

Geometry of irreversibility: The film of nonequilibrium states

Alexander N. Gorban^{1,2,3*},

Iliya V. Karlin^{1,2**},

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

A general geometrical framework of nonequilibrium thermodynamics is developed. The notion of *macroscopically definable ensembles* is developed. The thesis about macroscopically definable ensembles is suggested. This thesis should play the same role in the nonequilibrium thermodynamics, as the Church-Turing thesis in the theory of computability. The *primitive macroscopically definable ensembles* are described. These are ensembles with macroscopically prepared initial states. The method for computing trajectories of primitive macroscopically definable nonequilibrium ensembles is elaborated. These trajectories are represented as sequences of deformed equilibrium ensembles and simple quadratic models between them. The primitive macroscopically definable ensembles form the manifold in the space of ensembles. We call this manifold the *film of nonequilibrium states*. The equation for the film and the equation for the ensemble motion on the film are written down. The notion of the invariant film of non-equilibrium states, and the method of its approximate construction transform the the problem of nonequilibrium kinetics into a series of problems of equilibrium statistical physics. The developed methods allow us to solve the problem of macro-kinetics even when there are no autonomous equations of macro-kinetics.

*agorban@mat.ethz.ch, **ikarlin@mat.ethz.ch

Contents

Introduction	4
1 The problem of irreversibility	7
1.1 The phenomenon of the macroscopic irreversibility	7
1.2 Phase volume and dynamics of ensembles	7
1.3 Macroscopically definable ensembles and quasiequilibria	10
1.4 Irreversibility and initial conditions	13
1.5 Weak and strong tendency to equilibrium, shaking and short memory . . .	13
1.6 The essence of irreversibility in two words	15
1.7 Equivalence between trajectories and ensembles in the thermodynamic limit	15
1.8 Subjective time and irreversibility	15
2 Geometrization of irreversibility	16
2.1 Quasiequilibrium manifold	16
2.2 Thermodynamic projector	19
2.3 Quasiequilibrium approximation	22
3 Natural projector and models of nonequilibrium dynamics	25
3.1 Natural projector	25
3.2 One-dimensional model of nonequilibrium states	29
3.3 Stability of quasiequilibrium manifolds	32
3.4 Curvature and entropy production: Entropic circle and first kinetic equations	33
4 The film of non-equilibrium states	35
4.1 Equations for the film	35
4.2 Thermodynamic projector on the film	37
4.3 Fixed points and “right asymptotics” for the film equation	40
4.4 Coarse-graining projector	42
4.5 Choice of the coarse-graining projector, and layer-by-layer linearization . .	43
4.6 The failure of the simplest Galerkin approximations for conservative systems	45
4.7 Possible ways beyond the simplest Galerkin approximations	47
4.8 The film: Second order Kepler models	48
4.9 Minimal second order models: entropic parable, and entropic circle	49
4.10 The finite models: termination at the horizon points	51
4.11 The transversal restart lemma	52
4.12 The time replacement, and the invariance of the thermodynamic projector	55
4.13 Correction to the infinite models	56
4.14 The film, and the macroscopic equations	56
4.15 New in the separation of the relaxation times	59
5 Conclusion	60

6	Appendix	62
6.1	The method of invariant manifolds	62
6.2	Construction of the invariant sections	62
6.3	The entropic thermodynamic projectors	64
6.4	Method of invariant manifold for the positively invariant manifolds with fixed edge	65

Introduction

The goal of this paper is to discuss the nonlinear problems of irreversibility, and to revise the previous attempts to solve them. The interest to the problem of irreversibility persists during decades. It has been intensively discussed in the past, and nice accounts of these discussions can be found in the literature (see, for example, [1, 2, 4, 3]). Here, we intend to develop a more geometrical viewpoint on the subject. The paper consists of two parts. First, in section 1, we discuss in an informal way the origin of the problem, and demonstrate how the basic constructions arise. Second, in section 2, we give a consistent geometric formalization of these constructions. Our presentation is based on the notion of the natural projection introduced in section 3. We discuss in detail the method of natural projector as the consistent formalization of Ehrenfest's ideas of coarse-graining.

In section 3.2 we introduce a one-dimensional model of nonequilibrium states. In the background of many derivations of nonequilibrium kinetic equations there is present the following picture: Above each point of the quasiequilibrium manifold there is located a huge subspace of nonequilibrium distributions with the same values of the macroscopic variables, as in the quasiequilibrium point. It is as if the motion decomposes into two projections, above the point on the quasiequilibrium manifold, and in the projection on this manifold. The motion in each layer above the points is highly complicated, but fast, and everything quickly settles in this fast motion.

However, upon a more careful looking into the motions which start from the quasiequilibrium points, we will observe that, above each point of the quasiequilibrium manifold it is located *just a single curve*, and all the nonequilibrium (not-quasiequilibrium) states which come into the game form just a one-dimensional manifold.

The novel approach developed in section 3 allows to go beyond limitations of the short memory approximations through a study of stability of the quasiequilibrium manifold.

The one-dimensional models of nonequilibrium states form a *film of nonequilibrium states* over the quasiequilibrium manifold. In section 4 we present a collection of methods for the film construction. One of the benefits from this new technic is the possibility to solve the problem of macro-kinetic in cases when there are no autonomous equations of macro-kinetic for moment variables. The notion of the invariant film of non-equilibrium states, and the method of its approximate construction transform the the problem of nonequilibrium kinetics into a series of problems of equilibrium statistical physics. To describe a dynamics of nonequilibrium ensemble one should find series of deformed equilibrium ensembles.

In Appendix a short presentation of the method of invariant manifold for kinetic problems is given.

The most important results of the paper are:

1. The notion of *macroscopically definable ensembles* is developed.
2. The *primitive macroscopically definable ensembles* are described.

3. The method for computing trajectories of primitive macroscopically definable nonequilibrium ensembles is elaborated. These trajectories are represented as series of deformed equilibrium ensembles and simple quadratic models between them.

Let us give here an introductory description of these results.

The notion of macroscopically definable ensembles consists of three ingredients:

1. Macroscopic variables, the variables which values *can be controlled by us*;
2. Quasiequilibrium state, the conditional equilibrium state for fixed values of the macroscopic variables;
3. Natural dynamics of the system.

We use the simplest representation of the control: For some moments of time we fix some values of the macroscopic variables (of all these variables, or of part of them; for the whole system, or for macroscopically defined part of it; the current “natural”, or some arbitrary value of these variables), and the system obtains corresponding conditional equilibrium state. We can also keep fixed values of some macroscopic variables during a time interval.

These control operations are discrete in time. The continuous control can be created by the closure: the limit of a sequence of macroscopically definable ensembles is macroscopically definable too.

The role of the macroscopic variables for the irreversibility problem became clear to M. Leontovich and J. Lebowitz several decades ago [5, 6, 7, 8, 9]. But this was the first step. Now we do need the elaborate notion of ensembles which can be obtained by macroscopic tools. The Maxwell Demon gives the first clear picture of a difference between macroscopic and microscopic tools for ensembles control (there are books devoted to analysis of this Demon [10, 11]). Nevertheless, the further step to the analysis of the notion of macroscopic definability in context of constructive transition from microdynamics to macrokinetics equations had not done before the paper [12]. Our analysis pretends to be an analogue of the Church-Turing thesis [13, 14]. This thesis concerns the notion of an effective (or mechanical) method in mathematics. As a “working hypothesis”, Church proposed: A function of positive integers is effectively calculable only if recursive.

We introduce a class of “macroscopically definable ensembles” and formulate the thesis: An ensemble can be macroscopically obtained only if macroscopically definable in according to the introduced notion. This is a thesis about success of the formalization, as the Church-Turing thesis, and nobody can prove or disprove it in rigorous sense, as well, as this famous thesis.

Another important new notion is the “*macroscopically definable transformation*” of the ensemble: If one get an ensemble, how can he transform it? First, it is possible just let them evolve, second, it can be controlled by the macroscopic tools on the defined way (it is necessary just to keep values of some macroscopic variables during some time).

The *primitive macroscopically definable ensembles* are ensembles with quasiequilibrium initial states and without further macroscopic control. These ensembles are prepared macroscopically, and evolve due to natural dynamics. The significance of this class of ensembles is determined by the *hypothesis about the primitive macroscopically definable ensembles*: Any macroscopically definable ensemble can be approximated by primitive macroscopically definable ensembles with appropriate accuracy. Now we have no other effective way to describe the nonequilibrium state.

The primitive macroscopically definable ensembles form the manifold in the space of ensembles. We call this manifold the “film of nonequilibrium states”. The equation for the film and the equation for the ensemble motion on the film are written down.

The film of nonequilibrium states is the trajectory of the manifold of initial quasiequilibrium states due to the natural (microscopic) dynamics. For every value of macroscopic variables this film gives us a curve. The curvature of this curve defines kinetic coefficients and entropy production.

The main technical problem is the computation of this curve for arbitrary value of the macroscopic variables. We represent it as a sequence of special points and second-order polynomial (Kepler) models for trajectory between these points. The method elaborated for the computation is the further development of the method for initial layer problem in the Boltzmann kinetics [15, 16]. For dissipative Boltzmann microkinetics it was sufficient to use the first-order models (with or without smoothing). For conservative microkinetics it is necessary to use the highest-order models. Application of this method to the lattice kinetic equations gave the following possibilities:

- To create the Lattice-Boltzmann kinetics with H -theorem [17];
- To transform the Lattice-Boltzmann method into the numerically stable computational tool for fluid flows and other dissipative systems out of equilibrium [18];
- To develop the Entropic Lattice Boltzmann method as a starting basis for the formulation of a new class of turbulence models based on genuinely kinetic principles [19].

Now we extend the method elaborated for dissipative systems [15, 16] to the higher-order models for conservative systems. The iteration method for improvement of obtained approximations is proposed too. It is a version of the Method of invariant manifold for kinetic problems, developed in the series of papers [20, 21] (the almost exhaustive review of these works can be found in the paper [22]). The summary of this method is given in Appendix.

The constructing of the method of physically consistent computation is the central part of our paper. It is neither a philosophical opus, nor only discussion of foundations of science.

The main results of this paper were presented in the talk given on the First Mexican Meeting on Mathematical and Experimental Physics, Mexico City, September 10-14, 2001,

and in the lectures given on the V Russian National Seminar “Modeling of Nonequilibrium systems”, Krasnoyarsk, October 18-20, 2002 [49].

1 The problem of irreversibility

1.1 The phenomenon of the macroscopic irreversibility

The “stairs of reduction” (Fig. 1) lead from the reversible microdynamics to irreversible macrokinetics. The most mysterious is the first step: the appearance of irreversibility.

The best way to demonstrate the problem of irreversibility is the following *Gedankenexperiment*: Let us watch the movie: It’s raining, people are running, cars rolling. Let us now wind this movie in the opposite direction, and we will see a strange and funny picture: Drops of the rain are raising up to the clouds, which next condensate into the vapor on the pools, on the surfaces of rivers, people run with their backs forward, cars behave also quite strange, and so forth. This cannot be, and we “know” this for sure, we have never seen anything like this in our life. Let us now imagine that we watch the same movie with a magnitude of $10^8 - 10^9$ so that we can resolve individual particles. And all of the sudden we discover that we cannot see any substantial difference between the direct and the reverse demonstration: Everywhere the particles are moving, colliding, reacting according to the laws of physics, and nowhere there is a violation of anything. We cannot tell the direct progressing of the time from the reversed. So, we have the irreversibility of the macroscopic picture under the reversibility of the microscopic one.

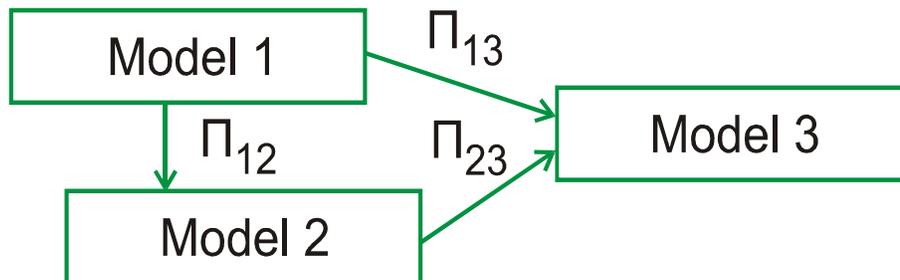
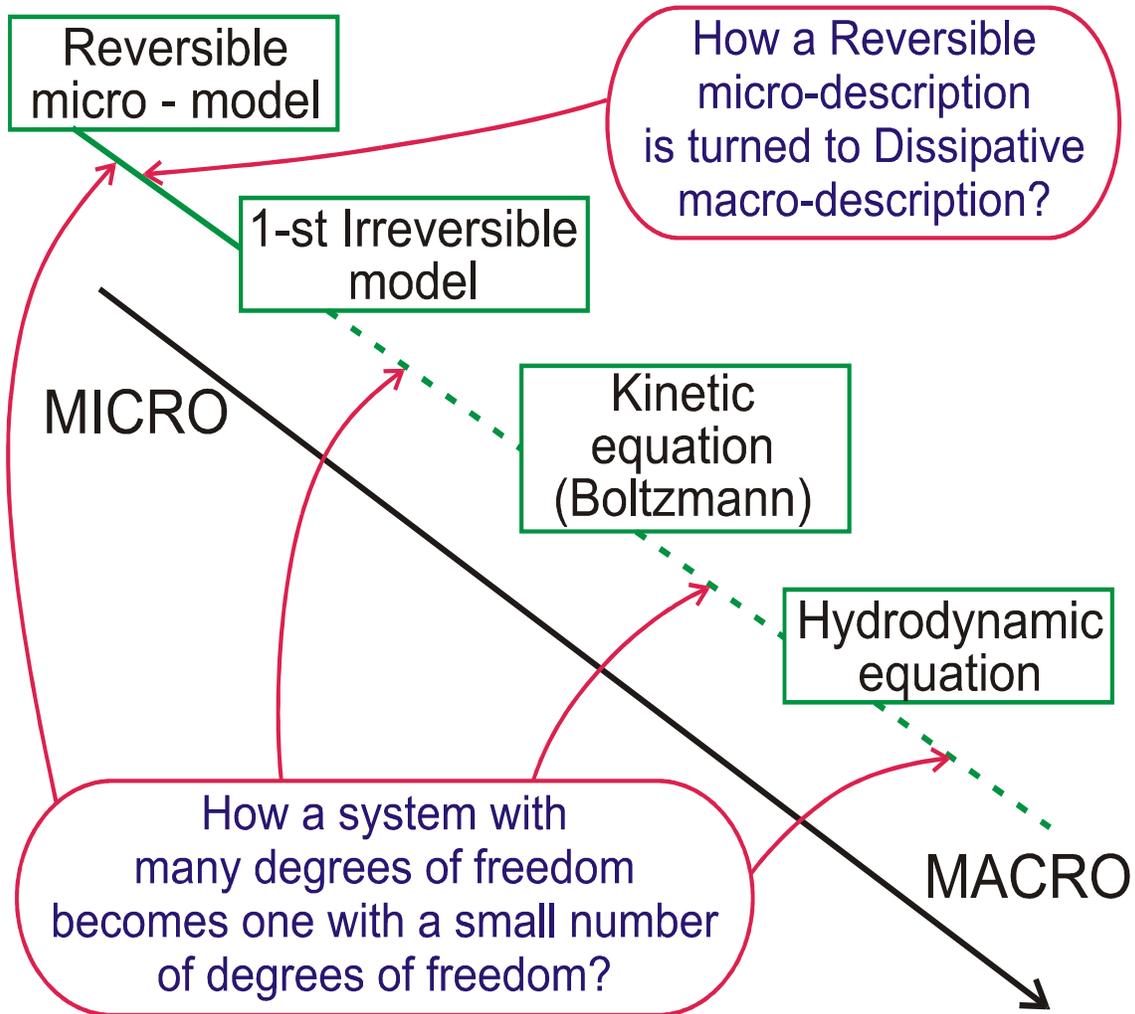
Rain, people, cars - this all is too complicated. One of the most simple examples of the irreversible macroscopic picture under the apparent reversibility of the microscopic picture (the “thermal ratchet”) is given by R. Feynman in his lectures on the character of physical law [23]. We easily label it as self-evident the fact that particles of different colors mix together, and we would see it as a wonder the reverse picture of a spontaneous decomposition of their mixture. However, itself an appreciation of one picture as usual, and of the other as unusual and wonderful - this is not yet the physics. It is desirable to measure somehow this transition from order to disorder.

1.2 Phase volume and dynamics of ensembles

Let there be n blue and n white particles in a box, and let the box is separated in two halves, the left and the right. Location of all the particles in the box is described by the assembly of $2n$ vectors of locations of individual particles. The set of all the assemblies is a “box” in the $6n$ -dimensional space. A point in this $6n$ -dimensional box describes a configuration. The motion of this point is defined by equations of mechanics.

“Order” is the configuration in which the blue particles are all in the right half, and all the white particles are in the left half. The set of all such configurations has a rather small volume. It makes only $(1/2)^{2n}$ of the total volume of the $6n$ -dimensional box. If $n = 10$, this is of the order of one per million of the total volume. It is practically unthinkable

STEPS OF REDUCTION



This diagram must be commutative:

$$\Pi_{13} = \Pi_{23} \circ \Pi_{12}$$

Figure 1: The stairs of reduction, step by step.

to get into such a configuration by chance. It is also highly improbable that, by forming more or less voluntary the initial conditions, we can observe that the system becomes ordered by itself. From this standpoint, the motion goes from the states of “order” to the state of “disorder”, just because there are many more states of “disorder”.

However, we have defined it in this way. The well known question of where is more order, in a fine castle or in a pile of stones, has a profound answer: It depends on which pile you mean. If “piles” are thought as all configurations of stones which are not castles, then there are many more such piles, and so there is less order in such a pile. However, if these are specially and uniquely placed stones (for example, a garden of stones), then there is the same amount of order in such a pile as in the fine castle. *Not a specific configuration is important but an assembly of configurations embraced by one notion.*

This transition from single configurations to their assemblies (ensembles) play the pivotal role in the understanding of irreversibility: The irreversible transition from the ordered configuration (blue particles are on the right, white particles are on the left) to the disordered one occurs simply because there are many more of the disordered (in the sense of the volume). Here, strictly speaking, we have to add also a reference to the Liouville theorem: The volume in the phase space which is occupied by the ensemble does not change in time as the mechanical system evolves. Because of this fact, the volume V is a good measure to compare the assemblies of configurations. However, more often the quantity $\ln V$ is used, this is called the entropy.

The point which represents the configuration, very rapidly leaves a small neighborhood and for a long time (in practice, never) does not come back into it. In this, seemingly idyllic picture, there are still two rather dark clouds left. First, the arrow of time has not appeared. If we move from the ordered initial state (separated particles) backwards in time, then everything will stay the same as when we move forward in time, that is, the order will be changing into the disorder. Second, let us wind the film backwards, let us shoot the movie about mixing of colored particles, and then let us watch in the reverse order their demixing. Then the initial configurations for the reverse motion will only seem to be disordered. Their “order” is in the fact that they were obtained from the separated mixture by letting the system to evolve for the time t . There are also very few such configurations, just the same number as of the ordered (separated particles) states. If we start with these configurations, then we obtain the ordered system after the time t . Then why this most obvious consequence of the laws of mechanics looks so improbable on the screen? Perhaps, it should be accepted that states which are obtained from the ordered state by a time shift, and by inversion of particle’s velocities (in order to initialize the reverse motion in time), cannot be prepared by using macroscopic means of preparation. In order to prepare such states, one would have to employ an army of Maxwell’s daemons which would invert individual velocities with sufficient accuracy (here, it is much more into the phrase “sufficient accuracy” but this has to be discussed separately and next time).

For this reason, we lump the distinguished initial conditions, for which the mixture

decomposes spontaneously (“piles” of special form, or “gardens of stones”) together with other configurations into *macroscopically definable ensembles*. And already for those ensembles the spontaneous demixing becomes improbable. This way we come to a new viewpoint: (i). We cannot prepare individual systems but only representatives of ensembles. (ii) We cannot prepare ensembles at our will but only “macroscopically definable ensembles”. What are these macroscopically definable ensembles? It seems that one has to give some constructions, the universality of which can only be proven by the time and experience.

1.3 Macroscopically definable ensembles and quasiequilibria

The main tool in the study of macroscopically definable ensembles is the notion of the macroscopic variables, and of the quasiequilibria. In the dynamics of the ensembles, the macroscopic variables are defined as linear functionals (moments) of the density distribution of the ensemble. Macroscopic variables M usually include hydrodynamic fields, density of particles, densities of momentum, and density of the energy, also the list may include stress tensor, reaction rates and other quantities. In the present context, it is solely important that the list the macroscopic variables is identified for the system under consideration.

A single system is characterized by a single point x in the phase space. The ensemble of the systems is defined by the probability density F on the phase space. Density F must satisfy a set of restrictions, the most important of which are: Nonnegativity, $F(x) \geq 0$, normalization,

$$\int_X F(x)dV(x) = 1, \quad (1)$$

and that the entropy is defined, that is, there exists the integral,

$$S(F) = - \int_X F(x) \ln F(x)dV(x). \quad (2)$$

(Function $F \ln F$ is continuously extended to zero values of F : $0 \ln 0 = 0$). Here $dV(x)$ is the invariant measure (phase volume).

The quasiequilibrium ensemble describes the “equilibrium under restrictions”. It is assumed that some external forcing keeps the given values of the macroscopic variables M , with this, “all the rest” comes the corresponding (generalized) canonic ensemble F which is the solution to the problem:

$$S(F) \rightarrow \max, \quad M(F) = M. \quad (3)$$

where $S(F)$ is the entropy, $M(F)$ is the set of macroscopic variables.

The thesis about the macroscopically definable ensembles. Macroscopically definable ensembles are obtained as the result of two operations:

(i). Bringing the system into the quasiequilibrium state corresponding to either the whole set of the macroscopic variables M , or to its subset.

(ii). Changing the ensemble according to the microscopic dynamics (due to the Liouville equation) during some time t .

These operations can be applied in the interchanging order any number of times, and for arbitrary time segments t . The limit of macroscopically definable ensembles will also be termed the macroscopically definable. One always starts with the operation (i).

In order to work out the notion of macroscopic definability, one has to pay more attention to partitioning the system into subsystems. This involves a partition of the phase space X with the measure dV on it into a direct product of spaces, $X = X_1 \times X_2$ with the measure $dV_1 dV_2$. To each admissible (“macroscopic”) partition into sub-systems, it corresponds the operation of taking a “partial quasiequilibrium”, applied to some density $F_0(x_1, x_2)$:

$$S(F) \rightarrow \max, \tag{4}$$

$$M(F) = M, \int_{X_2} F(x_1, x_2) dV_2(x_2) = \int_{X_2} F_0(x_1, x_2) dV_2(x_2).$$

where M is some subset of macroscopic variables (not necessarily the whole list of the macroscopic variables). In Eq. (4), the state of the first subsystem is not changing, whereas the second subsystem is brought into the quasiequilibrium. In fact, the problem (4) is a version of the problem (3) with additional “macroscopic variables”,

$$\int_{X_2} F(x_1, x_2) dV_2(x_2). \tag{5}$$

The extended thesis about macroscopically definable ensembles allows to use also operations (4) with only one restriction: The initial state should be the “true quasiequilibrium” that is, macroscopic variables related to all possible partitions into subsystems should appear only after the sequence of operations has started with the solution to the problem (3) for some initial M . This does not exclude a possibility of including operators (5) into the list of the basic macroscopic variables M . The standard example of such an inclusion are few-body distribution functions treated as macroscopic variables in derivations of kinetic equations from the Liouville equation.

