12 Geometry of Irreversibility: The Film of Nonequilibrium States

A geometrical framework of nonequilibrium thermodynamics is developed in this chapter. The notion of *macroscopically definable ensembles* is introduced. A thesis about macroscopically definable ensembles is suggested. This thesis should play the same role in the nonequilibrium thermodynamics, as the well-known Church-Turing thesis in the theory of computability. The *primitive macroscopically definable ensembles* are described. These are ensembles with macroscopically prepared initial states. A method for computing trajectories of primitive macroscopically definable nonequilibrium ensembles is elaborated. These trajectories are represented as sequences of deformed quasiequilibrium ensembles and simple quadratic models between them. The primitive macroscopically definable ensembles form a 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 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.

12.1 The Thesis About Macroscopically Definable Ensembles and the Hypothesis About Primitive Macroscopically Definable Ensembles

The goal of this chapter is to discuss the nonlinear problem of irreversibility, and to revise previous attempts to solve it. 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, [194, 195, 286, 287]). We here intend to develop a more geometrical viewpoint on the subject. First, in Sect. 12.2, we discuss in an informal way the origin of the problem, and demonstrate how the basic constructions arise. Second, in Sect. 12.3, we give a consistent geometric formalization of these constructions. Our presentation is based on the notion

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of the natural projection introduced in section 12.4. We discuss in detail the method of natural projector as the consistent formalization of Ehrenfests' ideas of coarse-graining.

In Sect. 12.4.2 we introduce a one-dimensional model of nonequilibrium states. In the background of many derivations of nonequilibrium kinetic equations one can imagine 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 state. It seems that the motion of the nonequilibrium ensemble decomposes into two projections, transversal to the quasiequilibrium manifold, and in the projection on this manifold. The motion in each layer above the quasiequilibrium points is highly complicated, but fast, and everything quickly settles in this fast motion.

However, upon a more careful looking into the motions of the ensembles which start from the quasiequilibrium points, we recognize that above each point of the quasiequilibrium manifold it is located *just a single and in some sense monotonic curve,* and all the relevant nonequilibrium (not-quasiequilibrium) states form just a one-dimensional manifold.

The one-dimensional models of nonequilibrium states form a *film of non-equilibrium states*. In Sect. 12.5 we present a collection of methods for the film construction. One of the benefits from this new technique is the possibility to solve the problem of macro-kinetics even 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 problem of nonequilibrium kinetics into a series of problems of equilibrium statistical physics.

The most important results of this chapter 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 a sequence of deformed quasiequilibrium ensembles connected by quadratic models.

Let us give here an introductory description of these results.

The notion of macroscopically definable ensembles consists of three ingredients:

1. The macroscopic variables, the variables which values *can be controlled by us*;
2. The quasiequilibrium state, the conditional equilibrium state for fixed values of the macroscopic variables;
3. The natural dynamics of the system, or the microscopic dynamics.

We use the simplest representation of the control: At certain moments of time we fix some values of the macroscopic variables (one can fix all of all these

macroscopic variables, or only a part of them; for the whole system, or for macroscopically defined part of it; the current values, or some arbitrary values of these variables), and the system settles in the 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 obtained by a closure: the limit of a sequence of macroscopically definable ensembles is macroscopically definable too.

The role of the macroscopic variables for the irreversibility problem was clarified by M. Leontovich and J. Lebowitz several decades ago [288–292]. This was the first step. Now we do need the elaborate notion of ensembles which can be obtained by the macroscopic tools. The Maxwell Demon gives the early clear picture of a difference between the macroscopic and microscopic tools for the ensembles control (books are devoted to the studies of this Demon [293, 294]). Nevertheless, a further step towards the notion of the macroscopic definability in the context of constructive transition from the microdynamics to macrokinetics was not done before the paper [33]. Our analysis is an analog of the Church-Turing thesis in the theory of computability [295, 296]. 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 according to the introduced notion. This is the thesis about the success of the formalization, as the Church-Turing thesis, and nobody can prove or disprove it in a rigorous sense, as well as this famous thesis.

Another important new notion is the *"macroscopically definable transformation"* of the ensemble: If one got an ensemble, how can he transform it? First, it is possible just to let them evolve due to the natural dynamics, second, it can be controlled by the macroscopic tools in the prescribed 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 the 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. After that there remains no other effective way to decribe 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 the entropy production.

The main technical problem is the computation of this curve for arbitrary values of the macroscopic variables. We represent it as a sequence of distinguished states and second-order polynomial (Kepler) models for the trajectory between these points. This can be viewed as a further development of the method for initial layer problem in the Boltzmann kinetics (see Sect. 9.3 and [26, 27]). For the 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 higher-order models. Applications of this method to the lattice kinetic equations (Sect. 2.7) allowed

- To create the lattice Boltzmann method with the H-theorem [137];
- To transform the lattice Boltzmann method into the numerically stable computational tool for fluid flows and other dissipative systems out of equilibrium [136];
- To develop the entropic lattice Boltzmann method as a basis for the formulation of a new class of turbulence models based on genuinely kinetic principles [66].

In this chapter we extend the method elaborated for dissipative systems [26,27] to the higher-order models for conservative systems. The constructing of the method of physically consistent computation is the central part of this chapter.

The main results of this chapter were presented in the talk given at the First Mexican Meeting on Mathematical and Experimental Physics, Mexico City, September 10–14, 2001 [33], and in the lectures given on the V Russian National Seminar "Modeling of Nonequilibrium systems", Krasnoyarsk, October 18–20, 2002 [298].

