0 = \langle \Psi_{\rm eq} m_0, \widetilde{\Psi} \rangle_{\rm s} = \int m_0 \widetilde{\Psi} {\rm d}\boldsymbol{Q},$$

$$\overset{\circ}{\mathbf{M}} = \langle \Psi_{\rm eq} m_1 \ \overset{\circ}{\mathbf{Q}\mathbf{Q}}, \widetilde{\Psi} \rangle_{\rm s} = \int m_1 \ \overset{\circ}{\mathbf{Q}\mathbf{Q}} \ \widetilde{\Psi} {\rm d}\boldsymbol{Q}. \quad (451)$$

Once a desired parameterization $\widetilde{\Psi}(M_0, \overset{\circ}{\mathbf{M}}, \mathcal{K})$ is obtained, the dynamic equations are found as:

$$\frac{DM_0}{D\widehat{t}} + \lambda_0 M_0 = \left\langle (\hat{\dot{\boldsymbol{\gamma}}} : \overset{\circ}{\mathbf{Q}\mathbf{Q}}) m_0' \right\rangle$$

$$\overset{\circ}{\mathbf{M}}_{[1]} + \lambda_1 \overset{\circ}{\mathbf{M}} = -\frac{1}{3}\mathbf{1}\hat{\dot{\boldsymbol{\gamma}}} : \overset{\circ}{\mathbf{M}} - \frac{1}{3}\hat{\dot{\boldsymbol{\gamma}}} \langle m_1 Q^2 \rangle + \left\langle \overset{\circ}{\mathbf{Q}\mathbf{Q}} \, (\hat{\dot{\boldsymbol{\gamma}}} : \overset{\circ}{\mathbf{Q}\mathbf{Q}}) m_1' \right\rangle, \quad (452)$$

where all averages are calculated with the d.f. $\widetilde{\Psi}$, i.e. $\langle \bullet \rangle = \int \bullet \widetilde{\Psi} \mathrm{d}\boldsymbol{Q}$, $m_{0,1}' = \partial m_{0,1}(Q^2)/\partial(Q^2)$ and subscript [1] represents the upper convective derivative of tensor:

$$\boldsymbol{\Lambda}_{[1]} = \frac{D\boldsymbol{\Lambda}}{D\widehat{t}} - \left\{ \widehat{\mathbf{k}} \cdot \boldsymbol{\Lambda} + \boldsymbol{\Lambda} \cdot \widehat{\mathbf{k}}^{\dagger} \right\}.$$

The parameters $\lambda_{0,1}$, which are absolute values of eigenvalues of operator J_{d}, are calculated by formulas (for definition of operators G_1 and G_2 see Appendix A):

$$\lambda_0 = -\frac{\langle m_0 G_0 m_0 \rangle_{\mathrm{e}}}{\langle m_0 m_0 \rangle_{\mathrm{e}}} > 0, \quad (453)$$

$$\lambda_1 = -\frac{\langle Q^4 m_1 G_1 m_1 \rangle_{\mathrm{e}}}{\langle m_1 m_1 Q^4 \rangle_{\mathrm{e}}} > 0, \quad (454)$$

where we have introduced the notation of the equilibrium average:

$$\langle y \rangle_{\mathrm{e}} = \int \Psi_{\mathrm{eq}} y \mathrm{d}\boldsymbol{Q}. \quad (455)$$

Equations on components of the polymeric stress tensor $\boldsymbol{\tau}_{\mathrm{p}}$ (416) are constructed as a change of variables $\{M_0, \overset{\circ}{\mathbf{M}}\} \to \boldsymbol{\tau}_{\mathrm{p}}$. The use of the projector $\widetilde{P}$ makes this operation straightforward:

$$\frac{D\boldsymbol{\tau}_{\mathrm{p}}}{D\widehat{t}} = -nk_{\mathrm{B}}T \int \boldsymbol{F}\boldsymbol{Q}\widetilde{P}J\widetilde{\Psi}(M_0(\boldsymbol{\tau}_{\mathrm{p}}, \mathcal{K}), \overset{\circ}{\mathbf{M}} (\boldsymbol{\tau}_{\mathrm{p}}, \mathcal{K}), \mathcal{K})\mathrm{d}\boldsymbol{Q}. \quad (456)$$

Here, the projector $\widetilde{P}$ is associated with the parameterization by the variables M_0 and $\overset{\circ}{\mathbf{M}}$:

$$\widetilde{P} = \frac{\partial \widetilde{\Psi}}{\partial M_0} \langle \Psi_{\mathrm{eq}} m_0, \bullet \rangle_{\mathrm{s}} + \sum_{kl} \frac{\partial \widetilde{\Psi}}{\partial \overset{\circ}{\mathbf{M}}_{kl}} \langle \Psi_{\mathrm{eq}} m_1 (\overset{\circ}{\mathbf{Q}\mathbf{Q}})_{kl}, \bullet \rangle_{\mathrm{s}}. \quad (457)$$

We note that sometimes it is easier to make transition to the variables $\boldsymbol{\tau}_{\mathrm{p}}$ after solving the equations (452) rather than to construct explicitly and solve equations in terms of $\boldsymbol{\tau}_{\mathrm{p}}$. It allows to avoid reverting the functions $\boldsymbol{\tau}_{\mathrm{p}}(M_0, \overset{\circ}{\mathbf{M}})$ and to deal with generally more simple equations.

Zero-order constitutive equation. In this subsection we derive the closure based on the zero–order manifold $\Psi_{(0)}$ found as appropriate solution to Eq. (450). Following the approach described in subsection, "Linear zero-order equations", we construct such a solution as the linear expansion near the equilibrium state Ψ_{eq} (444). After parameterization by the values of the variables M_0 and $\overset{\circ}{\mathbf{M}}$ associated with the eigenvectors $\Psi_{\mathrm{eq}} m_0$ and $\Psi_{\mathrm{eq}} m_1 \overset{\circ}{\mathbf{Q}\mathbf{Q}}$ we find:

$$\Psi_{(0)} = \Psi_{\mathrm{eq}} \left(1 + M_0 \frac{m_0}{\langle m_0 m_0 \rangle_{\mathrm{e}}} + \frac{15}{2} \overset{\circ}{\mathbf{M}} \colon \overset{\circ}{\mathbf{Q}\mathbf{Q}} \, \frac{m_1}{\langle m_1 m_1 Q^4 \rangle_{\mathrm{e}}} \right). \quad (458)$$

Then with the help of the projector (457):

$$P_M^{(0)} = \Psi_{\rm eq}\left\{\frac{m_0}{\langle m_0 m_0\rangle_{\rm e}}\langle m_0, \bullet\rangle_{\rm e} + \frac{15}{2}\frac{m_1}{\langle m_1 m_1 Q^4\rangle_{\rm e}}\,\overset{\circ}{\mathbf{Q}\mathbf{Q}} : \langle m_1\,\overset{\circ}{\mathbf{Q}\mathbf{Q}}, \bullet\rangle_{\rm e}\right\} \tag{459}$$

by the formula (456) we obtain:

$$\begin{aligned}
\frac{D\mathrm{tr}\boldsymbol{\tau}_{\rm p}}{D\widehat{t}} + \lambda_0 \mathrm{tr}\boldsymbol{\tau}_{\rm p} &= a_0\left(\overset{\circ}{\boldsymbol{\tau}}_{\rm p} : \hat{\dot{\boldsymbol{\gamma}}}\right), \qquad\qquad (460)\\
\overset{\circ}{\boldsymbol{\tau}}_{p[1]} + \lambda_0\,\overset{\circ}{\boldsymbol{\tau}}_{\rm p} &= b_0\left[\overset{\circ}{\boldsymbol{\tau}}_{\rm p}\cdot\hat{\dot{\boldsymbol{\gamma}}} + \hat{\dot{\boldsymbol{\gamma}}}\cdot\overset{\circ}{\boldsymbol{\tau}}_{\rm p}\right] - \frac{1}{3}\mathbf{1}(\overset{\circ}{\boldsymbol{\tau}}_{\rm p} : \hat{\dot{\boldsymbol{\gamma}}}) + (b_1\mathrm{tr}\boldsymbol{\tau}_{\rm p} - b_2 n k_{\rm B}T)\hat{\dot{\boldsymbol{\gamma}}},
\end{aligned}$$

where the constants b_i, a_0 are

$$\begin{aligned}
a_0 &= \frac{\langle f m_0 Q^2\rangle_{\rm e}\langle m_0 m_1 Q^4 m_1'\rangle_{\rm e}}{\langle f m_0 Q^4\rangle_{\rm e}\langle m_0^2\rangle_{\rm e}},\\
b_0 &= \frac{2}{7}\frac{\langle m_1 m_2' Q^6\rangle_{\rm e}}{\langle m_1^2 Q^4\rangle_{\rm e}},\\
b_1 &= \frac{1}{15}\frac{\langle f m_1 Q^4\rangle_{\rm e}}{\langle f m_0 Q^2\rangle_{\rm e}}\left\{2\frac{\langle m_0 m_2' Q^4\rangle_{\rm e}}{\langle m_1^2 Q^4\rangle_{\rm e}} + 5\frac{\langle m_0 m_1 Q^2\rangle_{\rm e}}{\langle m_1 m_1 Q^4\rangle_{\rm e}}\right\},\\
b_2 &= \frac{1}{15}\frac{\langle f m_1 Q^4\rangle_{\rm e}}{\langle m_1 m_1 Q^4\rangle_{\rm e}}\left\{2\left\langle m_2' Q^4\right\rangle_{\rm e} + 5\left\langle m_1 Q^2\right\rangle_{\rm e}\right\}.
\end{aligned} \tag{461}$$

We remind that $m_{0,1}' = \partial m_{0,1}/\partial(Q^2)$. These formulas were obtained by the use of the formulas from the Appendix B.

It is remarkable that being rewritten in terms of the full stresses $\boldsymbol{\tau} = -\nu_{\rm s}\dot{\boldsymbol{\gamma}} + \boldsymbol{\tau}_{\rm p}$ the dynamic system (460) takes a form:

$$\begin{aligned}
&\boldsymbol{\tau} + c_1\boldsymbol{\tau}_{[1]} + c_3\left\{\dot{\boldsymbol{\gamma}}\cdot\boldsymbol{\tau} + \boldsymbol{\tau}\cdot\dot{\boldsymbol{\gamma}}\right\} + c_5(\mathrm{tr}\boldsymbol{\tau})\dot{\boldsymbol{\gamma}} +\\
&\qquad \mathbf{1}\left(c_6\boldsymbol{\tau} : \dot{\boldsymbol{\gamma}} + c_8\mathrm{tr}\boldsymbol{\tau}\right) = -\nu\left\{\dot{\boldsymbol{\gamma}} + c_2\dot{\boldsymbol{\gamma}}_{[1]} + c_4\dot{\boldsymbol{\gamma}}\cdot\dot{\boldsymbol{\gamma}} + c_7(\dot{\boldsymbol{\gamma}} : \dot{\boldsymbol{\gamma}})\mathbf{1}\right\}
\end{aligned} \tag{462}$$

where the constants ν, c_i are given by the following relationships:

$$\begin{aligned}
&\nu = \lambda_{\rm r}\nu_{\rm s}\mu, \qquad \mu = 1 + nk_{\rm B}T\lambda_1 b_2/\nu_{\rm s},\\
&c_1 = \lambda_{\rm r}/\lambda_1, \qquad c_2 = \lambda_{\rm r}/(\mu\lambda_1),\\
&c_3 = -b_0\lambda_{\rm r}/\lambda_0, \qquad c_4 = -2b_0\lambda_{\rm r}/(\mu\lambda_1),\\
&c_5 = \frac{\lambda_{\rm r}}{3\lambda_1}(2b_0 - 3b_1 - 1), \qquad c_6 = \frac{\lambda_{\rm r}}{\lambda_1}(2b_0 + 1 - a_0),\\
&c_7 = \frac{\lambda_{\rm r}}{\lambda_1\mu}(2b_0 + 1 - a_0), \qquad c_8 = \frac{1}{3}(\lambda_0/\lambda_1 - 1).
\end{aligned} \tag{463}$$

In the last two formulas we returned to the original dimensional quantities: time t and gradient of velocity tensor $\boldsymbol{k} = \nabla\boldsymbol{v}$, and at the same time we kept the old notations for the dimensional convective derivative $\boldsymbol{\Lambda}_{[1]} = D\boldsymbol{\Lambda}/Dt - \boldsymbol{k}\cdot\boldsymbol{\Lambda} - \boldsymbol{\Lambda}\cdot\boldsymbol{k}^\dagger$.

If the constant c_8 were equal to zero, then the form of Eq. (462) would be recognized as *the Oldroyd 8 constant* model [202], proposed by Oldroyd about 40 years ago on a phenomenological basis. Nonzero c_8 indicates a presence of difference between $\lambda_{\rm r}/\lambda_0$ and $\lambda_{\rm r}/\lambda_1$ which are relaxation times of trace $\mathrm{tr}\boldsymbol{\tau}$ and traceless components $\overset{\circ}{\boldsymbol{\tau}}$ of the stress tensor $\boldsymbol{\tau}$.

Corrections. In this subsection we discuss the properties of corrections to the zero-order model (462). Let $P_M^{(0)}$ (459) be the projector onto the zero-order manifold $\Psi_{(0)}$ (458). The invariance equation (448) for the first-order correction $\Psi_{(1)} = \Psi_{(0)} + \Psi_1$ takes a form:

$$L\Psi_1 = -(1 - P_M^{(0)})(J_\mathrm{d} + J_\mathrm{h})\Psi_{(0)} \qquad (464)$$
$$P_M^{(0)}\Psi_1 = 0$$

where $L = (1 - P_M^{(0)})J_\mathrm{d}(1 - P_M^{(0)})$ is the symmetric operator. If the manifold $\Psi_{(0)}$ is parameterized by the functionals $M_0 = \int g_0 \Psi_{(0)} \mathrm{d}\boldsymbol{Q}$ and $\overset{\circ}{\mathbf{M}} = \int m_1 \overset{\circ}{\mathbf{QQ}} \Psi_{(0)}\mathrm{d}\boldsymbol{Q}$, where $\Psi_\mathrm{eq} m_0$ and $\Psi_\mathrm{eq} \overset{\circ}{\mathbf{QQ}} m_1$ are lowest eigenvectors of J_d, then the general form of the solution is given by:

$$\begin{aligned}\Psi_1 \;=\; \Psi_\mathrm{eq}\Big\{ & z_0 M_0(\dot{\boldsymbol{\gamma}} : \overset{\circ}{\mathbf{QQ}}) + z_1(\overset{\circ}{\mathbf{M}} : \overset{\circ}{\mathbf{QQ}})(\dot{\boldsymbol{\gamma}} : \overset{\circ}{\mathbf{QQ}}) + \\ & z_2\{\dot{\boldsymbol{\gamma}} \cdot \overset{\circ}{\mathbf{M}} + \overset{\circ}{\mathbf{M}} \cdot \dot{\boldsymbol{\gamma}}\} : \overset{\circ}{\mathbf{QQ}} + z_3 \dot{\boldsymbol{\gamma}} : \overset{\circ}{\mathbf{M}} + \frac{1}{2}\dot{\boldsymbol{\gamma}} : \overset{\circ}{\mathbf{QQ}} \Big\}. \end{aligned} \qquad (465)$$

The terms z_0 through z_3 are the functions of Q^2 found as the solutions to some linear differential equations.

We observe two features of the new manifold: first, it remains *linear* in variables M_0 and $\overset{\circ}{\mathbf{M}}$ and second it contains the dependence on the rate of strain tensor $\dot{\boldsymbol{\gamma}}$. As the consequence, the transition to variables $\boldsymbol{\tau}$ is given by the linear relations:

$$-\frac{\overset{\circ}{\boldsymbol{\tau}}_\mathrm{p}}{nk_\mathrm{B}T} = r_0 \overset{\circ}{\mathbf{M}} + r_1 M_0 \dot{\boldsymbol{\gamma}} + r_2\{\dot{\boldsymbol{\gamma}} \cdot \overset{\circ}{\mathbf{M}} + \overset{\circ}{\mathbf{M}} \cdot \dot{\boldsymbol{\gamma}}\} + r_3 \overset{\circ}{\overline{\dot{\boldsymbol{\gamma}} \cdot \dot{\boldsymbol{\gamma}}}}, \qquad (466)$$
$$-\frac{\mathrm{tr}\boldsymbol{\tau}_\mathrm{p}}{nk_\mathrm{B}T} = p_0 M_0 + p_1 \dot{\boldsymbol{\gamma}} : \overset{\circ}{\mathbf{M}},$$

where r_i and p_i are some constants. Finally the equations in terms of $\boldsymbol{\tau}$ should be also linear. Analysis shows that the first-order correction to the modified Oldroyd 8 constants model (462) will be transformed into the equations of the following general structure:

$$\begin{aligned}\boldsymbol{\tau} + c_1\boldsymbol{\tau}_{[1]} + \Big\{\boldsymbol{\Gamma}_1 \cdot \boldsymbol{\tau} \cdot \boldsymbol{\Gamma}_2 + \boldsymbol{\Gamma}_2^\dagger \cdot \boldsymbol{\tau} \cdot \boldsymbol{\Gamma}_1^\dagger\Big\} + & \\ \boldsymbol{\Gamma}_3(\mathrm{tr}\boldsymbol{\tau}) + \boldsymbol{\Gamma}_4(\boldsymbol{\Gamma}_5 : \boldsymbol{\tau}) \;&=\; -\nu_0 \boldsymbol{\Gamma}_6, \end{aligned} \qquad (467)$$

where $\boldsymbol{\Gamma}_1$ through $\boldsymbol{\Gamma}_6$ are tensors dependent on the rate-of-strain tensor $\dot{\boldsymbol{\gamma}}$ and its first convective derivative $\dot{\boldsymbol{\gamma}}_{[1]}$, constant c_1 is the same as in Eq. (463) and ν_0 is a positive constant.