Irreversibility is related to the choice of the initial conditions. The extended set of macroscopically definable ensembles is thus given by three objects:

(i). The set of macroscopic variables M which are linear (and, in an appropriate topology, continuous) mappings of the space of distributions onto the space of values of the macroscopic variables;

(ii). Macroscopically admissible partitions of the system into sub-systems;

(iii). Equations of microscopic dynamics (the Liouville equation, for example).

The choice of the macroscopic variables and of the macroscopically admissible partitions is a distinguished topic. The main question is: what variables are under the macroscopic control? Here the macroscopic variables are represented as formal elements of the construction, and the arbitrariness is removed only at solving specific problems.

Usual we can postulate some properties of macroscopic variables, for example, symmetry with respect to any permutation of equal micro-particles.

We have discussed the *prepared* ensembles. But there is another statement of problem too: Let us get an ensemble. The way how we get it may be different and unknown, for example, some demon or oracle¹ can give it to us. How can we transform this ensemble by macroscopic tools? First, it is possible just let them evolve, second, it can be controlled by the macroscopic tools on the defined way (it is necessary just to keep values of some macroscopic variables during some time).

The thesis about the macroscopically definable transformation of ensembles. Macroscopically definable transformation of ensembles are obtained as the result of two operations:

(i). Bringing the system into the quasiequilibrium state corresponding to either the whole set of the macroscopic variables M , or to its subset.

(ii). Changing the ensemble according to the microscopic dynamics (due to the Liouville equation, for example) during some time t .

These operations can be applied in the interchanging order any number of times, and for arbitrary time segments t . The limit of macroscopically definable transformations will also be termed the macroscopically definable. The main difference of this definition (macroscopically definable transformation) from the definition of the macroscopically definable ensembles is the absence of restriction on the initial state, one can start from arbitrary ensemble.

The class of macroscopically definable ensembles includes the more simple, but important class. Let us reduce the macroscopic control to preparation of quasiequilibrium ensemble: we just prepare the ensemble by macroscopic tools and then let them evolve due to natural dynamics (Liouville equation, for example). Let us call this class *the primitive macroscopically definable ensembles*. These ensembles appear as results (for $t > 0$) of motions which start from the quasiequilibrium state (at $t = 0$). The main technical results of our work concern the computation of the manifold of primitive macroscopically definable ensembles for a given system.

The importance of this class of ensembles is determined by the following hypothesis: **The hypothesis about the primitive macroscopically definable ensembles.** Any macroscopically definable ensemble can be approximated by primitive macroscopically definable ensembles with appropriate accuracy. In some limits we can attempt to say: “with any accuracy”. Moreover, this hypothesis with “arbitrary small accuracy” can be found as the basic but implicit foundation of all nonequilibrium kinetics theories which pretend to demonstrate a way from microdynamics to macrokinetics, for example in Zubarev nonequilibrium statistical operator theory [3], etc. This hypothesis allow to describe nonequilibrium state as a result of evolution of quasiequilibrium state in time. Now we have no other way to describe the nonequilibrium state²

¹In the theory of computation, if there is a device which could answer questions beyond those that a Turing machine can answer, then it would be called oracle.

²There exists a series of papers with discussion of Hamiltonian systems in so-called force thermostat,

The hypothesis about the primitive macroscopically definable ensembles is real hypothesis, it can hold for different systems with different accuracy, it can be true or false. In some limits the set of primitive macroscopically definable ensembles can be dense in the set of all macroscopically definable ensembles, or can be not dense, etc. There is the significant difference between this hypothesis and the *thesis* about macroscopically definable ensembles. The thesis can be accepted, or not, the reasons for acceptance can be discussed, but nobody can prove or disprove the definition, even the definition of the macroscopically definable ensembles.

1.4 Irreversibility and initial conditions

The choice of the initial state of the ensemble plays the crucial role in the thesis about the macroscopically definable ensembles. The initial state is always taken as the quasiequilibrium distribution which realizes the maximum of the entropy for given values of the macroscopic variables. The choice of the initial state splits the time axis into two semi-axes: moving forward in time, and moving backward in time, the observed non-order increases (the simplest example is the mixing of the particles of different colors).

In some works, in order to achieve the “true nonequilibrium”, that is, the irreversible motion along the whole time axis, the quasiequilibrium initial condition is shifted into $-\infty$ in time. This trick, however, casts some doubts, the major being this: Most of the known equations of macroscopic dynamics which describe irreversible processes have solutions which can be extended backwards in time only for finite times (or cannot be extended at all). Such equations as the Boltzmann kinetic equation, diffusion equation, equations of chemical kinetics and like do not allow for almost all their solutions to be extended backward in time for indefinitely long. All motions have a “beginning” beyond which some physical properties of a solution will be lost (often, positivity of distributions), although formally solutions may even exist, as in the case of chemical kinetics.

1.5 Weak and strong tendency to equilibrium, shaking and short memory

One aspect of irreversibility is the special choice of initial conditions. Roughly speaking, the arrow of time is defined by the fact that the quasiequilibrium initial condition was in the past.

This remarkably simple observation does not, however, exhaust the problem of transition from the reversible equations to irreversible macroscopic equations. One more aspect

or, in particular, isokinetic thermostat (see, for example, the review of D. Ruelle [24]). These thermostats were invented in computational molecular dynamics for acceleration of computations, as a technical trick. From physical point of view this is a theory about a friction of particles on the space, the “ether friction” (the “ether” is a theoretical substrate in the ancient physics). Of course, this theory is mathematically consistent and perhaps it may be useful as the theory of special computations methods, but a bridge between this theory and physics is desirable.

deserves a serious consideration. Indeed, distribution functions tend to the equilibrium state according to macroscopic equations in a strong sense: deviations from the equilibrium tends to zero in the sense of most relevant norms (in the L^1 sense, for example, or even uniformly). On the contrast, for the Liouville equation, tendency to equilibrium occurs (if at all) only in the weak sense: mean values of sufficiently “regular” functions on the phase space do tend to their equilibrium values but the distribution function itself does not tend to the equilibrium with respect to any norm, not even point-wise. This is especially easy to appreciate if the initial state has been taken as the equipartition over some small bounded subset of the phase space (the “phase drop” with small, but non-zero volume). This phase drop can mix over the phase space, but for all the times it will remain “the drop of oil in the water”, the density will always be taking only two values, 0 and $p > 0$, and the volume of the set where the density is larger than zero will not be changing in time, of course. So, how to arrive from the weak convergence (in the sense of the convergence of the mean values), to the strong convergence (to the L^1 or to the uniform convergence, for example)? In order to do this, there are two basic constructions: The coarse-graining (shaking) in the sense of Ehrenfests’, and the short memory approximation.

The idea of coarse-graining dates back to P. and T. Ehrenfests, and it has been most clearly expressed in their famous paper of 1911 [25]. Ehrenfests considered a partition of the phase space into small cells, and they have suggested to alter the motions of the phase space ensemble due to the Liouville equation with “shaking” - averaging of the density of the ensemble over the phase cells. In the result of this process, the convergence to the equilibrium becomes strong out of the weak. It is not difficult to recognize that ensembles with constant densities over the phase cells are quasiequilibria; corresponding macroscopic variables are integrals of the density over the phase cells (“occupation numbers” of the cells). This generalizes to the following: alternations of the motion of the phase ensemble due to microscopic equations with returns to the quasiequilibrium manifold, preserving the values of the macroscopic variables. It is precisely this construction which serves for the point of departure for many of the constructions below.

Another construction is the short memory approximation. The essence of it is the following: If one excludes microscopic variables and assumes quasiequilibrium initial conditions, then it is possible to derive integro-differential equations with retardation for the macroscopic variables (the way to do this is not unique). The form of the resulting equations is approximately this:

$$M(t) = \int_0^t K(t, t')[M(t')]dt',$$

where $K(t, t')$ is an operator (generally speaking, nonlinear) acting on $M(t')$. Once this equation is obtained, one assumes that the kernels of these integro-differential equations decay at a sufficiently high rate into the past (for example, exponentially, as $\|K(t, t')[M(t')]\| \leq \exp\{-(t-t')/\tau\}\|M(t')\|$). This can be interpreted in the spirit of Ehrenfests’: Every motion which has begun sufficiently recently (the “memory time” τ before now) can be

regarded as being started from the quasiequilibrium. Thus, after each time τ has elapsed, the system can be shaken in the sense of Ehrenfests - the result should not differ much.

1.6 The essence of irreversibility in two words

(i) The direction of the arrow of time is defined by the fact that only “macroscopically definable ensembles” can be taken as initial conditions, that is, only quasiequilibrium ensembles and what can be obtained from them when they are exposed to the true microscopic dynamics, or when partial quasiequilibria are taken in positive time. *We* are created in such a way that we prepare and control (in part) the present, and observe what happens in the future. (In a sense, this is a definition of the subjective time).

(ii) Microscopic dynamics can give only the weak convergence to the equilibrium, convergence of mean values. Macroscopic variables tend to the equilibrium in the strong sense. The passage from micro to macro occurs here with the help of Ehrenfests’ coarse-graining procedure or its analogs.

One might feel uneasy about the second of these points because the procedure of coarse-graining is not the result of the equations of motion, and therefore it is somehow voluntary. The only hope to lift this arbitrariness is that it may well happen that, in the limit of a very large number of particles, the perturbation caused by the coarse-graining can be made arbitrary small, for example, by increasing the time interval between coarse-graining.

1.7 Equivalence between trajectories and ensembles in the thermodynamic limit

In the preceding sections we were speaking about the dynamics of ensembles. This apparently contradicts the fact that the dynamics of a classical system goes along a single trajectory. Two arguments make it possible to proceed from the trajectories to ensembles:

(i) High sensitivity of trajectories to external perturbations when the number of particles is large. Arbitrary weak noise results in the stochastization of the motion.

(ii) In the thermodynamic limit, it is possible to partition the system into an arbitrary large number of small but still macroscopic sub-systems. Initial conditions in the sub-systems are independent from one sub-system to another, and they cannot be assigned completely voluntary but are taken from some distribution with a fixed sum of mean values (an analog of the macroscopic definability of ensembles). For spatially inhomogeneous systems, such small but still macroscopic subsystems are defined in small and “almost homogeneous” volumes.

1.8 Subjective time and irreversibility

In our discussion, the source of the arrow of time is, after all, the asymmetry of the subjective time of the experimentalist. *We prepare* initial conditions, and *after* that *we*

watch what will happen in the future but not what happened in the past. Thus, we obtain kinetic equations for specifically prepared systems. How is this related to the dynamics of the real world? These equations are applicable to real systems to the extent that the reality can be modeled with systems with specifically prepared quasiequilibrium initial conditions. This is anyway less demanding than the condition of quasi-staticity of processes in classical thermodynamics. For this reason, versions of nonequilibrium thermodynamics and kinetics based on this understanding of irreversibility allowed to include such a variety of situations, and besides that, they include all classical equations of nonequilibrium thermodynamics and kinetics.

2 Geometrization of irreversibility

2.1 Quasiequilibrium manifold

Let E be a linear space, and $U \subset E$ be a convex subset, with a nonempty interior $\text{int}U$. Let a twice differentiable concave functional S be defined in $\text{int}U$, and let S is continuous on U . According to the familiar interpretation, S is the entropy, E is an appropriate space of distributions, U is the cone of nonnegative distributions from E . Space E is chosen in such a way that the entropy is well defined on U .

Let L be a closed linear subspace of space E , and $m : E \rightarrow E/L$ be the natural projection on the factor-space. The factor-space E/L will further play the role of the space of macroscopic variables (in examples, the space of moments of the distribution).

For each $M \in \text{int}U/L$ we define the quasiequilibrium, $f_M^* \in \text{int}U$, as the solution to the problem,

$$S(f) \rightarrow \max, \quad m(f) = M. \quad (6)$$

We assume that, for each $M \in \text{int}U/L$, there exists the (unique) solution to the problem (6). This solution, f_M^* , is called the quasiequilibrium, corresponding to the value M of the macroscopic variables. The set of quasiequilibria f_M^* forms a manifold in $\text{int}U$, parameterized by the values of the macroscopic variables $M \in \text{int}U/L$ (Fig. 2).

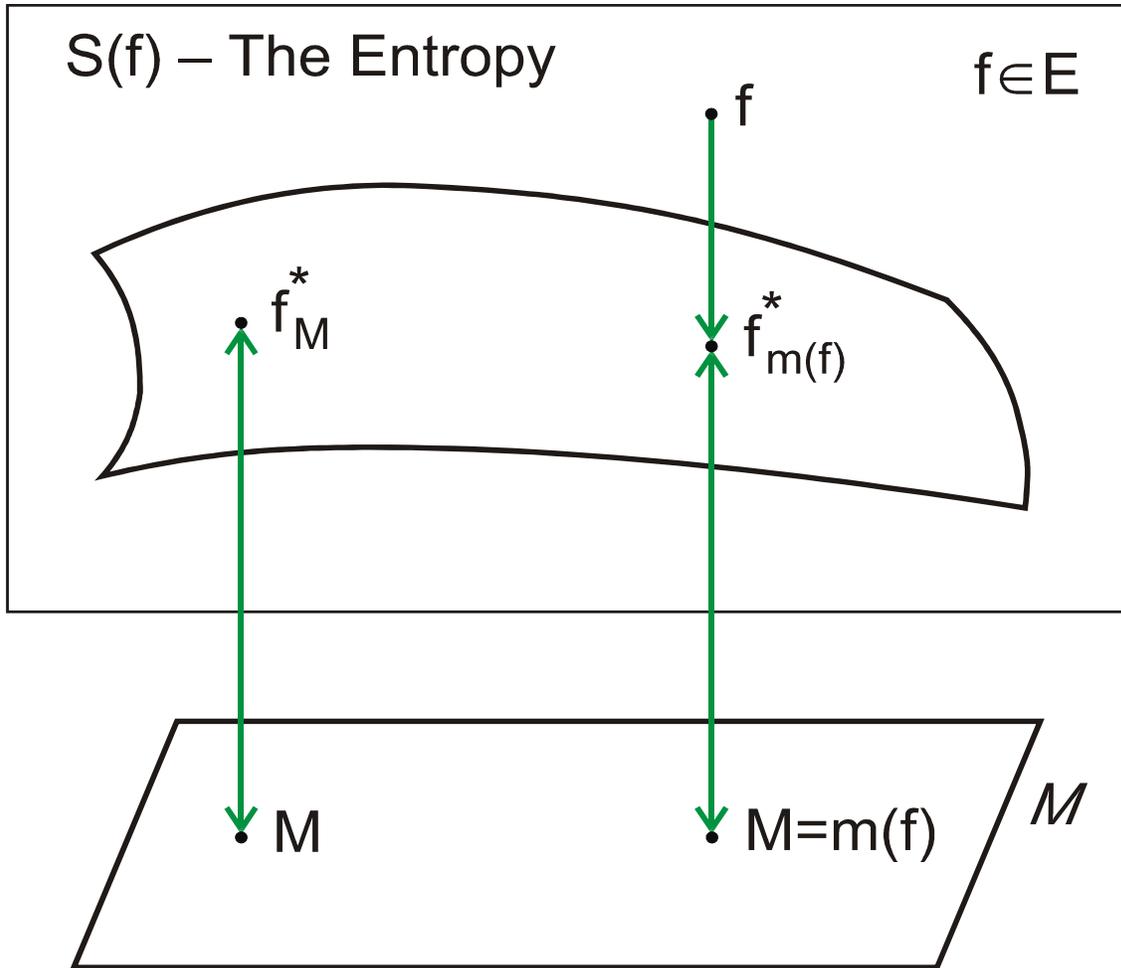
Let us specify some notations: E^T is the adjoint to the E space. Adjoint spaces and operators will be indicated by T , whereas notation $*$ is earmarked for equilibria and quasiequilibria.

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 $A : E_1 \rightarrow E_2$, the adjoint operator, $A^T : E_1^T \rightarrow E_2^T$ 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, $D_f S(f) \in E^T$ is the differential of the functional $S(f)$, $D^2 S(f)$ is the second differential of the functional $S(f)$. Corresponding quadratic functional $D^2 S(f)(x, x)$ on E is defined by the Taylor formula,

QE Manifold



$$f_M^* : \begin{cases} S(f) \rightarrow \max \\ m(f) = M \end{cases}$$

Figure 2: Relations between a microscopic state f , the corresponding macroscopic state $M = m(f)$, and quasiequilibria f_M^* .

$$S(f+x) = S(f) + [D_f S(f), x] + \frac{1}{2} D_f^2 S(f)(x, x) + o(\|x\|^2). \quad (7)$$

We keep the same notation for the corresponding symmetric bilinear form, $D_f^2 S(f)(x, y)$, and also for the linear operator, $D_f^2 S(f) : E \rightarrow E^T$, defined by the formula,

$$[D_f^2 S(f)x, y] = D_f^2 S(f)(x, y).$$

Here, on the left hand side there is the operator, on the right hand side there is the bilinear form. Operator $D_f^2 S(f)$ is symmetric on E , $D_f^2 S(f)^T = D_f^2 S(f)$.

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

A comment on the degree of rigor is in order: the statements which will be made below become theorems or plausible hypotheses in specific situations. Moreover, specialization is always done with an account for these statements in such a way as to simplify the proofs.

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

$$D_f S(f)|_{f_M^*} = \Lambda(M) \cdot m, \quad m(f_M^*) = M, \quad (8)$$

or

$$D_f S(f)|_{f_M^*} = m^T \cdot \Lambda(M), \quad m(f_M^*) = M. \quad (9)$$

From equation (9) we get,

$$m(D_M f_M^*) = 1_{(E/L)}, \quad (10)$$

where we have indicated the space in which the unit operator is acting. Next, using the latter expression, we transform the differential of the equation (8),

$$D_M \Lambda = (m(D_f^2 S)_{f_M^*}^{-1} m^T)^{-1}, \quad (11)$$

and, consequently,

$$D_M f_M^* = (D_f^2 S)_{f_M^*}^{-1} m^T (m(D_f^2 S)_{f_M^*}^{-1} m^T)^{-1}. \quad (12)$$

Notice that, elsewhere in equation (12), operator $(D_f^2 S)^{-1}$ acts on the linear functionals from imm^T . These functionals are precisely those which become zero on L (that is, on $\ker m$), or, which is the same, those which can be represented as functionals of macroscopic variables.

The tangent space to the quasiequilibrium manifold in the point f_M^* is the image of the operator $D_M f_M^*$:

$$\text{im}(D_M f_M^*) = (D_f^2 S)_{f_M^*}^{-1} \text{im} m^T = (D_f^2 S)_{f_M^*}^{-1} \text{Ann} L \quad (13)$$

where $\text{Ann} L$ (the annihilator of L) is the set of linear functionals which become zero on L . Another way to write equation (13) is the following:

$$x \in \text{im}(D_M f_M^*) \Leftrightarrow (D_f^2 S)_{f_M^*}(x, y) = 0, \quad y \in L \quad (14)$$

This means that $\text{im}(D_M f_M^*)$ is the orthogonal complement of L in E with respect to the scalar product,

$$\langle x|y \rangle_{f_M^*} = -(D_f^2 S)_{f_M^*}(x, y). \quad (15)$$

The entropic scalar product (15) appears often in the constructions below. (Usually, this becomes the scalar product indeed after the conservation laws are excluded). Let us denote as $T_{f_M^*} = \text{im}(D_M f_M^*)$ the tangent space to the quasiequilibrium manifold in the point f_M^* . An important role in the construction of quasiequilibrium dynamics and its generalizations is played by the quasiequilibrium projector, an operator which projects E on $T_{f_M^*}$ parallel to L . This is the orthogonal projector with respect to the entropic scalar product, $\pi_{f_M^*} : E \rightarrow T_{f_M^*}$:

$$\pi_{f_M^*} = (D_M f_M^*)_M m = (D_f^2 S)_{f_M^*}^{-1} m^T \left(m (D_f^2 S)_{f_M^*}^{-1} m^T \right)^{-1} m. \quad (16)$$

It is straightforward to check the equality $\pi_{f_M^*}^2 = \pi_{f_M^*}$, and the self-adjointness of $\pi_{f_M^*}$ with respect to entropic scalar product (15). Thus, we have introduced the basic constructions: quasiequilibrium manifold, entropic scalar product, and quasiequilibrium projector (Fig. 3).

2.2 Thermodynamic projector

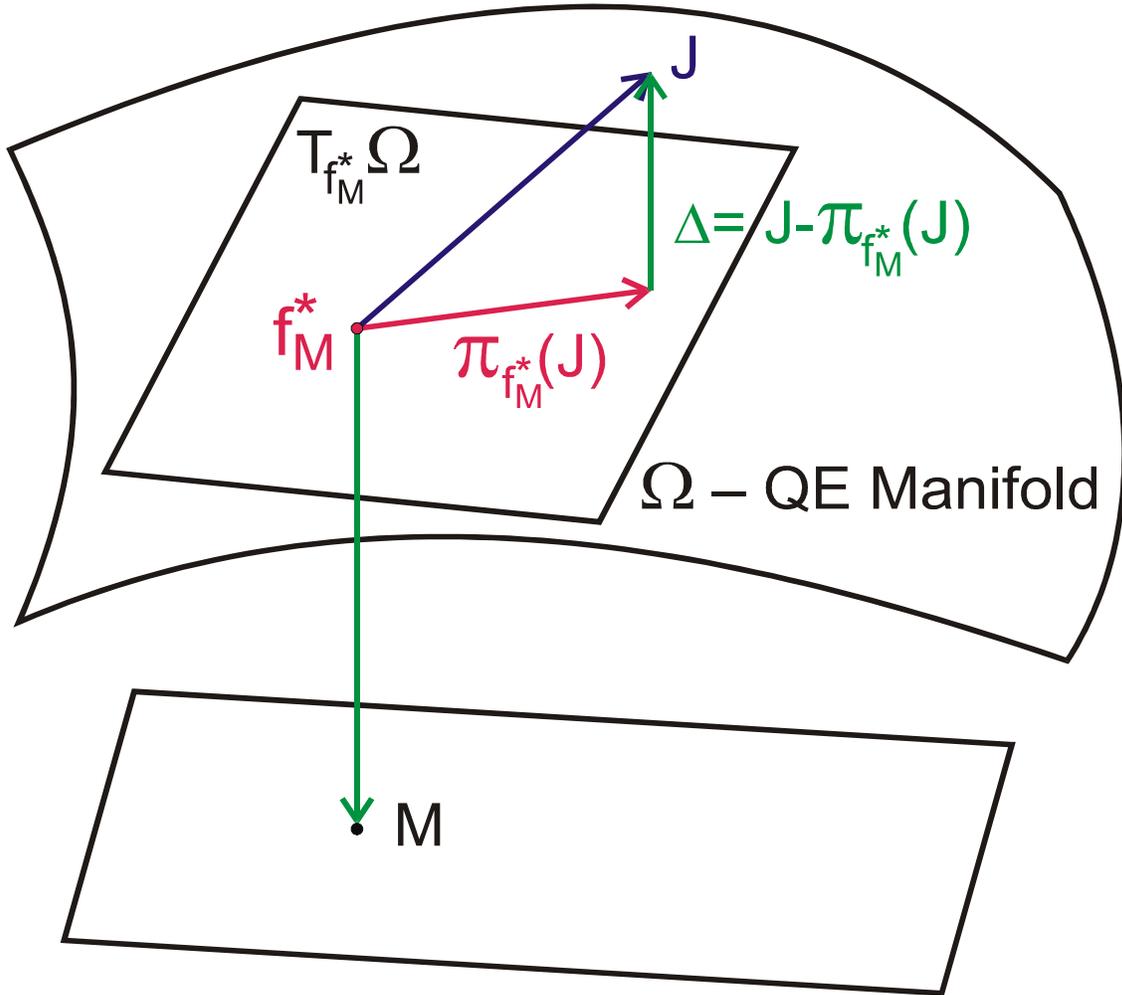
The construction of the quasiequilibrium allows for the following generalization: Almost every manifold can be represented as a set of minimizers of the entropy under linear constraints. However, in general, these linear constraints will depend on the point on the manifold.