12.2 The Problem of Irreversibility

12.2.1 The Phenomenon of the Macroscopic Irreversibility

The best way to get a feeling about the problem of irreversibility is the following thought experiment (*Gedankenexperiment*): Let us watch a movie: It's raining, people are running, cars rolling. Let us now wind this movie in the opposite direction, and we shall see a strange and funny picture: Drops of the rain are raising up to the clouds, people run with their backs forward, cars also behave quite strange, and so forth. This cannot be true, 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 notice any substantial difference between the direct and the reverse demonstration: Everywhere the particles move, collide, react 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 – all this is too complicated. One of the simplest examples of the irreversible macroscopic picture under the apparent reversibility of the microscopic picture is given by R. Feynman in his lectures on the character of physical law [297]. We easily label it as self-evident the fact that particles of different colors mix together, and we would deem it wonderful the reverse picture of a spontaneous decomposition of their mixture. However, by itself, an appreciation of one picture as usual, and of the other as unusual and wonderful – this is not yet physics. It is desirable to measure somehow this transition from order to disorder.

12.2.2 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 the 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 to land into such a configuration by a 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 what has more order, a fine castle or 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 a 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 phase 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 representing the configuration, very rapidly leaves a small neighborhood and for a long time (in practice, never) does not return 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 using macroscopic means* of preparation. In order to prepare such states, one would have to employ an army of Maxwell's Demons 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 that 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 these 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 time and experience.

There is one property that distinguishes an arbitrary ensemble with phase volume V and ensembles (with the same volume) that we usually associate with the order. This property is *observability*. Usually we can fix a configuration within some error only, this means that we cannot distinguish points, if the distance between them is less then some $\varepsilon > 0$. Hence, the *observable ensemble* should not change its volume significantly, if we replace all points by the ε-small balls (i.e. if we just add a small ball to the set of states, or, if the ensemble is presented by the distribution density, just average the density over such balls). This operation, averaging over small balls or cells, is called *coarse graining*. The observable state should not significantly change its volume after the coarse-graining. The ordered state (the blue particles are all in the right half, and all the white particles are in the left half, for example) is observable, but dynamics makes it unobservable after some time. Of course, the notion of macroscopically definable ensembles should meet the expectation concerning observability as well as implementability and controlability of these ensembles.

12.2.3 Macroscopically Definable Ensembles and Quasiequilibria

The main tool in the study of the 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 the hydrodynamic fields: density of particles, density of momentum, and density of energy. This list may also include the stress tensor, the 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 over the phase space. The density F must satisfy a set of restrictions, the most important of which are: Nonnegativity, $F(x) \geq 0$, normalization,

$$\int_X F(x)\,\mathrm{d}V(x) = 1\ , \tag{12.1}$$

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

$$S(F) = -\int_X F(x)\ln F(x)\,\mathrm{d}V(x)\ . \tag{12.2}$$

The function $F\ln F$ is continuously extended to zero values of F: $0\ln 0 = 0$). Here, $\mathrm{d}V(x)$ 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 to the equilibrium.

The corresponding (generalized) canonical ensemble F which is the solution to the problem:

$$S(F) \to \max,\ M(F) = M\ . \tag{12.3}$$

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:

1. Bringing the system into the quasiequilibrium state corresponding to either the whole set of the macroscopic variables M, or to its subset;
2. Evolution of 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 macroscopically definable. One always begins with the first operation.

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 $\mathrm{d}V$ into a direct product of spaces, $X = X_1 \times X_2$ with the measure $\mathrm{d}V_1\mathrm{d}V_2$. To each admissible ("macroscopic") partition into sub-systems, it corresponds the operation of taking a "partial quasiequilibrium", applied to some density $F_0(x_1, x_2)$:

$$\begin{aligned} &S(F) \to \max\ , \\ &M(F) = M,\ \int_{X_2} F(x_1, x_2)\,\mathrm{d}V_2(x_2) = \int_{X_2} F_0(x_1, x_2)\,\mathrm{d}V_2(x_2)\ . \end{aligned} \tag{12.4}$$

where M is some subset of macroscopic variables (not necessarily the whole list of the macroscopic variables). In (12.4), the state of the first subsystem is not changing, whereas the second subsystem is brought into the quasiequilibrium. In fact, the problem (12.4) is a version of the problem (12.3) with additional "macroscopic variables",

$$\int_{X_2} F(x_1, x_2)\,\mathrm{d}V_2(x_2)\ . \tag{12.5}$$

The *extended thesis* about the macroscopically definable ensembles allows to use also operations (12.4) 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 (12.3) for some initial M. This does not exclude a possibility of including operators (12.5) 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:

1. 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;
2. Macroscopically admissible partitions of the system into sub-systems;
3. Equations of the 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: which 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. Usually we can postulate some properties of macroscopic variables, for example, symmetry with respect to any permutation of equivalent particles.

We have discussed the *prepared* ensembles. But there is another statement of the problem: Let an ensemble be just given. The way it emerged it may be irrelevant or unknown, for example, some demon or *oracle*[1] can prepare the ensemble for us. How can we transform this ensemble by the macroscopic tools? First, it is possible just to let it evolve, second, it can be controlled by the macroscopic tools in the prescribed 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:

1. Bringing the system into the quasiequilibrium state corresponding to either the whole set of the macroscopic variables M, or to its subset.
2. 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 macroscopically definable. The main difference of this definition (macroscopically definable transformation) from the definition of the macroscopically definable ensembles is the absence of the restriction on the initial state, one can start from an arbitrary ensemble.

The class of macroscopically definable ensembles includes a simpler, but important subclass. Let us reduce the macroscopic control to preparation of the initial quasiequilibrium ensemble: we just prepare the ensemble by macroscopic tools and then let it evolve due to the natural dynamics (Liouville

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

equation, for example). Let us call this class *the primitive macroscopically definable ensembles*. These ensembles appear as the results (for $t > 0$) of motions which start from the quasiequilibrium state (at $t = 0$). The main technical focus of our work concerns the computation of the manifold of primitive macroscopically definable ensembles for a given system.