Because the explicit form of the tensors $\boldsymbol{\Gamma}_i$ is quite extensive we do not present them in this section. Instead we give several general remarks about the structure of the first- and higher-order corrections:

1) Since the manifold (465) does not depend on the vorticity tensor $\omega = \boldsymbol{k} - \boldsymbol{k}^\dagger$ the latter enters the equations (467) only via convective derivatives of $\boldsymbol{\tau}$ and $\dot{\boldsymbol{\gamma}}$. This is

sufficient to acquire the frame indifference feature, since all the tensorial quantities in dynamic equations are indifferent in any time dependent reference frame [201].

2) When $\boldsymbol{k}=0$ the first order equations (467) as well as equations for any order reduce to linear relaxation dynamics of slow modes:

$$
\begin{aligned}
\frac{D\overset{\circ}{\boldsymbol{\tau}}}{Dt}+\frac{\lambda_1}{\lambda_{\mathrm{r}}}\overset{\circ}{\boldsymbol{\tau}}&=0,\\
\frac{D\mathrm{tr}\boldsymbol{\tau}}{Dt}+\frac{\lambda_0}{\lambda_{\mathrm{r}}}\mathrm{tr}\boldsymbol{\tau}&=0,
\end{aligned}
$$

which is obviously concordant with the dissipativity and the slowness requirements.

3) In all higher-order corrections one will be always left with linear manifolds if the projector associated with functionals $M_0[\Psi]$ and $\overset{\circ}{\mathbf{M}}[\Psi]$ is used in every step. It follows that the resulting constitutive equations will always take a linear form (467), where all tensors $\boldsymbol{\Gamma}_i$ depend on higher order convective derivatives of $\dot{\boldsymbol{\gamma}}$ (the highest possible order is limited by the order of the correction). Similarly to the first and zero orders the frame indifference is guaranteed if the manifold does not depend on the vorticity tensor unless the latter is incorporated in any frame invariant time derivatives. It is reasonable to eliminate the dependence on vorticity (if any) at the stage of constructing the solution to iteration equations (448).

4) When the force $\boldsymbol{F}$ is linear $\boldsymbol{F}=\boldsymbol{Q}$ our approach is proven to be also correct since it leads the Oldroyd–B model (Eq. (462) with $c_i=0$ for $i=3,\dots,8$). This follows from the fact that the spectrum of the corresponding operator J_{d} is more degenerated, in particular $\lambda_0=\lambda_1=1$ and the corresponding lowest eigenvectors comprise a simple dyad $\Psi_{\mathrm{eq}}\boldsymbol{QQ}$.

Tests on the FENE dumbbell model

In this section we specify the choice of the force law as the FENE springs (419) and present results of test calculations for the revised Oldroyd 8 constants (460) equations on the examples of two simple viscometric flows.

We introduce the extensibility parameter of FENE dumbbell model b:

$$
b=\widehat{\mathbf{Q}}_0^2=\frac{H\boldsymbol{Q}_0^2}{k_{\mathrm{B}}T}. \tag{468}
$$

It was estimated [86] that b is proportional to the length of polymeric molecule and has a meaningful variation interval 50–1000. The limit $b\to\infty$ corresponds to the Hookean case and therefore to the Oldroyd-B constitutive relation.

In our test calculations we will compare our results with the Brownian dynamic (BD) simulation data made on FENE dumbbell equations [203], and also with one popular approximation to the FENE model known as *FENE–P* (FENE–Peterelin) model [204, 86, 205]. The latter is obtained by selfconsistent approximation to FENE force:

$$
\boldsymbol{F}=\frac{1}{1-\left\langle \boldsymbol{Q}^2\right\rangle/b}\boldsymbol{Q}. \tag{469}
$$

This force law like Hookean case allows for the exact moment closure leading to nonlinear constitutive equations [86, 205]. Specifically we will use the modified variant of FENE-P model, which matches the dynamics of original FENE in near equilibrium region better than the classical variant. This modification is achieved by a slight modification of Kramers definition of the stress tensor:

$$\boldsymbol{\tau}_{\mathrm{p}} = nk_{\mathrm{B}}T(1-\theta b)\mathbf{1} - \langle \boldsymbol{F}\boldsymbol{Q} \rangle \,. \tag{470}$$

The case $\theta = 0$ gives the classical definition of FENE-P, while more thorough estimation [194, 205] is $\theta = (b(b+2))^{-1}$.

Constants

The specific feature of the FENE model is that the length of dumbbells $\boldsymbol{Q}$ can vary only in a bounded domain of $\mathbf{R}^3$, namely inside a sphere $S_b = \{Q^2 \le b\}$. The sphere S_b defines the domain of integration for averages $\langle \bullet \rangle_{\mathrm{e}} = \int_{S_b} \Psi_{\mathrm{eq}} \bullet \mathrm{d}\boldsymbol{Q}$, where the equilibrium distribution reads $\Psi_{\mathrm{eq}} = c^{-1}\left(1 - Q^2/b\right)^{b/2}$, $c = \int_{S_b} \left(1 - Q^2/b\right)^{b/2} \mathrm{d}\boldsymbol{Q}$.

In order to find constants for the zero-order model (460) we do the following: First we analytically compute the lowest eigenfunctions of operator J_{d}: $g_1(Q^2)\, \overset{\circ}{\mathbf{Q}\mathbf{Q}}$ and $g_0(Q^2)$ without account of the hydrodynamic interaction ($\kappa = 0$). The functions g_0 and g_1 are computed by a procedure presented in Appendix A with the help of the symbolic manipulation software *Maple V.3* [206]. Then we calculate the perturbations terms $h_{0,1}$ by formulas (484) introducing the account of hydrodynamic interaction. The Table 4 presents the constants $\lambda_{0,1}$, a_i, b_i (454) (461) of the zero-order model (460) without inclusion of hydrodynamic interaction $\kappa = 0$ for several values of extensibility parameter b. The relative error $\delta_{0,1}$ (see Appendix A) of approximation for these calculations did not exceed the value 0.02. The Table 5 shows the linear correction terms for constants from Tab. 4 which account a hydrodynamic interaction effect: $\lambda_{0,1}^{\mathrm{h}} = \lambda_{0,1}(1 + \kappa(\delta\lambda_{0,1}))$, $a_i^{\mathrm{h}} = a_i(1 + \kappa(\delta a_i))$, $b_i^{\mathrm{h}} = b_i(1 + \kappa(\delta b_i))$. The latter are calculated by substituting the perturbed functions $m_{0,1} = g_{0,1} + \kappa h_{0,1}$ into (454) and (461), and expanding them up to first-order in κ. One can observe, since $\kappa > 0$, the effect of hydrodynamic interaction results in the reduction of the relaxation times.

Dynamic problems

The rest of this section concerns the computations for two particular flows. The shear flow is defined by

$$\boldsymbol{k}(t) = \dot{\gamma}(t) \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{471}$$

where $\dot{\gamma}(t)$ is the shear rate, and the elongation flow corresponds to the choice:

$$\boldsymbol{k}(t) = \dot{\varepsilon}(t) \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1/2 & 0 \\ 0 & 0 & -1/2 \end{bmatrix}, \tag{472}$$

where $\dot{\varepsilon}(t)$ is the elongation rate.

Table 4: Values of constants to the revised Oldroyd 8 constants model computed on the base of the FENE dumbbells model

b	λ_0	λ_1	b_0	b_1	b_2	a_0
20	1.498	1.329	-0.0742	0.221	1.019	0.927
50	1.198	1.135	-0.0326	0.279	1.024	0.982
100	1.099	1.068	-0.0179	0.303	1.015	0.990
200	1.050	1.035	0.000053	0.328	1.0097	1.014
∞	1	1	0	1/3	1	1

Table 5: Corrections due to hydrodynamic interaction to the constants of the revised Oldroyd 8 constants model based on FENE force

b	$\delta\lambda_0$	$\delta\lambda_1$	δb_0	δb_1	δb_2	δa_0
20	-0.076	-0.101	0.257	-0.080	-0.0487	-0.0664
50	-0.0618	-0.109	-0.365	0.0885	-0.0205	-0.0691
100	-0.0574	-0.111	-1.020	0.109	-0.020	-0.0603

In test computations we will look at so called viscometric material functions defined through the components of the polymeric part of the stress tensor $\boldsymbol{\tau}_{\rm p}$. Namely, for shear flow they are the shear viscosity ν, the first and the second normal stress coefficients ψ_1, ψ_2, and for elongation flow the only function is the elongation viscosity $\bar{\nu}$. In dimensionless form they are written as:

$$\widehat{\nu} = \frac{\nu - \nu_{\rm s}}{nk_{\rm B}T\lambda_{\rm r}} = -\frac{\boldsymbol{\tau}_{\rm p,12}}{\overline{\gamma}nk_{\rm B}T}, \tag{473}$$

$$\widehat{\psi}_1 = \frac{\psi_1}{nk_{\rm B}T\lambda_{\rm r}^2} = \frac{\boldsymbol{\tau}_{\rm p,22} - \boldsymbol{\tau}_{\rm p,11}}{\overline{\gamma}^2 nk_{\rm B}T}, \tag{474}$$

$$\widehat{\psi}_2 = \frac{\psi_2}{nk_{\rm B}T\lambda_{\rm r}^2} = \frac{\boldsymbol{\tau}_{p,33} - \boldsymbol{\tau}_{p,22}}{\overline{\gamma}^2 nk_{\rm B}T}, \tag{475}$$

$$\vartheta = \frac{\bar{\nu} - 3\nu_{\rm s}}{nk_{\rm B}T\lambda_{\rm r}} = \frac{\boldsymbol{\tau}_{\rm p,22} - \boldsymbol{\tau}_{\rm p,11}}{\overline{\varepsilon}nk_{\rm B}T}, \tag{476}$$

where $\overline{\gamma} = \dot{\gamma}\lambda_{\rm r}$ and $\overline{\varepsilon} = \dot{\varepsilon}\lambda_{\rm r}$ are dimensionless shear and elongation rates. Characteristic values of latter parameters $\overline{\gamma}$ and $\overline{\varepsilon}$ allow to estimate the parameter ε_1 (427). For all flows considered below the second flow parameter (Deborah number) ε_2 is equal to zero.

Let us consider the steady state values of viscometric functions in steady shear and elongation flows: $\dot{\gamma} = const$, $\dot{\varepsilon} = const$. For the shear flow the steady values of these functions are found from Eqs. (460) as follows:

$$\widehat{\nu} = b_2/(\lambda_1 - c\overline{\gamma}^2), \qquad \widehat{\psi}_1 = 2\widehat{\nu}/\lambda_1, \qquad \widehat{\psi}_2 = 2b_0\widehat{\nu}/\lambda_1,$$

where $c = 2/3(2b_0^2 + 2b_0 - 1)/\lambda_1 + 2b_1a_0/\lambda_0$. Estimations for the constants (see Table

Table 6: Singular values of elongation rate

b	20	50	100	120	200	∞
$\overline{\varepsilon}^*$	0.864	0.632	0.566	0.555	0.520	0.5

I) shows that $c \leq 0$ for all values of b (case $c = 0$ corresponds to $b = \infty$), thus all three functions are monotonically decreasing in absolute value with increase of quantity $\overline{\gamma}$, besides the case when $b = \infty$. Although they qualitatively correctly predict the shear thinning for large shear rates due to power law, but the exponent -2 of power dependence in the limit of large $\overline{\gamma}$ from the values -0.66 for parameter $\widehat{\nu}$ and -1.33 for $\widehat{\psi}_1$ observed in Brownian dynamic simulations [203]. It is explained by the fact that slopes of shear thining lie out of the applicability domain of our model. A comparison with BD simulations and modified FENE-P model is depicted in Fig. 14.

The predictions for the second normal stress coefficient indicate one more difference between revised Oldroyd 8 constant equation and FENE–P model. FENE–P model shows identically zero values for $\widehat{\psi}_2$ in any shear flow, either steady or time dependent, while the model (460), as well as BD simulations (see Fig. 9 in Ref. [203]) predict small, but nonvanishing values for this quantity. Namely, due to the model (460) in shear flows the following relation $\widehat{\psi}_2 = b_0\widehat{\psi}_1$ is always valid, with proportionality coefficient b_0 small and mostly negative, what leads to small and mostly negative values of $\widehat{\psi}_2$.

In the elongation flow the steady state value to ϑ is found as:

$$\vartheta = \frac{3b_2}{\lambda_1 - \frac{5}{6}(2b_0+1)\overline{\varepsilon} - 7b_1a_0\overline{\varepsilon}^2/\lambda_0}. \tag{477}$$

The denominator has one root on positive semi–axis

$$\overline{\varepsilon}_* = -\frac{5\lambda_0(2b_0+1)}{84b_1a_0} + \left(\left(\frac{5\lambda_0(2b_0+1)}{84b_1a_0}\right)^2 + \frac{\lambda_1\lambda_0}{7b_1a_0}\right)^{1/2}, \tag{478}$$

which defines a singularity point for the dependence $\vartheta(\overline{\varepsilon})$. The BD simulation experiments [203] on the FENE dumbbell models shows that there is no divergence of elongation viscosity for all values of elongation rate (see Fig. 15). For Hookean springs $\overline{\varepsilon}_* = 1/2$ while in our model (460) the singularity point shifts to higher values with respect to decreasing values of b as it is demonstrated in Table 6.

The Figure 16 gives an example of dynamic behavior for elongation viscosity in the instant start-up of the elongational flow. Namely it shows the evolution of initially vanishing polymeric stresses after instant jump of elongation rate at the time moment $t = 0$ from the value $\overline{\varepsilon} = 0$ to the value $\overline{\varepsilon} = 0.3$.

It is possible to conclude that the revised Oldroyd 8 constants model (460) with estimations given by (461) for small and moderate rates of strain up to $\varepsilon_1 = \lambda_{\rm r}|\dot{\boldsymbol{\gamma}}|/(2\lambda_1) \sim 0.5$ yields a good approximation to original FENE dynamics. The quality of the approximation in this interval is the same or better than the one of the nonlinear FENE-P model.

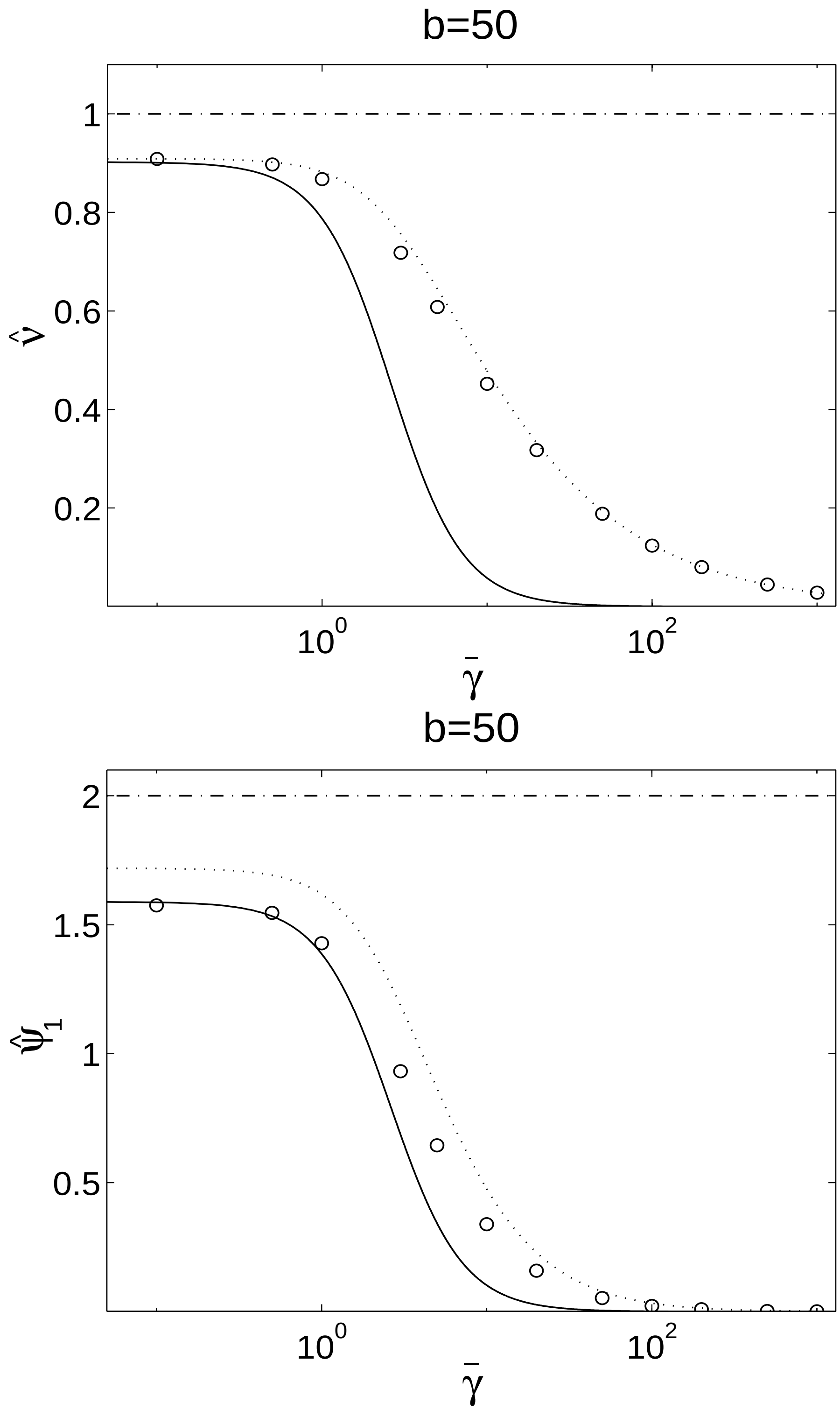


Figure 14: Dimensionless shear viscosity $\widehat{\nu}$ and first normal stress coefficient $\widehat{\psi}_1$ vs. shear rate: (———) revised Oldroyd 8 constants model; $(\cdots\cdots)$ FENE-P model; $(\circ\circ\circ)$ BD simulations on the FENE model; $(-\cdot-\cdot-)$ Hookean dumbbell model.