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

$$S(f) \rightarrow \max, \quad m(f) = M. \quad (17)$$

For each point f_M , we identify $T_M \in E$, the tangent space to the manifold Ω in f_M , and subspace $L_M \subset E$, which depends smoothly on M , and which has the property, $L_M \oplus T_M = E$. Let us define $m(f)$ in the neighborhood of f_M in such a way, that

QE Projector



$$\pi_{f_M^*} = (D^2 S)^{-1} m^T (m (D^2 S)^{-1} m^T)^{-1} m$$

$$\Delta = J - \pi_{f_M^*}(J)$$

Figure 3: Quasiequilibrium manifold Ω , tangent space $T_{f_M^*} \Omega$, quasiequilibrium projector $\pi_{f_M^*}$, and defect of invariance, $\Delta = \Delta_{f_M^*} = J - \pi_{f_M^*}(J)$.

$$m(f) = M, \text{ if } f - f_M \in L_M. \quad (18)$$

The point f_M will be the solution of the quasiequilibrium problem (17) if and only if

$$D_f S(f)|_{f_M} \in \text{Ann } L_M. \quad (19)$$

That is, if and only if $L_M \subset \ker D_f S(f)|_{f_M}$. It is always possible to construct subspaces L_M with the properties just specified, at least locally, if the functional $D_f S(f)|_{f_M}$ is not identically equal to zero on T_M .

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_M parallel to L_M , and this preserves intact the basic properties of the quasiequilibrium approximations.

It was proven [26, 22] the **theorem of uniqueness of the the thermodynamic projector**: There exists 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).

Thermodynamic projector is constructed in the following way: Assume that the manifold $\Omega \subset U$ is given, $f \in \Omega$ and T is the tangent space to the manifold Ω in the point f . Let us describe the construction of the thermodynamic projector onto tangent space T in the point f .

Let us consider T_0 that is a subspace of T and which is annulled by the differential S in the point f :

$$T_0 = \{a \in T | (D_f S)(a) = 0\} \quad (20)$$

If $T_0 = T$, then the thermodynamic projector is the orthogonal projector on T with respect to the entropic scalar product $\langle | \rangle_f$ (15). Suppose that $T_0 \neq T$. Let $e_g \in T$, $e_g \perp T_0$ with respect to the entropic scalar product $\langle | \rangle_f$, and $(D_f S)(e_g) = 1$. These conditions define vector e_g uniquely.

The projector onto T is defined by the formula

$$P(J) = P_0(J) + e_g(D_f S)(J) \quad (21)$$

where P_0 is the orthogonal projector with respect to the entropic scalar product $\langle | \rangle_f$. For example, if T a finite-dimensional space, then the projector (21) is constructed in the following way. Let e_1, \dots, e_n be a basis in T , and for definiteness, $(D_f S)(e_1) \neq 0$.

1) Let us construct a system of vectors

$$b_i = e_{i+1} - \lambda_i e_1, (i = 1, \dots, n-1), \quad (22)$$

where $\lambda_i = (D_f S)(e_{i+1}) / (D_f S)(e_1)$, and hence $(D_f S)(b_i) = 0$. Thus, $\{b_i\}_1^{n-1}$ is a basis in T_0 .

2) Let us orthogonalize $\{b_i\}_1^{n-1}$ with respect to the entropic scalar product $\langle | \rangle_f$ (15). We have got an orthonormal with respect to $\langle | \rangle_f$ basis $\{g_i\}_1^{n-1}$ in T_0 .

3) We find $e_g \in T$ from the conditions:

$$\langle e_g | g_i \rangle_f = 0, (i = 1, \dots, n - 1), (D_f S)(e_g) = 1. \quad (23)$$

and, finally we get

$$P(J) = \sum_{i=1}^{n-1} g_i \langle g_i | J \rangle_f + e_g (D_f S)(J) \quad (24)$$

If $(D_f S)(T) = 0$, then the projector P is simply the orthogonal projector with respect to the entropic scalar product. This is possible, for example, if f is the global maximum of entropy point (equilibrium). Then

$$P(J) = \sum_{i=1}^n g_i \langle g_i | J \rangle_f, \langle g_i | g_j \rangle = \delta_{ij}. \quad (25)$$

If $(D_f S)(T) = 0$ and f is not equilibrium (Ω is tangent to the level of the entropy), then the dynamic $\dot{f} = J(f)$ can be projected on Ω with preservation of dissipation only if $(D_f S)(J(f)) = 0$ in this point.

2.3 Quasiequilibrium approximation

Let a kinetic equation be defined in U :

$$\frac{df}{dt} = J(f). \quad (26)$$

(This can be the Liouville equation, the Boltzmann equation, and so on, dependent on which level of precision is taken for the microscopic description.) One seeks the dynamics of the macroscopic variables M . If we adopt the thesis that the solutions of the equation (26) of interest for us begin on the quasiequilibrium manifold, and stay close to it for all the later times, then, as the first approximation, we can take the quasiequilibrium approximation. It is constructed this way: We regard f as the quasiequilibrium, and write,

$$\frac{dM}{dt} = m(J(f_M^*)). \quad (27)$$

With this, the corresponding to M point on the quasiequilibrium manifold moves according to the following equation:

$$\frac{df_{M(t)}^*}{dt} = (D_M f_M^*) m(J(f_M^*)) = \pi_{f_M^*} J(f_M^*), \quad (28)$$

where $\pi_{f_M^*}$ is the quasiequilibrium projector (16). It is instructive to represent solutions to equations of the quasiequilibrium approximation (28) in the following way: Let $T_\tau(f)$ be the shift operator along the phase flow of equation (26) (that is, $T_\tau(f)$ is solution to

equation (26) at the time $t = \tau$ with the initial condition f at $t = 0$). Let us take the initial point $f_0 = f_{M_0}^*$, and set, $f_{1/2} = T_\tau(f_0)$, $M_1 = m(f_{1/2})$, $f_1 = f_{M_1}^*$, \dots , $f_{n+1/2} = T_\tau(f_n)$, $M_{n+1} = m(f_{n+1/2})$, \dots . The sequence f_n will be termed the *Ehrenfest's chain*. We set, $f_\tau(n\tau) = f_n$. Then, $f_\tau(t) \rightarrow f(t)$, where $f(t)$ is the solution to the quasiequilibrium approximation (28), as $\tau \rightarrow 0$, $n \rightarrow \infty$, $n\tau = t$.

Let us notice that the way the entropy evolves in time according to the Ehrenfests' chain is defined in the limit $\tau \rightarrow 0$ solely by the way it evolves along trajectories of the kinetic equation (26). Indeed, f_M^* is the point of maximum of the entropy on the subspace defined by equation, $m(f) = M$. Therefore, for

$$S(f_{n+1/2}) - S(f_{n+1}) = o(\|f_{n+1/2} - f_{n+1}\|) = o(\tau),$$

it holds

$$\sum_n |S(f_{n+1/2}) - S(f_{n+1})| = o(n\tau) \rightarrow 0,$$

for $\tau \rightarrow 0$, $n \rightarrow \infty$, $n\tau = \text{const}$. This simple observation has a rather important implication: Let us denote as $dS(f)/dt$ the entropy production due to the original kinetic equation (26), and as $(dS(f_M^*)/dt)_1$ its derivative due to the quasiequilibrium system (28). Then,

$$(dS(f_M^*)/dt)_1 = dS(f)/dt|_{f=f_M^*}. \quad (29)$$

Let us give a different formulation of the latter identity. Let us term function $S(M) = S(f_M^*)$ the *quasiequilibrium entropy*. Let us denote as $dS(M)/dt$ the derivative of the quasiequilibrium entropy due to the quasiequilibrium approximation (27). Then,

$$\frac{dS(M)}{dt} = \frac{dS(f)}{dt} \Big|_{f=f_M^*}. \quad (30)$$

From the identity (29), it follows **the theorem about preservation of the type of dynamics**:

(i) If, for the original kinetic equation (26), $dS(f)/dt = 0$ at $f = f_M^*$, then the entropy is conserved due to the quasiequilibrium system (28).

(ii) If, for the original kinetic equation (26), $dS(f)/dt \geq 0$ at $f = f_M^*$, then, at the same points, f_M^* , $dS(M)/dt \geq 0$ due to the quasiequilibrium system (27).

The theorem about the preservation of the type of dynamics³ demonstrates that, if there was no dissipation in the original system (26) (if the entropy was conserved) then

³This is a rather old theorem, one of us had published this theorem in 1984 already as textbook material ([27], chapter 3 "Quasiequilibrium and entropy maximum", p. 37, see also the paper [29]), but from time to time different particular cases of this theorem are continued to be published as new results.

Another old theorem which was rediscovered many times is the theorem about **quasiequilibrium entropy growth** for quasiequilibrium initial conditions: If $f(t)$ is the solution of initial kinetic equations (26), $f(0)$ is a quasiequilibrium state, $f(0) = f = f_{m(f(0))}^*$, and $J(f(0))$ is not tangent to quasiequilibrium manifold, then the quasiequilibrium entropy $S(f_{m(f(t))}^*)$ for conservative system (26) strictly monotonically increase on some time interval $[0, T]$, $T > 0$. One of us had published this theorem in 1986 as a textbook material [28], see also the papers [12, 29, 30, 42].

Ehrenfestics

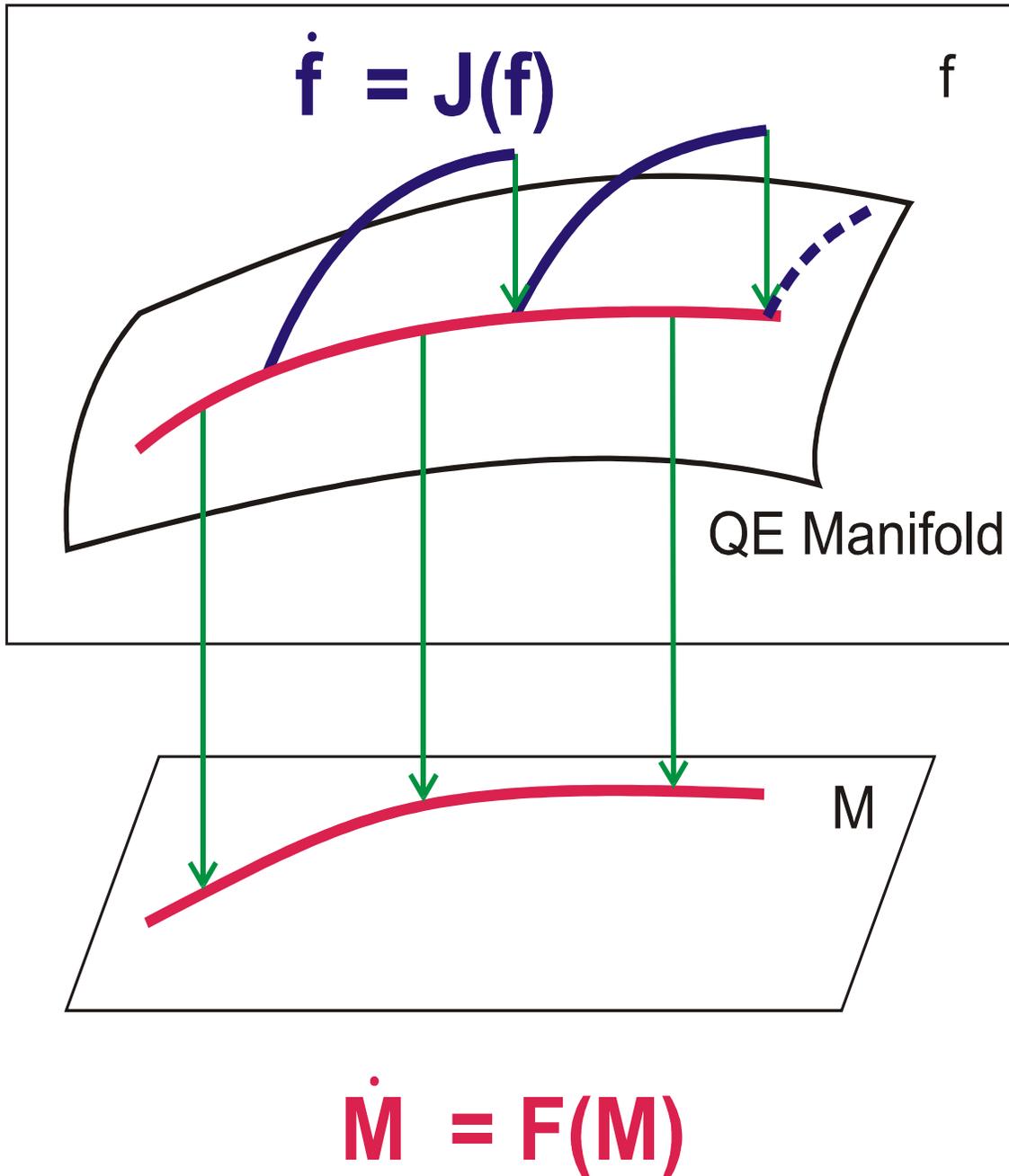


Figure 4: Ehrenfest's chain over the quasiequilibrium manifold, and trajectory of the macroscopic dynamics, $\dot{M} = F(M)$.

there is also no dissipation in the quasiequilibrium approximation. The passage to the quasiequilibrium does not introduce irreversibility (the reverse may happen, for example, there is no dissipation in the quasiequilibrium approximation for hydrodynamic variables as obtained from the Boltzmann kinetic equation; though dissipation is present in the Boltzmann equation, it occurs in different points but on the quasiequilibrium manifold of local Maxwellians the entropy production is equal to zero). The same statement also hold for the thermodynamic projectors described in Section 2.2. On the other hand, the entropy production in the quasiequilibrium state is the same, as for the quasiequilibrium system in the corresponding point, hence, if the initial system is dissipative, then quasiequilibrium entropy production is nonnegative.

Usually, the original dynamics (26) does not leave the quasiequilibrium manifold invariant, that is, vector field $J(f)$ is not tangent to the quasiequilibrium manifold in all its points f_M^* . In other words, the *condition of invariance*,

$$(1 - \pi_{f_M^*})J(f_M^*) = 0, \quad (31)$$

is not satisfied. The left hand side of the invariance condition (31) is of such an outstanding importance that it deserves a separate name. We call it the *defect of invariance*, and denote it as $\Delta_{f_M^*}$. It is possible to consider the invariance condition as an equation, and to compute corrections to the quasiequilibrium approximation f_M^* in such a way as to make it “more invariant”. In those cases where the original equation (26) is already dissipative, this route of corrections, supplemented by the construction of the thermodynamic projector as in Section 2.2, leads to an appropriate macroscopic kinetics [21].

However, here, we are mainly interested in the route “from the very beginning”, from conservative systems to dissipative. And here solving of the invariance equation does not help since it will lead us to, while “more invariant”, but still conservative dynamics. In all the approaches to this problem (passage from the conservative to the dissipative systems), dissipation is introduced in a more or less explicit fashion by various assumptions about the “short memory”. The originating point of our constructions will be the absolutely transparent and explicit approach of Ehrenfests.

3 Natural projector and models of nonequilibrium dynamics

3.1 Natural projector

So, let the original system (26) be conservative, and thus, $dS(f)/dt = 0$. The idea of Ehrenfests is to supplement the dynamics (26) by “shakings”. Shakings are external perturbations which are applied periodically with a fixed time interval τ , and which lead to a “forgetting” of the small scale (nonequilibrium) details of the dynamics. For us here the shaking is the replacement of f with the quasiequilibrium distribution $f_{m(f)}^*$. In the particular case which was originally considered in by Ehrenfests, the macroscopic

variables $m(f)$ were the averages of f over cells in the phase space, while $f_{m(f)}^*$ was the cell-homogeneous distribution with with the constant density within each cell equal to the corresponding cell-average of f . As we have already mentioned it, in the limit $\tau \rightarrow 0$, one gets back the quasiequilibrium approximation - and the type of the dynamics is preserved. In this limit we obtain just the usual projection of the vector field $J(f)$ (26) on the tangent bundle to the quasiequilibrium manifold. So, the natural question appears: What will happen, if we will not just send τ to zero but will consider finite, and even large, τ ? In such an approach, not just the vector fields are projected but segments of trajectories. We shall term this way of projecting the *natural*. Let us now pose the problem of the *natural projector* formally. Let $T_t(f)$ be the phase flow of the system (26). We must derive a phase flow of the macroscopic system, $\Theta_t(M)$ (that is, the phase flow of the macroscopic system, $dM/dt = F(M)$), which we are looking for), such that, for any M ,

$$m(T_\tau(f_M^*)) = \Theta_\tau(M). \quad (32)$$

That is, when moving along the macroscopic trajectory, after the time τ we must obtain the same values of the macroscopic variables as if we were moving along the true microscopic trajectory for the same time τ , starting with the quasiequilibrium initial condition (Fig. 5).

It is instructive to remark that, at finite τ , the entropy growth follows immediately from equation (32) because $S(f) < S(f_{m(f)}^*)$. The difference of the values of the entropy is of the order $\|f - f_{m(f)}^*\|^2$, for the time τ , thus, the first non-vanishing order in the entropy production will be of the order of τ . Let us find it.

We shall seek F in terms of a series in τ . Let us expand F and *both* the sides of the equation (32) in powers of τ to second order, and find the expansion coefficients of F [31]⁴:

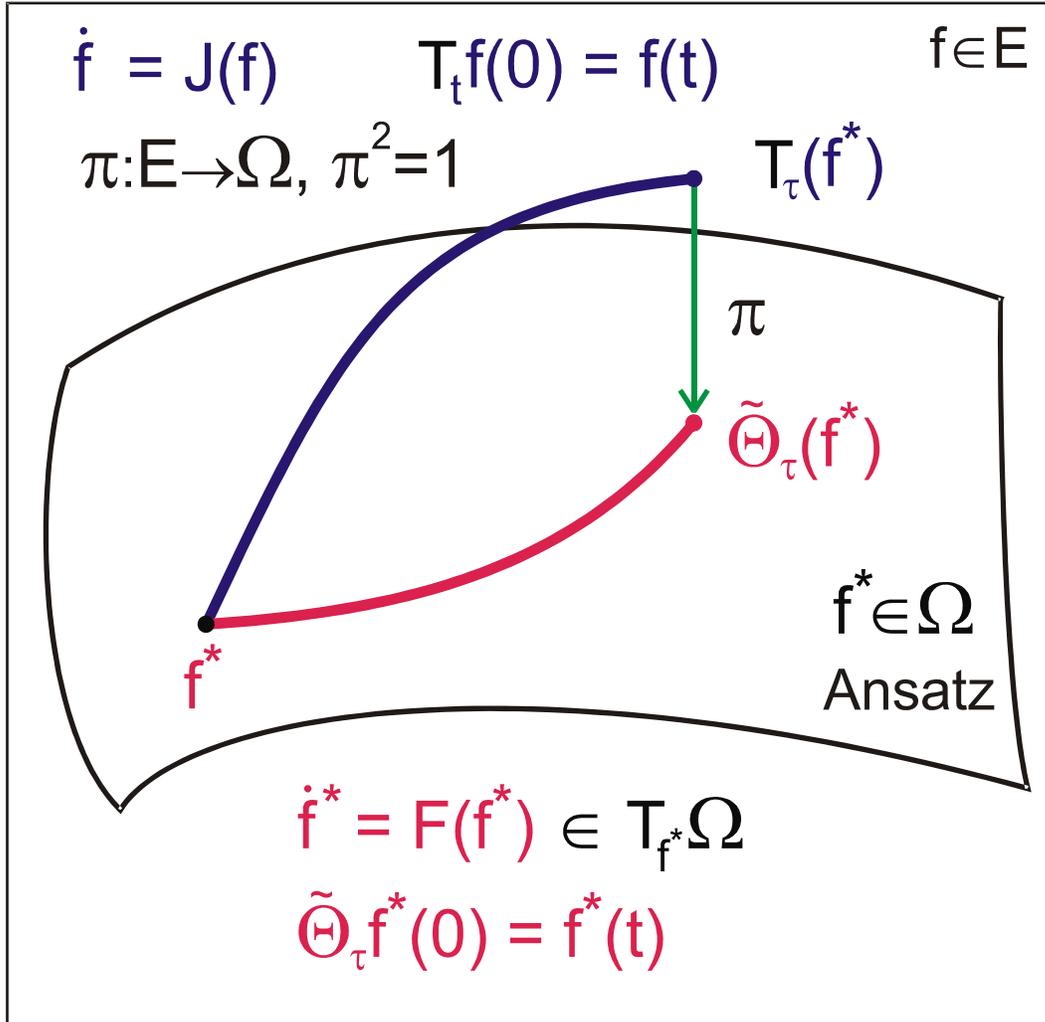
$$\begin{aligned} T_\tau(f_0^*) &= f_0 + df/dt|_{f_0}\tau + d^2f/dt^2|_{f_0}(\tau^2/2) + o(\tau^2), \\ \Theta_\tau(M_0) &= M_0 + dM/dt|_{M_0}\tau + d^2M/dt^2|_{M_0}(\tau^2/2) + o(\tau^2), \\ df/dt|_{f_0} &= J(f_0), \quad d^2f/dt^2|_{f_0} = D_f J(f)|_{f_0} J(f_0), \\ dM/dt|_{M_0} &= F(M_0), \quad d^2M/dt^2|_{M_0} = D_M F(M)|_{M_0} F(M_0), \\ F(M) &= F_0(M) + \tau F_1(M) + o(\tau). \end{aligned}$$

Using these expansions in the condition for natural projector (32), we get,

$$f_0 = f_{M_0}^*,$$

⁴In this well known work [31] Lewis expanded only the right hand side of equation (32), and did not do the same also with the left hand side. There were some hidden reason for this ‘‘inconsistency’’: it was impossible to obtain the Boltzmann equation without such a deformation of expansion. We stress that our approach of matched expansion for exploring the coarse-graining condition is, in fact, the exact (formal) statement that the unknown macroscopic dynamics which causes the shift of M on the left hand side of equation (32) 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.

Natural projector



$$\forall f^* \in \Omega \quad \pi(T_\tau f^*) = \tilde{\Theta}_\tau(f^*)$$

Figure 5: Projection of segments of trajectories: The microscopic motion above the manifold Ω and the macroscopic motion on this manifold. If these motions began in the same point on Ω , then, after time τ , projection of the microscopic state onto Ω should coincide with the result of the macroscopic motion on Ω . For quasiequilibrium Ω projector $\pi : E \rightarrow \Omega$ acts as $\pi(f) = f_{m(f)}^*$.

$$\begin{aligned}
& m(f_0) + \tau m(J(f_0)) + (\tau^2/2)D_f J(f)|_{f_0} J(f_0) + o(\tau^2) \\
& = M_0 + \tau F_0(M_0) + \tau^2 F_1(M_0) + (\tau^2/2)D_M F(M)|_{M_0} F(M_0) + o(\tau^2),
\end{aligned}$$

whereupon,

$$\begin{aligned}
F_0(M) &= m(J(f_M^*)), \\
F_1(M) &= (1/2) \left\{ m(D_f J(f)|_{f_M^*} J(f_M^*)) - D_M F_0(M)|_M F_0(M) \right\}.
\end{aligned}$$

Thus, the approximation F_0 is the quasiequilibrium, and using this fact in the expression for F_1 , after some transformation, we derive,

$$\begin{aligned}
F_1 &= (1/2) \left\{ m(D_f J(f)|_{f_M^*} J(f_M^*)) - D_M(m(J(f_M^*)))m(J(f_M^*)) \right\} \\
&= (1/2) \left\{ m(D_f J(f)|_{f_M^*} J(f_M^*)) - m(D_f J(f)|_{f_M^*} D_M f_M^*)m(J(f_M^*)) \right\} \\
&= (1/2)m \left(D_f J(f)|_{f_M^*} [J(f_M^*) - D_M f_M^* m(J(f_M^*))] \right) \\
&= (1/2)m \left(D_f J(f)|_{f_M^*} [1 - \pi_{f_M^*}]J(f_M^*) \right) \\
&= (1/2)m \left(D_f J(f)|_{f_M^*} \Delta_{f_M^*} \right).
\end{aligned}$$

Thus, the final form of the equation for the macroscopic variables M may be written:

$$\frac{dM}{dt} = F(M) = m(J(f_M^*)) + (\tau/2)m(D_f J(f)|_{f_M^*} \Delta_{f_M^*}) + o(\tau^2). \quad (33)$$

It is remarkable the appearance of the defect of invariance in the second term (proportional to τ): If the quasiequilibrium manifold is invariant with respect to the microscopic dynamics, then $F(M)$ is quasiequilibrium.