The importance of this subclass 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 an appropriate accuracy. In certain limits we can attempt to say: "with any accuracy". Moreover, this hypothesis with "arbitrary accuracy" can be found as the basic but implicit foundation of all nonequilibrium kinetics theories which claim derivation the macrokinetics from microdymamics, for example Zubarev's nonequilibrium statistical operator theory [195]. This hypothesis allows us to describe nonequilibrium state as a result of evolution of quasiequilibrium state in time.

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

12.2.4 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. In both cases the observed disorder 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 to $-\infty$ in time. This trick, however, casts some doubts, the major being this: Most of the known equations of the macroscopic dynamics describing 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 ordinary differential equations of chemical kinetics.

12.2.5 Weak and Strong Tendency to Equilibrium, Shaking and Short Memory

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

This remarkably simple observation does not, however, exhaust the problem of transition from the reversible equations to the irreversible macroscopic equations. One more aspect deserves a serious consideration. Indeed, distribution functions tend to the equilibrium state according to the 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, the tendency to equilibrium occurs (if at all) only in the weak sense: the average 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 was 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 be always 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 [15]. Ehrenfests considered a partition of the phase space into small cells, and they have suggested to supplement 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. The formalization of this idea was given in the previous chapter.

12.2.6 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 moreover, they include all classical equations of nonequilibrium thermodynamics and kinetics.

12.3 Geometrization of Irreversibility

12.3.1 Quasiequilibrium Manifold

We remind here some of the constructions from Chap. 5. Let E be a linear space, and $U \subset E$ be a convex subset, with a nonempty interior $\mathrm{int}U$. Let a twice differentiable concave functional S be defined in $\mathrm{int}U$, and S be 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 K be a closed linear subspace of space E, and $m : E \to E/K$ be the natural projection on the factor-space. The factor-space $L = E/K$ will further play the role of the space of macroscopic variables (in examples, the space of moments of the distribution).

For each $M \in \mathrm{int}m(U)$ we define the quasiequilibrium, $f^*_M \in \mathrm{int}U$, as the solution to the problem,

$$S(f) \to \max,\ m(f) = M\ . \tag{12.6}$$

We assume that, for each $M \in m(U)$, there exists the (unique) solution to the problem (12.6). 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 $\mathrm{int}U$, parameterized by the values of the macroscopic variables $M \in \mathrm{int}U/L$ (Fig. 12.1).

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

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

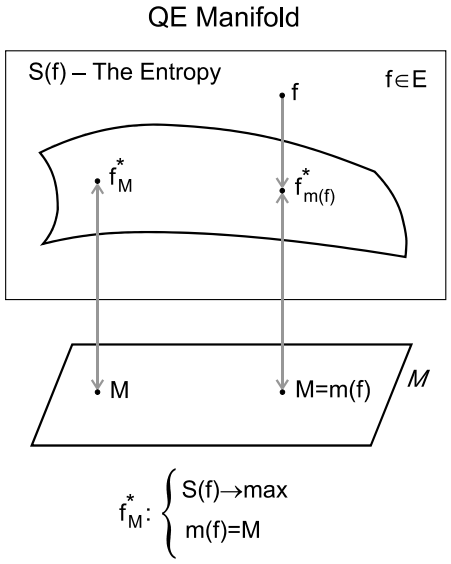

Fig. 12.1. Relations between a microscopic state f, the corresponding macroscopic state $M = m(f)$, and quasiequilibria f^*_M

operator, $A^T : E_1^T \to E_2^T$ is defined by the following relation: For any $l \in E_2^T$ and $x \in E_1$,

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

Next, $D_f S(f) \in E^T$ is the differential of the functional $S(f)$, $D^2_f S(f)$ is the second differential of the functional $S(f)$. Corresponding quadratic functional $D^2_f S(f)(x, x)$ on E is defined by the Taylor formula,

$$S(f + x) = S(f) + \big[D_f S(f), x\big] + \frac{1}{2} D^2_f S(f)(x, x) + o(\|x\|^2) \; . \qquad (12.7)$$

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

$$[D^2_f S(f)x, y] = D^2_f S(f)(x, y) \; .$$

In this formula, on the left hand side there is the operator, on the right hand side there is the bilinear form. Operator $D^2_f S(f)$ is symmetric on E, $D^2_f S(f)^T = D^2_f S(f)$.

Concavity of S means that for any $x \in E$ the inequality holds,

$$D^2_f S(f)(x, x) \le 0 \; ;$$

in the restriction onto the affine subspace parallel to $K = \ker m$ we assume the strict concavity,

$$D_f^2 S(f)(x,x) < 0 \text{ if } x \in K \text{ and } x \neq 0 \, .$$

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 $\Lambda(M) \in L^T$, that

$$D_f S(f)\big|_{f_M^*} = \Lambda(M) \cdot m, \;\; m(f_M^*) = M \, , \tag{12.8}$$

or

$$D_f S(f)\big|_{f_M^*} = m^T \cdot \Lambda(M), \;\; m(f_M^*) = M \, . \tag{12.9}$$

From equation (12.9) we get,

$$m(D_M f_M^*) = 1_{(L)} \, , \tag{12.10}$$

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 (12.8),

$$D_M \Lambda = (m(D_f^2 S)^{-1}_{f_M^*} m^T)^{-1} \, , \tag{12.11}$$

and, consequently, from (12.9)

$$D_M f_M^* = (D_f^2 S)^{-1}_{f_M^*} m^T (m(D_f^2 S)^{-1}_{f_M^*} m^T)^{-1} \, . \tag{12.12}$$

Notice that, elsewhere in equation (12.12), operator $(D_f^2 S)^{-1}$ acts on the linear functionals from $\mathrm{im}(m^T)$. These functionals are precisely those which become zero on K (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 $D_M f_M^*$:

$$\mathrm{im}\,(D_M f_M^*) = (D_f^2 S)^{-1}_{f_M^*} \mathrm{im}(m^T) = (D_f^2 S)^{-1}_{f_M^*} \mathrm{Ann} K \tag{12.13}$$

where $\mathrm{Ann}K$ (the annulator of K) is the set of linear functionals which become zero on K. Another way to write equation (12.13) is the following:

$$x \in \mathrm{im}\,(D_M f_M^*) \Leftrightarrow (D_f^2 S)_{f_M^*}(x,y) = 0, \;\; y \in K \tag{12.14}$$