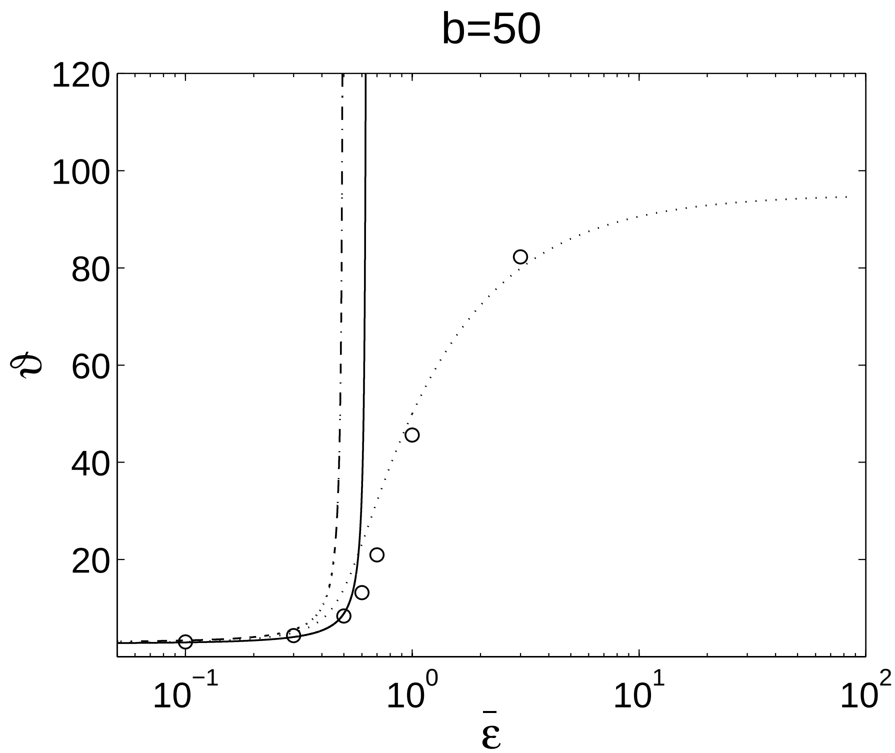


Figure 15: Dimensionless elongation viscosity vs. elongation rate: (——) revised Oldroyd 8 constants model, $(\cdots\cdots)$ FENE-P model, $(\circ\circ\circ)$ BD simulations on the FENE model; $(-\cdot-\cdot-)$ Hookean dumbbell model.

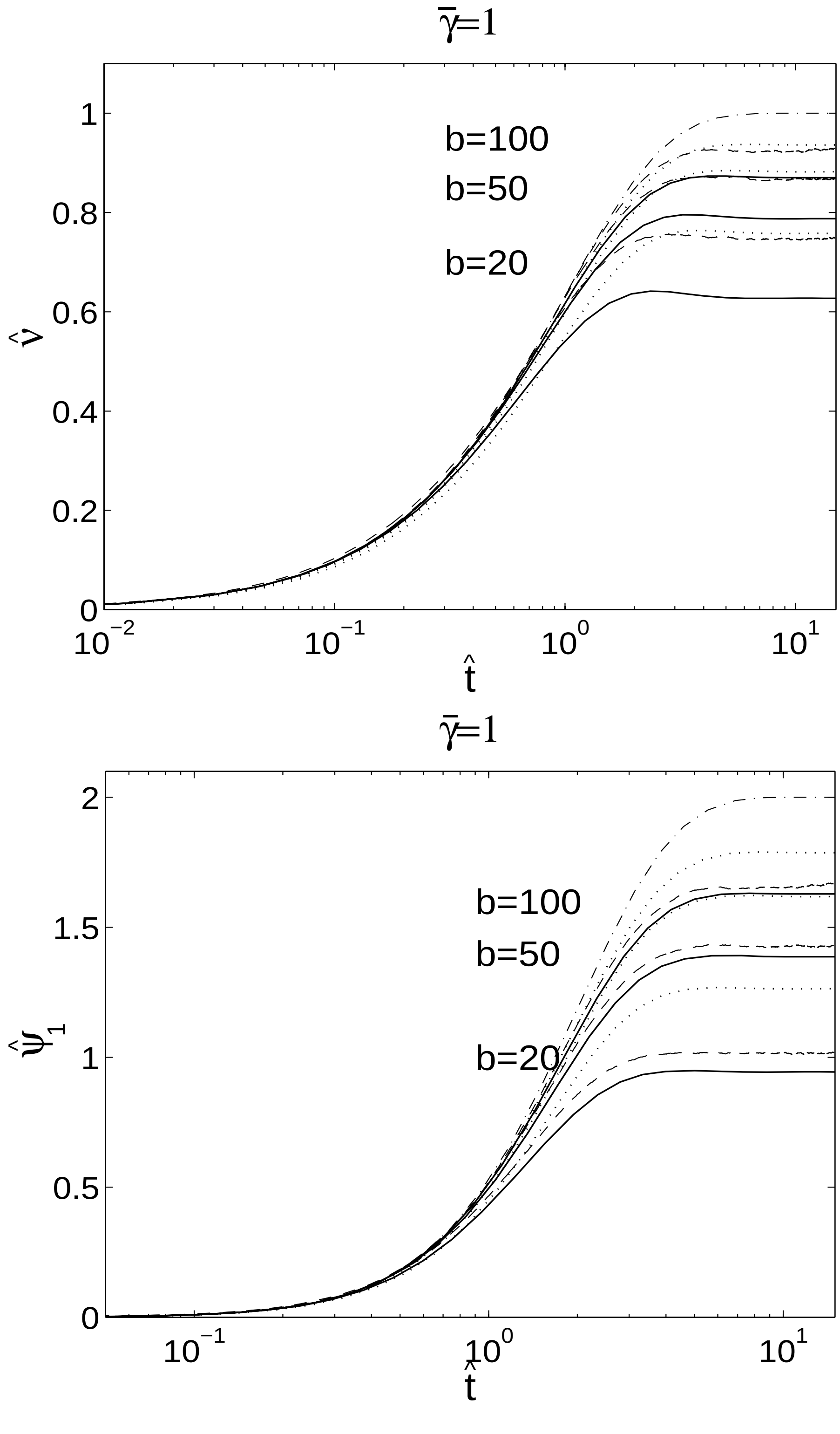


Figure 16: Time evolution of elongation viscosity after inception of the elongation flow with elongation rate $\bar{\varepsilon} = 0.3$: (———) revised Oldroyd 8 constants model, $(\cdots\cdots)$ FENE-P model, $(-\ \ -\ \ -)$ BD simulations on FENE model; $(-\cdot-\cdot-)$ Hookean dumbbell model.

The main results of this Example are as follows:

(i) We have developed a systematic method of constructing constitutive equations from the kinetic dumbbell models for the polymeric solutions. The method is free from a'priori assumptions about the form of the spring force and is consistent with basic physical requirements: frame invariance and dissipativity of internal motions of fluid. The method extends so-called the method of invariant manifold onto equations coupled with external fields. Two characteristic parameters of fluid flow were distinguished in order to account for the effect of the presence of external fields. The iterative Newton scheme for obtaining a slow invariant manifold of the system driven by the flow with relatively low values of both characteristic parameters was developed.

(ii) We demonstrated that the revised phenomenological Oldroyd 8 constants constitutive equations represent the slow dynamics of microscopic elastic dumbbell model with any nonlinear spring force in the limit when the rate of strain and frequency of time variation of the flow are sufficiently small and microscopic states at initial time of evolution are taken not far from the equilibrium.

(iii) The corrections to the zero-order manifold lead generally to linear in stresses equations but with highly nonlinear dependence on the rate of strain tensor and its convective derivatives.

(iv) The zero-order constitutive equation is compared to the direct Brownian dynamics simulation for FENE dumbbell model as well as to predictions of FENE-P model. This comparison shows that the zero-order constitutive equation gives the correct predictions in the domain of its validity, but does not exclude qualitative discrepancy occurring out of this domain, particularly in elongation flows.

This discrepancy calls for a further development, in particular, the use of nonlinear manifolds for derivation of zero-order model. The reason is in the necessity to provide concordance with the requirement of the positivity of distribution function. It may lead to nonlinear constitutive equation on any order of correction. These issues are currently under consideration and results will be reported separately.

Approximations to eigenfunctions of the Fokker-Planck operator

In this appendix we discuss the question how to find the lowest eigenvectors $\Psi_{\rm eq} m_0(Q^2)$ and $\Psi_{\rm eq} m_1(Q^2)\ \overset{\circ}{\mathbf{Q}\mathbf{Q}}$ of the operator $J_{\rm d}$ (422) in the classes of functions having a form: $w_0(Q)$ and $w_1(Q)\ \overset{\circ}{\mathbf{Q}\mathbf{Q}}$. The results presented in this Appendix were used in the subsections: "Constitutive equations" and "Tests on the FENE dumbbell model". It is directly verified that:

$$J_{\rm d} w_0 = G_0^{\rm h} w_0,$$
$$J_{\rm d} w_1\ \overset{\circ}{\mathbf{Q}\mathbf{Q}} = (G_1^{\rm h} w_1)\ \overset{\circ}{\mathbf{Q}\mathbf{Q}},$$

where the operators G_0^{h} and G_1^{h} are given by:

$$G_0^{\mathrm{h}} = G_0 - \kappa H_0, \qquad G_1^{\mathrm{h}} = G_1 - \kappa H_1. \tag{479}$$

The operators $G_{0,1}$ and $H_{0,1}$ act in the space of isotropic functions (i.e. dependent only on $Q = (\boldsymbol{Q} \cdot \boldsymbol{Q})^{1/2}$) as follows:

$$G_0 = \frac{1}{2}\left(\frac{\partial^2}{\partial Q^2} - fQ\frac{\partial}{\partial Q} + \frac{2}{Q}\frac{\partial}{\partial Q}\right), \tag{480}$$

$$G_1 = \frac{1}{2}\left(\frac{\partial^2}{\partial Q^2} - fQ\frac{\partial}{\partial Q} + \frac{6}{Q}\frac{\partial}{\partial Q} - 2f\right), \tag{481}$$

$$H_0 = \frac{2}{Q}\left(\frac{\partial^2}{\partial Q^2} - fQ\frac{\partial}{\partial Q} + \frac{2}{Q}\frac{\partial}{\partial Q}\right), \tag{482}$$

$$H_1 = \frac{2}{Q}\left(\frac{\partial^2}{\partial Q^2} - fQ\frac{\partial}{\partial Q} + \frac{5}{Q}\frac{\partial}{\partial Q} - 2f + \frac{1}{Q^2}\right). \tag{483}$$

The following two properties of the operators $G_{0,1}^{\mathrm{h}}$ are important for our analysis: Let us define two scalar products $\langle \bullet, \bullet \rangle_0$ and $\langle \bullet, \bullet \rangle_1$:

$$\langle y, x \rangle_0 = \langle xy \rangle_{\mathrm{e}},$$

$$\langle y, x \rangle_1 = \langle xyQ^4 \rangle_{\mathrm{e}}.$$

Here $\langle \bullet \rangle_{\mathrm{e}}$ is the equilibrium average as defined in (455). Then we state that for sufficiently small κ the operators G_0^{h} and G_1^{h} are symmetric and nonpositive in the scalar products $\langle \bullet, \bullet \rangle_0$ and $\langle \bullet, \bullet \rangle_1$ respectively. Thus for obtaining the desired eigenvectors of the operator J_{d} we need to find the eigenfunctions m_0 and m_1 related to the lowest nonzero eigenvalues of the operators $G_{0,1}^{\mathrm{h}}$.

Since we regard the parameter κ small it is convenient, first, to find lowest eigenfunctions $g_{0,1}$ of the operators $G_{0,1}$ and, then, to use standard perturbation technique in order to obtain $m_{0,1}$. For the perturbation of the first order one finds [207]:

$$\begin{aligned} m_0 &= g_0 + \kappa h_0, \qquad & h_0 &= -g_0\frac{\langle g_0 H_0 G_0 g_0 \rangle_0}{\langle g_0, g_0 \rangle_0} - G_0 H_0 g_0; \\ m_1 &= g_1 + \kappa h_1, \qquad & h_1 &= -g_1\frac{\langle g_1 H_1 G_1 g_1 \rangle_1}{\langle g_1, g_1 \rangle_1} - G_1 H_1 g_1. \end{aligned} \tag{484}$$

For the rest of this appendix we describe one recurrent procedure for obtaining the functions m_0 and m_1 in a constructive way. Let us solve this problem by minimizing the functionals $\boldsymbol{\Lambda}_{0,1}$:

$$\Lambda_{0,1}[m_{0,1}] = -\frac{\langle m_{0,1}, G_{0,1}^{\mathrm{h}} m_{0,1} \rangle_{0,1}}{\langle m_{0,1}, m_{0,1} \rangle_{0,1}} \longrightarrow \min, \tag{485}$$

by means of the *gradient descent method.*

Let us denote $e_{0,1}$ the eigenfunctions of the zero eigenvalues of the operators $G_{0,1}^{\mathrm{h}}$. Their explicite values are $e_0 = 1$ and $e_1 = 0$. Let the initial approximations $m_{0,1}^{(0)}$ to the lowest eigenfunctions $m_{0,1}$ be chosen so that $\langle m^{(0)}_{0,1}, e_{0,1}\rangle_{0,1} = 0$. We define the variation derivative $\delta\Lambda_{0,1}/\delta m_{0,1}$ and look for the correction in the form:

$$m^{(1)}_{0,1} = m^{(0)}_{0,1} + \delta m^{(0)}_{0,1}, \qquad \delta m^{(0)}_{0,1} = \alpha \frac{\delta\Lambda_{0,1}}{\delta m_{0,1}}, \tag{486}$$

where scalar parameter $\alpha < 0$ is found from the condition:

$$\frac{\partial \Lambda_{0,1}[m^{(1)}_{0,1}(\alpha)]}{\partial\alpha} = 0.$$

In the explicit form the result reads:

$$\delta m^{(0)}_{0,1} = \alpha^{(0)}_{0,1}\Delta^{(0)}_{0,1},$$

where

$$\begin{aligned}
\Delta^{(0)}_{0,1} &= \frac{2}{\langle m^{(0)}_{0,1}, m^{(0)}_{0,1}\rangle_{0,1}}\left(m^{(0)}_{0,1}\lambda^{(0)}_{0,1} - G^{\mathrm{h}}_{0,1} m^{(0)}_{0,1}\right),\\
\lambda^{(0)}_{0,1} &= \frac{\langle m^{(0)}_{0,1}, G^{\mathrm{h}}_{0,1} m^{(0)}_{0,1}\rangle_{0,1}}{\langle m^{(0)}_{0,1}, m^{(0)}_{0,1}\rangle_{0,1}},\\
\alpha^{(0)}_{0,1} &= q_{0,1} - \sqrt{q^2_{0,1} + \frac{\langle m^{(0)}_{0,1}, m^{(0)}_{0,1}\rangle_{0,1}}{\langle \Delta^{(0)}_{0,1}, \Delta^{(0)}_{0,1}\rangle_{0,1}}},\\
q_{0,1} &= \frac{1}{\langle \Delta^{(0)}_{0,1}, \Delta^{(0)}_{0,1}\rangle_{0,1}}\left(\frac{\langle m^{(0)}_{0,1}, G^{\mathrm{h}}_{0,1} m^{(0)}_{0,1}\rangle_{0,1}}{\langle m^{(0)}_{0,1}, m^{(0)}_{0,1}\rangle_{0,1}} - \frac{\langle \Delta^{(0)}_{0,1}, G^{\mathrm{h}}_{0,1} \Delta^{(0)}_{0,1}\rangle_{0,1}}{\langle \Delta^{(0)}_{0,1}, \Delta^{(0)}_{0,1}\rangle_{0,1}}\right).
\end{aligned} \tag{487}$$

Having the new correction $m^{(1)}_{0,1}$ we can repeat the procedure and eventually generate the recurrence scheme. Since by the construction all iterative approximations $m^{(n)}_{0,1}$ remain orthogonal to zero eigenfunctions $e_{0,1}$: $\langle m^{(n)}_{0,1}, e_{0,1}\rangle_{0,1} = 0$ we avoid the convergence of this recurrence procedure to the eigenfunctions $e_{0,1}$.