Let us compute the production of the quasiequilibrium entropy $S(M) = S(f_M^*)$ due to macroscopic equations (33), neglecting the higher-order term $o(\tau^2)$.

$$dS(f_M^*)/dt = (\tau/2)D_f S(f)|_{f_M^*} \pi_{f_M^*} D_f J(f)|_{f_M^*} \Delta_{f_M^*}.$$

We notice that,

$$D_f S(f)|_{f_M^*} \pi_{f_M^*} = D_f S(f)|_{f_M^*},$$

because $\pi_{f_M^*}$ is a projector, and also because the thermodynamic condition

$$\ker \pi_{f_M^*} \subset \ker D_f S(f)|_{f_M^*}$$

which follows from the definition of quasiequilibrium (6). Next, by our assumption, the system (26) conserves the entropy,

$$dS(f)/dt = D_f S(f)|_f J(f) = 0.$$

Let us differentiate the latter identity:

$$D_f^2 S(f)|_f J(f) + D_f S(f)|_f D_f J(f)|_f = 0. \quad (34)$$

Thus, due to the right hand side of equation (33),

$$\begin{aligned}
\frac{dS(f_M^*)}{dt} &= (\tau/2)D_f S(f)|_{f_M^*} D_f J(f)|_{f_M^*} \Delta_{f_M^*} \\
&= -(\tau/2) \left(D_f^2 S(f)|_{f_M^*} J(f_M^*) \right) \Delta_{f_M^*} \\
&= (\tau/2) \langle J(f_M^*) | \Delta_{f_M^*} \rangle_{f_M^*},
\end{aligned}$$

where we have used notation for entropic scalar product (15). Finally,

$$\Delta_{f_M^*} = (1 - \pi_{f_M^*})J(f_M^*) = (1 - \pi_{f_M^*})^2 J(f_M^*),$$

whereas projector $\pi_{f_M^*}$ is self-adjoint in the entropic scalar product (15). Thus, $\langle J(f_M^*) | \Delta_{f_M^*} \rangle_{f_M^*} = \langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}$, and

$$\frac{dS(f_M^*)}{dt} = (\tau/2) \langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}. \quad (35)$$

Thus, the quasiequilibrium entropy increases due to equation of macroscopic dynamics (33) in those points of the quasiequilibrium manifold where the defect of invariance is not equal to zero. This way we see how the problem of the natural projector (projected are not vector fields but segments of trajectories) results in the dissipative equations. For specific examples see [30] where the second term in equation (33) results in viscous terms in the Navier-Stokes equations, diffusion and other dissipative contributions. However, it remains the undetermined coefficient τ . Formula (35) gives the entropy production just proportional to the time interval between subsequent coarse-graining. Of course, this could be true only for small enough τ , whereas we are mostly interested in the limit $\tau \rightarrow \infty$. It is only in this limit where one can get rid of the arbitrariness in the choice of τ present in equations (33) and (35). In order to do this, we need to study more carefully the structure of the trajectories which begin on the quasiequilibrium manifold.

3.2 One-dimensional model of nonequilibrium states

In the background of many derivations of nonequilibrium kinetic equations there is present the following picture: Above each point of the quasiequilibrium manifold there is located a huge subspace of nonequilibrium distributions with the same values of the macroscopic variables, as in the quasiequilibrium point. It is as if the motion decomposes into two projections, above the point on the quasiequilibrium manifold, and in the projection on this manifold. The motion in each layer above the quasiequilibrium points is extremely complicated, but fast, and everything quickly settles in this fast motion.

However, upon a more careful looking into the motions which begin in the quasiequilibrium points, we will observe that, above each point of the quasiequilibrium manifold it is located just a single curve, and all the nonequilibrium (not-quasiequilibrium) states which come into the game form just a one-dimensional manifold. It is namely this curve the construction of which we shall be dealing with in this section.

This is the curve of *the primitive macroscopically definable ensembles*. These ensembles appear as the result (for $t > 0$) of motions which start from the quasiequilibrium state (at $t = 0$).

For each value of the macroscopic variables M , and for each time τ , we define $M_{-\tau}$ by the following equality:

$$m(T_\tau(f_{M_{-\tau}}^*)) = M. \quad (36)$$

In other words, $M_{-\tau}$ are those values of macroscopic variables which satisfy $\Theta_\tau(M_{-\tau}) = M$ for the natural projector (32). Of course, it may well happen that such $M_{-\tau}$ exists not for every pair (M, τ) but we shall assume here that for every M there exists such $\tau_M > 0$ that there exists $M_{-\tau}$ for $0 < \tau < \tau_M$.

A set of distributions, $q_{M,\tau} = T_\tau(f_{M_{-\tau}}^*)$, forms precisely the desired curve of nonequilibrium states with given values of M . Notice that, for each τ , it holds, $m(q_{M,\tau}) = M$. The set $\{q_{M,\tau}\}$ for all possible M and τ is positive invariant: If the motion of the system starts on it at some time t_0 , it stays on it also at $t > t_0$. If the dependence $q_{M,\tau}$ is known, equations of motion in the coordinate system (M, τ) have a simple form:

$$\begin{aligned} \frac{d\tau}{dt} &= 1, \\ \frac{dM}{dt} &= m(J(q_{M,\tau})). \end{aligned} \quad (37)$$

The simplest way to study $q_{M,\tau}$ is through a consideration of a sequence of its derivatives with respect to τ at fixed M . The first derivative is readily written as,

$$\left. \frac{dq_{M,\tau}}{d\tau} \right|_{\tau=0} = J(f_M^*) - \pi_{f_M^*} J(f_M^*) = \Delta_{f_M^*}. \quad (38)$$

By the construction of the quasiequilibrium manifold (we remind that $L = \ker m$), for any $x \in L$,

$$S(f_M^* + \tau x) = S(f_M^*) - (\tau^2/2)\langle x|x \rangle_{f_M^*} + o(\tau^2).$$

Therefore,

$$S(q_{M,\tau}) = S(f_M^*) - (\tau^2/2)\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*} + o(\tau^2).$$

Thus, to first order in τ , we have, as expected.

$$q_{M,\tau} = f_M^* + \tau \Delta_{f_M^*} + o(\tau).$$

Let us find $q_{M,\tau}$ to the accuracy of the order $o(\tau^2)$. To this end, we expand all the functions in equation (36) to the order of $o(\tau^2)$. With

$$M_{-\tau} = M - \tau m(J(f_M^*)) + \tau^2 B(M) + o(\tau^2),$$

where function B is yet unknown, we write:

$$f_{M-\tau}^* = f_M^* - \tau D_M f_M^* m(J(f_M^*)) + \tau^2 D_M f_M^* B(M) + (\tau^2/2)A_2(M) + o(\tau^2),$$

where

$$A_2(M) = \left. \frac{d^2 f_{M+tm(J(f_M^*))}^*}{dt^2} \right|_{t=0}, \quad (39)$$

and

$$\begin{aligned} T_\tau(x + \tau\alpha) &= x + \tau\alpha + \tau J(x) + \tau^2 D_x J(x)|_x \alpha \\ &\quad + (\tau^2/2) D_x J(x)|_x J(x) + o(\tau^2), \\ T_\tau(f_{M-\tau}^*) &= f_M^* - \tau D_M f_M^* m(J(f_M^*)) + \tau^2 D_M f_M^* B(M) + (\tau^2/2)A_2(M) \\ &\quad + \tau J(f_M^*) - \tau^2 D_f J(f)|_{f_M^*} D_M f_M^* m(J(f_M^*)) \\ &\quad + (\tau^2/2) D_f J(f)|_{f_M^*} J(f_M^*) + o(\tau^2) \\ &= f_M^* + \tau \Delta_{f_M^*} + (\tau^2/2)A_2(M) + (\tau^2/2) D_f J(f)|_{f_M^*} (1 - 2\pi_{f_M^*}) J(f_M^*) \\ &\quad + \tau^2 D_M f_M^* B(M) + o(\tau^2). \end{aligned}$$

The latter somewhat lengthy expression simplifies significantly under the action of m . Indeed,

$$\begin{aligned} m(A_2(M)) &= d^2[M + tm(J(f_M^*))]/dt^2 = 0, \\ m(1 - \pi_{f_M^*}) &= 0, \\ m(D_M f_M^*) &= 1. \end{aligned}$$

Thus,

$$\begin{aligned} m(T_\tau(f_{M-\tau}^*)) &= M + (\tau^2/2)m(D_f J(f)|_{f_M^*} (1 - 2\pi_{f_M^*}) J(f_M^*)) + \tau^2 B(M) + o(\tau^2), \\ B(M) &= (1/2)m(D_f J(f)|_{f_M^*} (2\pi_{f_M^*} - 1) J(f_M^*)). \end{aligned}$$

Accordingly, to second order in τ ,

$$\begin{aligned} q_{M,\tau} &= T_\tau(f_{M-\tau}^*) \\ &= f_M^* + \tau \Delta_{f_M^*} + (\tau^2/2)A_2(M) \\ &\quad + (\tau^2/2)(1 - \pi_{f_M^*}) D_f J(f)|_{f_M^*} (1 - 2\pi_{f_M^*}) J(f_M^*) + o(\tau^2). \end{aligned} \quad (40)$$

Notice that, besides the dynamic contribution of the order of τ^2 (the last term), there appears also the term A_2 (39) which is related to the curvature of the quasiequilibrium manifold along the quasiequilibrium trajectory.

Let us address the behavior of the entropy production in the neighborhood of f_M^* . Let $x \in L$ (that is, $m(x) = 0$). The production of the quasiequilibrium entropy, $\sigma_M^*(x)$, equals, by definition,

$$\sigma_M^*(x) = D_M S(f_M^*) \cdot m(J(f_M^* + x)). \quad (41)$$

Equation (41) gives the rate of entropy change under the motion of the projection of the state onto the quasiequilibrium manifold if the true trajectory goes through the point $f_M^* + x$. In order to compute the right hand side of equation (41), we use essentially the same argument, as in the proof of the entropy production formula (35). Namely, in the point f_M^* , we have $L \subset \ker D_f S(f)|_{f_M^*}$, and thus $D_f S(f)|_{f_M^*} \pi_{f_M^*} = D_f S(f)|_{f_M^*}$. Using this, and the fact that entropy production in the quasiequilibrium approximation is equal to zero, equation (41) may be written,

$$\sigma_M^*(x) = D_f S(f)|_{f_M^*} (J(f_M^* + x) - J(f_M^*)). \quad (42)$$

To the linear order in x , the latter expression reads:

$$\sigma_M^*(x) = D_f S(f)|_{f_M^*} D_f J(f)|_{f_M^*} x. \quad (43)$$

Using the identity (34), we obtain in equation (43),

$$\sigma_M^*(x) = -D_f^2 S(f)|_{f_M^*} (J(f_M^*), x) = \langle J(f_M^*) | x \rangle_{f_M^*}. \quad (44)$$

Because $x \in L$, we have $(1 - \pi_{f_M^*})x = x$, and

$$\begin{aligned} \langle J(f_M^*) | x \rangle_{f_M^*} &= \langle J(f_M^*) | (1 - \pi_{f_M^*})x \rangle_{f_M^*} \\ &= \langle (1 - \pi_{f_M^*})J(f_M^*) | x \rangle_{f_M^*} = \langle \Delta_{f_M^*} | x \rangle_{f_M^*}. \end{aligned}$$

Thus, finally, the entropy production in the formalism developed here, to the linear order reads,

$$\sigma_M^*(x) = \langle \Delta_{f_M^*} | x \rangle_{f_M^*}. \quad (45)$$

3.3 Stability of quasiequilibrium manifolds

The notion of stability does not cause essential difficulties when it goes about an invariant manifold, it is stable if, for any $\epsilon > 0$, there exist such $\delta > 0$ that a motion which has started at $t = 0$ at the distance (in some appropriate sense) less than δ from the manifold will not go away further than ϵ at any $t > 0$.

However, this is not so for a non-invariant manifold, and, probably, it is not possible to give a useful for all the cases formalization of the notion of *stability of the quasiequilibrium manifold*, in the spirit of motions going not far away when started sufficiently close to the manifold (indeed, what is here “sufficiently close” and “not far”?). In spite of that, expression (40) gives important opportunity to measure the stability. Indeed, let us consider how the entropy production depends on τ , that is, let us study the function,

$$\sigma_M(\tau) = \langle \Delta_{f_M^*} | q_{M,\tau} \rangle_{f_M^*}. \quad (46)$$

It is natural to expect that $\sigma_M(\tau)$ initially increases, and then it saturates to some limiting value. The question is, however, how function $\sigma_M(\tau)$ behaves at $t = 0$, is it concave or is it convex in this point? If function $\sigma_M(\tau)$ is concave, $d^2 \sigma_M(\tau)/d\tau^2|_{\tau=0} < 0$, then the

speed with which it grows reduces immediately, and one can even estimate the limiting value,

$$\sigma_M^* = \lim_{\tau \rightarrow \infty} \sigma_M(\tau),$$

using the first Padé approximate:

$$\begin{aligned} \sigma_M(\tau) &= a\tau/(1 + b\tau) = a\tau - ab\tau^2 + \dots \\ \sigma_M^* &= a/b = -\frac{2(d\sigma_M(\tau)/d\tau|_{\tau=0})^2}{d^2\sigma_M(\tau)/d\tau^2|_{\tau=0}}. \end{aligned} \quad (47)$$

Concavity of $\sigma_M(\tau)$ at $\tau = 0$ ($d^2\sigma_M(\tau)/d\tau^2|_{\tau=0} < 0$) is analogous to a soft instability: The motion does not run too far away, and it is possible to estimate where it will stop, see equation (47). However, if $d^2\sigma_M(\tau)/d\tau^2|_{\tau=0} > 0$, then this is analogous to a hard instability, and none of the estimates like (47) work. Thus, everything is defined by the sign of the scalar product,

$$\left. \frac{d^2\sigma_M(\tau)}{d\tau^2} \right|_{\tau=0} = \langle \Delta_{f_M^*} | A_2(M) + D_f J(f)|_{f_M^*} (1 - 2\pi_{f_M^*}) J(f_M^*) \rangle_{f_M^*}. \quad (48)$$

If this expression is negative, then the Padé estimate (47) gives:

$$\sigma_M^* = -\frac{2\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}^2}{\langle \Delta_{f_M^*} | A_2(M) + D_f J(f)|_{f_M^*} (1 - 2\pi_{f_M^*}) J(f_M^*) \rangle_{f_M^*}}. \quad (49)$$

In the opposite case, if the sign of the expression (48) is *positive*, we call the quasiequilibrium manifold *unstable*.

Equation (49) allows us to estimate the parameter τ in the equations of the method of natural projector. To this end, we make use of equation (35):

$$(\tau/2)\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*} = \sigma_M^*,$$

whereupon,

$$\tau \approx -\frac{4\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}}{\langle \Delta_{f_M^*} | A_2(M) + D_f J(f)|_{f_M^*} (1 - 2\pi_{f_M^*}) J(f_M^*) \rangle_{f_M^*}}, \quad (50)$$

if the denominator assumes negative values. In this case, there are no free parameters left in equation (33).

Above, the parameter τ , or the time of “leaving the initial quasiequilibrium condition”, has been appearing explicitly in the equations. Except for the case of linear quasiequilibrium manifolds where the formal limit $\tau \rightarrow \infty$ can be addressed to derive generalized fluctuation-dissipation relations [32], this may be not the best way to do in the general, nonlinear case.

3.4 Curvature and entropy production: Entropic circle and first kinetic equations

In a consequent geometric approach to the problem of constructing the one-dimensional model of nonequilibrium states it is sufficient to consider the entropic parameter, $\delta S =$

$S^*(M) - S$. Within this parameterization of the one-dimensional curve of the nonequilibrium states, one has to address functions $\sigma_M(\Delta S)$, rather than $\sigma_M(\tau)$ (46), whereas their Padè approximates can be constructed, in turn, from expansions in τ .

In order to give an example here, we notice that the simplest geometric estimate amounts to approximating the trajectory $q_{M,\tau}$ with a second order curve. Given $\dot{q}_{M,\tau}$ and $\ddot{q}_{M,\tau}$ (40), we construct a tangent circle (in the entropic metrics, $\langle | \rangle_{f_M^*}$, since the entropy is the integral of motion of the original equations). For the radius of this circle we get,

$$R = \frac{\langle \dot{q}_{M,0} | \dot{q}_{M,0} \rangle_{f_M^*}}{\sqrt{\langle \ddot{q}_{\perp M,0} | \ddot{q}_{\perp M,0} \rangle_{f_M^*}}}, \quad (51)$$

where

$$\begin{aligned} \dot{q}_{M,0} &= \Delta_{f_M^*}, \\ \ddot{q}_{\perp M,0} &= \ddot{q}_{M,0} - \frac{\langle \ddot{q}_{M,0} | \Delta_{f_M^*} \rangle_{f_M^*} \Delta_{f_M^*}}{\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}}, \\ \ddot{q}_{M,0} &= (1 - \pi_{f_M^*}) D_f J(f) |_{f_M^*} (1 - 2\pi_{f_M^*}) J(f_M^*) + (D_M \pi_{f_M^*}) m(J(f_M^*)). \end{aligned}$$

Let us represent the microscopic motion as a circular motion along this entropic circle with constant velocity $\dot{q}_{M,0} = \Delta_{f_M^*}$. When the microscopic motion passed the quarter of the circle, the entropy production started to decrease and it became zero after the halve of the circle. Hence, after passing the quarter of the circle, this model should be changed. The time of the motion along the quarter of the model entropic circle is:

$$\tau \approx \frac{\pi}{2} \sqrt{\frac{\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}}{\langle \ddot{q}_{\perp M,0} | \ddot{q}_{\perp M,0} \rangle_{f_M^*}}}. \quad (52)$$

After averaging on the 1/4 of this circle circular motion we obtain the macroscopic equations⁵

$$\begin{aligned} \frac{dM}{dt} &= m \left(J \left(f_M^* + \frac{2}{\pi} R \frac{\Delta_{f_M^*}}{\|\Delta_{f_M^*}\|} + \left(1 - \frac{2}{\pi} \right) R \frac{\ddot{q}_{\perp M,0}}{\|\ddot{q}_{\perp M,0}\|} \right) \right) = m(J(f_M^*)) + \\ &+ \frac{2}{\pi} \frac{R}{\|\Delta_{f_M^*}\|} m \left(D_f J(f) |_{f_M^*} (\Delta_{f_M^*}) \right) + \left(1 - \frac{2}{\pi} \right) \frac{R}{\|\ddot{q}_{\perp M,0}\|} m \left(D_f J(f) |_{f_M^*} (\ddot{q}_{\perp M,0}) \right) + o(R). \end{aligned} \quad (53)$$

where $\|y\| = \sqrt{\langle y | y \rangle_{f_M^*}}$.

Equations (53) contain no undetermined parameters. This is the simplest example of the general macroscopic equations obtained by the natural projector. The coefficients ($2/\pi$, etc.) can be corrected, but the form is more universal. The entropy production for equations (53) is proportional both to the defect of invariance and to the radius of curvature:

$$\sigma_M = \frac{2}{\pi} R \|\Delta_{f_M^*}\|. \quad (54)$$

⁵This averaging makes sense for *conservative* microdynamics, and for dissipative microdynamics the model of uniform circular motion along the entropic circle should be improved by taking into account the acceleration along the circle.

This equation demonstrates the thermodynamical sense of curvature of the curve of nonequilibrium states. The combination $\frac{\text{defect of invariance}}{\text{curvature}}$ is the dissipation. (It should be remained that all the scalar products and norms are *entropic*).

4 The film of non-equilibrium states

4.1 Equations for the film

The set $q_{M,\tau}$ in a space E generates a surface parameterized by “two variables”: A scalar, $\tau \geq 0$, and value of macroscopic variables, M , with condition

$$M = m(q_{M,\tau}). \quad (55)$$

We call this surface *the film of non-equilibrium states* or simply *the film*. It consists of *the primitive macroscopically definable ensembles*, the results (for $t > 0$) of motions which start from the quasiequilibrium state (at $t = 0$).

For each $\tau \geq 0$ *the section of the film* is defined: the set, $q_{M,\tau}$, for given τ . It is parameterized by the value of M . For $\tau = 0$ the section of the film coincides with the quasiequilibrium manifold. The film itself can be considered as a trajectory of motion of the section under variation of $\tau \in [0; +\infty)$ (Fig. 6). It is not difficult to write down equations of this motion using definition of $q_{M,\tau}$:

$$q_{M,\tau} = T_\tau f_{M-\tau}^*, \quad (56)$$

where T_τ is shift in time in accordance with the original dynamical system, $M_{-\tau}$ is defined with equation (36).

For small $\Delta\tau$

$$q_{M,\tau+\Delta\tau} = q_{M-\Delta M,\tau} + J(q_{M,\tau})\Delta\tau + o(\Delta\tau), \quad (57)$$

where $\Delta M = mJ(q_{M,\tau})\Delta\tau$. Hence,

$$\frac{dq_{M,\tau}}{dt} = (1 - D_M q_{M,\tau} m) J(q_{M,\tau}). \quad (58)$$

Initial condition for equation (58) is the quasiequilibrium

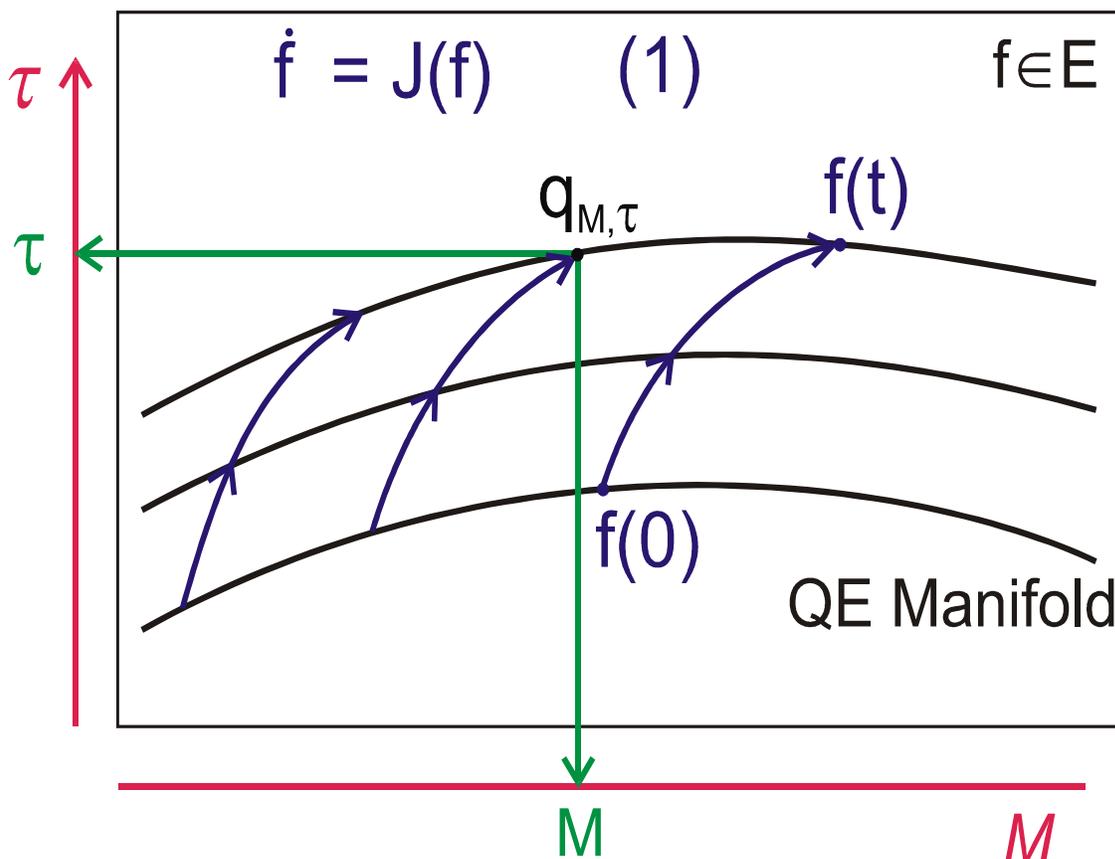
$$q_{M,0} = f_M^*. \quad (59)$$

Equation (58) under initial condition (59) defines the film of non-equilibrium states in the space E . This film is a minimal positive invariant set (i.e invariant with respect to shift T_τ by positive times $\tau > 0$), including the quasiequilibrium manifold, f_M^* . The kinetics we are interested in occurs only on this film.