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

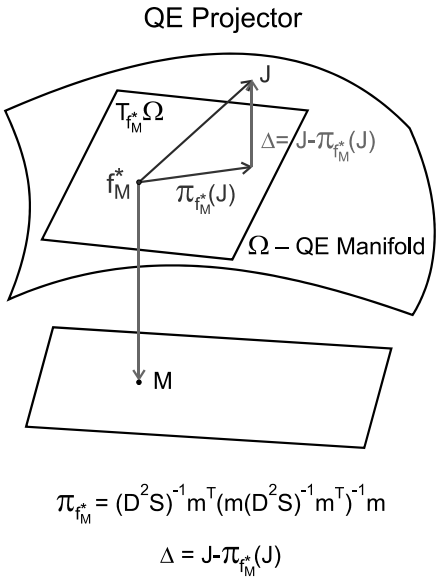

Fig. 12.2. Quasiequilibrium manifold Ω, tangent space $T_{f^*_M}\Omega$, quasiequilibrium projector $\pi_{f^*_M}$, and defect of invariance, $\Delta = \Delta_{f^*_M} = J - \pi_{f^*_M}(J)$

$$\langle x|y\rangle_{f^*_M} = -(D^2_f S)_{f^*_M}(x,y)\ . \tag{12.15}$$

The entropic scalar product (12.15) appears often in the constructions below. (Usually, this becomes the scalar product indeed after the conservation laws are excluded). Let us denote as $T_{f^*_M} = \mathrm{im}(D_M f^*_M)$ 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 K. This is the orthogonal projector with respect to the entropic scalar product, $\pi_{f^*_M} : E \to T_{f^*_M}$:

$$\pi_{f^*_M} = (D_M f^*_M)_M\, m = \left(D^2_f S\right)^{-1}_{f^*_M} m^T \left(m \left(D^2_f S\right)^{-1}_{f^*_M} m^T\right)^{-1} m\ . \tag{12.16}$$

It is straightforward to check the equality $\pi^2_{f^*_M} = \pi_{f^*_M}$, and the self-adjointness of $\pi_{f^*_M}$ with respect to entropic scalar product (12.15). Thus, we have introduced the basic constructions: quasiequilibrium manifold, entropic scalar product, and quasiequilibrium projector (Fig. 12.2).

12.3.2 Quasiequilibrium Approximation

Let a kinetic equation be defined in U:

$$\frac{\mathrm{d}f}{\mathrm{d}t} = J(f)\ . \tag{12.17}$$

(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 (12.17) 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,

$$\frac{\mathrm{d}M}{\mathrm{d}t} = m\left(J\left(f^*_M\right)\right) \ . \tag{12.18}$$

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

$$\frac{\mathrm{d}f^*_{M(t)}}{\mathrm{d}t} = (D_M f^*_M) m(J(f^*_M)) = \pi_{f^*_M} J(f^*_M) \ , \tag{12.19}$$

where $\pi_{f^*_M}$ is the quasiequilibrium projector (12.16).

Let us term function $S(M) = S(f^*_M)$ *the quasiequilibrium entropy*. Let us denote as $\mathrm{d}S(M)/\mathrm{d}t$ the derivative of the quasiequilibrium entropy due to the quasiequilibrium approximation (12.18). Then,

$$\frac{\mathrm{d}S(M)}{\mathrm{d}t} = \left.\frac{\mathrm{d}S(f)}{\mathrm{d}t}\right|_{f=f^*_M} \ . \tag{12.20}$$

From the identity (12.20), it follows **the theorem about preservation of the type of dynamics:**

(i) If for the original kinetic equation (12.17) $\mathrm{d}S(f)/\mathrm{d}t = 0$ at $f = f^*_M$, then the entropy is conserved due to the quasiequilibrium system (12.19).

(ii) If for the original kinetic equation (12.17) $\mathrm{d}S(f)/\mathrm{d}t \geq 0$ at $f = f^*_M$, then, at the same points f^*_M, $\mathrm{d}S(M)/\mathrm{d}t \geq 0$ due to the quasiequilibrium system (12.18).

The theorem about the preservation of the type of dynamics[2] demonstrates that if there was no dissipation in the original system (12.17) (if the entropy was conserved) then 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 (the compressible Euler equations). 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 holds for

[2] This is a rather old theorem, one of us had published this theorem in 1984 already as a textbook material ([115], 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.

the thermodynamic projectors described in Sect. 5.3. 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 (12.17) does not leave the quasiequilibrium manifold invariant, that is, the vector field $J(f)$ is not tangent to the quasiequilibrium manifold in all its points f^*_M. In other words, the *condition of invariance* (see Chap. 3),

$$(1 - \pi_{f^*_M})J(f^*_M) = 0 \,, \tag{12.21}$$

is not satisfied on the quasiequilibrium manifold. The left hand side of the invariance condition (12.21) is the *defect of invariance*, and we denote it as $\Delta_{f^*_M}$ (Chap. 3). 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". If the original equation (12.17) is already dissipative, this route of corrections, supplemented by the construction of the projector as in Sect. 5.3, leads to an appropriate macroscopic kinetics [11].

However, here, we are mainly interested in the route "from the very beginning", from conservative systems to dissipative. And here solving the invariance equation does not help since it will lead us to "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 is the absolutely transparent and explicit approach of Ehrenfests.