The quantities $\delta^{(n)}_{0,1}$:

$$\delta^{(n)}_{0,1} = \frac{\langle \Delta^{(n)}_{0,1}, \Delta^{(n)}_{0,1}\rangle_{0,1}}{\langle m^{(n)}_{0,1}, m^{(n)}_{0,1}\rangle_{0,1}}$$

can serve as relative error parameters for controlling the convergence of the iteration procedure (486).

Integration formulas

Let Ω be a sphere in $\mathbf{R}^3$ with the center at the origin of the coordinate system or be the entire space $\mathbf{R}^3$. For any function $s(x^2)$, where $x^2 = \boldsymbol{x}\cdot\boldsymbol{x}$, $\boldsymbol{x} \in \mathbf{R}^3$, and any square 3×3 matrices $\mathbf{A}$, $\boldsymbol{B}$, $\boldsymbol{C}$ independent of $\boldsymbol{x}$ the following integral relations are valid:

$$\int_\Omega s(x^2)\, \overset{\circ}{\mathbf{x}\mathbf{x}}\, (\overset{\circ}{\mathbf{x}\mathbf{x}} : \mathbf{A})\mathrm{d}\boldsymbol{x} = \frac{2}{15}\,\overset{\circ}{\mathbf{A}} \int_\Omega s x^4 \mathrm{d}\boldsymbol{x};$$

$$\int_\Omega s(x^2)\, \overset{\circ}{\mathbf{x}\mathbf{x}}\, (\overset{\circ}{\mathbf{x}\mathbf{x}} : \mathbf{A})(\overset{\circ}{\mathbf{x}\mathbf{x}} : \boldsymbol{B})\mathrm{d}\boldsymbol{x} = \frac{4}{105}\, (\mathbf{A}\cdot\boldsymbol{B} \overset{\circ}{+} \boldsymbol{B}\cdot\mathbf{A}) \int_\Omega s x^6 \mathrm{d}\boldsymbol{x};$$

$$\int_\Omega s(x^2)\, \overset{\circ}{\mathbf{x}\mathbf{x}}\, (\overset{\circ}{\mathbf{x}\mathbf{x}} : \mathbf{A})(\overset{\circ}{\mathbf{x}\mathbf{x}} : \boldsymbol{B})(\overset{\circ}{\mathbf{x}\mathbf{x}} : \boldsymbol{C})\mathrm{d}\boldsymbol{x} =$$

$$\frac{4}{315}\left\{ \overset{\circ}{\mathbf{A}}\, (\boldsymbol{B} : \boldsymbol{C}) + \overset{\circ}{\mathbf{B}}\, (\mathbf{A} : \boldsymbol{C}) + \overset{\circ}{\mathbf{C}}\, (\mathbf{A} : \boldsymbol{B}) \right\} \int_\Omega s x^8 \mathrm{d}\boldsymbol{x}.$$

Example 13: Explosion of invariant manifold and limits of macroscopic description for polymer molecules

Derivation of macroscopic equations from the simplest dumbbell models is revisited [66]. It is demonstrated that the onset of the macroscopic description is sensitive to the flows. For the FENE-P model, small deviations from the Gaussian solution undergo a slow relaxation before the macroscopic description sets on. Some consequences of these observations are discussed.

Dumbbell models and the problem of the classical Gaussian solution stability

Dumbbell models of dilute polymeric solutions are the simplest kinetic (microscopic) models of complex fluids [86]. The macroscopic description in this context is an equation for the stress tensor (the constitutive equation). Since simple models form a basis for our understanding of how the macroscopic description sets on within the kinetic picture, it makes sense to study the derivation of the macroscopic description in every detail for those cases.

In this Example, we revisit the derivation of the constitutive equation from the simplest (solvable) dumbbell models. We focus our attention on the following question: *How well is the macroscopic description represented by the classical Gaussian solution?* It appears that the answer to this question is sensitive to the flow. For weak enough flows, all microscopic solutions approach rapidly the Gaussian solution which manifests validity of the standard macroscopic description. However, for strong flows, relaxation to the Gaussian solution becomes much slower, significant deviations persist over long times, in which case the macroscopic description is less valid. We discuss a possible impact of this observation on the statement of the problem of macroscopic description in related more complicated problems.

We consider the following simplest one-dimensional kinetic equation for the configuration distribution function $\Psi(q,t)$, where q is the reduced vector connecting the beads of the dumbbell:

$$\partial_t \Psi = -\partial_q \{\alpha(t) q \Psi\} + \frac{1}{2}\partial_q^2 \Psi. \tag{488}$$

Here

$$\alpha(t) = \kappa(t) - (1/2) f(M_1(t)), \tag{489}$$

$\kappa(t)$ is the given time-dependent velocity gradient, t is the reduced time, and the function $-fq$ is the reduced spring force. Function f may depend on the second moment of the distribution function $M_1 = \int q^2 \Psi(q,t) dq$. In particular, the case $f \equiv 1$ corresponds to the linear Hookean spring, while $f = [1 - M_1(t)/b]^{-1}$ corresponds to the self-consistent finite extension nonlinear elastic spring (the FENE-P model, first introduced in [205]). The second moment M_1 occurring in the FENE-P force f is the result of the pre-averaging approximation to the original FENE model (with nonlinear spring force $f = [1 - q^2/b]^{-1}$). Leading to closed constitutive equations, the FENE-P model is frequently used in simulations of complex rheological flows as well as the reference for more sophisticated closures to the FENE model [208]. The parameter b changes the characteristics of the force law from Hookean at small extensions to a confining force for $q^2 \to b$. Parameter b is roughly equal to the number of monomer units represented by the dumbbell and should therefore be a large number. In the limit $b \to \infty$, the Hookean spring is recovered. Recently, it has been demonstrated that the FENE-P model appears as first approximation within a systematic self-consistent expansion of nonlinear forces [209, 13].

Eq. (488) describes an ensemble of non-interacting dumbbells subject to a pseudo-elongational flow with fixed kinematics. As it is well known, the Gaussian distribution function,

$$\Psi^{\mathrm{G}}(M_1) = (1/\sqrt{2\pi M_1}) \exp[-q^2/(2M_1)], \tag{490}$$

solves Eq. (488) provided the second moment M_1 satisfies

$$\frac{dM_1}{dt} = 1 + 2\alpha(t)M_1. \tag{491}$$

Solution (490) and (491) is the valid macroscopic description if all other solutions of the Eq. (488) are rapidly attracted to the family of Gaussian distributions (490). In other words [3], the special solution (490) and (491) is the macroscopic description if Eq. (490) is the stable invariant manifold of the kinetic equation (488). If not, then the Gaussian solution is just a member of the family of solutions, and Eq. (491) has no meaning of the macroscopic equation. Thus, the complete answer to the question of validity of the Eq. (491) as the macroscopic equation requires a study of dynamics in the neighborhood of the manifold (490). Because of the simplicity of the model (488), this is possible to a satisfactory level even for M_1-dependent spring forces.

Dynamics of the moments and explosion of the Gaussian manifold

Let $M_n = \int q^{2n}\Psi dq$ denote the even moments (odd moments vanish by symmetry). We consider deviations $\mu_n = M_n - M_n^{\mathrm{G}}$, where $M_n^{\mathrm{G}} = \int q^{2n}\Psi^{\mathrm{G}} dq$ are moments of the Gaussian distribution function (490). Let $\Psi(q, t_0)$ be the initial condition to the Eq. (488) at time $t = t_0$. Introducing functions,

$$p_n(t, t_0) = \exp\left[2n \int_{t_0}^{t} \alpha(t')dt'\right], \tag{492}$$

where $t \geq t_0$, and $n \geq 2$, the *exact* time evolution of the deviations μ_n for $n \geq 2$ reads

$$\mu_2(t) = p_2(t, t_0)\mu_2(t_0), \tag{493}$$

and

$$\mu_n(t) = \left[\mu_n(t_0) + n(2n-1)\int_{t_0}^{t} \mu_{n-1}(t')p_n^{-1}(t', t_0)dt'\right] p_n(t, t_0), \tag{494}$$

for $n \geq 3$. Equations (492), (493) and (494) describe evolution near the Gaussian solution for arbitrary initial condition $\Psi(q, t_0)$. Notice that explicit evaluation of the integral in the Eq. (492) requires solution to the moment equation (491) which is not available in the analytical form for the FENE-P model.

It is straightforward to conclude that any solution with a non-Gaussian initial condition converges to the Gaussian solution asymptotically as $t \to \infty$ if

$$\lim_{t\to\infty} \int_{t_0}^{t} \alpha(t')dt' < 0. \tag{495}$$

However, even if this asymptotic condition is met, deviations from the Gaussian solution may survive for considerable *finite* times. For example, if for some finite time T, the integral in the Eq. (492) is estimated as $\int_{t_0}^{t} \alpha(t')dt' > \alpha(t-t_0)$, $\alpha > 0$, $t \le T$, then the Gaussian solution becomes exponentially unstable during this time interval. If this is the case, the moment equation (491) cannot be regarded as the macroscopic equation. Let us consider specific examples.

For the Hookean spring ($f \equiv 1$) under a constant elongation ($\kappa = \text{const}$), the Gaussian solution is exponentially stable for $\kappa < 0.5$, and it becomes exponentially unstable for $\kappa > 0.5$. The exponential instability in this case is accompanied by the well known breakdown of the solution to the Eq. (491) due to infinite stretching of the dumbbell. Similar instability has been found numerically in three-dimensional flows for high Weissenberg numbers [210, 211].

A more interesting situation is provided by the FENE-P model. As it is well known, due to the singularity of the FENE-P force, the infinite stretching is not possible, and solutions to the Eq. (491) are always well behaved. Thus, in this case, non-convergence to the Gaussian solution (if any), does not interfere with the collapse of the solution to the Eq. (491).

Eqs. (491) and (493) were integrated by the 5-th order Runge-Kutta method with adaptive time step. The FENE-P parameter b was set equal to 50. The initial condition was $\Psi(q,0) = C(1-q^2/b)^{b/2}$, where C is the normalization (the equilibrium of the FENE model, notoriously close to the FENE-P equilibrium [203]). For this initial condition, in particular, $\mu_2(0) = -6b^2/[(b+3)^2(b+5)]$ which is about 4% of the value of M_2 in the Gaussian equilibrium for $b = 50$. In Fig. 17 we demonstrate deviation $\mu_2(t)$ as a function of time for several values of the flow. Function $M_1(t)$ is also given for comparison. For small enough κ we find an adiabatic regime, that is μ_2 relaxes exponentially to zero. For stronger flows, we observe an initial *fast runaway* from the invariant manifold with $|\mu_2|$ growing over three orders of magnitude compared to its initial value. After the maximum deviation has been reached, μ_2 relaxes to zero. This relaxation is exponential as soon as the solution to Eq. (491) approaches the steady state. However, the time constant for this exponential relaxation $|\alpha_\infty|$ is very small. Specifically, for large κ,

$$\alpha_\infty = \lim_{t\to\infty} \alpha(t) = -\frac{1}{2b} + O(\kappa^{-1}). \tag{496}$$

Thus, the steady state solution is unique and Gaussian but the stronger is the flow, the larger is the initial runaway from the Gaussian solution, while the return to it thereafter becomes flow-independent. Our observation demonstrates that, though the stability condition (495) is met, *significant deviations from the Gaussian solution persist over the times when the solution of Eq.* (491) *is already reasonably close to the stationary state.* If we

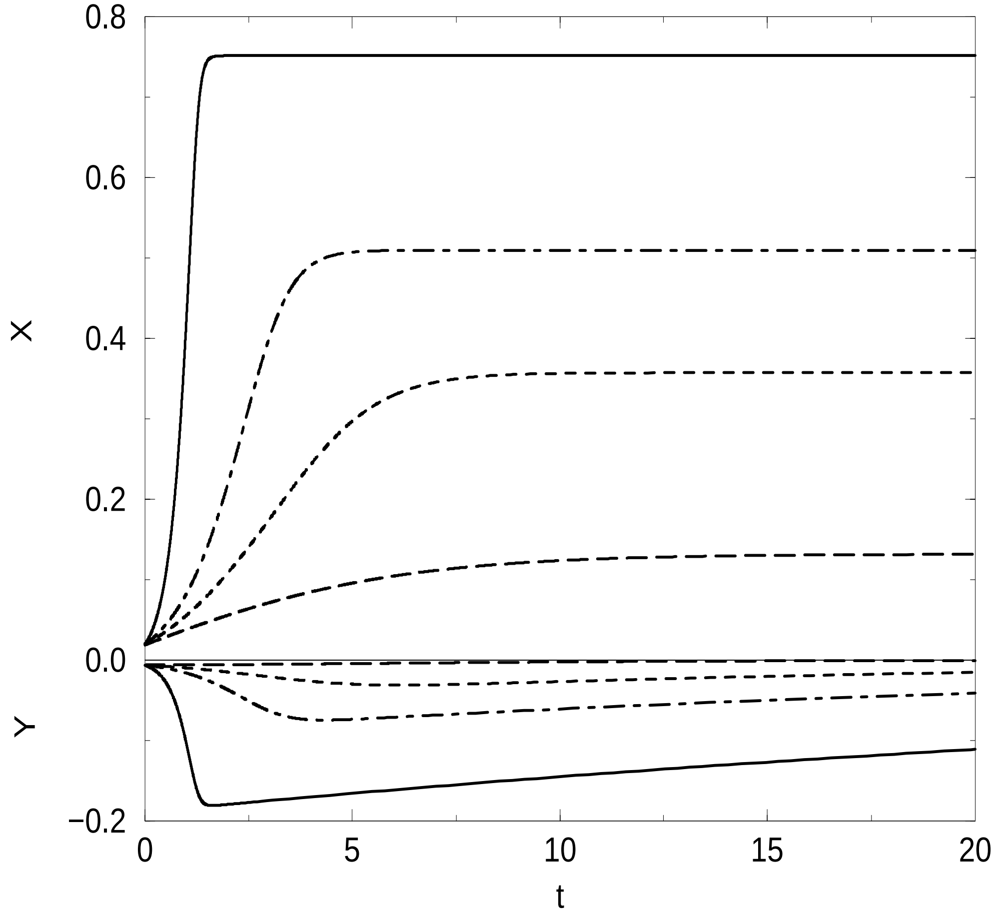


Figure 17: Deviations of reduced moments from the Gaussian solution as a function of reduced time t in pseudo-elongation flow for the FENE-P model. Upper part: Reduced second moment $X = M_1/b$. Lower part: Reduced deviation of fourth moment from Gaussian solution $Y = -\mu_2^{1/2}/b$. Solid: $\kappa = 2$, dash-dot: $\kappa = 1$, dash: $\kappa = 0.75$, long dash: $\kappa = 0.5$.

accept the usually quoted physically reasonable minimal value of parameter b of the order 20 then the minimal relaxation time is of order 40 in the reduced time units of Fig. 17. We should also stress that the two limits, $\kappa \to \infty$ and $b \to \infty$, are not commutative, thus it is not surprising that the estimation (496) does not reduce to the above mentioned Hookean result as $b \to \infty$. Finally, peculiarities of convergence to the Gaussian solution are even furthered if we consider more complicated (in particular, oscillating) flows $\kappa(t)$. We close this Example with several comments.

(i). From the standpoint of a general theory of macroscopic description [3], the set of Gaussian distributions (490) is the invariant manifold of the kinetic equation (488), while Eq. (491) is the dynamic equation on the invariant manifold written in natural internal variables of this manifold. This macroscopic description is supplemented by Eqs. (493), (494) which give the dynamics near the invariant manifold. Though the models we have considered here are simple, our observations demonstrate that relaxation to the invariant manifold may be very slow depending on the flow.

(ii). For more difficult models, such as the FENE model, finding invariant manifold is a difficult task. However, there exist methods to derive approximate invariant manifolds by iteration procedures [3]. It has been shown recently that the macroscopic description of any dumbbell model is a revised Oldroyd 8-constant model for low Deborah number flows [5]. For strong flows, *ad hoc* closures are frequently used and little is known about their stability and whether they respect the invariance principle. It would be interesting to find out whether good closure approximations correspond to invariant manifolds, identify them and learn about their stability.