Investigation of non-equilibrium kinetics can be separated into two problems:

i) Construction of the film of non-equilibrium states: solution of equation (58) under initial conditions (59).

Invariant Film



The Film $q_{M,\tau}$ is the trajectory of QEM moved by system (1)

Figure 6: The film of nonequilibrium states as the trajectory of motion of the quasiequilibrium manifold due to microscopic dynamics.

ii) Investigation of the motion of the system on the film.

Naturally, it should be assumed that the film will be constructed only approximately. Therefore, the second problem should be separated in two again:

ii1) Construction of projection of initial vector field, J , on the approximately found film, and construction of equations for M and τ .

ii2) Investigation and solution of equations for M and τ .

It should be especially emphasized that existence of the film is not significantly questionable (though, of course, the deriving of the theorems of existence and uniqueness for (58), (59) can turn into a complicated mathematical problem). In contrast, existence of kinetic coefficients (viscosity etc.), and generally, the fast convergence of dM/dt to a certain dependence $dM/dt(M)$ is essentially a hypothesis which is not always true.

Below we will be solving, mainly, the problem of construction of equations: problems ii1) and ii2). And we will begin with the problem ii2). Thus, let the film be approximately constructed.

4.2 Thermodynamic projector on the film

We need the projector in order to project the vector field on the tangent space. The idea of thermodynamic projector [20] consists of a description of every manifold (subject to certain requirements of transversality) as the quasiequilibrium one. For this, one constructs a projection of a neighborhood of the manifold on it, and later, the required projector is obtained by linearization.

The projection of the neighborhood on the manifold should satisfy essentially only one condition: a point of manifold must be the point of maximum of the entropy on its preimage. If the preimage of point f^* is a domain in the affine subspace, $L_{f^*} \subset E$, then required condition is:

$$D_f S^*(L_{f^*} - f^*) \equiv 0. \quad (60)$$

where $L_{f^*} - f^*$ is already the linear subspace in E .

For such projections, a dissipative vector field is projected into a dissipative one, and a conservative vector field (with the entropy conservation) is projected into a conservative one, i.e. the entropy balance is exact. Thus, let the film, $q_{M,\tau}$, be defined. Let us construct for it a thermodynamic projector.

Under small variation of variables M and τ

$$\begin{aligned} \Delta q_{M,\tau} &= D_M q_{M,\tau} \Delta M + D_\tau q_{M,\tau} \Delta \tau + o(\Delta M, \Delta \tau), \\ \Delta S &= D_f S|_{q_{M,\tau}} \Delta q_{M,\tau} + o(\Delta M, \Delta \tau). \end{aligned} \quad (61)$$

After simple transformations we obtain:

$$\begin{aligned}\Delta\tau &= \frac{1}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} + o(\Delta M, \Delta S), \\ \Delta q_{M,\tau} &= \left[1 - \frac{D_\tau q_{M,\tau} D_f S|_{q_{M,\tau}}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} \right] D_M q_{M,\tau} \Delta M \\ &+ \frac{1}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} D_\tau q_{M,\tau} \Delta S + o(\Delta M, \Delta S).\end{aligned}\quad (62)$$

From this formulae we obtain thermodynamic projector for J , π_{td} :

$$\pi_{\text{td}}|_{q_{M,\tau}} J = \left[1 - \frac{D_\tau q_{M,\tau} D_f S|_{q_{M,\tau}}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} \right] D_M q_{M,\tau} m J + \frac{D_\tau q_{M,\tau} D_f S|_{q_{M,\tau}}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} J. \quad (63)$$

For conservative systems the second term in (63) vanishes and we obtain:

$$\pi_{\text{td}}|_{q_{M,\tau}} J = \left[1 - \frac{D_\tau q_{M,\tau} D_f S|_{q_{M,\tau}}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} \right] D_M q_{M,\tau} m J. \quad (64)$$

The equation for M corresponding to (64) has the form:

$$\dot{M} = m \pi_{\text{td}}|_{q_{M,\tau}} J(q_{M,\tau}) = m \left[1 - \frac{D_\tau q_{M,\tau} D_f S|_{q_{M,\tau}}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} \right] D_M q_{M,\tau} m J = m J(q_{M,\tau}). \quad (65)$$

It should be supplemented with the equation for S :

$$\frac{dS}{dt} = 0, \quad (66)$$

or for τ , in accordance with (62),

$$\frac{d\tau}{dt} = \frac{\dot{S} - D_f S|_{q_{M,\tau}} D_M q_{M,\tau} \dot{M}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} = - \frac{D_f S|_{q_{M,\tau}} D_M q_{M,\tau} \dot{M}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}}, \quad (67)$$

where \dot{M} is defined in accordance with (65). The numerator in (67) has a simple meaning: it is the rate of the entropy production by dynamic equations (65) when τ is constant (for frozen τ). Expression (67) can be obtained from the condition of the constant entropy for the motion on the film in accordance with (65,67). Equations (65,67) describe dynamics on the film (Fig. 7).

Let us further assume that condition (38) is satisfied:

$$q_{M,\tau} = f_M^* + \tau \Delta f_M^* + o(\tau).$$

In expressions (62,65,67) the denominator, $D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}$, is present. For $\tau \rightarrow 0$ this expression vanishes:

$$\begin{aligned}D_\tau q_{M,\tau}|_{\tau=0} &= \Delta f_M^*, \\ D_f S|_{f=f_M^*} x &= 0, \quad \text{for } x \in \ker m,\end{aligned}\quad (68)$$

Dynamic Equation on The Film

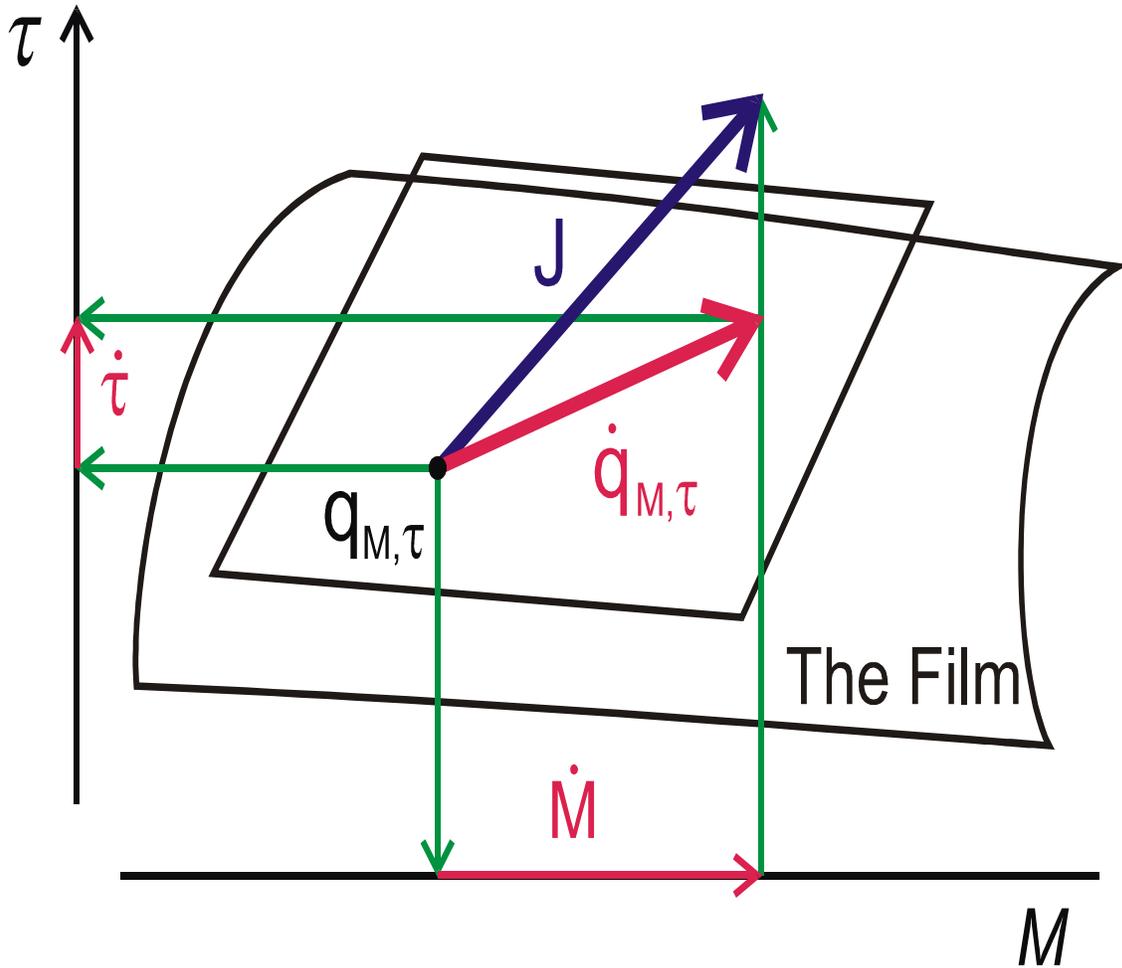


Figure 7: Dynamics on the film: $\dot{M} = mJ(q_{M,\tau})$, $\dot{\tau} = -\frac{D_f S|_{q_{M,\tau}} D_M q_{M,\tau} \dot{M}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}}$.

$m(\Delta_{f_M^*}) = 0$, therefore $D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau} \rightarrow 0$ for $\tau \rightarrow 0$. For $\tau \rightarrow 0$ indeterminate forms $0/0$ appear in expressions (62-64,66,67). Let us resolve the indeterminate forms and calculate the corresponding limits.

Two indeterminate forms are present:

$$N_1 = \frac{(D_\tau q_{M,\tau})(D_f S|_{q_{M,\tau}}) D_M q_{M,\tau} m J}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} \quad (69)$$

and right hand side of equation (67). Let us evaluate the indeterminate form (69) with the L'Hôpital rule. We obtain:

$$N_1(\tau) \rightarrow_{\tau \rightarrow 0} \frac{\Delta_{f_M^*} D_f S|_{f_M^*} \pi_{f_M^*} D_f J(f)|_{f_M^*}}{\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}} \quad (70)$$

using identity (34), similar to (35), we obtain:

$$N_1(\tau) \rightarrow_{\tau \rightarrow 0} - \frac{\Delta_{f_M^*} \langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}}{\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}} = -\Delta_{f_M^*}.$$

In such a way, for $\tau \rightarrow 0$

$$\pi_{\text{td}}|_{q_{M,\tau}} J(q_{M,\tau}) \rightarrow D_M f_M^* m J(f_M^*) + \Delta_{f_M^*} = \pi_{f_M^*} J(f_M^*) + (1 - \pi_{f_M^*}) J(f_M^*) = J(f_M^*). \quad (71)$$

Similarly, after simple calculations we obtain that:

$$\frac{d\tau}{dt} \rightarrow 1, \text{ for } \tau \rightarrow 0. \quad (72)$$

The fact that for $\tau \rightarrow 0$ the action of the thermodynamic projector on J becomes trivial, $\pi_{\text{td}} J = J$, can be obtained (without calculations) from the construction of $q_{M,\tau}$ in vicinity of zero. We have chosen this dependence in such a way that $J(q_{M,\tau})$ becomes transverse to the film for $\tau \rightarrow 0$. This follows from the condition (38). Let us emphasise, however, that derivation of the formulas (64-67) themselves was not based on (38), and they are applicable to any ansatz, $q_{M,\tau}$, not necessarily with the right behavior near the quasiequilibrium (if one needs such ansatzes for anything).

4.3 Fixed points and “right asymptotics” for the film equation

What is the dynamics of the film in accordance with equation (58)? A naive expectation that $q_{M,\tau}$ tends to the stable point of equation (58) leads to strange consequences. Stable point (58) is the invariant manifold q_M . On this manifold

$$J(q_M) = D_M q_M m J(q_M), \quad (73)$$

i.e. the projection of the vector field, J , onto q_M coincides with J . Were the condition $q_{M,\tau} \rightarrow q_M$ satisfied for $\tau \rightarrow \infty$, the dynamics would become more and more conservative. On the limit manifold q_M , the entropy should be conserved. This could lead to unusual consequences. The first of them is limited extendability backwards “in the entropy”.

Let us consider the set of points $M_{-\tau}$ for given M . Because of the existence of the limit, $T_\tau M_{-\tau} \rightarrow q_M$, for $\tau \rightarrow 0$, the difference, $S(M) - S(M_{-\tau}) = \Delta S_\tau$, is bounded on the half-axis, $\tau \in [0; +\infty) : \Delta S_\tau < \Delta S_\infty(M)$. this means that it is impossible to get into the values of macroscopic variables, M , from the quasiequilibrium initial conditions, M_1 , for that $S(M) - S(M_1) > \Delta S_\infty(M)$. Assuming additionally a smoothness of q_M and $M_{-\tau}$, we see that it is impossible to get into ε -neighborhood of the quasiequilibrium state, M^* , (over macro-variables) from the outside, from the quasiequilibrium initial conditions M_0 , if $S(M_0) < S_\varepsilon$, where S_ε is ε dependent threshold of the entropy. Thus, possible stable points of the equation (58), regardless of their obvious interest, likely demonstrate exotic possibilities. The following “right asymptotics” correspond to our qualitative expectations for large τ . Namely, it is expected that for the quite large τ , \dot{M} becomes, within a good precision, a function of M , and later does not depend on τ :

$$m(J(q_{M,\tau})) \rightarrow \dot{M}(M); \quad (74)$$

with the entropy production:

$$\sigma(q_{M,\tau}) = D_M S(M) mJ(q_{M,\tau}) \rightarrow \sigma(M) > 0, \quad (75)$$

and, correspondingly, $S(q_{M,\tau}) \rightarrow -\infty$, $\tau \rightarrow \infty$.

Already simple examples (linear in J) demonstrate that it is not so simple to construct such an asymptotic. Moreover, for reasonably built systems it probably does not exist. Indeed, let $J(q) = Lq$, we search for “the right asymptotic” in the form $q_{M,\tau} = a(M) + \tau b(M) + o(1)$. We obtain:

$$\begin{aligned} mb = mLb &= 0, \\ ma(M) &= M, \\ Lb(M) - D_M b(M) mL(a(M)) &= 0, \\ La(M) - D_M a(M) mL(a(M)) &= b(M). \end{aligned} \quad (76)$$

Acting with the operator mL on the first equation, we obtain $mL^2 b(M) = 0$; further, acting with the operator mL^2 , we obtain $mL^3 b(M) = 0$, and so on.

Thus,

$$b(M) \subset \bigcap_{k=0}^{\infty} \ker mL^k = H. \quad (77)$$

Space H is L -invariant, therefore, it is possible to pass from the initial dynamics, $\dot{f} = Lf$, to the dynamics in the factor-space. This does not change the dynamics of macroscopic variables because of the definition of H (77).

In such a way, instead of the right asymptotic equations, (76) leads us again to the equation of the invariant manifold ($b = 0$, $a(M)$ determines the invariant manifolds.)

4.4 Coarse-graining projector

A construction of an exact projection of the microscopic dynamics on the macroscopic is meaningless, it has meaning only as an intermediate result. Really, generically, such a projection (finite segment of the trajectory $M(t)$) contains practically all the information about the Liouville equation. This is a bit too much.

Moreover, there are no invariant manifolds with the dissipative dynamics for the finite-dimensional conservative systems. The conclusion is: every time explicitly, or sometimes implicitly, coarse-graining, or replacing of the system with something different, takes place.

For example, there is no invariant manifold for the Liouville equation parameterized with the one-particle distribution function with dissipative dynamics on this manifold. The derivation of the Boltzmann equation requires some limit transitions.

A few ways of coarse-graining are known, but essentially only two exist. The first one is related to distinguishing a manifold, M , and a projector, Π , on it; the manifold, M , with the projector, Π , separate the “microscopic” ($\ker \Pi$) from the macroscopic, M . In particular, $m(f) = m(\Pi f)$. Then, a “new microscopic dynamic” is parameterized: instead of $\dot{M} = m(J(f))$ the equality

$$\dot{M} = m(J(\Pi f)) \quad (78)$$

is used.

Equation (78) determines, for example, quite different system of relations in the chain of derivatives M, \dot{M}, \ddot{M} (original system can contain no such relations). For construction of “right asymptotics” relation (76) is much more appropriate then the correct initial relation: for example, instead of mL^k in (77) one can get $m(L\Pi)^k$, and the kernel $(L\Pi)^k$ always contains the kernel Π .

If the coarse-graining projector, Π , and manifold, M , are postulated, then the *hypothesis of existence of the thermodynamic limit* consists of existence of the limit:

$$\Pi q_{M,\tau} \rightarrow f_M^\# \quad \text{for } \tau \rightarrow \infty. \quad (79)$$

Nevertheless, one should not expect a precise fulfillment of equality (79), this is still the case of exact projection (on M). For $\tau \rightarrow \infty$ one can expect realistically only the smallness of the remainder:

$$\delta(\tau, M, N) = \Pi q_{M,\tau} - f_M^\#, \quad (80)$$

and its elimination for $N \rightarrow \infty$, where N is number of particles.

For a more precise formalization of this condition one should estimate δ under $\tau \rightarrow \infty$, for example, such as:

$$\varepsilon(M, N) = \sqrt{\lim_{\tau \rightarrow \infty} \frac{1}{\theta} \int_0^\theta \|\delta(\tau, M, N)\|^2 d\tau} \quad (81)$$

and, further, investigate the thermodynamic limit $N \rightarrow \infty$.

So far, however, the number of particles was not taken into consideration, and we dealt with only one fixed system. In this case we can't help but to assume that the value of $\varepsilon(M)$ (81) is "sufficiently small". We notice that the problem of determining the dynamic for the thermodynamic limit of infinite systems is a very difficult problem. For infinite system even determining the energy, entropy, and other characteristics is not clear. We are talking not about the limit does not exist (the number of particles is always finite), but about the asymptotics for large N , therefore, strictly speaking, one needs not only to know the limits, but to estimate the reminding terms too.

The second coarse-graining method consists of a decomposition of the system into small subsystems, and introduction of two incomparable time scales: micro and macro. The main assumption is that during an arbitrarily small macroscopic time period a small part of the system passes the micro-evolution within an infinitely long time. This leads to a quasi-chemical description: within each period a number of elementary atomic processes (events) takes place. For example, the derivation of the Boltzmann equation in frames of all formalisms is, in fact, reduced to this. We will return to considering this approach, but for now we'll concern ourselves with the coarse-graining projector for the film.

4.5 Choice of the coarse-graining projector, and layer-by-layer linearization

The simplest choice of the coarse-graining projector is

$$\Pi(f) = (M(f), \dot{M}(f)) = (mf, mJ(f)). \quad (82)$$

For many problems, for example, to investigate the invariance defect (78) it is not necessary to place the manifold M in the initial space E , it is sufficient to investigate $\dot{M}_M^\#$.

In the cases when one needs, after all, to have corresponding elements of E , a good choice could be the quasiequilibrium manifold corresponding to Π . The quasiequilibrium manifolds have an evident but important property. Let

$$f \xrightarrow{m_1} M_1 \xrightarrow{m_2} M_2, \quad f \xrightarrow{m_1 m_2} M_2, \quad (83)$$

be a sequence of linear mappings, where m_1, m_2 are mappings "on", their images are whole corresponding spaces.

Let, furthermore, $\mathbf{M}_1 \subset E$ be a quasiequilibrium manifold in E , corresponding to m_1 , \mathbf{M}_2 be a quasiequilibrium manifold of macro-variables, M_2 , corresponding to m_2 , \mathbf{M}_{21} be a quasiequilibrium manifold in E corresponding to $m_2 m_1$. Then

$$m_1(\mathbf{M}_{21}) = m_2, \quad \text{or} \quad \mathbf{M}_{21} = m_1^{-1}(\mathbf{M}_{21}). \quad (84)$$

For the transition to the quasiequilibrium approximation this property reads simpler:

$$U_2 U_1 = U_{21}, \quad (85)$$

where U_i the corresponding to m_i procedure of the taking of the quasiequilibrium approximation.

For each M_2 both the point of the quasiequilibrium, $M_1^*(M_2)$, and the linear manifold, $m_2^{-1}(M_2)$, containing this point are defined. For each M_1 the quasiequilibrium, $f_1^*(M_1)$, and the linear manifold, $m_1^{-1}(M_1)$ containing this point are defined. As well $f_2^*(M_2)$, and containing them $(m_2 m_1)^{-1}(M_2)$ are defined.

Relations:

$$\begin{aligned} f_2^*(M_2) &= f_1^*(M_1^*(M_2)), \\ m_1^{-1}(m_2^{-1}(M_2)) &= (m_2 m_1)^{-1}(M_2). \end{aligned} \quad (86)$$

are fulfilled.

The quasiequilibrium manifold, $f_2^*(M_2) \subset E$ parameterized by M_2 lies on the quasiequilibrium manifold, $f_1^*(M_1) \subset E$ parameterized by M_1 . For each M_2 the set

$$\{f_1^*(M_1) | f_1^*(M_1) \subseteq (m_2 m_1)^{-1}(M_2)\} \quad (87)$$

forms the quasiequilibrium manifold in $(m_2 m_1)^{-1}(M_2)$ with the set of macroscopic variables, $m_2^{-1}(M_2)$, and the same entropy. For the projector, $\Pi(f) = (M(f), \dot{M}(f))$, it means that for each M in the linear manifold, on that $m(f) = M$, the quasiequilibrium manifold corresponding to the macroscopic variables $\dot{M}(f) = mJ(f)$ (if $J(f)$ is a linear mapping on this manifold) is defined.

The last remark leads us to an important construction named by us “*layer-by-layer linearization*”. The field $J(f)$ could be presented in the form:

$$J_L(f) = J(f_{m(f)}^*) + D_f J(f) |_{f_{m(f)}^*} (f - f_{m(f)}^*). \quad (88)$$

The “*layer-by-layer quadratic entropy*” has special importance for the theory of non-linear equations (88) :

$$S_L(f) = S(f_{m(f)}^*) - (1/2) \langle f - f_{m(f)}^* | f - f_{m(f)}^* \rangle_{f_{m(f)}^*}. \quad (89)$$

Let us remind that the bilinear form, $\langle | \rangle_{f_{m(f)}^*}$, is generated by the negative second differential of the entropy at the point f .