12.4 Natural Projector and Models of Nonequilibrium Dynamics

12.4.1 Natural Projector

So, let the original system (12.17) be conservative, and thus, $\mathrm{d}S(f)/\mathrm{d}t = 0$. The idea of Ehrenfests is to supplement the dynamics (12.17) by coarse-graining ("shakings"). The coarse-graining steps are external perturbations which are applied periodically with a fixed time interval τ, and which lead to "forgetting" of the small scale (nonequilibrium) details of the dynamics. For us here the coarse-graining is the replacement of f by 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 the constant density within each cell equal to the corresponding cell-average of f. In the limit $\tau \to 0$, 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 $J(f)$ (12.17) on the tangent bundle to the quasiequilibrium manifold.

So, the natural question appears: What will happen, if we shall 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 (12.17). We must derive a phase flow of the macroscopic system, $\Theta_t(M)$ (that is, the phase flow of the macroscopic system, $\mathrm{d}M/\mathrm{d}t = F(M)$, which we are looking for), such that, for any M,

$$m(T_\tau(f^*_M)) = \Theta_\tau(M)\ . \tag{12.22}$$

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. 12.3).

The final form of the equation for the macroscopic variables M (see Chap. 11) may be written:

$$\frac{\mathrm{d}M}{\mathrm{d}t} = F(M) = m(J(f^*_M)) + (\tau/2)m(D_f J(f)\big|_{f^*_M}\Delta_{f^*_M}) + o(\tau^2)\ . \tag{12.23}$$

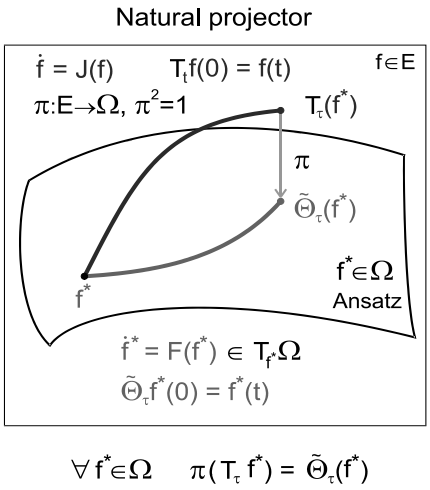

Fig. 12.3. Projection of segments of trajectories: The microscopic motion above the manifold Ω and the macroscopic motion on this manifold. If these motions began in the same point on Ω, then, after time τ, projection of the microscopic state onto Ω should coincide with the result of the macroscopic motion on Ω. For quasiequilibrium Ω, projector $\pi : E \to \Omega$ acts as $\pi(f) = f^*_{m(f)}$

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 the quasiequilibrium state.

The formula for the entropy production follows from (12.23):

$$\frac{\mathrm{d}S(f_M^*)}{\mathrm{d}t} = (\tau/2)\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*} \ . \tag{12.24}$$

The quasiequilibrium entropy increases due to the equation of the macroscopic dynamics (12.23) 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] and Chap. 11. The second term in equation (12.23) results in viscosity and heat conductivity terms in the Navier–Stokes equations, diffusion and other dissipative contributions. However, it remains the undetermined parameter τ. Formula (12.24) gives the entropy production just proportional to the time interval between subsequent coarse-grainings. Of course, this could be true only for small enough τ, whereas we are mostly interested in the limit $\tau \to \infty$. It is only in this limit where one can eliminate the arbitrariness in the choice of τ present in equations (12.23) and (12.24). In order to do this, we need to study more carefully the structure of the trajectories which begin on the quasiequilibrium manifold.

12.4.2 One-Dimensional Model of Nonequilibrium States

In the background of many derivations of nonequilibrium kinetic equations one can recognize 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. 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 quasiequilibria 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 shall observe that, above each point of the quasiequilibrium manifold it is located just a single and in certain sense monotonic curve. All the nonequilibrium (not-quasiequilibrium) states which come into the game form just a one-dimensional manifold. 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 $t = 0$). It is namely this curve the construction of which we shall be dealing with in this chapter.

For each value of the macroscopic variables M, and for every time $\tau \geq 0$, we define $M_{-\tau}$ by the following equality:

$$m(T_\tau(f^*_{M_{-\tau}})) = M \ . \tag{12.25}$$

In other words, $M_{-\tau}$ are those values of macroscopic variables which satisfy $\Theta_\tau(M_{-\tau}) = M$ for the natural projector (12.22). 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 $\tau_M > 0$, so 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 the 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:

$$\begin{aligned} \frac{\mathrm{d}\tau}{\mathrm{d}t} &= 1 \ , \\ \frac{\mathrm{d}M}{\mathrm{d}t} &= m(J(q_{M,\tau})) \ . \end{aligned} \tag{12.26}$$

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,

$$\left.\frac{\mathrm{d}q_{M,\tau}}{\mathrm{d}\tau}\right|_{\tau=0} = J(f^*_M) - \pi_{f^*_M} J(f^*_M) = \Delta_{f^*_M} \ . \tag{12.27}$$

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

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

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 (12.25) 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

$$A_2(M) = \left.\frac{\mathrm{d}^2 f^*_{M+tm(J(f^*_M))}}{\mathrm{d}t^2}\right|_{t=0} , \tag{12.28}$$

and

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

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

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

Thus,

$$m(T_\tau(f^*_{M_{-\tau}})) = M + (\tau^2/2) m(D_f J(f)\big|_{f^*_M} (1 - 2\pi_{f^*_M}) J(f^*_M)) + \tau^2 B(M) + o(\tau^2) ,$$

$$B(M) = (1/2) m(D_f J(f)\big|_{f^*_M} (2\pi_{f^*_M} - 1) J(f^*_M)) .$$

Accordingly, to second order in τ,

$$\begin{aligned}
q_{M,\tau} &= T_\tau(f^*_{M_{-\tau}}) \\
&= f^*_M + \tau \Delta_{f^*_M} + (\tau^2/2) A_2(M) \\
&\quad + (\tau^2/2)(1 - \pi_{f^*_M}) D_f J(f)\big|_{f^*_M} (1 - 2\pi_{f^*_M}) J(f^*_M) + o(\tau^2) .
\end{aligned} \tag{12.29}$$