12 Accuracy estimation and postprocessing in invariant manifolds constructing

Suppose that for the dynamical system (34) the approximate invariant manifold has been constructed and the slow motion equations have been derived:

$$\frac{dx_{sl}}{dt} = P_{x_{sl}}(J(x_{sl})), x_{sl} \in M, \tag{497}$$

where $P_{x_{sl}}$ is the corresponding projector onto the tangent space $T_{x_{sl}}$ of M. Suppose that we have solved the system (497) and have obtained $x_{sl}(t)$. Let's consider the following two questions:

- How well this solution approximates the real solution $x(t)$ given the same initial conditions?
- How is it possible to use the solution $x_{sl}(t)$ for it's refinement without solving the system (497) again?

These two questions are interconnected. The first question states the problem of the *accuracy estimation*. The second one states the problem of *postprocessing*.

The simplest ("naive") estimation is given by the "invariance defect":

$$\Delta_{x_{sl}} = (1 - P_{x_{sl}})J(x_{sl}) \tag{498}$$

compared with $J(x_{sl})$. For example, this estimation is given by $\epsilon = \|\Delta_{x_{sl}}\|/\|J(x_{sl})\|$ using some appropriate norm.

Probably, the most comprehensive answer for this question can be given by solving the following equation:

$$\frac{d(\delta x)}{dt} = \Delta_{x_{sl}(t)} + D_x J(x)|_{x_{sl}(t)} \delta x. \tag{499}$$

This linear equation describes the dynamics of the deviation $\delta x(t) = x(t) - x_{sl}(t)$ using the linear approximation. The solution with zero initial conditions $\delta x(0) = 0$ allows estimating x_{sl} robustness as well as the error value. Substituting $x_{sl}(t)$ for $x_{sl}(t) + \delta x(t)$ gives the required solution refinement. This *dynamical postprocessing* [193] allows to refine the solution substantially and to estimate it's accuracy and robustness. However, the price for this is solving the equation (499) with variable coefficients. Thus, this dynamical postprocessing can be followed by the whole hierarchy of simplifications, both dynamical and static. Let's mention some of them, starting from the dynamical ones.

1) **Freezing the coefficients**. In the equation (499) the linear operator $D_x J(x)|_{x_{sl}(t)}$ is replaced by it's value in some distinguished point x^* (for example, in the equilibrium) or it is frozen somehow else. As a result, one gets the equation with constant coefficients and the explicit integration formula:

$$\delta x(t) = \int_0^t exp(D^*(t-\tau))\Delta_{x_{sl}(\tau)}d\tau, \tag{500}$$

where D^* is the "frozen" operator and $\delta x(0) = 0$.

Another important way of freezing is substituting (499) for some *model equation*, i.e. substituting $D_x J(x)$ for $-\frac{1}{\tau^*}$, where τ^* is the relaxation time. In this case the formula for $\delta x(t)$ has very simple form:

$$\delta x(t) = \int_0^t e^{\frac{\tau - t}{\tau^*}}\Delta_{x_{sl}(\tau)}d\tau. \tag{501}$$

2) **One-dimensional Galerkin-type approximation.** Another "scalar" approximation is given by projecting (499) on $\Delta(t) = \Delta_{x_{sl}(t)}$:

$$\delta x(t) = \delta(t)\cdot\Delta(t),\ \frac{d\delta(t)}{dt} = 1 + \delta\frac{\langle\Delta|D\Delta\rangle - \langle\Delta|\dot{\Delta}\rangle}{\langle\Delta|\Delta\rangle}, \tag{502}$$

where $\langle|\rangle$ is an appropriate scalar product, which can depend on the point x_{sl} (for example, the entropic scalar product), $D = D_x J(x)|_{x_{sl}(t)}$ or the self-adjoint linearizarion of this operator, or some approximation of it.

The "hybrid" between equations (502) and (499) has the simplest form (but is more difficult for computation than eq. (502)):

$$\frac{d(\delta x)}{dt} = \Delta(t) + \frac{\langle\Delta|D\Delta\rangle}{\langle\Delta|\Delta\rangle}\delta x. \tag{503}$$

Here one uses the normalized matrix element $\frac{\langle\Delta|D\Delta\rangle}{\langle\Delta|\Delta\rangle}$ instead of the linear operator $D = D_x J(x)|_{x_{sl}(t)}$.

Both equations (502) and (503) can be solved explicitly:

$$\delta(t) = \int_0^t d\tau \exp\left(\int_\tau^t k(\theta)d\theta\right), \tag{504}$$

$$\delta x(t) = \int_0^t \Delta(\tau)d\tau \exp\left(\int_\tau^t k_1(\theta)d\theta\right), \tag{505}$$

where $k(t) = \frac{\langle\Delta|D\Delta\rangle - \langle\Delta|\dot{\Delta}\rangle}{\langle\Delta|\Delta\rangle}$, $k_1(t) = \frac{\langle\Delta|D\Delta\rangle}{\langle\Delta|\Delta\rangle}$.

3) For a **static postprocessing** one uses stationary points of dynamical equations (499) or their simplified versions (500),(502). Instead of (499) one gets:

$$D_x J(x)|_{x_{sl}(t)}\delta x = -\Delta_{x_{sl}(t)} \tag{506}$$

with one additional condition $P_{x_{sl}}\delta x = 0$. This is exactly the iteration equation of the Newton's method in solving the invariance equation.

The corresponding stationary problems for the model equations and for the projections of (499) on Δ are evident. We only mention that in the projection on Δ one gets a step of the relaxation method for the invariant manifold construction.

For the static postprocessing with frozen parameters the "naive" estimation given by the "invariance defect" (498) makes sense.

In the following example it will be demonstrated how one can utilize Δ in the accuracy estimation of macroscopic equations and we will provide one example of such utilization for polymer solution dynamics.

Example 14: Defect of invariance estimation and switching from the microscopic simulations to macroscopic equations

A method which recognizes the onset and breakdown of the macroscopic description in microscopic simulations was developed in [13, 212]. The method is based on the invariance of the macroscopic dynamics relative to the microscopic dynamics, and it is demonstrated for a model of dilute polymeric solutions where it decides switching between Direct Brownian Dynamics simulations and integration of constitutive equations.

Invariance principle and micro-macro computations

Derivation of reduced (macroscopic) dynamics from the microscopic dynamics is the dominant theme of non–equilibrium statistical mechanics. At the present time, this very old theme demonstrates new facets in view of a massive use of simulation techniques on various levels of description. A two–side benefit of this use is expected: On the one hand, simulations provide data on molecular systems which can be used to test various theoretical constructions about the transition from micro to macro description. On the other hand, while the microscopic simulations in many cases are based on limit theorems [such as, for example, the central limit theorem underlying the Direct Brownian Dynamics simulations (BD)] they are extremely time–consuming in any real situation, and a timely recognition of the onset of a macroscopic description may considerably reduce computational efforts.

In this section, we aim at developing a 'device' which is able to recognize the onset and the breakdown of a macroscopic description in the course of microscopic computations.

Let us first present the main ideas of the construction in an abstract setting. We assume that the microscopic description is set up in terms of microscopic variables ξ. In the examples considered below, microscopic variables are distribution functions over the configuration space of polymers. The microscopic dynamics of variables ξ is given by the microscopic time derivative $\dot{\xi}(\xi)$. We also assume that the set of macroscopic variables $\boldsymbol{M}$ is chosen. Typically, the macroscopic variables are some lower-order moments if the microscopic variables are distribution functions. The reduced (macroscopic) description assumes (a) The dependence $\xi(\boldsymbol{M})$, and (b) The macroscopic dynamics $\dot{\boldsymbol{M}}(\boldsymbol{M})$. We do not discuss here in any detail the way one gets the dependence $\xi(\boldsymbol{M})$, however, we should remark that, typically, it is based on some (explicit or implicit) idea about decomposition of motions into slow and fast, with M as slow variables. With this, such tools as maximum entropy principle, quasi-stationarity, cumulant expansion etc. become available for constructing the dependence $\xi(\boldsymbol{M})$.

Let us compare the microscopic time derivative of the function $\xi(\boldsymbol{M})$ with its macroscopic time derivative due to the macroscopic dynamics:

$$\Delta(\boldsymbol{M}) = \frac{\partial \xi(\boldsymbol{M})}{\partial \boldsymbol{M}} \cdot \dot{\boldsymbol{M}}(\boldsymbol{M}) - \dot{\xi}(\xi(\boldsymbol{M})). \tag{507}$$

If the *mismatch* $\Delta(\boldsymbol{M})$ (507) is equal to zero on the set of admissible values of the macroscopic variables M, it is said that the reduced description $\xi(\boldsymbol{M})$ is invariant. Then the function $\xi(\boldsymbol{M})$ represents the invariant manifold in the space of microscopic variables. The invariant manifold is relevant if it is stable. Exact invariant manifolds are known in a very few cases (for example, the exact hydrodynamic description in the kinetic Lorentz gas model [114], in Grad's systems [20, 21], and one more example will be mentioned below). Corrections to the approximate reduced description through minimization of the mismatch is a part of the so–called method of invariant manifolds [3]. We here consider a different application of the invariance principle for the purpose mentioned above.

The time dependence of the macroscopic variables can be obtained in two different ways: First, if the solution of the microscopic dynamics at time t with initial data at t_0 is ξ_{t,t_0}, then evaluation of the macroscopic variables on this solution gives $\boldsymbol{M}^{\text{micro}}_{t,t_0}$. On the other hand, solving dynamic equations of the reduced description with initial data at t_0 gives $\boldsymbol{M}^{\text{macro}}_{t,t_0}$. Let $\|\Delta\|$ be a value of mismatch with respect to some norm, and $\epsilon > 0$ is a fixed tolerance level. Then, if at the time t the following inequality is valid,

$$\|\Delta(\boldsymbol{M}^{\text{micro}}_{t,t_0})\| < \epsilon, \tag{508}$$

this indicates that the accuracy provided by the reduced description is not worse than the true microscopic dynamics (the macroscopic description *sets on*). On the other hand, if

$$\|\Delta(\boldsymbol{M}^{\text{macro}}_{t,t_0})\| > \epsilon, \tag{509}$$

then the accuracy of the reduced description is insufficient (the reduced description *breaks down*), and we must use the microscopic dynamics.

Thus, evaluating the mismatch (507) on the current solution to macroscopic equations, and checking the inequality (509), we are able to answer the question whether we can trust the solution without looking at the microscopic solution. If the tolerance level is not exceeded then we can safely integrate the macroscopic equation. We now proceed to a specific example of this approach. We consider a well–known class of microscopic models of dilute polymeric solutions

Application to dynamics of dilute polymer solution

A well–known problem of the non–Newtonian fluids is the problem of establishing constitutive equations on the basis of microscopic kinetic equations. We here consider a model introduced by Lielens *et al.* [208]:

$$\dot{f}(q,t) = -\partial_q \left\{ \kappa(t) q f - \frac{1}{2} f \partial_q U(q^2) \right\} + \frac{1}{2}\partial_q^2 f. \tag{510}$$

With the potential $U(x) = -(b/2)\ln(1 - x/b)$ Eq. (510) becomes the one–dimensional version of the FENE dumbbell model which is used to describe the elongational behavior of dilute polymer solutions.

The reduced description seeks a closed time evolution equation for the stress $\tau = \langle q\partial_q U(q^2)\rangle - 1$. Due to its non–polynomial character, the stress τ for the FENE potential depends on all moments of f. We have shown in [209] how such potentials can

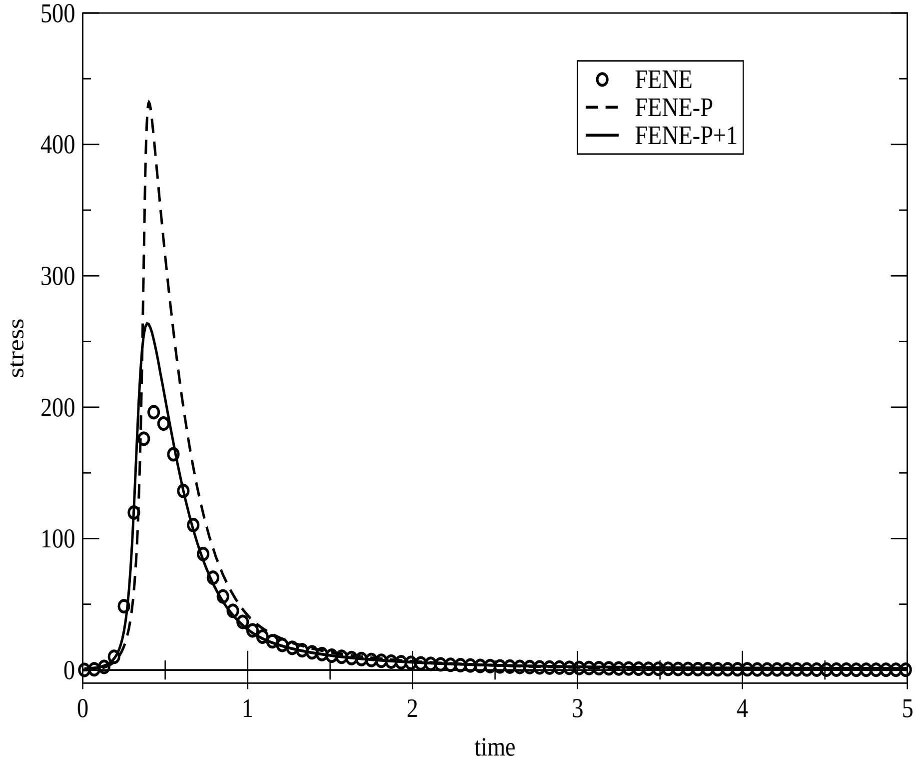


Figure 18: Stress τ versus time from direct Brownian dynamics simulation: symbols – FENE, dashed line – FENE–P, solid line – FENE-P+1.

be approximated systematically by a set of polynomial potentials $U_n(x) = \sum_{j=1}^{n} \frac{1}{2j} c_j x^j$ of degree n with coefficients c_j depending on the even moments $M_j = \langle q^{2j} \rangle$ of f up to order n, with $n = 1, 2, \ldots$, formally converging to the original potential as n tends to infinity. In this approximation, the stress τ becomes a function of the first n even moments of f, $\tau(\boldsymbol{M}) = \sum_{j=1}^{n} c_j M_j - 1$, where the set of macroscopic variables is denoted by $\boldsymbol{M} = \{M_1, \ldots, M_n\}$.

The first two potentials approximating the FENE potential are:

$$
\begin{aligned}
U_1(q^2) &= U'(M_1) q^2 && (511)\\
U_2(q^2) &= \frac{1}{2}(q^4 - 2M_1 q^2) U''(M_1) + \frac{1}{2}(M_2 - M_1^2) q^2 U'''(M_1), && (512)
\end{aligned}
$$

where U', U'' and U''' denote the first, second and third derivative of the potential U, respectively. The potential U_1 corresponds to the well–known FENE–P model. The kinetic equation (510) with the potential U_2 (512) will be termed the FENE–P+1 model below. Direct Brownian Dynamics simulation (BD) of the kinetic equation (510) with the potential U_2 for the flow situations studied in [208] demonstrates that it is a reasonable approximation to the true FENE dynamics whereas the corresponding moment chain is of a simpler structure. In [13] this was shown for a periodic flow, while Fig. 18 shows results for the flow

$$
\kappa(t) = \begin{cases} 100t(1-t)e^{-4t} & 0 \le t \le 1 \\ 0 & \text{else} \end{cases} \qquad (513)
$$

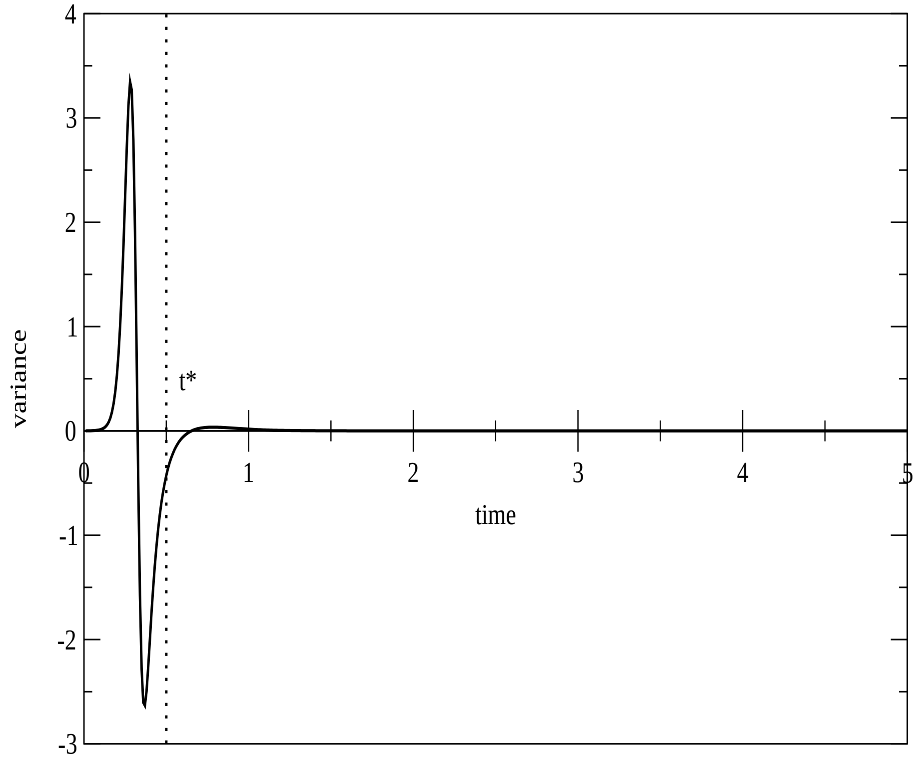


Figure 19: Mismatch Δ_3/b^3, Eq. (517), versus time extracted from BD simulation (the FENE–P+1 model) for the flow situation of Eq. (513).