The layer-by-layer linearized equations allowed us to add more moment equations and construct the quasiequilibrium approximations using the entropy (89). This is especially important for the moments which are time derivatives \dot{M} , \ddot{M} and so on.

Application of the layer-by-layer linearized equations (85) together with the layer-by-layer quadratic entropy (89) allowed us to construct a thermodynamically consistent theory of the moment equations for the Boltzmann equation [33, 34].

It is convenient to supplement the quasiequilibrium, f_M^* , with the quasiequilibrium for additional macro-variables \dot{M} ,

$$\dot{M}(f) = m(D_f J(f) |_{f_{m(f)}^*} f), \quad (90)$$

in two stages: i) supplementing by the entropy production, ii) and later by the conserving part of the entropy.

i) We supplement M by the entropy production. In the layer-by-layer linear approximation

$$\sigma(f) = \langle \Delta_{f_{m(f)}^*} | f - f_{m(f)}^* \rangle_{f_{m(f)}^*} \quad (91)$$

(as was already determined, see (45)). The quasiequilibrium manifold corresponding to σ in the layer over f_M^* has the form:

$$f_{M,\sigma}^* = f_M^* + \frac{\sigma(f) \Delta_{f_M^*}}{\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}}. \quad (92)$$

Quasiequilibrium projector in the layer is:

$$\pi_\sigma = \frac{|\Delta_{f_M^*}\rangle \langle \Delta_{f_M^*}|}{\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}}$$

ii) We distinguish in $L = DJ(f)|_{f_M^*}$ the conservative (conserving the entropy) part over f_M^* :

$$L_M^C \varphi = L_M(\varphi - \pi_\sigma \varphi).$$

This corresponds to the situation when we have fixed $\sigma(f) = \langle \Delta_{f_M^*} | \varphi \rangle$, and we consider the motion in the layer for fixed σ . For this:

$$L_M \varphi = L_M^C \varphi + \frac{L_M \Delta_{f_M^*} \langle \Delta_{f_M^*} | \varphi \rangle}{\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}} = L_M^C \varphi + \frac{\sigma(\varphi)}{\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}}. \quad (93)$$

The quasiequilibrium manifold corresponding to L_M^C in the layer over f_M^* could be constructed in the following way: we search for the kernel of L_M^C , in L (the set of all solutions to equations $L_M^C \varphi = 0$, $m\varphi = 0$). We define it as K . The orthogonal complement, K^\perp , to K in the scalar product, $\langle | \rangle_{f_M^*}$, is the corresponding manifold. For each point from the image, L_M , on L , $\psi \in L_M^C(L)$, there exists unique $\varphi \in K_{f_M^*}^\perp$ such that $L_M \varphi = \psi$. We define it as $\varphi = (L_M^C)^{-1}(\psi)$. As a result, for every $\psi \in L_M^C(L)$

$$f_{M,\sigma,\psi}^* = f_M^* + \frac{\sigma \Delta_{f_M^*}}{\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}} + (L_M^C)^{-1} \psi. \quad (94)$$

The second and third terms in (94) are reciprocally orthogonal in the scalar product $\langle | \rangle_{f_M^*}$.

4.6 The failure of the simplest Galerkin approximations for conservative systems

The simplest approach to the problem is connected to the Galerkin approaches: one considers a projection of the vector field, $J(f)$, onto the manifold in question and investigates

the obtained motion equations. It is not difficult to make sure that for conservative systems such an approach is unfruitful. If the orthogonal projection, $\langle | \rangle_{f_M^*}$, is taken, then in the linear within the layer approximation only quasiequilibrium approximations with increased number of moments could be obtained. For the dissipative systems, in contrast, such a way leads to quite satisfactory results. Thus, if for the Boltzmann equation and the hydrodynamic moments the invariant manifold is to be searched in the form $f_M^\# = f_M^* + a(M)\Delta_{f_M^*}$, then we obtain the Navier-Stokes equations with the viscosity calculated within the first Sonine polynomials approximation. Using another scalar product simply leads to unphysical results.

In order to specify appearing problems, let us give an example with a linear field, $J(f) = Af$, and quadratic entropy, $S(f) = (1/2)\langle f|f \rangle$. The conservativity of J means that for each f

$$\langle f|Af \rangle = 0 \quad (95)$$

is fulfilled.

The quasiequilibrium subspace corresponding to the moments $M = mf$ is the orthogonal complement, $\ker M$. The quasiequilibrium projector, π , is an orthogonal projector on this subspace, and does not depend on the point. For the defect of invariance $\Delta_{f_M^*}$ we obtain:

$$\Delta_{f_M^*} = (A - \pi A)f_M^*. \quad (96)$$

Under Galerkin approximation we write

$$q_{M,\tau} = f_M^* + a(M, \tau)\Delta_{f_M^*}. \quad (97)$$

Projector of the vector field on $\Delta_{f_M^*}$ is

$$\frac{|\Delta_{f_M^*}\rangle\langle\Delta_{f_M^*}|}{\langle\Delta_{f_M^*}|\Delta_{f_M^*}\rangle}. \quad (98)$$

Thus, we pass from the equation of motion of the film (58) to the Galerkin approximation for $a(M, \tau)$.

$$\begin{aligned} \dot{a} = 1 + & \quad (99) \\ a \frac{\langle\Delta_{f_M^*}|A\Delta_{f_M^*}\rangle}{\langle\Delta_{f_M^*}|\Delta_{f_M^*}\rangle} - a \frac{\langle\Delta_{f_M^*}|A\pi A\Delta_{f_M^*}\rangle}{\langle\Delta_{f_M^*}|\Delta_{f_M^*}\rangle} - a^2 \frac{\langle\Delta_{f_M^*}|A\pi A\Delta_{f_M^*}\rangle}{\langle\Delta_{f_M^*}|\Delta_{f_M^*}\rangle} - (D_M a)m \frac{Af_M^* + aA\Delta_{f_M^*}}{\langle\Delta_{f_M^*}|\Delta_{f_M^*}\rangle}. \end{aligned}$$

One can try to find the fixed points (solving $\dot{a} = 0$). This is the projected invariance equation. Due to the properties of the operator A , and the self-adjoint projector, π , we obtain for conservative systems

$$\langle\Delta_{f_M^*}|A\Delta_{f_M^*}\rangle = 0, \quad (100)$$

$$\langle\Delta_{f_M^*}|A\pi A\Delta_{f_M^*}\rangle = -\langle\pi A\Delta_{f_M^*}|(\pi A^2 - (\pi A)^2)\Delta_{f_M^*}\rangle. \quad (101)$$

On the other hand, for the dissipative systems the form (100) is negatively definite, and it is this form that determines the Navier-Stokes equations (in the first Sonine's polynomials approximation) for derivation of these equations from the Boltzmann equation. For the conservative equations this main part vanishes, and the second term in equation (100), generally speaking, is sign-indefinite.

The failure of the Galerkin approximations is even more obvious in the equations of motions on the film. Here everything is very simple:

$$\dot{a} = 1 + a \frac{\langle \Delta f_M^* | A \Delta f_M^* \rangle}{\langle \Delta f_M^* | \Delta f_M^* \rangle}. \quad (102)$$

For the dissipative systems under frozen M , a relaxes to the stable point

$$a = - \frac{\langle \Delta f_M^* | \Delta f_M^* \rangle}{\langle \Delta f_M^* | A \Delta f_M^* \rangle}. \quad (103)$$

This fixed point is “the leading order term” in the solution of the invariance equation, $\dot{a} = 0$ (100).

For the conservative systems $\dot{a} = 1$. This result was evident beforehand from the entropy production formula (35), and

$$-S(f) = (1/2)\langle f|f \rangle = (1/2)\langle \pi f | \pi f \rangle + (1/2)\langle (1 - \pi)f | (1 - \pi)f \rangle.$$

4.7 Possible ways beyond the simplest Galerkin approximations

The first way is an application of the projection operators methods [4]. The film equation (56) is considered for two sets of “variables”: slow “macro-variables”, Πq , and rapid “micro-variables”, $(1 - \Pi)q$ (where Π is a coarse-graining projector, see subsection 4.4).

Next the rapid variables are eliminated, and the equation with retardation for the slow variables is written. This formally exact equation becomes tractable only after a sequence of additional approximations (“short memory”, “Markovian models” etc.). The method is applicable to linear (linear within the layer) vector fields, $J(q) = L_M q$. The main problem is the computation of the coefficients including averaging along the trajectories of the rapid motion.

The second way is an introduction of the dissipative part (using the thermodynamic limit) into the vector field, $J(q_{M,\tau})$. One adds into (58) either a “relaxation” operator

$$-\gamma(q_{M,\tau} - f_M^*), \quad (104)$$

or operator γP , simulating a random process. For example, if f is a function on a space X , then the typical form of P with the “detailed equilibrium” is f_M^*

$$P(f) = \int Q(x, x') \left(\frac{f(x')}{f_M^*(x')} - \frac{f(x)}{f_M^*(x)} \right) dx' \quad (105)$$

with non-negative kernel $Q(x, x') \geq 0$, $\int Q(x, x') dx' \equiv 0$.

As a result, the system becomes dissipative, and one can construct for it invariant manifolds that are stationary solutions for the film equation. They could be found either as a sequence [35, 36] or, more effectively, based on the Newton method with the incomplete linearization [21, 29]. It becomes possible to use the Galerkin approximations, and so on.

After this one makes the transition to the thermodynamic limit. It is suggested that the thermodynamic limit exists for the found invariant manifold, $q_M^\#(\gamma)$, and, if later γ tends to zero, that a finite limit, $\Pi q_M^\#(\gamma)$ exists. This limit is suggested for the definition of the macroscopic variables M .

In some problems of dissipative kinetics (namely, in the problem of initial layer for the Boltzmann equation) it was found to be effective to approximate the trajectories by segments (with further smoothing and corrections, or without them). These segments were constructed in the following way: the initial direction of motion was taken, and f evolved along this direction for as long as it was possible to conserve the smooth evolution of the entropy. Further, the procedure was repeated from the obtained point (for details see [15, 16]).

Unfortunately, in the problem of the initial layer for the conservative systems there are no stop points during the motion along the straight line (more precisely, the start of the motion itself can be considered as a stop point because under the linear approximation the relation (100) is valid). In the initial layer for the dissipative systems the motion of the system along the straight line $x = \tau\Delta$ in any case increases the entropy. For the conservative systems one needs to “rotate the phase”, and the models of motion are to be arcs of ellipses (in linear space), or the constant entropy lines, instead of the straight lines. In the film problem, as even the simplest examples show, the simplest good model is a general conic section. A simple example: $J(f) = Af$, A is generator of rotation around the axis with direction $\vec{r} = \vec{e}_x + \alpha\vec{e}_y$, $M = x$, the film is the lateral surface of the cone, obtained by rotation of the quasiequilibrium manifold, the axis $\{x\vec{e}_x\}$, around the axis $\{\varphi\vec{r}\}$. For $\alpha < 1$ the curve $q_{M,\tau}$ is an ellipse, for $\alpha > 1$ it is a hyperbole, for $\alpha = 1$ it is a parable.

4.8 The film: Second order Kepler models

The curve $q_{M,\tau}$ is a section of two manifolds: one of them is the result of motion of the quasiequilibrium manifold along the vector field $J(f)$, and another one is the linear manifold $f_M^* + \ker m$.

Already in the finite-dimensional space, and under linear approximation (J is linear, S is quadratic) we have an interesting geometrical picture: quasiequilibrium manifold is an orthogonal complement to $\ker m$, A is the rotation generator. $(\ker m)^\perp$ is rotated under action of $e^{A\tau}$, unknown curve is the section:

$$(f_M^* + \ker m) \cap e^{AR_+}(\ker m)^\perp, \quad (106)$$

where $R_+ = [0; \infty)$, $f_M^* \in (\ker m)^\perp$.

The simplest model motion is a second order curve. However, it is not sufficient to know the first and the second derivatives. We need information about the third derivative. If we consider the curve $q_{M,\tau}$ as a trajectory in the Kepler problem, then the location, r , of the center of attraction (repulsion) is (Fig. 8):

$$r = q_0 - \ddot{q} \frac{\langle \dot{q}_\perp | \dot{q}_\perp \rangle}{\langle \ddot{q} | \dot{q}_\perp \rangle}, \quad (107)$$

where r_0 is the initial point where all the derivatives are taken. The force is:

$$F = \alpha \frac{r - q}{\langle r - q | r - q \rangle^{3/2}};$$

$$\alpha^2 = \langle \ddot{q} | \ddot{q} \rangle \langle r - q | r - q \rangle^2 = \langle \ddot{q} | \ddot{q} \rangle^3 \frac{\langle \ddot{q}_\perp | \ddot{q}_\perp \rangle^4}{\langle \ddot{q} | \dot{q}_\perp \rangle^4}; \quad (108)$$

$$\begin{aligned} \alpha > 0 & \quad (\text{attraction}) & \text{if} & \quad \langle \ddot{q} | \dot{q}_\perp \rangle < 0; \\ \alpha < 0 & \quad (\text{repulsion}) & \text{if} & \quad \langle \ddot{q} | \dot{q}_\perp \rangle > 0. \end{aligned} \quad (109)$$

It is necessary to specifically note that the Kepler problem defines an approximation of the trajectory $q_{M,\tau}$, but not the dependence on τ .

An important question is the finiteness of the film. Is the modeling motion finite?

The answer is simple in terms of the Kepler problem [37]:

$$\frac{\|\dot{q}\|^2}{2} < \frac{\alpha}{\|r - q_0\|},$$

or

$$\frac{\|\dot{q}\|^2 |\langle \dot{q}_\perp | \ddot{q} \rangle|}{2 \|\dot{q}_\perp\|^2 \|\ddot{q}\|^2} < 1. \quad (110)$$

Here $\|\cdot\| = (\langle \cdot | \cdot \rangle_{f_M^*})^{1/2}$ is the norm in the entropic scalar product, as it is usual.

4.9 Minimal second order models: entropic parable, and entropic circle

In accordance with the film equation (58), the following derivatives

$$\begin{aligned} \dot{q}_{M,\tau} &= \partial q_{M,\tau} / \partial \tau; \\ \ddot{q}_{M,\tau} &= \partial^2 q_{M,\tau} / \partial \tau^2; \\ \dddot{q}_{M,\tau} &= \partial^3 q_{M,\tau} / \partial \tau^3; \end{aligned}$$

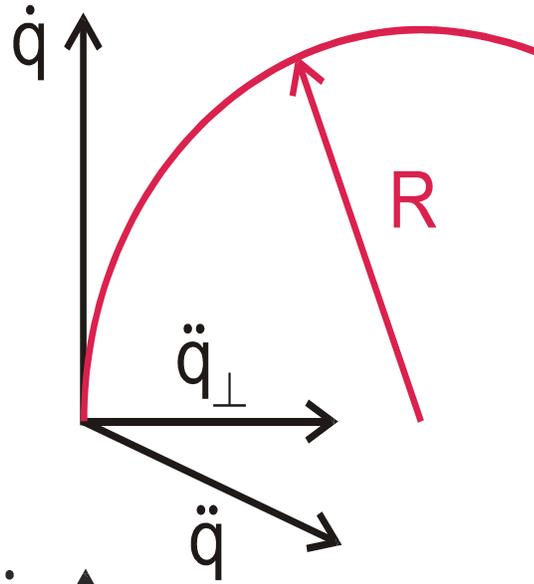
contribute to the construction of the second order Kepler models.

There is a rougher construction leading to the two distinguished simplest second order models that uses only two derivatives. One of them is finite (the entropic circle), another one is infinite (the entropic parable). Both could be constructed for every point of the

Second order models

1. The circle

$$R = \frac{\langle \dot{q} | \dot{q} \rangle}{\sqrt{\langle \ddot{q}_\perp | \ddot{q}_\perp \rangle}}$$



2. Kepler models

$$r = -\ddot{q} \frac{\langle \dot{q}_\perp | \dot{q}_\perp \rangle}{\langle \ddot{q}_\perp | \dot{q}_\perp \rangle}$$

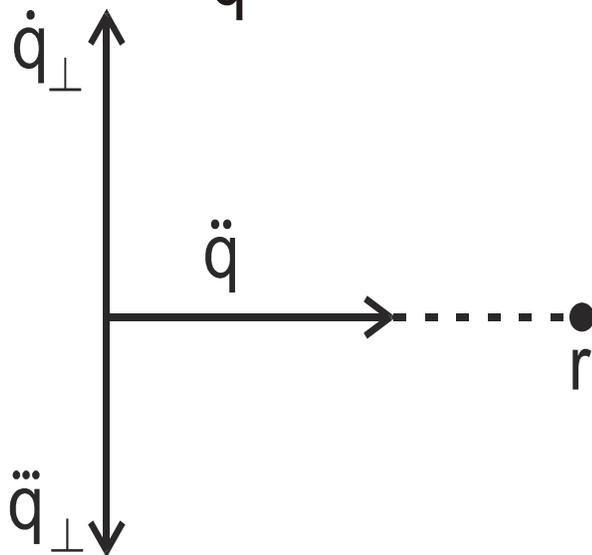


Figure 8: The definition of the second-order models.

film (if $\ddot{q}_\perp \neq 0$, otherwise, all second order models turn into straight lines). The circle was already used by us in subsection 3.3 in order to estimate stabilizing value of σ . Let us remind that:

$$R = \frac{\langle \dot{q} | \dot{q} \rangle}{\sqrt{\langle \ddot{q}_\perp | \ddot{q}_\perp \rangle}} \quad (111)$$

where $\dot{q} = \partial q_{M,\tau} / \partial \tau$, $\ddot{q} = \partial^2 q_{M,\tau} / \partial \tau^2$

$$\ddot{q}_\perp = \ddot{q} - \frac{\dot{q} \langle \dot{q} | \ddot{q} \rangle}{\langle \dot{q} | \dot{q} \rangle}$$

$\langle | \rangle$ is the entropic scalar product corresponding to the extension of the entropy at the point q_{M,τ_0} , or, for the linear (as well as linear within the layer) systems, at the point f_M^* .

The concentric motion could be presented as:

$$\begin{aligned} q_{M,\tau} - q_{M,\tau_0} &= \dot{q} \frac{R}{\|\dot{q}\|} \sin \left(\frac{\|\dot{q}\|}{R} (\tau - \tau_0) \right) + \ddot{q}_\perp \frac{R}{\|\ddot{q}_\perp\|} \left(1 - \cos \left(\frac{\|\dot{q}\|}{R} (\tau - \tau_0) \right) \right) \\ &= \dot{q} \sqrt{\frac{\langle \dot{q} | \dot{q} \rangle}{\langle \ddot{q}_\perp | \ddot{q}_\perp \rangle}} \sin \left[\sqrt{\frac{\langle \ddot{q}_\perp | \ddot{q}_\perp \rangle}{\langle \dot{q} | \dot{q} \rangle}} (\tau - \tau_0) \right] \\ &+ \ddot{q}_\perp \frac{\langle \dot{q} | \dot{q} \rangle}{\langle \ddot{q}_\perp | \ddot{q}_\perp \rangle} \left(1 - \cos \left[\sqrt{\frac{\langle \ddot{q}_\perp | \ddot{q}_\perp \rangle}{\langle \dot{q} | \dot{q} \rangle}} (\tau - \tau_0) \right] \right) \end{aligned} \quad (112)$$

The parable could be constructed simpler:

$$q_{M,\tau} - q_{M,\tau_0} = \dot{q} (\tau - \tau_0) + (1/2) \ddot{q}_\perp (\tau - \tau_0)^2, \quad (113)$$

or even as:

$$q_{M,\tau} - q_{M,\tau_0} = \dot{q} (\tau - \tau_0) + (1/2) \ddot{q} (\tau - \tau_0)^2, \quad (114)$$

The difference between (113) and (114) is this: in the formula (113) the angle between $\partial q_{M,\tau} / \partial \tau|_{\varepsilon=\tau_0}$ and $\partial q_{M,\tau} / \partial \tau$ tends to $\pi/2$ for $\tau \rightarrow \infty$, in the model (114) this occurs too if $\langle \dot{q} | \ddot{q} \rangle \neq 0$.

Note. In expressions (112-114) τ coincides with the true τ of the motion on the film only in the zeroth and the first orders. For the further calculations it could be necessary to recalculate τ using true values of \dot{q} in the projection on the trajectory. This is discussed below.

4.10 The finite models: termination at the horizon points

In order to construct a step-by-step approximation it is necessary to be able to solve two problems: the choice of the direction of the next step, and the choice of the value of this step.

If the motion $q_{M,\tau}$ is along the straight line (dissipative systems), the direction of the next step is \dot{q}_{M,τ_0} (let us remind that \dot{q}_{M,τ_0} is the defect of the invariance of the manifold

$q_M = q_{M,\tau_0}$ under fixed $\tau = \tau_0$), and the value of the step should be taken in the direction to the stable point: to the point where direction of $\dot{q}_{M,\tau}$ becomes orthogonal to initial one, \dot{q}_{M,τ_0} (Fig. 9). Naturally, the current direction of $\dot{q}_{M,\tau}$ is calculated with (58), but approximately, with the frozen projector ($D_M q_{M,\tau_0}$ instead of $D_m q_{M,\tau} m$).

For the conservative systems we have chosen the second order models instead of the linear ones. For finiteness of the models we need to define the moments of stop. It is suggested to operate in a manner similar to the case of the dissipative systems: to stop at the moment when the direction of motion is orthogonal to the initial one. In this case we will take the direction of motion along the model.

Thus, if q_{M,τ_0} is a starting point of motion, and $\tilde{q}_{M,\tau_0+\theta}$ is a motion on the finite second order model, then condition for the transition to the next model is

$$\langle \dot{q}_{M,\tau_0} | \frac{d\tilde{q}_{M,\tau_0+\theta}}{d\theta} \rangle = 0 \quad (115)$$

(in the entropic scalar product).

Let us call *the horizon points* such points, $q_{M,\tau_0+\theta_0}$, where the scalar product (115) for the first time becomes zero (for $0 \leq \theta < \theta_0$ this scalar product is positive). This notion is motivated by the fact that for $\theta > \theta_0$ the motion on the second order model “disappears behind the horizon”, and its orthogonal projection on the line parallel to \dot{q}_{M,τ_0} starts to move back passing the same points for the second time.

The convention about the change of the model in the horizon points seemed quite natural. The following sequence of calculations suggests itself (Fig. 10):

- 1) we pose that $q_{M,0} = f_M^*$;
- 2) we calculate $\dot{q}_{M,0}, \ddot{q}_{M,0}, \dots$ in accordance with equation (50);
- 3) we construct the (finite) second order models, $q_{M,\theta}$;
- 4) we find the horizon points, $q_{M,\theta_0(M)}$;
- 5) then we take the manifold of the horizon points as a new initial manifold, and so on.

At the first glance, this sequence contradicts the original statement of the film problem. The manifold $q_{M,\theta_0(M)}$ does not have the form of $q_{M,\tau}$ for a fixed τ and is not a shift of the quasiequilibrium manifold by the given time along the true microscopic equations of motion.