Notice that, besides the dynamic contribution of the order of τ^2 (the last term), there appears also the term A_2 (12.28) 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 $x \in K$ (that is, $m(x) = 0$). The production of the quasiequilibrium entropy, $\sigma^*_M(x)$, equals, by definition,

$$\sigma^*_M(x) = D_M S(f^*_M) \cdot m(J(f^*_M + x)) . \tag{12.30}$$

Equation (12.30) gives the rate of the entropy change under the motion of the projection of the state onto the quasiequilibrium manifold if the true trajectory passes the point $f^*_M + x$. In order to compute the right hand side of equation (12.30), we use essentially the same argument, as in the proof of the entropy production formula (12.24). Namely, in the point f^*_M, we have $K \subset \ker D_f S(f)\big|_{f^*_M}$, and thus $D_f S(f)\big|_{f^*_M} \pi_{f^*_M} = D_f S(f)\big|_{f^*_M}$. Using this, and the fact that the entropy production in the quasiequilibrium approximation is equal to zero, equation (12.30) may be written,

$$\sigma^*_M(x) = D_f S(f)\big|_{f^*_M} (J(f^*_M + x) - J(f^*_M)) \; . \tag{12.31}$$

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

$$\sigma^*_M(x) = D_f S(f)\big|_{f^*_M} D_f J(f)\big|_{f^*_M} x \; . \tag{12.32}$$

Using the identity

$$D^2_f S(f)\big|_f J(f) + D_f S(f)\big|_f D_f J(f)\big|_f = 0 \; , \tag{12.33}$$

we obtain in equation (12.32),

$$\sigma^*_M(x) = -D^2_f S(f)\big|_{f^*_M} (J(f^*_M), x) = \langle J(f^*_M)|x\rangle_{f^*_M} \; . \tag{12.34}$$

Because $x \in K$, 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,

$$\sigma^*_M(x) = \langle \Delta_{f^*_M}|x\rangle_{f^*_M} \; . \tag{12.35}$$

The above consideration gives us the simplest way to study the primitive macroscopically definable ensembles using Taylor expansion in τ. This way has obvious limitations because τ remains a parameter of the theory.

12.4.3 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 more relevant to consider the entropic parameter, $\delta S = S^*(M) - S$ instead of τ. Within this parameterization of the one-dimensional curve of the nonequilibrium states one has to address functions $\sigma_M(\Delta S)$, rather than $\sigma_M(\tau)$.

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[3]. Given $\dot{q}_{M,\tau}$ and $\ddot{q}_{M,\tau}$ (12.29), 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 compute

$$R = \frac{\langle \dot{q}_{M,0}|\dot{q}_{M,0}\rangle_{f^*_M}}{\sqrt{\langle \ddot{q}_{\perp\ M,0}|\ddot{q}_{\perp\ M,0}\rangle_{f^*_M}}} , \tag{12.36}$$

where

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

Let us represent the microscopic motion as a circular motion along this entropic circle with the constant "linear velocity" $\dot{q}_{M,0} = \Delta_{f^*_M}$. After the microscopic motion passed the quarter of the circle, the entropy production begins decreasing and it becomes equal to zero after passing the semicircle. Hence, after passing the quarter of the circle, this model should be changed. The time of the motion along the quarter of the entropic circle is:

$$\tau \approx \frac{\pi}{2}\sqrt{\frac{\langle \Delta_{f^*_M}|\Delta_{f^*_M}\rangle_{f^*_M}}{\langle \ddot{q}_{\perp\ M,0}|\ddot{q}_{\perp\ M,0}\rangle_{f^*_M}}} . \tag{12.37}$$

After averaging over the 1/4 of this circle we obtain the macroscopic equations

$$\begin{aligned}
\frac{\mathrm{d}M}{\mathrm{d}t} &= m\left(J\left(f^*_M + \frac{2}{\pi}R\frac{\Delta_{f^*_M}}{\|\Delta_{f^*_M}\|} + \left(1-\frac{2}{\pi}\right)R\frac{\ddot{q}_{\perp\ M,0}}{\|\ddot{q}_{\perp\ M,0}\|}\right)\right) \\
&= m(J(f^*_M)) + \frac{2}{\pi}\frac{R}{\|\Delta_{f^*_M}\|}m\left(D_f J(f)\big|_{f^*_M}(\Delta_{f^*_M})\right) \\
&\quad + \left(1-\frac{2}{\pi}\right)\frac{R}{\|\ddot{q}_{\perp\ M,0}\|}m\left(D_f J(f)\big|_{f^*_M}(\ddot{q}_{\perp\ M,0})\right) + o(R) .
\end{aligned} \tag{12.38}$$

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

Equations (12.38) contain no undetermined parameters. This is the simplest example of a 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 (12.38) is proportional both to the defect of invariance and to the radius of curvature:

[3] We shall argue below in detail, why the first-order estimates, $q_{M,\tau} = f^*_M + \tau\Delta_{f^*_M}$, are insufficient in the case of the conservative dynamics.

$$\sigma_M = \frac{2}{\pi} R \| \Delta_{f^*_M} \| \ . \tag{12.39}$$

This equation demonstrates the thermodynamical sense of curvature of the curve of the nonequilibrium states. The combination

$$\frac{\textbf{defect of invariance}}{\textbf{curvature}} \tag{12.40}$$

is the dissipation (recall that all the scalar products and norms are *entropic*).

12.5 The Film of Non-Equilibrium States

12.5.1 Equations for the Film

The set $q_{M,\tau}$ in the space E forms a "surface" parameterized by "two variables": A scalar, $\tau \geq 0$, and the value of the macroscopic variables, M, subject to the condition

$$M = m(q_{M,\tau}) \ . \tag{12.41}$$

We call this surface *the film of non-equilibrium states* or simply *the film*. It consists of *the primitive macroscopically definable ensembles*, the result (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 a 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 the variation of $\tau \in [0; +\infty)$. It is not difficult to write down equations of this motion using the definition of $q_{M,\tau}$:

$$q_{M,\tau} = T_\tau f^*_{M_{-\tau}} \ , \tag{12.42}$$

where T_τ is the phase flow of the microscopic dynamical system, $M_{-\tau}$ is defined with equation (12.25).