The quality of the approximation indeed increases with the order of the polynomial.

For any potential U_n, the invariance equation can be studied directly in terms of the full set of the moments, which is equivalent to studying the distribution functions. The kinetic equation (510) can be rewritten equivalently in terms of moment equations,

$$\begin{aligned} \dot{M}_k &= F_k(M_1, \dots, M_{k+n-1}) \\ F_k &= 2k\kappa(t)M_k + k(2k-1)M_{k-1} - k\sum_{j=1}^{n} c_j M_{k+j-1}. \end{aligned} \tag{514}$$

We seek functions $M_k^{\mathrm{macro}}(\boldsymbol{M})$, $k = n+1, \dots$ which are form–invariant under the dynamics:

$$\sum_{j=1}^{n} \frac{\partial M_k^{\mathrm{macro}}(\boldsymbol{M})}{\partial M_j} F_j(\boldsymbol{M}) = F_k(M_1, \dots, M_n, M_{n+1}(\boldsymbol{M}), \dots, M_{n+k}(\boldsymbol{M})). \tag{515}$$

This set of invariance equations states the following: The time derivative of the form $M_k^{\mathrm{macro}}(\boldsymbol{M})$ when computed due to the closed equation for $\boldsymbol{M}$ (the first contribution on the left hand side of Eq. (515), or the 'macroscopic' time derivative) equals the time derivative of M_k as computed by true moment equation with the same form $M_k(\boldsymbol{M})$ (the second contribution, or the 'microscopic' time derivative), and this equality should hold whatsoever values of the moments $\boldsymbol{M}$ are.

Equations (515) in case $n = 1$ (FENE–P) are solvable exactly with the result

$$M_k^{\mathrm{macro}} = a_k M_1^k, \qquad \text{with} \quad a_k = (2k-1)a_{k-1}, \; a_0 = 1.$$

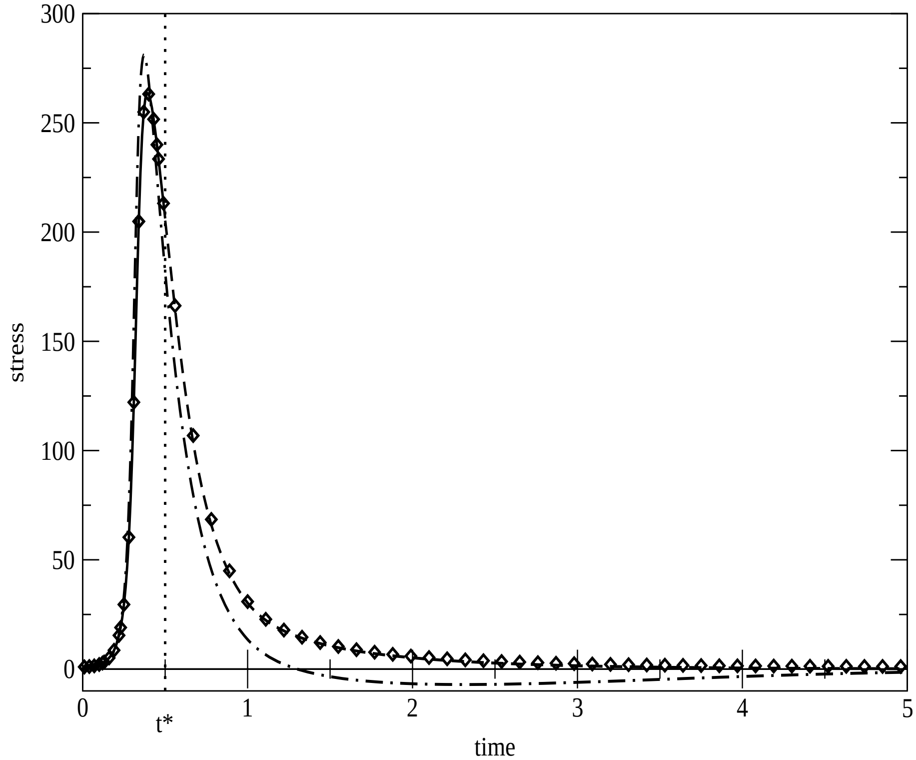


Figure 20: Switching from the BD simulations to macroscopic equations after the mismatch has reached the given tolerance level (the FENE–P+1 model): symbols – the BD simulation, solid line – the BD simulation from time $t = 0$ up to time $t = t^*$, dashed line – integration of the macroscopic dynamics with initial data from BD simulation at time $t = t^*$. For comparison, the dot–dashed line gives the result for the integration of the macroscopic dynamics with equilibrium conditions from $t = 0$. Inset: Transient dynamics at the switching from BD to macroscopic dynamics on a finer time scale.

This dependence corresponds to the Gaussian solution in terms of the distribution functions. As expected, the invariance principle give just the same result as the usual method of solving the FENE–P model.

Let us briefly discuss the potential U_2, considering a simple closure approximation

$$M_k^{\mathrm{macro}}(M_1, M_2) = a_k M_1^k + b_k M_2 M_1^{k-2}, \tag{516}$$

where $a_k = 1 - k(k-1)/2$ and $b_k = k(k-1)/2$. The function M_3^{macro} closes the moment equations for the two independent moments M_1 and M_2. Note, that M_3^{macro} differs from the corresponding moment M_3 of the actual distribution function by the neglect of the 6–th cumulant. The mismatch of this approximation is a set of functions Δ_k where

$$\Delta_3(M_1, M_2) = \frac{\partial M_3^{\mathrm{macro}}}{\partial M_1} F_1 + \frac{\partial M_3^{\mathrm{macro}}}{\partial M_2} F_2 - F_3, \tag{517}$$

and analogously for $k \geq 3$. In the sequel, we make all conclusions based on the mismatch Δ_3 (517).

It is instructive to plot the mismatch Δ_3 versus time, assuming the functions M_1 and M_2 are extracted from the BD simulation (see Fig. 19). We observe that the mismatch is a nonmonotonic function of the time, and that there are three pronounced domains: From $t_0 = 0$ to t_1 the mismatch is almost zero which means that the ansatz is reasonable. In the intermediate domain, the mismatch jumps to high values (so the quality of approximation is poor). However, after some time $t = t^*$, the mismatch again becomes negligible, and remains so for later times. Such behavior is typical of so–called "kinetic layer".

Instead of attempting to improve the closure, the invariance principle can be used directly to switch from the BD simulation to the solution of the macroscopic equation without loosing the accuracy to a given tolerance. Indeed, the mismatch is a function of M_1 and M_2, and it can be easily evaluated both on the data from the solution to the macroscopic equation, and the BD data. If the mismatch *exceeds* some given tolerance on the macroscopic solution this signals to switch to the BD integration. On the other hand, if the mismatch becomes *less* than the tolerance level on the BD data signals that the BD simulation is not necessary anymore, and one can continue with the integration of the macroscopic equations. This reduces the necessity of using BD simulations only to get through the kinetic layers. A realization of this hybrid approach is demonstrated in Fig. 20: For the same flow we have used the BD dynamics only for the first period of the flow while integrated the macroscopic equations in all the later times. The quality of the result is comparable to the BD simulation whereas the total integration time is much shorter. The *transient dynamics* at the point of switching from the BD scheme to the integration of the macroscopic equations (shown in the inset in Fig. 20) deserves a special comment: The initial conditions at t^* are taken from the BD data. Therefore, we cannot expect that at the time t^* the solution is already on the invariant manifold, rather, at best, close to it. Transient dynamics therefore signals the *stability* of the invariant manifold we expect: Even though the macroscopic solution starts not on this manifold, it nevertheless attracts to it. The transient dynamics becomes progressively less pronounced if the switching is done at later times. The stability of the invariant manifold in case of the FENE–P model is studied in detail in [66].

The present approach of combined microscopic and macroscopic simulations can be realized on the level of moment closures (which then needs reconstruction of the distribution function from the moments at the switching from macroscopic integration to BD procedures), or for parametric sets of distribution functions if they are available [208].

13 Conclusion

To construct slow invariant manifolds is useful. Effective model reduction becomes impossible without them for complex kinetic systems.

Why to reduce description in the times of supercomputers?

First, in order to gain understanding. In the process of reducing the description one is often able to extract the essential, and the mechanisms of the processes under study become more transparent.

Second, if one is given the detailed description of the system, then one should be able also to solve the initial-value problem for this system. But what should one do in the case where the system is representing just a small part of the huge number of interacting systems? For example, a complex chemical reaction system may represent only a point in a three-dimensional flow.

Third, without reducing the kinetic model, it is impossible to construct this model. This statement seems paradoxal only at the first glance: How come, the model is first simplified, and is constructed only after the simplification is done? However, in practice, the typical for a mathematician statement of the problem, (Let the system of differential equations be *given*, then ...) is rather rarely applicable for detailed kinetics. Quite on the contrary, the thermodynamic data (energies, enthalpies, entropies, chemical potentials etc) for sufficiently rarefied systems are quite reliable. Final identification of the model is always done on the basis of comparison with the experiment and with a help of fitting. For this purpose, it is extremely important to reduce the dimension of the system, and to reduce the number of tunable parameters.

And, finally, for every supercomputer there exist too complicated problems. Model reduction makes these problems less complicated and sometimes gives us the possibility to solve them.

It is useful to apply thermodynamics and the quasiequilibrium concept while seeking slow invariant manifolds. Though the open systems are important for many applications, however, it is useful to begin their study and model reduction with the analysis of closed (sub)sustems. Then the thermodynamics equips these systems with Lyapunov functions (entropy, free energy, free enthalpy, depending on the context). These Lyapunov functions are usually known much better than the right hand sides of kinetic equations (in particular, this is the case in reaction kinetics). Using this Lyapunov function, one constructs the initial approximation to the slow manifold, that is, the quasiequilibrium manifold, and also one constructs the thermodynamic projector.

The thermodynamic projector is the unique operator which transforms the arbitrary vector field equipped with the given Lyapunov function into a vector field with the same Lyapunov function (and also this happens on any manifold which is not tangent to the level of the Lyapunov function).

The quasi-chemical approximation is an extremely rich toolbox for assembling equations. It enables to construct and study wide classes of evolution equations equipped with prescribed Lyapunov functions, with Onsager reciprocity relations and like.

Slow invariant manifolds of thermodynamically closed systems are useful for constructing slow invariant manifolds of corresponding open systems. The necessary technic is developed.

Postprocessing of the invariant manifold construction is important both for estimation of the accuracy and for the accuracy improvement.

The main result of this work can be formulated as follows: **It is possible indeed to construct invariant manifolds.** The problem of constructing invariant manifolds can be formulated as the invariance equation, subject to additional conditions of slowness (stability). The Newton method with incomplete linearization, relaxation methods, the method of natural projector, and the method of invariant grids enables educated approximations to the slow invariant manifolds.

Studies on invariant manifolds were initiated by A. Lyapunov [98] and H. Poincare [99] (see [100]). Essential stages of the development of these ideas in the XX century are reflected in the books [100, 214, 183, 182]. It becomes more and more evident at the present time that the constructive methods of invariant manifold are useful on a host of subjects, from applied hydrodynamics [215] to physical and chemical kinetics.

References

[1] Gorban, A. N., Karlin, I. V., The constructing of invariant manifolds for the Boltzmann equation, *Adv. Model. and Analysis C*, **33(3)** (1992), 39-54.

[2] Gorban, A. N., Karlin, I. V., Thermodynamic parameterization, *Physica A*, **190** (1992), 393-404.

[3] Gorban, A. N., Karlin, I. V., Method of invariant manifolds and regularization of acoustic spectra. *Transport Theory and Stat. Phys.*, **23** (1994), 559-632.

[4] Karlin, I. V., Dukek, G., Nonnenmacher, T. F., Invariance principle for extension of hydrodynamics: Nonlinear viscosity. *Phys. Rev. E*, **55(2)** (1997), 1573-1576.

[5] Zmievskii, V. B., Karlin, I. V., Deville, M., The universal limit in dynamics of dilute polymeric solutions. *Physica A*, **275(1-2)** (2000), 152-177.

[6] Karlin, I. V., Gorban, A. N., Dukek, G., Nonnenmacher, T. F. Dynamic correction to moment approximations. *Phys. Rev. E*, **57** (1998), 1668–1672.

[7] Gorban, A. N., Karlin, I. V., Method of invariant manifold for chemical kinetics, Chem. Eng. Sci., to appear. Preprint online: http://arxiv.org/abs/cond-mat/0207231, 9 Jul 2002.

[8] Gorban, A. N., Karlin, I. V., Zmievskii, V. B., Dymova S. V., Reduced description in reaction kinetics. *Physica A*, **275(3-4)** (2000), 361–379.

[9] Karlin, I. V., Zmievskii, V. B., Invariant closure for the Fokker-Planck equation, 1998. Preprint online: http://arxiv.org/abs/adap-org/9801004 4 Feb 1998.

[10] Foias, C., Jolly, M. S., Kevrekidis, I. G., Sell, G. R., Titi, E. S. On the computation of inertial manifolds, Physics Letters A, **131**, 7-8 (1988), 433-436.

[11] Gorban, A. N., Karlin, I. V., Zmievskii, V. B., Nonnenmacher, T. F., Relaxational trajectories: global approximations. *Physica A*, **231** (1996), 648-672.

[12] Gorban, A. N., Karlin, I. V., Zmievskii, V. B., Two–step approximation of space–independent relaxation. *Transp. Theory Stat. Phys.*. **28(3)** (1999), 271–296.

[13] Gorban, A. N., Karlin, I. V., Ilg, P. and Öttinger, H. C., Corrections and enhancements of quasi-equilibrium states, J. Non-Newtonian Fluid Mech. **96** (2001), 203–219.

[14] Gorban, A. N., Karlin, I. V., Öttinger, H. C. , and Tatarinova, L. L., Ehrenfests argument extended to a formalism of nonequilibrium thermodynamics, Phys. Rev. E **63** (2001), 066124(1-6).

[15] Gorban, A. N., Karlin, I. V., Reconstruction lemma and fluctuation-dissipation theorem, Revista Mexicana de Fisica **48**, Supl. 1 (2002), 238-242.

[16] Gorban, A. N., Karlin, I. V., Macroscopic dynamics through coarse-graining: A solvable example *Phys. Rev. E*, **56** (2002), 026116(1-5).

[17] Gorban, A. N., Karlin, I. V., Geometry of irreversibility, in: Recent Developments in Mathematical and Experimental Physics, Volume C: Hydrodynamics and Dynamical Systems, Ed. F. Uribe (Kluwer, Dordrecht, 2002), 19–43.

[18] Karlin, I. V., Tatarinova, L. L., Gorban, A. N., Öttinger, H. C., Irreversibility in the short memory approximation, Physica A, to appear. Preprint online: http://arXiv.org/abs/cond-mat/0305419 v1 18 May 2003.

[19] Karlin, I. V., Ricksen, A., Succi, S., Dissipative Quantum Dynamics from Wigner Distributions, in: Quantum Limits to the Second Law: First International Conference on Quantum Limits to the Second Law, San Diego, California (USA), 29-31 July 2002, AIP Conference Proceedings, **643**, 19-24.

[20] Gorban, A. N., Karlin, I. V., Short-Wave Limit of Hydrodynamics: A Soluble Example, Phys. Rev. Lett. **77** (1996), 282-285.

[21] Karlin, I. V., Gorban, A. N., Hydrodynamics from Grad's equations: What can we learn from exact solutions?, Ann. Phys. (Leipzig) **11** (2002), 783-833. Online: http://arXiv.org/abs/cond-mat/0209560.

[22] Gorban, A. N., Karlin, I. V., Structure and Approximations of the Chapman-Enskog Expansion, Sov. Phys. JETP **73** (1991), 637-641.

[23] Gorban, A. N., Karlin, I. V., Structure and approximations of the Chapman-Enskog expansion for linearized Grad equations, *Transport Theory and Stat. Phys.* **21** (1992), 101-117.

[24] Karlin, I. V., Simplest nonlinear regularization, *Transport Theory and Stat. Phys.* **21** (1992), 291-293.

[25] Kolmogorov, A. N., On conservation of conditionally periodic motions under small perturbations of the Hamiltonian. Dokl. Akad. Nauk SSSR, **98** (1954), 527-530.

[26] Arnold, V. I., Proof of a theorem of A N Kolmogorov on the invariance of quasi-periodic motions under small perturbations of the Hamiltonian. (English translation) Russian Math Surveys, **18** (1963), 9-36.