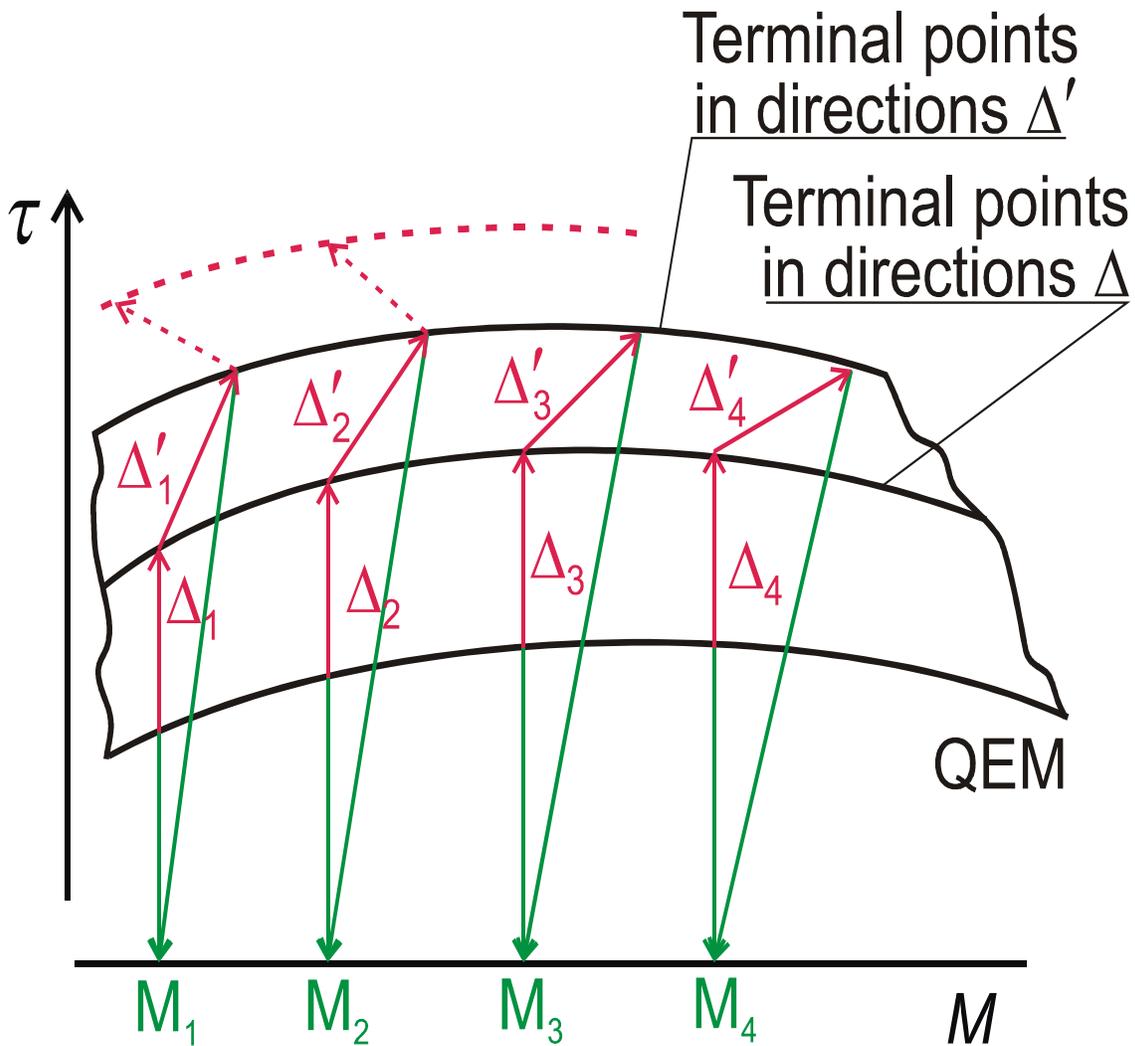
The second difficulty was already mentioned: the time of motion along the modeling curve does not coincide with the true time, τ . More precisely, it coincides only within the second order. However, global, not local approximation are constructed. Therefore, global corrections to the time, or ways to circumvent these corrections, are required.

The following two sections are devoted to the elimination of these difficulties.

4.11 The transversal restart lemma

Let $q_{M,\tau}$ ($\tau \in [0; +\infty)$) be the solution to (58) under initial condition (59) (the film). We call *the transverse section* of the film, $q_{M,\tau}$, the manifold, $q_{M,\theta(M)}$, where $\theta(M)$ is a smooth function $0 \leq \theta(M) \leq t < \infty$.

The Film for dissipative systems: step by step



But ... there are no terminal points
in directions Δ for conservative systems

Figure 9: The stepwise construction of the film for dissipative system. First-order models:
The motion along the defect of invariance.

The Film for conservative systems: second order steps

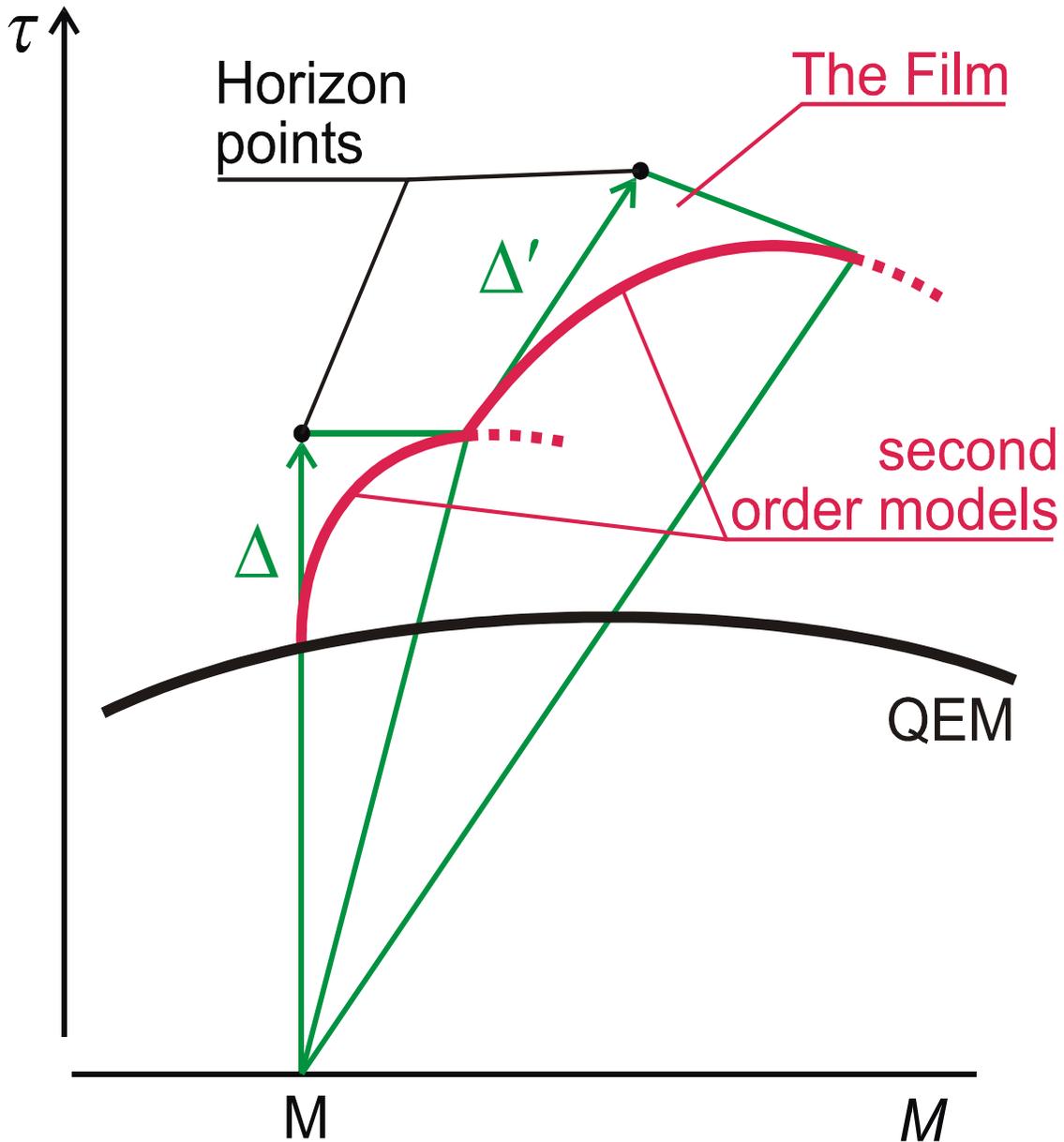


Figure 10: The stepwise construction of the film for dissipative system. Finite second-order models: The motion starts in the direction of the defect of invariance, and stops when the direction of motion becomes orthogonal to the defect of invariance.

Let the *transverse condition* be fulfilled. Namely, for every finite patch, M , that does not exclude equilibrium exists, $\varepsilon > 0$ such that in this patch

$$\frac{\|J(q_{M,\theta(M)}) - D_M q_{M,\theta(M)} m J(q_{M,\theta(M)})\|}{\|J(q_{M,\theta(M)})\|} > \varepsilon \quad (116)$$

in an appropriate (for example, entropic) norm. Let $\tilde{q}_{M,\tau}$ be the solution to (58) under the initial condition $\tilde{q}_{M,0} = q_{M,\theta(M)}$. Then the following *transverse restart lemma* is valid:

$$q_{M,[0;+\infty)} = q_{M,[0;\theta(M)]} \bigcup \tilde{q}_{M,[0;+\infty)}. \quad (117)$$

here $q_{M,[a;b]} = \{q_{M,\tau} | \tau \in [a;b]\}$.

In order to prove⁶ this lemma, we notice that it is equivalent to the following statement. For every M the segment of the trajectory, $T_\tau f_M^*$ ($\tau \in [0;t]$), crosses the manifold $q_{M,\theta(M)}$, and only once.

In order to demonstrate the unicity of the section, we consider the film in another coordinates, for each point q we set M and τ ,: $q = T_\tau f_M^*$.

In these coordinates the transverse condition excludes pleats on $q_{M,\theta(M)}$.

In order to demonstrate the existence of the segment $T_\tau f_M^*$ ($\tau \in [0;t]$) for the cross point, q^* , with $q_{M,\theta(M)}$, we define in the neighborhood of the point f_M^* on the quasiequilibrium manifold the mapping into the neighborhood of this section point. Image of the point f_M^* is section of the trajectory $T_\tau f_M^*$ ($\tau \in [0;t]$) with the manifold $q_{M,\theta(M)}$ in the neighborhood of q^* . Due to the transverse condition, it performs an isomorphism of the neighborhoods. Therefore, the set of M for which the section of the trajectory with $q_{M,\theta(M)}$ exists is open. Furthermore, it is closed, because the limit of section points is a section point (and segment $[0;t]$ is compact). Obviously, it is not empty. Consequently, it is the set of all possible M .

4.12 The time replacement, and the invariance of the thermodynamic projector

Let the film be constructed as $\tilde{q}_{M,\theta}$, where relation between θ and τ is unknown; $\tau = \tau(M, \theta)$, $\theta = \theta(M, \tau)$, in order to determine this functions one needs to solve the equation obtaining from (58) with substitution $q_{M,\tau} = \tilde{q}_{M,\theta(M,\tau)}$ (and projection, therefore, \tilde{q} is only an approximation). The calculation itself does not contain principal difficulties. However, a question arises: is it possible to escape the reverse replacing of time for the derivation of the kinetic equations? Another words, could we use the constructed geometrical object, the film, without an exact reconstruction of the time, τ , on it?

For positive answer to this question it is sufficient to demonstrate that the equations of motion, constructed with the thermodynamic projector (65-67), describes the same motion on the film after the time replacement.

⁶Let us remind that in the degree of generality being used there are no proofs to the theorems of existence and uniqueness

This property of the thermodynamic projector is evident: deriving equations (65-67), we did not use that τ is the “true time” from the equation (58), and made the local replacement of variables, passing from $\Delta M, \Delta\tau$ to $\Delta M, \Delta S$.

In such a way, the thermodynamic projector is invariant with respect to the time replacement, and, constructing equations of motion, it is not necessary to restore the “true time”.

Results of this, and previous sections allow to apply the sequence of operations suggested in subsection 4.10.

4.13 Correction to the infinite models

Let an infinite model $q_{M,\theta}$, ($\theta \in [0; +\infty)$), $q_{M,0} = f_M^*$ be constructed for the film. Actually, it means that an approximation is constructed for the whole film $q_{M,\tau}$ (but not for its initial fragment, as it was for the finite models). Naturally, there arises a problem of correction to this initial approximation, and, in general, construction of a step-by-step computational procedure.

The thermodynamic projector on the film is defined (64). Correspondingly, the invariance defect of the film is determined too

$$\Delta q_{M,\theta} = (1 - \pi_{\text{id}}|_{q_{M,\theta}})J(q_{M,\theta}) = \left[1 - \left(1 - \frac{D_\theta q_{M,\theta} D_f S|_{q_{M,\theta}}}{D_f S|_{q_{M,\theta}} D_\theta q_{M,\theta}} \right) D_M q_{M,\theta} m \right] J(q_{M,\theta}) \quad (118)$$

It is easy to verify, that if $q_{M,\theta}$ is a solution to (58), then $\Delta q_{M,\theta} \equiv 0$.

Subsequently we calculate the corrections to $q_{M,\tau}$ using an iterative method for the manifold with edge (see Appendix).

Generally speaking, one could (and should) calculate these corrections for the finite models. However, the infinite models are distinguished, because they require such corrections.

4.14 The film, and the macroscopic equations

Let a film be constructed. What next? There are two routes.

i) Investigation of the conservative dynamics of “ $N + 1$ ” variables, where “ N ” is moments, M , and “ $+ 1$ ” is τ on the film;

ii) Derivation of the macroscopic equations for M .

Actually, the second route is more desirable, it leads to the usual classes of equations. The first one, however, is always available, because the film exists always (at least formally) but the existence of equations for M is not guaranteed.

The route of obtaining equations for M is the same one, suggested by us [29],[30]-[12] following Ehrenfest [25], and Zubarev [3].

i) One chooses a time T .

ii) For arbitrary M_0 one solves the problem of the motion on the film (65), (67) under initial conditions $M(0) = M_0$, $\tau(0) = \tau_0$ on the segment $t \in [0; T]$. The solution is $M(t, M_0)$.

iii) For the mapping $M_0 \rightarrow M(T)$ the system $dM/dt = F(M)$ is constructed. It has the property that for its phase flow, $\theta_t(M)$, the identity

$$\theta_T(M_0) \equiv M(T, M_0) \quad (119)$$

is satisfied, for defined T and all M_0 . This is a natural projector again (see (32), and whole section).

In this sequence of actions there are two nontrivial problems: solution to the equations on the film, and reconstruction of the vector field by transformation of the phase flow, θ_T , under fixed T .

The natural method for solving the first problem is the averaging method. The equations of motion on the film read

$$\dot{M} = \varepsilon P(M, \tau); \quad \dot{\tau} = Q(M, \tau) \quad (120)$$

where ε is (formally) small parameter.

Assuming that the motion of M is slow, one can write down the series of the Bogoliubov-Krylov averaging method [38]. The first term of this series is a simple averaging over the period T : $\tau_1(T, M)$ is solution to the equation $\dot{\tau} = Q(M, \tau)$ under fixed M ,

$$M_1(t, M_0) = M_0 + \varepsilon t \left(\frac{1}{T} \int_0^T P(M_0, \tau_1(\theta, M_0)) d\theta \right) \quad (121)$$

for $t \in [0; T]$, and

$$M_1(T, M_0) = M_0 + \varepsilon \int_0^T P(M_0, \tau(\theta, M_0)) d\theta, \quad (122)$$

correspondingly.

The first correction to reconstruction of the vector field, $F(M)$, by the transformation of the phase flow, $\theta_T(M)$, is very simple too:

$$F_1(M) = \frac{1}{T} (\theta_T(M) - M). \quad (123)$$

Hence, we obtain the first correction to the macroscopic equations:

$$\dot{M} = F_1(M) = \frac{1}{T} \int_0^T m(J(q_{M, \tau(t, M)})) dt, \quad (124)$$

where $\tau(t, M)$ is a solution to the equation (67) under fixed M (actually, $mJ(q_{M, \tau})$ should be substituted into (67) instead of \dot{M}).

The second and higher approximations are much more cumbersome, but their construction is not a significant problem.

Let us demonstrate an explicit expression for \dot{M} (124) for the modeling motion on the entropic circle (51), (112) for the linear in layer system (88).

The original system is

$$\dot{f} = J(f_{m(f)}^*) + L_{m(f)}(f - f_{m(f)}^*),$$

where $L_M = (D_f J(f))|_{f_M^*}$.

The macroscopic equations are (see also equations (53)):

$$\begin{aligned}
\dot{M} &= m(J(f_M^*)) + (1/\omega)m(L_M(\dot{q}))\frac{2\omega}{\pi} \int_0^{\pi/2\omega} \sin(\omega t) dt \\
&+ (1/\omega^2)m(L_M(\ddot{q}_\perp))\frac{2\omega}{\pi} \int_0^{\pi/2\omega} (1 - \cos(\omega t)) dt \\
&= m(J(f_M^*)) + \frac{2\omega}{\pi}m(L_M(\dot{q})) + (1/\omega^2)(1 - 2/\pi)m(L_M(\ddot{q}_\perp)), \tag{125}
\end{aligned}$$

where $\dot{q} = \Delta_{f_M^*} = J(f_M^*) - \pi_{f_M^*} J(f_M^*)$, and $\pi_{f_M^*}$ is the quasiequilibrium projector (16),

$$\begin{aligned}
\ddot{q} &= (1 - \pi_{f_M^*})L_M((1 - 2\pi_{f_M^*})J(f_M^*)) + D_M \pi_{f_M^*} m(J(f_M^*)), \\
\ddot{q}_\perp &= \ddot{q} - \frac{\langle \ddot{q} | \dot{q} \rangle_{f_M^*}}{\langle \dot{q} | \dot{q} \rangle_{f_M^*}} \dot{q}.
\end{aligned}$$

$\langle | \rangle_{f_M^*}$ is the entropic scalar product related with quadratic approximation to the entropy f_M^* :

$$\begin{aligned}
S(f) &= S(f_M^*) + DS|_{f_M^*}(f - f_M^*) - (1/2)\langle f - f_M^* | f - f_M^* \rangle_{f_M^*} + o(\|f - f_M^*\|^2), \\
\omega &= \frac{\langle \ddot{q}_\perp | \ddot{q}_\perp \rangle_{f_M^*}}{\langle \dot{q} | \dot{q} \rangle_{f_M^*}}.
\end{aligned}$$

Note. In (125), in accordance with (67), the model of motion on the circle (112) is taken without recalculating the time. Such a recalculation changes the values of the coefficients without a change in the structure of the equation: instead of $2/\pi$ and $(1 - 2/\pi)$, other numbers appear.

The entropy production for equations (125) has the form $const \frac{\text{defect of invariance}}{\text{curvature}}$ (54).

In general, equations such as (125) are determined accurately to the values of the coefficients simply by the sequence of the horizon points of the second order finite Kepler models, and corresponding \dot{q}_i, \ddot{q}_i

$$\dot{M} = m(J(f_M^*)) + \sum_i (\alpha_i m(L_M(\dot{q}_i)) + \beta_i m(L_M(\ddot{q}_i))), \tag{126}$$

with $\alpha_i, \beta_i > 0$.

The last comment on the positivity of the “kinetic constants” α_i and β_i is important, and cannot be easily verified every time. However, in the case under consideration it follows from the next theorem.

The theorem about the positivity of kinetic constants. The motion on the Kepler ellipse from start to the horizon point always satisfies the property

$$q - q_0 = \alpha \dot{q} + \beta \ddot{q}; \quad \alpha, \beta > 0, \tag{127}$$

where q_0 is a starting point, \dot{q} , and \ddot{q} are velocity, and acceleration correspondingly.

This theorem follows from elementary theorems about analytical geometry of second-order curves.

For the modeling motion on the circle, strictly speaking, this is not so every time. Positivity of the coefficients is guaranteed only for $m(L(\dot{q}))$, and $m(L(\ddot{q}_\perp))$.

Two phenomena can be related to the increase of the number of terms in (126): i) alteration of the kinetic constants (terms are not orthogonal to each other, therefore, new terms contribute to the previous processes), ii) appearance of new processes.

Motion on an infinite film can lead to the stabilization of kinetic constants as functions of M , but it can also lead to their permanent transformation. In the second case one has to introduce into macroscopic equations an additional variable, the coordinate, τ , on the film.

From the applications point of view, another form of equations of motion on the film could be more natural. In these equations kinetic coefficients are used as dynamic variables. Essentially, this is just another representation of equations (65), (67). For every kinetic coefficient, k , expression $dk/dt = \psi_k(\tau, M) = \varphi_k(k, M)$ is calculated in accordance with (65), (67). Substitution of variables $(\tau, M) \rightarrow (k, M)$ in this equation is possible (at least locally) if value k does not stabilize during the motion on the film. Finally, we have the system in the form:

$$\dot{M} = m(J(f_M^*)) + \sum_j k_j F_j(M); \quad \dot{k}_j = \varphi_j(k_j, M). \quad (128)$$

For the motion starting from the quasiequilibrium state the initial conditions are $k_j = 0$.

4.15 New in the separation of the relaxation times

The classical Bogoliubov's concept about separation of the relaxation times does not agree well with the thesis of the quasiequilibrium initial conditions.

Originally, there are no dissipative processes in the quasiequilibrium state (the theorem of preservation of the type of dynamics for the quasiequilibrium approximation).

The first thing that occurs during the motion out of the quasiequilibrium initial conditions is appearance of the dissipation. It can be described (in the first non-vanishing approximation) by equation (33). It is of special importance here that there is still no separation into processes with various kinetic coefficients. This occurs at further relaxation stages: Various processes appear, their kinetic coefficients are determined (see, for example, (126)) (or, in some cases, the dynamics of the kinetic coefficients is determined). And just after this the "hydrodynamic" relaxation occurs, which is the motion of the macroscopic variables to their equilibrium values.

Generalizing, we can distinguish three stages:

- i) appearance of dissipation;
- ii) branching of dissipation: appearance of various processes;
- iii) macroscopic relaxation.

It is important to notice in this schema that the determination of the kinetic coefficients can occur at both stages: at the second stage when macroscopic (hydrodynamic) relaxation can be described in the usual form with kinetic coefficient as functions of the macroscopic parameters, as well as in the third phase (motion on the film), when the hydrodynamic description includes dynamics of the kinetic coefficients also.

5 Conclusion

To solve the problem of irreversibility we have introduced the notion of the macroscopically definable ensembles. They are result of evolution of ensembles from the quasiequilibrium initial conditions under macroscopic control. The quasiequilibria (ensembles of conditional maximum of the entropy under fixed macro-variables) are intensively used in statistical mechanics after Jaynes [45]. Papers of Rosonoer and Kogan [46]-[48] significantly affected our initial investigation. The primitive macroscopically definable ensembles appear as results (for $t > 0$) of motions which start from the quasiequilibrium state (at $t = 0$). The hypothesis of the primitive macroscopically definable ensembles is very important from constructive point of view: Any macroscopically definable ensemble can be approximated by primitive macroscopically definable ensembles with appropriate accuracy. In accordance to this hypothesis it is possible to study the one curve for every value of macroscopic variables. These curves form the film of nonequilibrium states.

The hypothesis about the primitive macroscopically definable ensembles is real hypothesis, it can be true or false. There is the significant difference between this hypothesis and the *thesis* about macroscopically definable ensembles. The thesis can be accepted, or not, but nobody can prove the definition, even the definition of the macroscopically definable ensembles.

Technically, the solution to the problem of irreversibility looks as follows: we can operate only with the macroscopically definable ensembles; the class of these ensembles is not invariant with respect to the time inversion. The notion of the macroscopically definable ensembles moves the problem of irreversibility into a new setting. It could be called a control theory point of view. The key question is: Which parameters can we control? It is those parameters that are fixed until “all the rest” come to an equilibrium. The quasiequilibrium states are obtained in such a way.

The further development of this direction must lead to an investigation of the macrodynamics under controlled macro-parameters. This will be a supplement of the postulated quasiequilibrium initial conditions with an investigation of a general case of an evolution of the controlled ensembles: The initial condition is quasiequilibrium, after which one carries out on the system by available control influences.