For small $\Delta\tau$

$$q_{M,\tau+\Delta\tau} = q_{M-\Delta M,\tau} + J(q_{M,\tau})\Delta\tau + o(\Delta\tau) \ , \tag{12.43}$$

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

$$\frac{\mathrm{d}q_{M,\tau}}{\mathrm{d}\tau} = (1 - D_M q_{M,\tau} m) J(q_{M,\tau}) \ . \tag{12.44}$$

The initial condition for equation (12.44) is the quasiequilibrium

$$q_{M,0} = f^*_M \ . \tag{12.45}$$

Equation (12.44), subject to the initial condition (12.45), 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 the shift T_τ for positive times $\tau > 0$), including the quasiequilibrium manifold, f^*_M. All of the macroscopic kinetics take place only on this film.

Thus, the study of the non-equilibrium kinetics can be separated into two problems:

1. Construction of the film of non-equilibrium states: solution of equation (12.44) with the initial condition (12.45).
2. Investigation of the motion of the system on the film.

Of course, one should assume that the film will be constructed only approximately. Therefore, the second problem in turn should be separated in two subproblems:

– Construction of projection of the microscopic vector field J on the approximately found film, and construction of equations for M and τ.
– Investigation and solution of equations for M and τ.

It should be emphasized that the existence of the film is not significantly questionable (though, of course, proving theorems about existence and uniqueness for (12.44), (12.45) can turn into a hard mathematical problem). In a contrast, existence of kinetic coefficients (viscosity etc.), and generally, of the fast convergence of $\mathrm{d}M/\mathrm{d}t$ to a certain dependence $\mathrm{d}M/\mathrm{d}t$ of M is essentially a hypothesis which is not expected to always be true.

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

12.5.2 Thermodynamic Projector on the Film

We need the projector in order to project the vector field on the tangent space. The method of the thermodynamic projector ([9,10] and Chap. 5) allows to characterize every manifold (subject to certain requirements of transversality) as the quasiequilibrium one. This is achieved by a construction of a projection of a neighborhood of the manifold. The projection of the neighborhood on the manifold should satisfy essentially only one condition: a point of the manifold must be the point of maximum of the entropy on its preimage. If the preimage of the point f^* is a domain in the affine subspace, $K_{f^*} \subset E$, then the required condition is the property **A** (5.37):

$$(D_f S)_{f^*}(K_{f^*} - f^*) \equiv 0\,. \tag{12.46}$$

where $K_{f^*} - f^*$ is the linear subspace in E because $f^* \in K_{f^*}$.

For the projections with the property **A** (5.37), 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, and let us construct for it the projector.

Under small variation of variables M and τ

$$\begin{aligned} \Delta q_{M,\tau} &= D_M q_{M,\tau} \Delta M + D_\tau q_{M,\tau} \Delta\tau + o(\Delta M, \Delta\tau) \,, \\ \Delta S &= D_f S \,\big|_{q_{M,\tau}} \, \Delta q_{M,\tau} + o(\Delta M, \Delta\tau) \,. \end{aligned} \tag{12.47}$$

After simple transformations we obtain:

$$\begin{aligned} \Delta\tau &= \frac{\Delta S - D_f S|_{q_{M,\tau}} D_M q_{M,\tau} \Delta M}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} + o(\Delta M, \Delta S) \,, \\ \Delta q_{M,\tau} &= \left[1 - \frac{D_\tau q_{M,\tau} D_f S|_{q_{M,\tau}}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}}\right] D_M q_{M,\tau} \Delta M \\ &\quad + \frac{D_\tau q_{M,\tau} \Delta S}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} + o(\Delta M, \Delta S) \,. \end{aligned} \tag{12.48}$$

From this formulae we obtain the projector with the property **A** for J, π_{A}:

$$\begin{aligned} \pi_{\mathrm{A}}|_{q_{M,\tau}} J &= \left[1 - \frac{D_\tau q_{M,\tau} D_f S|_{q_{M,\tau}}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}}\right] D_M q_{M,\tau} m J \\ &\quad + \frac{D_\tau q_{M,\tau} D_f S|_{q_{M,\tau}}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} J \,. \end{aligned} \tag{12.49}$$

It is straightforward to check the equality $\pi_{\mathrm{A}}^2 = \pi_{\mathrm{A}}$. For the conservative vector fields $J(f)$, the second term in (12.49) vanishes because $D_f S|_f(J(f)) = 0$, and

$$\pi_{\mathrm{A}}|_{q_{M,\tau}} J = \left[1 - \frac{D_\tau q_{M,\tau} D_f S|_{q_{M,\tau}}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}}\right] D_M q_{M,\tau} m J \,. \tag{12.50}$$

The equation for M corresponding to (12.50) has the form:

$$\begin{aligned} \frac{\mathrm{d}M}{\mathrm{d}t} &= m(\pi_{\mathrm{A}}|_{q_{M,\tau}}(J(q_{M,\tau}))) \\ &= m \left[1 - \frac{D_\tau q_{M,\tau} D_f S|_{q_{M,\tau}}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}}\right] D_M q_{M,\tau} m J(q_{M,\tau}) \\ &= m J(q_{M,\tau}) \,. \end{aligned} \tag{12.51}$$