[27] Moser J. Convergent series expansions for quasi-periodic motions, Math. Ann., **169** (1967), 136-176.

[28] Jones, D. A., Stuart, A. M., Titi, E. S., Persistence of Invariant Sets for Dissipative Evolution Equations, Journal of Mathematical Analysis and Applications, **219**, 2 (1998), 479-502.

[29] Beyn, W.-J., Kless, W. Numerical Taylor expansions of invariant manifolds in large dynamical systems, Numerische Mathematik **80** (1998), 1-38.

[30] Kazantzis, N., Singular PDEs and the problem of finding invariant manifolds for nonlinear dynamical systems. Physics Letters, A **272** (4) (2000), 257-263.

[31] Shirkov, D. V., Kovalev, V. F., Bogoliubov Renormalization Group and Symmetry of Solution in Mathematical Physics, Phys. Rept. **352** (2001). 219-249. Online: http://arxiv.org/abs/hep-th/0001210

[32] Zinn-Justin, J., Quantum Field Theory and Critical Phenomena (Clarendon Press, Oxford, 1989).

[33] Pashko O., Oono, Y., The Boltzmann equation is a renormalization group equation, *Int. J. Mod. Phys. B* **14** (2000), 555-561.

[34] Kunihiro T., A Geometrical Formulation of the Renormalization Group Method for Global Analysis, Prog. Theor. Phys. **94** (1995), 503-514; Erratum: ibid. **95** (1996), 835. Online: http://arxiv.org/abs/hep-th/9505166

[35] Ei, S.-I., Fujii, K., Kunihiro, T., Renormalization-Group Method for Reduction of Evolution Equations; Invariant Manifolds and Envelopes, Annals Phys. **280** (2000), 236-298. Online: http://arxiv.org/abs/hep-th/9905088

[36] Hatta Y., Kunihiro T. Renormalization Group Method Applied to Kinetic Equations: roles of initial values and time, Annals Phys. **298** (2002), 24-57. Online: http://arxiv.org/abs/hep-th/0108159

[37] Degenhard A., Rodrigues-Laguna J. Towards the evaluation of the Relevant Degrees of Freedom in Nonlinear Partial Differential Equations, J. Stat. Phys., **106**, No. 516 (2002), 1093-1119.

[38] Forster, D., Nelson D. R., Stephen, M. J., Long-Time Tails and the Large-Eddy Behavior of a Randomly Stirred Fluid, Phys. Rev. Lett. **36** (1976), 867-870.

[39] Forster, D., Nelson D. R., Stephen, M. J., Large-distance and long-time properties of a randomly stirred fluid, Phys. Rev. A **16** (1977), 732-749.

[40] Adzhemyan, L. Ts., Antonov, N. V., Kompaniets, M. V., Vasil'ev, A. N., Renormalization-Group Approach To The Stochastic Navier Stokes Equation: Two-Loop Approximation, International Journal of Modern Physics B, **17**, 10 (2003), 2137-2170.

[41] Bricmont, J., Gawedzki, K., Kupiainen, A., KAM theorem and quantum field theory. Commun. Math. Phys. **201** (1999), 699-727. E-print mp_arc 98-526, online: http://mpej.unige.ch/mp_arc/c/98/98-517.ps.gz

[42] Gorban, A. N., Karlin, I. V., Methods of nonlinear kinetics, Contribution to the "Encyclopedia of Life Support Systems" (EOLSS Publishers, Oxford, to appear). Online: http://arXiv.org/abs/cond-mat/0306062

[43] Chapman, S., Cowling, T., *Mathematical Theory of Non-Uniform Gases*, Third edition (Cambridge University Press, Cambridge, 1970).

[44] Hilbert, D. Begrndung der kinetischen Gastheorie, Mathematische Annalen, **72** (1912), 562-577.

[45] Bobylev, A. V., The Chapman-Enskog and Grad Methods for Solving the Boltzmann Equation, Sov. Phys. Dokl., **27** (1982), No. 1, 29-31.

[46] Bowen, J. R., Acrivos, A., Oppenheim, A. K., Singular Perturbation Refinement to Quasi-Steady State Approximation in Chemical Kinetics. Chemical Engineering Science, **18** (1963), 177-188.

[47] Segel, L. A., Slemrod, M., The quasi-steady-state assumption: A case study in perturbation. SIAM Rev., **31** (1989), 446-477.

[48] Fraser, S. J., The steady state and equilibrium approximations: A geometrical picture. J. Chem. Phys., **88**(8) (1988), 4732-4738.

[49] Roussel, M. R., Fraser, S. J., Geometry of the steady-state approximation: Perturbation and accelerated convergence methods. J. Chem. Phys., **93** (1990), 1072-1081.

[50] Yablonskii, G. S., Bykov, V. I., Gorban, A. N., Elokhin, V. I., Kinetic models of catalytic reactions. Comprehensive Chemical Kinetics, Vol. 32, Compton R. G. ed., Elsevier, Amsterdam (1991).

[51] Vasil'eva A. B., Butuzov V. F., Kalachev L. V., The boundary function method for singular perturbation problems, SIAM (1995).

[52] Strygin V. V., Sobolev V. A., Spliting of motion by means of integral manifolds. Nauka, Moscow (1988).

[53] Roos, H. G., Stynes, M., Tobiska, L., Numerical Methods for Singularly Perturbed Differential Equations: Convection-Diffusion and Flow Problems, Springer Verlag, 1996.

[54] Mishchenko, E. F., Kolesov, Y. S., Kolesov, A. U., Rozov, N. Kh., Asymptotic Methods in Singularly Perturbed Systems, Consultants Bureau, 1994.

[55] Novozhilov, I. V., Fractional Analysis: Methods of Motion Decomposition, Birkhauser, 1997.

[56] Milik, A., Singular Perturbation on the Web, 1997. http://www.ima.umn.edu/~milik/singdir.html#geo:sing

[57] Gear, C. W., Numerical Initial Value Problems in Ordinary Differential Equations. Prentice-Hall, Englewood Cliffs, NJ (1971).

[58] Rabitz, H., Kramer, M., Dacol, D., Sensitivity analysis in chemical kinetics. Ann. Rev. Phys. Chem., 34, 419-461 (1983).

[59] Lam, S.H., Goussis, D. A., The CSP Method for Simplifying Ki- netics. International Journal of Chemical Kinetics, **26** (1994), 461-486.

[60] Maas, U., Pope, S. B. Simplifying chemical kinetics: intrinsic low- dimensional manifolds in composition space. Combustion and Flame, **88** (1992), 239-264.

[61] Dellnitz, M., Junge, O., Set Oriented Numerical Methods for Dynamical Systems, in: B. Fiedler, G. Iooss and N. Kopell (eds.): Handbook of Dynamical Systems II: Towards Applications, World Scientific, 2002, 221-264, . http://math-www.upb.de/~agdellnitz/papers/handbook.pdf

[62] Dellnitz, M., Hohmann, A. The computation of unstable manifolds using subdivision and continuation, in H.W. Broer et al. (eds.), Progress in Nonlinear Differential Equations and Their Applications 19:449-459, Birkhauser Verlag, Basel / Switzerland, 1996.

[63] Broer, H. W., Osinga, H. M. and Vegter, G. Algorithms for computing normally hyperbolic invariant manifolds, Z. angew. Math. Phys. **48** (1997), 480–524.

[64] Garay, B. M., Estimates in Discretizing Normally Hyperbolic Compact Invariant Manifolds of Ordinary Differential Equations, Computers and Mathematics with Applications, **42** (2001), 1103-1122.

[65] Gorban, A. N., Karlin, I. V., Zinovyev, A. Yu., Invariant grids for reaction kinetics, Preprint, Institut des Hautes tude Scientifiques, 2003. Online: http://www.ihes.fr/PREPRINTS/P03/Resu/resu-P03-42.html

[66] Ilg P., Karlin, I. V., Validity of macroscopic description in dilute polymeric solutions, Phys. Rev. E **62** (2000), 1441-1443.

[67] Ilg, P., De Angelis, E., Karlin, I. V., Casciola, C. M., Succi, S. Polymer dynamics in wall turbulent flow, Europhys. Lett., **58** (2002), 616-622.

[68] Boltzmann L. Lectures on gas theory, University of California Press, 1964.

[69] Cercignani, C. *The Boltzmann Equation and its Applications* (Springer, New York, 1988).

[70] Cercignani C., Illner R., Pulvirent M. The Mathematical theory of Dilute Gases, Springer, New York, 1994.

[71] P. L. Bhatnagar, E. P. Gross, and M. Krook, A Model for Collision Processes in Gases. I. Small Amplitude Processes in Charged and Neutral One-Component Systems, Phys. Rev. **94**, 3 (1954), 511-525.

[72] Gorban, A. N., Karlin, I. V., General approach to constructing models of the Boltzmann equation. *Physica A*, **206** (1994), 401-420.

[73] Lebowitz, J., Frisch, H., Helfand, E., Non-equilibrium Distribution Functions in a Fluid. Physics of Fluids, **3** (1960), 325.

[74] DiPerna R.J., Lions P.L. On the Cauchy problem for Boltzmann equation: Global existence and weak stability, Ann. Math, **130** (1989), 321-366.

[75] Enskog D. Kinetische theorie der Vorange in massig verdunnten Gasen. I Allgemeiner Teil, Almqvist and Wiksell, Uppsala, 1917.

[76] Broadwell J.E. Study of shear flow by the discrete velocity method, J. Fluid Mech. **19** (1964), 401-414.

[77] Robertson, B., Equations of motion in nonequilibrium statistical mechanics, Phys. Rev., **144** (1966), 151-161.

[78] Bird G.A. Molecular Gas Dynamics and the Direct Simulation of gas Flows, Clarendon Press, Oxford, 1994.

[79] Gatignol R. Theorie cinetique des gaz a repartition discrete de vitesses. Lecture notes in physics, V.36, Springer, Berlin, etc, 1975.

[80] Frisch U., Hasslacher B. and Pomeau Y. (1986). Lattice-gas automata for the Navier-Stokes equation, Phys.Rev.Lett., 56, 1505-1509. [Introduction of the Lattice Gas models for hydrodynamics]

[81] Chen S. and Doolen G.D. Lattice Boltzmann method for fluid flows, Annu. Rev. Fluid. Mech. **30** (1998), 329-364.

[82] Succi S., The Lattice Boltzmann Equation for Fluid Dynamics and Beyond. Clarendon Press, Oxford, 2001.

[83] Succi S., Karlin I.V., and Chen H. Role of the H theorem in lattice Boltzmann hydrodynamic simulations, Rev. Mod. Phys. **74** (2002), 1203-1220.

[84] van Kampen, N. G., Stochastic Processes in Physics and Chemistry, North-Holland, Amsterdam 1981.

[85] Risken, H., The Fokker-Planck Equation, Springer, Berlin, 1984.

[86] Bird, R. B., Curtiss, C. F., Armstrong, R. C. and Hassager, O., Dynamics of Polymer Liquids, 2nd edn., Wiley, New York, 1987.

[87] Doi, M., Edwards, S. F., The Theory of Polymer Dynamics, Clarendon Press, Oxford, 1986.

[88] Öttinger, H. C., Stochastic Processes in Polymeric Fluids, Springer, Berlin, 1996.

[89] Grmela, M., Öttinger, H. C. Dynamics and thermodynamics of complex fluids. I. Development of a general formalism, Phys. Rev. E **56** (1997), 6620-6632.

[90] Öttinger, H. C., Grmela, M., Dynamics and thermodynamics of complex fluids. II. Illustrations of a general formalism, Phys. Rev. E, **56** (1997), 6633-6655.

[91] Lifshitz E.M. and Pitaevskii L.P., Physical kinetics (Landau L.D. and Lifshitz E.M. Course of Theoretical Physics, V.10), Pergamon Press, Oxford, 1968.

[92] Ryashko, L. B., Shnol, E. E., On exponentially attracting invariant manifolds of ODEs, Nonlinearity, **16** (2003), 147-160.

[93] Walter, W. An elementary proof of the Cauchy–Kovalevsky Theorem, Amer. Math. Month- ly **92** (1985), 115-126.

[94] Evans, L. C. Partial Differential Equations, AMS, Providence, RI, USA, 1998.

[95] Dubinskii, Ju. A. Analytic Pseudo-Differential Operators and their Applications. Kluwer Academic Publishers, Book Series: Mathematics And its Applications Soviet Series: Volume 68, 1991.

[96] Levermore, C.D., Oliver, M. Analyticity of solutions for a generalized Euler equation, J. Differential Equations **133** (1997), 321-339.

[97] Oliver, M., Titi, E. S., On the domain of analyticity for solutions of second order analytic nonlinear differential equations, J. Differential Equations **174** (2001), 55-74.

[98] Lyapunov A. M., The general Problem of the Stability of Motion, Taylor & Francis, 1992.

[99] Poincaré, H.: Les méthodes nouvelles de la mécanique céleste. Vols. 1-3. Paris: Gauthier-Villars. (1892/1893/1899).

[100] Arnold, V. I., Geometrical Methods in the Theory of Differential Equations, Springer- Verlag, New York-Berlin, 1983.

[101] Kazantzis, N., Kravaris, C., Nonlinear observer design using Lyapunovs auxiliary theorem, Systems Control Lett., **34** (1998), 241-247.

[102] Krener, A. J., Xiao, M., Nonlinear observer design in the Siegel domain, SIAM J. Control Optim. Vol. **41**, 3 (2002), 932-953.

[103] Kazantzis, N., Good, Th., Invariant manifolds and the calculation of the long-term asymptotic response of nonlinear processes using singular PDEs, Computers and Chemical Engineering **26** (2002), 999-1012.

[104] Onsager, L. Reciprocal relations in irreversible processes. I. Phys. Rev. **37** (1931), 405-426; II. Phys. Rev. **38** (1931), 2265-2279.

[105] Wehrl, A., General properties of entropy, Rev. Mod. Phys. **50**, 2 (1978), 221-260.

[106] Schlögl, F., Stochastic measures in nonequilibrium thermodynamics, Phys. Rep. **62**, 4 (July 1980), 267-380.

[107] Gorban, A. N., *Equilibrium Encircling. Equations of Chemical Kinetics and Their Thermodynamic Analysis*, Nauka, Novosibirsk, 1984.

[108] Jaynes E. T., Information theory and statistical mechanics, in: *Statistical Physics. Brandeis Lectures, V. 3* 160-185 (1963).

[109] Grabert, H. *Projection Operator Techniques in Nonequilibrium Statistical Mechanics* (Springer Verlag, Berlin, 1982).

[110] Zubarev, D., Morozov, V., Röpke, G. *Statistical Mechanics of Nonequilibrium Processes*, V. 1, *Basic Concepts, Kinetic Theory* (Akademie Verlag, Berlin, 1996), V. 2, *Relaxation and Hydrodynamic Processes* (Akademie Verlag, Berlin, 1997)

[111] Öttinger, H. C. Derivation of Two-Generator Framework of Nonequilibrium Thermodynamics for Quantum Systems, Phys. Rev. E **62** (2000), 4720-4724.

[112] Uhlenbeck, G. E. in: *Fundamental Problems in Statistical Mechanics II*, edited by E. G. D. Cohen, (North Holland, Amsterdam, 1968).

[113] Grad, H. On the kinetic theory of rarefied gases, *Comm. Pure and Appl. Math.* **2(4)** (1949), 331–407.

[114] Hauge, E. H. Phys. Fluids **13** (1970), 1201.

[115] Titulaer, U. M. A systematic solution procedure for the Fokker-Planck equation of a Brownian particle in the high-friction case, Physica A, **91**, 3-4 (May 1978), 321-344.

[116] Widder, M. E., Titulaer, U. M. Two kinetic models for the growth of small droplets from gas mixtures, Physica A: Statistical and Theoretical Physics, **167**, 3 (1990), 663-675.

[117] Karlin, I. V., Dukek, G., Nonnenmacher, T. F., Gradient expansions in kinetic theory of phonons, Phys. Rev. B **55** (1997), 6324-6329.

[118] Karlin, I. V., Exact summation of the Chapman-Enskog expansion from moment equations, J. Phys. A: Math. Gen. **33** (2000), 8037-8046.

[119] Slemrod M., Constitutive relations for monatomic gases based on a generalized rational approximation to the sum of the Chapman-Enskog expansion, Arch. Rat. Mech. Anal, **150** (1) (1999), 1-22.

[120] Slemrod M., Renormalization of the Chapman-Enskog expansion: Isothermal fluid flow and Rosenau saturation J. Stat. Phys, **91**, 1-2 (1998), 285-305.

[121] Gibbs, G. W. *Elementary Principles of Statistical Mechanics*, Dover, 1960.

[122] Kogan, A. M., Rozonoer, L. I. On the macroscopic description of kinetic processes, *Dokl. AN SSSR* **158** (3) (1964), 566–569.

[123] Kogan, A. M. Derivation of Grad–type equations and study of their properties by the method of entropy maximization, *Prikl. Math. Mech.* **29** (1) (1965), 122–133.