The method of the natural projector allows us to construct an approximate dynamics of macro-variables. Under tendency of the time of projection, τ , to infinity, these equations should tend to the actual equations of macro-dynamics, if the latter exist. This a hypothesis about their existence for the thermodynamic limit (first, the number of par-

ticles $N \rightarrow \infty$, and then, the time of projection $\tau \rightarrow \infty$) is the basis of the Zubarev statistical operator [3]. Here, however, we need to make a note. Frequently, physicists use objects whose existence and unicity are not proven: solution to the hydro- gaso-dynamics, kinetic equations etc. Often, the failure to prove the theorems of existence and unicity is treated as an absence of an adequate mathematical statement of the problem (definition of spaces etc.). For all this, it is assumed, that substantial obstacles either are absent, or can be distinguished separately, independently on the theorem proof in physically trivial situations. Existence (or non-existence) of the macroscopic dynamics is a problem of an absolutely different kind. This question is substantial: the cases of non-existence can be found as frequently as the usual existence.

The notion of the invariant film of non-equilibrium states, and the method of its approximate construction allow us to solve the problem of macro-kinetic even in cases when there are no autonomous equations of macro-kinetic. The existence of the film appears to be one of the physically trivial problems of existence and uniqueness of solutions.

Using the Taylor's expansions of the natural projector, the first applications already have been constructed [30, 43, 44]. Particularly, the post-Navier-Stokes hydrodynamic, replacing the Burnett equations, have been found. It is free from unphysical singularities [30, 42].

The formula for entropy production

$$\sigma = \text{const} \frac{\text{defect of invariance}}{\text{curvature}}$$

makes the geometrical sense of dissipation clear.

Nevertheless, at least one important problem remains unsolved. This is a *problem of undivisible events*: For macroscopically small time small microscopic subsystems can go through “the whole life”, from the beginning to the limit state (or, more accurate, to the limit behaviour which may be not only a state, but a type of motion, etc.). The microscopic evolution of the system in a small interval of macroscopic time can not be written in the form

$$\Delta f = \dot{f} \Delta t,$$

if it is really the system with microscopic structure, and consists of a large number of microscopic subsystems. The evolution of microscopic subsystems in a macroscopically small time Δt should be described as a “ensemble of undivisible events”. An excellent hint gives us the Boltzmann equation with undivisible collisions, another good hint gives the chemical kinetics with undivisible events of elementary reactions. The useful formalism for description such ensembles of undivisible events is developed. It is the “quasi-chemical” representation (see elsewhere, for example, the review [22]). But the way from a general systems to such ensembles remains unclear. It is a challenge to the following works.

6 Appendix

6.1 The method of invariant manifolds

The aim of this appendix is to give a short presentation of the method of invariant manifold, including positive-invariant manifolds with the fixed edge.

6.2 Construction of the invariant sections

Let E be a vector space, in the patch $U \subset E$ the vector field (microscopic system)

$$\dot{f} = J(f), \quad (f \in U). \quad (129)$$

is defined.

J is assumed to be smoothly continued to the closure of U positively invariantly with respect to (129). It means that every solution to (129), $f(t)$, starting under $t = 0$ in U , is to be found within U for every $t \in [0; +\infty)$.

Let B be a vector field (of macroscopic variables), and a surjective mapping $m : E \rightarrow B$ is defined.

It is required to construct such a mapping

$$M \mapsto f_M^\# \quad (M \in m(U), f_M^\# \in U), \quad (130)$$

that $m(f_M^\#) \equiv M$, and $f_M^\#$ is a positive invariant manifold of the system (129) (since U is positive-invariant, it is sufficient to verify a local condition: the field $J(f_M^\#)$ is tangent to the manifold $f_M^\#$ for each $M \in m(U)$).

Actually, we continue to keep such a level of strictness (unstrictness) of reasoning when such details as topology in E and B etc. are not discussed. If necessary, it could be made for particular realizations.

We call the mapping (130) a section, and the problem of construction of positive invariant manifold, $f_M^\#$, an invariant section problem.

It could be solved with many methods. Here are some of them:

i) the Taylor expansion over the degrees of an appropriate parameter in a neighborhood of the initial approximation (for example the Chapman-Enskog method [39]);

ii) the Newton method (as in the KAM-theory [40], [41] but with a incomplete linearization, as in the original formulation of the method of invariant manifolds for dissipative systems [21]).

iii) the implementation of Galerkin approximations for each iteration.

Omitting the well known expansions of the perturbation theory, we consider the direct methods.

In order to make one step of the Newton method with incomplete linearization, we need:

- i) an approximate manifold, $f_M^\#$, which we call Ω ;
- ii) projector P mapping a neighborhood of Ω on Ω .

For each $f_M^\#$ the projector, $\pi_{f_M^\#}$, mapping E on the tangent space, $T_{f_M^\#}\Omega$, is $\pi_{f_M^\#} = D_f P_\Omega|_{f_M^\#}$ (π is differential of P_Ω).

Usually, the projector P_Ω is defined in such a way that the layers (prototypes of points $f_M^\#$ under projection) could be patches on affine subspaces of E .

For each $f_M^\#$ we define the invariance defect

$$\Delta_{f_M^\#} = J(f_M^\#) - \pi_{f_M^\#} J(f_M^\#). \quad (131)$$

The invariance equation

$$\Delta_{f_M^\#} = 0 \quad (132)$$

is solved with the Newton method with incomplete linearization: for every M we search for $\delta f_M^\#$, such as:

$$\begin{cases} P_\Omega(f_M^\# + \delta f_M^\#) = f_M^\#, \\ (1 - \pi_{f_M^\#})DJ(f)|_{f_M^\#} \delta f_M^\# = -\Delta_{f_M^\#}. \end{cases} \quad (133)$$

If the layers of P_Ω are patches on the affine manifolds, then (133) is a system of linear equations. Another form of this system is

$$\begin{cases} \pi_{f_M^\#} \delta f_M^\# = 0, \\ (1 - \pi_{f_M^\#})DJ(f)|_{f_M^\#} \delta f_M^\# = -\Delta_{f_M^\#}. \end{cases} \quad (134)$$

It should be stressed that in equation (133) incomplete (in contrast to the Newton method) linearization has been used. We did not differentiate $\pi_{f_M^\#}$ in $\Delta_{f_M^\#}$ in (131).

The discussion is given in (8). We note only that for the simplest stable self-adjoint linear systems with incomplete linearization equations (133) lead generically to an invariant subspace with the largest (i.e. closest to zero) eigenvalues. In contrast, procedures with whole linearization lead in this case to the subspace closest to the initial approximation.

As soon as $\delta f_M^\#$ is found from equations (133), we substitute $f_M^\#$ for $f_M^\# + \delta f_M^\#$; construct new projectors and repeat the procedure.

Solution to the invariance equation (132) by the Newton method with incomplete linearisation can turn into a difficult problem. In spite of their linearity, equations (133) cannot be solved easily every time. One can try to simplify the problem passing from the invariance equations to the Galerkin approximations. The simplest example is one-dimensional approximations when $\delta f_M^\# = \delta_M \Delta_{f_M^\#}$, and equation is solved in the projection on Δ :

$$\langle \Delta_{f_M^\#} | (1 - \pi_{f_M^\#})J(f_M^\# + \delta_M \Delta_{f_M^\#}) \rangle_{f_M^\#} = 0. \quad (135)$$

The entropic scalar product $\langle | \rangle_{f_M^\#} = -D^2 S(f)|_{f_M^\#}$ is used.

Solving (135) with the Newton method, we obtain at the first iteration:

$$\delta M = -\frac{\langle \Delta_{f_M^\#} | \Delta_{f_M^\#} \rangle_{f_M^\#}}{\langle \Delta_{f_M^\#} | DJ(f)_{f_M^\#} \Delta_{f_M^\#} \rangle_{f_M^\#}}. \quad (136)$$

More often for the dissipative systems the denominator is negative, and this allows us to move on. For the conservative systems the one-dimensional Galerkin approximations lead to an unsatisfactory result, at least, in the combination with the Newton method (with the incomplete linearization).

6.3 The entropic thermodynamic projectors

The simplest choice of P_Ω is obvious:

$$P_\Omega(f) = f_M^\#; \quad (137)$$

for each value of f the values of macroscopic variables, $m(f)$, can be calculated. Based on these values, the corresponding point with the same value of $m(f)$ on the manifold can be obtained.

However, projector (137) does not satisfy the physical constraints every time.

On the set U a concave function, the entropy, S , is defined. Two kinds of systems are under consideration: i) (129) dissipative, for which $dS/dt \leq 0$, in accordance with the system, ii) conservative, for which $dS/dt = 0$. The quasiequilibrium manifolds, f_M^* , are physically distinguished. They are the solution to the variational problem

$$\begin{aligned} S(f) &\rightarrow \max, \\ m(f) &= M. \end{aligned} \quad (138)$$

Application of the simplest projector (137) leads to the fact that the vector field, $\pi_{f_M^*} J(f_M^*)$, preserves the type of dynamics of the system on the quasiequilibrium manifold. For the conservative J it is conservative, and for the dissipative systems it is dissipative too (with the same entropy). Such a preservation of the type of dynamics by the projector is guaranteed only for the quasiequilibrium manifolds.

However, practically for every manifold $\Omega = \{f_M^\#\}$ it is possible to construct such a projector, P_Ω , that every $f_M^\#$ is a solution to the problem

$$\begin{aligned} S(f) &\rightarrow \max, \\ P_\Omega(f) &= f_M^\# \end{aligned} \quad (139)$$

in a neighborhood of Ω . For this it would be sufficient that for every M the functional $DS(f)|_{f_M^\#}$ eliminate $\ker \pi_{f_M^\#}$:

$$DS(f)|_{f_M^\#}(\ker \pi_{f_M^\#}) = 0. \quad (140)$$

Thus, in order to control the physical sense of obtained approximations, one needs to consider the projector depending on the manifold [21].

6.4 Method of invariant manifold for the positively invariant manifolds with fixed edge

In the problem of construction of invariant sections the position of points $f_M^\#$ was not fixed. Only fulfillment of condition $m(f_M^\#) \equiv M$ was important. There is another kind of problems where one needs to find a positive invariant manifold with a fixed edge. Practically, this is a problem of construction of a trajectory of the edge in accordance with (129) for $t \in [0; +\infty)$.

These problems include the problem of initial layer [15], [16], as well as the problem of construction of the film of non-equilibrium states discussed in this paper.

The iterative methods described above cannot be implemented here, because they destroy the boundary conditions on the edge of the manifold. If the invariance conditions are fulfilled on the edge of the initial approximation, $f_M^\#$, accurate to the k -th derivative in time, then the Newton method leads to the fact that after the $(k + 1)$ -th iteration the edges of the manifold will be changed (the film tears off the edge).

In the previous paper devoted to the problem of initial layer [15] we have technically overcome this difficulty. To do this, we simulated the trajectory as an elastic beam with a rigidly fixed end. In the mechanical equilibrium this beam had the form of an approximate trajectory. Later, it was elastically attracted to the result of the Newton iterations. Even though that this technique allows to avoid the separation of contact between the edge and the film, its technical artificiality forces us to continue to search for new methods.

The application of the Picard iterative procedure allows to conserve initial conditions. For the film equation we write: let $q_{M,\tau}^0$ be an approximation for the film, then the Picard iteration gives:

$$q_{M,\tau}^1 = q_{M,0} + \int_0^\tau \frac{\partial q_{M,\tau}}{\partial \theta} \Big|_{q_{M,\theta}^0} d\theta. \quad (141)$$

Here $\partial q_{M,\tau} / \partial \theta|_{q_{M,\theta}^0}$ is the right hand side of (58) taken at the point $q_{M,\theta}^0$.

Let us define, as usual, $\Delta_{M,\theta} = \partial q_{M,\tau} / \partial \theta|_{q_{M,\theta}^0} - \partial q_{M,\tau}^0 / \partial \theta$ as the difference of the vector field and its projection on the approximate manifold, then the Picard iteration obtains the form:

$$q_{M,\tau}^1 = q_{M,\tau}^0 + \int_0^\tau \Delta_{M,\theta} d\theta. \quad (142)$$

The Picard iteration gives a good result for small τ but can be too radical for large one. It is possible to use the Picard iterations together with the weight which ensures essential dependence of the correction, $q_{M,\tau}^1$, not from all $\Delta_{M,\theta}$, $0 \leq \theta \leq \tau$, but from those within a segment $\theta \in [\tau - h; \tau]$. For example,

$$q_{M,\tau}^1 = q_{M,\tau}^0 + \int_0^\tau e^{(\theta-\tau)/h} \Delta_{M,\theta} d\theta. \quad (143)$$

Another choice of the weight function is possible. For large τ and sufficiently small h and $\Delta \neq 0$, the formula (143) gives:

$$q_{M,\tau}^1 = q_{M,\tau}^0 + h\Delta_{M,\tau} + o(h). \quad (144)$$

For small τ we obtain:

$$q_{M,\tau}^1 = q_{M,\tau}^0 + \frac{\tau}{k+1} \Delta_{M,\tau} + o(\tau \Delta). \quad (145)$$

where k is order of zero of $\Delta_{M,\tau}$ at the point $\tau = 0$.

Joining (144) and (145), we obtain:

$$q_{M,\tau}^1 \approx q_{M,\tau}^0 + \frac{h\tau}{(k+1)h + \tau} \Delta_{M,\tau}. \quad (146)$$

In all cases the question of how to choose the step arises. The simplest solution exists for (146): it is possible to take the step, h , depending on the point:

$$q_{M,\tau}^1 \approx q_{M,\tau}^0 + \lambda_{M,\tau} \Delta_{M,\tau}. \quad (147)$$

where $\lambda_{M,\tau} = \min\{\tau/(k+1), \delta_{M,\tau}\}$, and $\delta_{M,\tau}$ is to be found from the condition of stopping in the direction of Δ (135).

Various combinations of the Picard and Newton iterations can generate a separate subject for investigation. Their simplest hybridisation consists of the following. Let for each (M, τ) the step, $\delta_{M,\tau}$, is found according to the Newton method (133).

Define

$$q_{M,\tau}^1 = q_{M,\tau}^0 + 1/h \int_0^\tau e^{(\theta-\tau)/h} \delta q_{M,\theta} d\theta. \quad (148)$$

In order to have the step value on the direction $\delta q_{M,\theta}$ close to 1 for large τ , the multiplier $1/h$ has been used. An analog to (146) is

$$q_{M,\tau}^1 = q_{M,\tau}^0 + \frac{\tau}{(k+1)h + \tau} \delta q_{M,\theta}. \quad (149)$$

The typical time scale, which separates in (137) and (138) the Picard (small times, $\tau \ll h$), and Newton (large time, $\tau \gg h$) iterations, can be estimated by the curvature radius (52) (in general, from the relations $\|\dot{q}\|/\|\ddot{q}\|$ or $\|\dot{q}\|/\|\ddot{q}_\perp\|$).

Further development of the methods will be determined by particular applications.

Acknowledgments. A.N.G. is thankful to G. Sh. Fridman for stimulating discussions and encouragement. A.N.G. thanks Institut des Hautes Études Scientifiques, where parts of this work have been developed, for hospitality. I.V.K. is thankful to the organizers of the First Mexican Meeting on Mathematical and Experimental Physics, where parts of this work have been presented, and especially to Leo García-Colín and Francisco Uribe for discussions. I.V.K. acknowledges stimulating discussions with Miroslav Grmela. Finally, it is our pleasure to thank Misha Gromov and Hans Christian Öttinger for stimulating discussions.

S. Ansumali, P. Gorban, V. Ilyushchenko, and L. Tatarinova helped us to prepare the manuscript.

References

- [1] *Studies in Statistical Mechanics, V. IX*, Eds. E. W. Montroll and J. L. Lebowitz, (North-Holland, 1981).
- [2] Del Río-Correa, J. L., García-Colín, L. S., *Phys. Rev. E* **48** (1993) 891;
- [3] Zubarev, D., Morosov, V., Röpke, G., *Statistical Mechanics of Nonequilibrium Processes*, Akademie Verlag, Berlin, Vol. 1. (1996).
- [4] Grabert, H., *Projection Operator Techniques in Nonequilibrium Statistical Mechanics*, Springer, Berlin, 1982.
- [5] Leontovich, M. A., *An Introduction to thermodynamics*, GITTL Publ., Moscow, 1950 (in Russian).
- [6] Lebowitz, J. L., Bergmann, P. G., New approach to nonequilibrium processes, *Phys. Rev.* **99** (1955), 578-587.
- [7] Lebowitz, J. L., Bergmann, P. G., Irreversible Gibbsian Ensembles, *Annals of Physics*, 1:1, 1957.
- [8] Lebowitz, J. L., Stationary Nonequilibrium Gibbsian Ensembles, *Phys. Rev.*, **114** (1959), 1192-1202.
- [9] Lebowitz, J. L., Boltzmann's entropy and time's arrow, *Physics Today*, **46** 9 (1993), 32-38.
- [10] *Maxwell's Demon 2: Entropy, Classical and Quantum Information, Computing*. 2nd edition. H. S. Leff, A. F. Rex, eds. IOP, Philadelphia, 2003.
- [11] Von Baeyer, H. C., *Maxwell's Demon: Why Warmth Disperses and Time Passes*, Random House, 1998.
- [12] Gorban, A. N., Karlin, I. V., Geometry of irreversibility, in: *Recent Developments in Mathematical and Experimental Physics, Volume C: Hydrodynamics and Dynamical Systems*, F. Uribe. Kluwer, Dordrecht, 19 (2002).
- [13] Pour-El, M. B., Richards, J. I., *Computability in Analysis and Physics*. Springer Verlag, 1989.
- [14] Copeland, B. J., The Church-Turing Thesis, In: The Stanford Encyclopedia of Philosophy (Fall 2002 Edition),
On-line: <http://plato.stanford.edu/archives/fall2002/entries/church-turing/>.
- [15] Gorban, A. N., Karlin, I. V., Zmievskii, V. B., Nonnenmacher, T. F., Relaxational trajectories: global approximations *Physica A*, **231** (1996), 648-672.

- [16] 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.
- [17] Karlin, I. V., Gorban, A. N., Succi, S., Boffi, V., Maximum Entropy Principle for Lattice Kinetic Equations, *Phys. Rev. Lett.*, **81**, 1 (1998), 6–9
- [18] 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.
- [19] Karlin, I. V., Ansumali, S., De Angelis, E., Öttinger, H. C., Succi, S. Entropic Lattice Boltzmann Method for Large Scale Turbulence Simulation, E-print,
On-line: <http://arxiv.org/abs/cond-mat/0306003>.
- [20] Gorban, A. N., Karlin, I. V., Thermodynamic parameterization *Physica A*, **190** (1992), 393–404.
- [21] Gorban, A. N., Karlin, I. V., Method of invariant manifolds and regularization of acoustic spectra, *Transport Theory and Stat. Phys.*, **23** (1994), 559–632.
- [22] Gorban, A. N., Karlin, I. V., Zinovyev, A. Yu. Constructive Methods of Invariant Manifolds for Kinetic Problems, Preprint IHES/M/03/50, Institut des Hautes tudes Scientifiques in Bures-sur-Yvette (France), 2003.
On-line: <http://agorban.fatal.ru/kinetics/pdf/cmimprobeta.pdf>,
http://mpej.unige.ch/mp_arc/c/03/03-335.pdf.
- [23] Feynman, R., *The Character of Physical Law*, Cox and Wyman, London, 1965. Lecture No. 5.
- [24] Ruelle, D., Smooth Dynamics and New Theoretical Ideas in Nonequilibrium Statistical Mechanics, *Journal of Statistical Physics*, **95** (1-2) (1999), 393–468.
- [25] Ehrenfest, P., *Collected Scientific Papers*, North-Holland, Amsterdam, 1959, pp. 213–300.
- [26] 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.
- [27] Gorban, A. N., Equilibrium Encircling. Equations of Chemical Kinetics and Their Thermodynamic Analysis, Nauka, Novosibirsk, 1984. [In Russian]
- [28] Gorban, A. N., Bykov, V. I., Yablonskii, G. S., Essays on chemical relaxation, Nauka, Novosibirsk, 1986. [In Russian]
- [29] Gorban, A. N., Karlin, I. V., Ilg, P., Öttinger, H. C., Corrections and enhancements of quasi-equilibrium states *J. Non-Newtonian Fluid Mech.*, **96(1-2)** (2001), 203–219.

- [30] Gorban, A. N., Karlin, I. V., Öttinger, H. C., Tatarinova, L. L., Ehrenfest's argument extended to a formalism of nonequilibrium thermodynamics, *Phys. Rev. E*, **63** 066124 (2001).
- [31] Lewis, R. M., A unifying principle in statistical mechanics, *J. Math. Phys.* **8** (1967), 1448-1460.
- [32] Gorban, A. N., Karlin, I. V., Macroscopic dynamics through coarse-graining: A solvable example, *Phys. Rev. E* **65** (2002), 026116(1-5).
- [33] Gorban, A. N., Karlin, I. V., Quasi-equilibrium approximations and non-standard expansions in the theory of the Boltzmann kinetic equation, *Mathematical Modeling in Biology and Chemistry (New Approaches)*, R. G. Khlebopros, ed., Nauka, Novosibirsk, 1992, 69–117. [In Russian]
- [34] Gorban, A. N., Karlin, I. V., Quasi-Equilibrium Closure Hierarchies for The Boltzmann Equation [Translation of the first part of the paper [33]]. Preprint, 2003, Online: <http://arXiv.org/abs/cond-mat/0305599>.
- [35] Kazantzis, N., Singular PDEs and the problem of finding invariant manifolds for nonlinear dynamical systems *Physics Letters, A* **272(4)** (2000), 257–263.
- [36] Beyn, W.-J., Kless, W., Numerical Taylor expansions of invariant manifolds in large dynamical systems, *Numerische Mathematik*, **80** (1989), 1–38.
- [37] Arnold, V. I., Vogtmann, K., Weinstein, A., *Mathematical methods of classical mechanics*, Springer Verlag, 1989.
- [38] Bogoliubov, N. N., Mitropolskii, Yu. A., *Asymptotic Methods in the Theory of Non-linear Oscillations*, Fizmatgiz, Moscow, 1958 (in Russian).
- [39] Chapman, S., Cowling, T. G., *The Mathematical Theory of Non-uniform Gases*, Cambridge University Press, Cambridge, (1970).
- [40] Kolmogorov, A. N., On conservation of conditionally periodic motions under small perturbations of the Hamiltonian. *Dokl. Akad. Nauk SSSR*, **98** (1954), 527–530.
- [41] 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.
- [42] Karlin, I. V., Tatarinova, L. L., Gorban, A. N., Öttinger, H. C., Irreversibility in the short memory approximation, *Physica A*, to appear. Online: <http://arXiv.org/abs/cond-mat/0305419>.
- [43] Gorban, A. N., Karlin, I. V., Macroscopic dynamics through coarse-graining: A solvable example *Phys. Rev. E*, **56** 026116(1-5) (2002).

- [44] Gorban, A. N., Karlin, I. V., Reconstruction lemma and fluctuation-dissipation theorem *Revista Mexicana de Fisica*, **48** 1 (2002), 238–242.
- [45] Jaynes, E. T., Information theory and statistical mechanics, in: *Statistical Physics. Brandeis Lectures, V. 3*, 1963. 160-185.
- [46] Kogan, A. N., Rosonoer, L. I., On the macroscopic description of kinetic processes, *Dokl. AN SSSR* **158** (3) (1964), 566–569.
- [47] Rosonoer, L. I., Thermodynamics of nonequilibrium processes far from equilibrium, in: *Thermodynamics and Kinetics of Biological Processes* (Nauka, Moscow, 1980), 169-186.
- [48] 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.
- [49] Gorban, A. N., Karlin, I. V., *Geometry of irreversibility: Film of nonequilibrium states*, The lecture given on the V Russian National Seminar “Modeling of Nonequilibrium systems”, Krasnoyarsk, Oct. 18-20, 2002, Printed by Krasnoyarsk State Technical University Press, 2002. [In Russian].