[124] Rozonoer, L. I. Thermodynamics of nonequilibrium processes far from equilibrium, in: *Thermodynamics and Kinetics of Biological Processes* (Nauka, Moscow, 1980), 169-186.

[125] Karkheck, J., Stell, G., Maximization of entropy, kinetic equations, and irreversible thermodynamics Phys. Rev. A **25**, 6 (1984), 3302-3327.

[126] Bugaenko, N. N., Gorban, A. N., Karlin, I. V. Universal Expansion of the Triplet Distribution Function, Teoreticheskaya i Matematicheskaya Fisika, **88**, 3 (1991), 430-441 (Transl.: Theoret. Math. Phys. (1992) 977-985).

[127] Levermore C. D., Moment Closure Hierarchies for Kinetic Theories, J. Stat. Phys. **83** (1996), 1021–1065.

[128] Balian, R., Alhassid, Y. and Reinhardt, H. Dissipation in many-body systems: A geometric approach based on information theory, Phys. Reports **131**, 1 (1986), 1–146.

[129] Gorban, A. N., Karlin, I. V., Quasi-equilibrium approximation and non-standard expansions in the theory of the Boltzmann kinetic equation, in: "Mathematical Modelling in Biology and Chemistry. New Approaches", ed. R. G. Khlebopros, Nauka, Novosibirsk, P.69-117 (1991).[in Russian]

[130] Gorban, A. N., Karlin, I. V., Quasi-Equilibrium Closure Hierarchies for The Boltzmann Equation [Translation of the first part of the paper [129]]. Preprint, 2003, Online: http://arXiv.org/abs/cond-mat/0305599

[131] Jou, D., Casas-Vázquez, J., Lebon, G., Extended Irreversible Thermodynamics, Springer, Berlin, 1993.

[132] A. Gorban and I. Karlin, New Methods for Solving the Boltzmann Equations, AMSE Press, Tassin, France, 1994.

[133] Hirschfelder, J. O., Curtiss C. F., Bird, R. B. *Molecular Theory of Gases and Liquids*, (J. Wiley, NY, 1954).

[134] Dorfman, J., van Beijeren, H., in: Statistical Mechanics B, B. Berne, ed., Plenum, NY, 1977.

[135] Résibois, P., De Leener, M., Classical Kinetic Theory of Fluids, Wiley, NY, 1977.

[136] Ford, G., Foch, J., in: Studies in Statistical Mechanics, G. Uhlenbeck and J. de Boer, eds., V. 5, North Holland, Amsterdam, 1970.

[137] Van Rysselberge, P., Reaction rates and affinities, J. Chem. Phys., **29**, 3 (1958), 640-642.

[138] Feinberg, M., Chemical kinetics of a sertain class, Arch. Rat. Mech. Anal., **46**, 1 (1972), 1-41.

[139] Bykov, V. I., Gorban, A. N., Yablonskii, G. S., Description of nonisothermal reactions in terms of Marcelin – de Donder kinetics and its generalizations, React. Kinet. Catal. Lett., **20**, 3-4 (1982), 261-265.

[140] Karlin, I. V., On the relaxation of the chemical reaction rate, in: Mathematical Problems of Chemical Kinetics, eds. K. I. Zamaraev and G. S. Yablonskii, Nauka, Novosibirsk, 1989, 7–42. [In Russian].

[141] Karlin, I. V. The problem of reduced description in kinetic theory of chemically reacting gas, Modeling, Measurement and Control C, **34(4)** (1993), 1-34.

[142] Gorban, A. N., Karlin, I. V., Scattering rates versus moments: Alternative Grad equations, Phys. Rev. E **54** (1996), R3109.

[143] Treves, F., Introduction to Pseudodifferential and Fourier Integral Operators, Plenum, NY, (1982).

[144] Shubin, M. A., Pseudodifferential Operators and Spectral Theory, Nauka, Moscow, (1978).

[145] Dedeurwaerdere, T., Casas-Vzquez, J., Jou, D., Lebon, G., Foundations and applications of a mesoscopic thermodynamic theory of fast phenomena Phys. Rev. E, **53**, 1 (1996), 498-506.

[146] Rodríguez, R. F., García-Colín, L. S., Lpez de Haro, M., Jou, D., Prez-Garca, C., The underlying thermodynamic aspects of generalized hydrodynamics, Phys. Lett. A, **107**, 1 (1985), 17-20.

[147] Struchtrup, H., Torrilhon M., Regularization of Grad's 13 Moment Equations: Derivation and Linear Analysis, Phys. Fluids, accepted (2003).

[148] Ilg, P., Karlin, I. V., Öttinger H. C., Canonical distribution functions in polymer dynamics: I. Dilute solutions of flexible polymers, Physica A, **315** (2002), 367-385.

[149] Ilg, P., Karlin, I. V., Kröger, M. , Öttinger H. C., Canonical distribution functions in polymer dynamics: II Liquid-crystalline polymers, Physica A, **319** (2003), 134-150.

[150] Courant, R., Friedrichs, K. O. and Lewy, H. On the partial difference equations of mathematical physics. IBM Journal (March 1967), 215–234.

[151] Ames, W.F., Numerical Methods for Partial Differential Equations, 2nd ed. (New York: Academic Press), 1977.

[152] Richtmyer, R.D., and Morton, K.W., Difference Methods for Initial Value Problems, 2nd ed. (New York: Wiley-Interscience), 1967.

[153] Gorban, A.N., Zinovyev, A.Yu. Visualization of data by method of elastic maps and its applications in genomics, economics and sociology. Institut des Hautes Etudes Scientifiques, Preprint. IHES M/01/36. (2001) . Online- version: http://www.ihes.fr/PREPRINTS/M01/Resu/resu-M01-36.html.

[154] Jolliffe, I. T. Principal Component Analysis. Springer-Verlag, 1986.

[155] Callen, H. B. Thermodynamics and an Introduction to Thermostatistics (Wiley, New York), 1985.

[156] Use of Legendre Transforms in Chemical Thermodynamics (IUPAC Technical Report), Prepared for publication by R. A. Alberty. Pure Appl.Chem., **73**, 8 (2001), pp.1349–1380. www.iupac.org/publications/pac/2001/pdf/7308x1349.pdf

[157] Grmela, M., Reciprocity relations in thermodynamics, Physica A, **309**, 3-4 (2002), 304-328.

[158] Aizenberg, L., Carleman's Formulas in Complex Analysis: Theory and Applications. (Mathematics and Its Applications; V. 244) Kluwer, 1993.

[159] Gorban, A. N., Rossiev, A. A., Wunsch, D. C. II, Neural network modeling of data with gaps: method of principal curves, Carleman's formula, and other, The talk was given at the USA-NIS Neurocomputing opportunities workshop, Washington DC, July 1999 (Associated with IJCNN'99). Online: http://arXiv.org/abs/cond-mat/0305508

[160] Gorban, A. N., Rossiev, A. A., Neural network iterative method of principal curves for data with gaps, Journal of Computer and System Sciences Intrnational, **38(5)** (1999), 825-831.

[161] Dergachev, V. A., Gorban, A. N., Rossiev, A. A., Karimova, L. M., Kuandykov, E. B., Makarenko, N. G., Steier, P., The filling of gaps in geophysical time series by artificial neural networks, Radiocarbon, **43**, 2A (2001), 365 - 371.

[162] Gorban A., Rossiev A., Makarenko N., Kuandykov Y., Dergachev V. Recovering data gaps through neural network methods. International Journal of Geomagnetism and Aeronomy, **3**, 2 (2002), 191-197.

[163] Ehrenfest, P., Collected Scientific Papers, North-Holland, Amsterdam, 1959, pp. 213-300.

[164] Lewis, R. M., A unifying principle in statistical mechanics, *J. Math. Phys.,* **8** (1967), 1448-1460.

[165] McKean, H. P. Jr., J. Math. Phys. **8**, 547 (1967).

[166] Ansumali S., Karlin, I. V. Single relaxation time model for entropic Lattice Boltzmann methods. *Phys. Rev. E,* **65** (2002), 056312(1-9).

[167] Gorban, A. N., Bykov, V. I., Yablonskii, G. S., Essays on chemical relaxation, Novosibirsk: Nauka, 1986.

[168] Verbitskii, V. I., Gorban, A. N., Utjubaev, G. Sh., Shokin, Yu. I. Moore effect in interval spaces, Dokl. AN SSSR. **304**, 1 (1989), 17-21.

[169] Bykov, V. I., Verbitskii, V. I., Gorban, A. N., On one estimation of solution of Cauchy problem with uncertainty in initial data and rigt part, Izv. vuzov, Ser. mat. N. 12 (1991), 5-8.

[170] Verbitskii, V. I., Gorban, A. N. Simultaneously dissipative operators and their applications, Sib. Mat. Jurnal, **33**, 1 (1992), 26–31.

[171] Gorban, A. N., Shokin, Yu. I., Verbitskii, V. I. Simultaneously dissipative operators and the infinitesimal Moore effect in interval spaces, Preprint (1997). Online: http://arXiv.org/abs/physics/9702021

[172] Gorban, A. N., Bykov, V. I., Yablonskii, G. S. Thermodynamic function analogue for reactions proceeding without interaction of various substances, Chemical Engineering Science, **41**, 11 (1986), 2739-2745.

[173] Grassberger, P., On the Hausdorff Dimension of Fractal Attractors, J. Stat. Phys. **26** (1981), 173-179.

[174] Grassberger, P. and Procaccia, I., Measuring the Strangeness of Strange Attractors, Physica D **9** (1983), 189-208.

[175] Frederickson, P. , Kaplan, J. L., Yorke, E. D., Yorke, J. A., The Lyapunov dimension of strange attractors. J. Differ. Equations **49** (1983), 185-207.

[176] Ledrappier F., Young, L.-S., The metric entropy of diffeomorphisms: I. Characterization of measures satisfying Pesin's formula; II. Relations between entropy, exponents and dimensions, Annals of Mathematics, **122** (1985), 509-539, 540-574.

[177] Hentschel, H. G. E., Procaccia, I., The infinite number of generalized dimensions of fractals and strange attractors, Physica D: Nonlinear Phenomena, **8** 3 (1983), 435-444.

[178] Ilyashenko, Yu. S., On dimension of attractors of k-contracting systems in an infinite dimensional space, Vest. Mosk. Univ. Ser. 1 Mat. Mekh., No. 3 (1983), 52-58.

[179] Nicolis, C., Nicolis, G., Is there a climate attractor?, Nature, **311** (1984), 529-532.

[180] Foias, C., Manley, O. P., Temam, R., An estimate of the Hausdorff dimension of the attractor for homogeneous decaying turbulence, Physics Letters A, **122** 3-4 (1987), 140-144.

[181] Foias, C., Sell, G. R., Temam R., Inertial manifolds for dissipative nonlinear evolution equations, Journal of Differential Equations, **73** (1988), 309-353.

[182] Temam R., Infinite-Dimensional Dynamical Systems in Mechanics and Physics, Applied Math. Sci., 1988, Vol 68 (Springer Verlag, New York) (Second edition, 1997).

[183] Constantin, P., Foias, C., Nicolaenko, B., Temam, R., Integral manifolds and inertial manifolds for dissipative partial differential equations, Applied Math. Sci., 1988, Vol. 70 (Springer Verlag, New York).

[184] Foias, C., Sell, G. R., Titi, E. S., Exponential tracking and approximation of inertial manifolds for dissipative nonlinear equations Journal of Dynamics and Differential Equations, **1** (1989), 199-244.

[185] Vishik, M. I., Asymptotic Behaviour of Solutions of Evolutionary Equations, Cambridge University Press, 1993.

[186] Jones, D. A., Titi, E. S., C^1 Approximations of Inertial Manifolds for Dissipative Nonlinear Equations, Journal of Differential Equations, **127**, 1 (1996), 54-86.

[187] Christofides, P. D., Nonlinear and Robust Control of Partial Differential Equation Systems: Methods and Applications to Transport-Reaction Processes, 248 pages, Birkhäuser, Boston, 2001.

[188] Chepyzhov, V. V., Ilyin, A. A., A note on the fractal dimension of attractors of dissipative dynamical systems, Nonlinear Analysis, **44** (2001), 811-819.

[189] Marion, M., Temam, R., Nonlinear Galerkin methods, SIAM J. Numer. Anal., **26** (1989), 1139-1157.

[190] Jones, C., Kaper, T., Kopell, N., Tracking invariant manifolds up to exponentially small errors, SIAM J. Math., Anal. 27 (1996), 558-577.

[191] Yinnian He, Mattheij, R. M. M., Stability and convergence for the reform postprocessing Galerkin method, Nonlinear Anal. Real World Appl., **4** (2000), 517-533.

[192] Garsia-Archilla, B., Novo, J., Titi E. S., Postprocessing the Galerkin method: a novel approach to approximate inertial manifolds, SIAM J. Numer. Anal., **35** (1998), 941-972.

[193] Margolin, L. G., Titi, E. S., Wynne, S. The postprocessing Galerkin and nonlinear Galerkin methods – a truncation analysis point of view, SIAM, Journal of Numerical Analysis, (to appear) Online: http://math.uci.edu/%7Eetiti/Publications/Wynne/DPP/DPP_final_revised.pdf

[194] Bird, R. B., Wiest, J. M., Constitutive equations for polymeric liquids, Annu. Rev. Fluid Mech. **27** (1995), 169.

[195] Warner, H. R., Kinetic theory and rheology of dilute suspensions of finitely extendible dumbbells, Ind. Eng. Chem. Fundamentals **11** (1972), 379.

[196] Oseen, C. W., Ark. f. Mat. Astr. og Fys. **6** No. 29 (1910) 1.

[197] Burgers, J. M., Verhandelingen Koninkl. Ned. Akad. Wetenschap. **16** (Section 1, Chapter 3) (1938), 113.

[198] Rotne, J., Prager, S., Variational treatment of hydrodynamic interaction, J. Chem. Phys. **50** (1969) 4831.

[199] Yamakawa, H., Transport properties of polymer chain in dilute solution: Hydrodynamic interaction, J. Chem. Phys. **53** (1970), 436.

[200] Noll, W., A mathematical theory of the mechanical behavior of continuous media, Arch. Ratl. Mech. Anal. **2** (1958), 197.

[201] Astarita, G., Marrucci, G., Principles of Non-Newtonian Fluid Mechanics, McGraw-Hill, London, 1974.

[202] Oldroyd, J. G., Non-Newtonian effects in steady motion of some idealized elastico-viscous liquids, Proc. Roy. Soc. A245 (1958), 278.

[203] Herrchen M., Öttinger, H.C., A detailed comparison of various FENE dumbbell models, J. Non-Newtonian Fluid Mech. **68** (1997), 17.

[204] Kröger, M., Simple models for complex nonequilibrium fluids, Phys. Reports, submitted (2003).
Online: http://owl.ethz.ch/d-werk/oettinger/MK_DIR/pmk80/paper.ps.

[205] Bird, R. B., Dotson, R. B., Jonson, N. J., Polymer solution rheology based on a finitely extensible bead-spring chain model, J. Non-Newtonian Fluid Mech. **7** (1980), 213-235; Corrigendum **8** (1981), 193,

[206] Char B. W., et al., Maple V Language Reference Manual, Springer–Verlag, New York, 1991.

[207] Kato, T., Perturbation Theory for Linear Operators, Springer-Verlag, Berlin, 1976.

[208] Lielens, G., Halin, P., Jaumin, I. Keunings, R. Legat, V., New closure approximations for the kinetic theory of finitely extensible dumbbells, J. Non–Newtonian Fluid Mech. **76** (1998), 249-279.

[209] Ilg, P., Karlin, I. V., Öttinger, H. C., Generating moment equations in the Doi model of liquid-crystalline polymers, Phys. Rev. E **60** (1999), 5783-5787.

[210] Phan-Thien, N., Goh, C. G., Atkinson, J. D., The motion of a dumbbell molecule in a torsional flow is unstable at high Weissenberg number, J. Non-Newtonian Fluid Mech. **18**, 1 (1985), 1-17.

[211] Goh, C. G., Phan-Thien, N., Atkinson, J. D., On the stability of a dumbbell molecule in a continuous squeezing flow, Journal of Non-Newtonian Fluid Mechanics, **18**, 1 (1985), 19-23.

[212] Karlin, I. V., Ilg, P., Öttinger, H. C. Invariance principle to decide between micro and macro computation, in: Recent Developments in Mathematical and Experimental Physics, Volume C: Hydrodynamics and Dynamical Systems, Ed. F. Uribe (Kluwer, Dordrecht, 2002), 45-52.

[213] Novo, J., Titi, E.S., Wynne, S. Efficient methods using high accuracy approximate inertial manifolds, Numerische Mathematik, **87** (2001), 523–554.

[214] Hirsch, M. W., Pugh, C. and Shub, M. Invariant Manifolds, volume 583 of Lecture Notes in Mathematics, Springer, 1977.

[215] Jones, Cr., Winkler, S. Do Invariant Manifolds Hold Water?, Handbook of Dynamical Systems III: Towards Applications, B. Fiedler, G. Iooss, N. Koppell, Eds. World Scientific, to appear.
Online: http://www.cfm.brown.edu/people/sean/JonesWinkler.ps.zip