By the definition of the projector with the property **A** the equation for M (12.51) should be supplemented with the equation for S:

$$\frac{\mathrm{d}S}{\mathrm{d}t} = 0 \,, \tag{12.52}$$

or for τ, in accordance with (12.48),

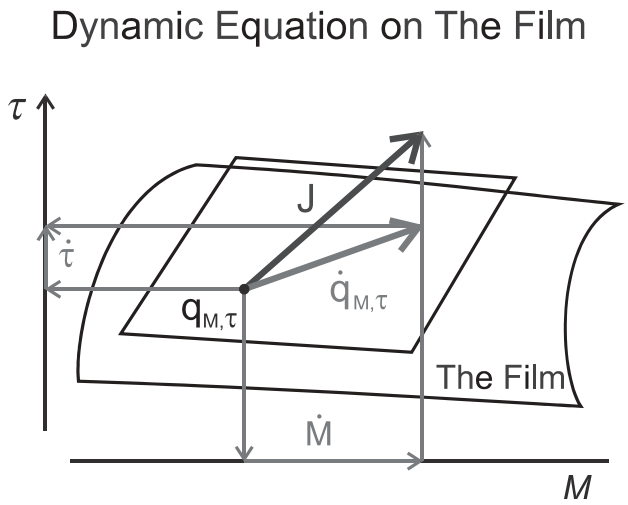

Fig. 12.4. Dynamics on the film: $\dot{M} = mJ(q_{M,\tau})$, $\dot{\tau} = -\frac{D_f S|_{q_{M,\tau}} D_M q_{M,\tau} \dot{M}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}}$

$$\frac{\mathrm{d}\tau}{\mathrm{d}t} = \frac{\dot{S} - D_f S|_{q_{M,\tau}} D_M q_{M,\tau} \dot{M}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} = -\frac{D_f S|_{q_{M,\tau}} D_M q_{M,\tau} \dot{M}}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} \,, \quad (12.53)$$

where $\dot{M}$ is defined in accordance with (12.51). The numerator in (12.53) has a simple meaning: it is the rate of the entropy production by dynamic equations (12.51) when τ is constant (for frozen τ). Expression (12.53) can be obtained from the condition of the constant entropy for the motion on the film in accordance with (12.51,12.53). Equations (12.51,12.53) describe dynamics on the film (Fig. 12.4).

The system of equations (12.51,12.53) has a very simple sense:

$$\frac{\mathrm{d}M}{\mathrm{d}t} = mJ(q_{M,\tau}); \; \frac{\mathrm{d}S}{\mathrm{d}t} = 0 \,. \quad (12.54)$$

It is just the standard moment equation supplied by the equation of entropy production (in this case by the equation of entropy conservation).

It should be emphasized that the projector with the property **A** is not unique, and here we made the simplest choice.

Let us further assume that condition (12.27) is satisfied:

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

In expressions (12.48,12.51,12.53) the denominator, $D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}$, is present. For $\tau \to 0$ this expression vanishes:

$$\begin{aligned} &D_\tau q_{M,\tau}|_{\tau=0} = \Delta_{f^*_M} \,, \\ &D_f S|_{f=f^*_M} x = 0, \text{ for } x \in \ker m \,, \end{aligned} \quad (12.55)$$

$m(\Delta_{f_M^*}) = 0$, therefore $D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau} \to 0$ for $\tau \to 0$. For $\tau \to 0$ indeterminate forms $0/0$ appear in expressions (12.48–12.50,12.52,12.53). Let us resolve the indeterminate forms and calculate the corresponding limits.

Two indeterminate forms are present:

$$N_1 = \frac{(D_\tau q_{M,\tau})(D_f S|_{q_{M,\tau}}) D_M q_{M,\tau} m J}{D_f S|_{q_{M,\tau}} D_\tau q_{M,\tau}} \tag{12.56}$$

and the right hand side of equation (12.53), $N_2(\tau)$. Let us evaluate the form (12.56). We obtain:

$$\lim_{\tau\to 0} N_1(\tau) = \frac{\Delta_{f_M^*} D_f S|_{f_M^*} \pi_{f_M^*} D_f J(f)|_{f_M^*}}{\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}} \tag{12.57}$$

using identity (12.33), similar to (12.24), we obtain:

$$\lim_{\tau\to 0} N_2(\tau) = -\frac{\Delta_{f_M^*} \langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}}{\langle \Delta_{f_M^*} | \Delta_{f_M^*} \rangle_{f_M^*}} = -\Delta_{f_M^*} \, .$$

Therefore, for $\tau \to 0$

$$\begin{aligned} \pi_{\mathrm{A}}|_{q_{M,\tau}} J(q_{M,\tau}) &\to D_M f_M^* m J(f_M^*) + \Delta_{f_M^*} \\ &= \pi_{f_M^*} J(f_M^*) + (1 - \pi_{f_M^*}) J(f_M^*) = J(f_M^*) \, . \end{aligned} \tag{12.58}$$

Similarly, after simple calculations we obtain that:

$$\frac{\mathrm{d}\tau}{\mathrm{d}t} \to 1, \ \text{ for } \ \tau \to 0 \, . \tag{12.59}$$

The fact that for $\tau \to 0$ the action of the projector π_{A} on J becomes trivial, $\pi_{\mathrm{A}} J = J$, can be obtained (without calculations) from the construction of $q_{M,\tau}$ in the vicinity of zero. We have chosen this dependence in such a way that $J(q_{M,\tau})$ becomes transverse to the film for $\tau \to 0$. This follows from the condition (12.27). Let us emphasize, however, that derivation of the formulas (12.50–12.53) themselves was not based on (12.27), and they are applicable to any ansatz, $q_{M,\tau}$, not necessarily with the right behavior near the quasiequilibrium (if one needs such an ansatz for anything).

12.5.3 Fixed Points of the Film Equation

What features can one expect from the dynamics of the film according to equation (12.44)? A naive expectation that $q_{M,\tau}$ tends to a stable fixed point of equation (12.44) leads to somewhat strange consequences. Fixed point for equation (12.44) is the invariant manifold q_M. On this manifold,

$$J(q_M) = D_M q_M m J(q_M) \, , \tag{12.60}$$

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

Indeed, let us consider the set of points $M_{-\tau}$ (12.25) for a given M. There exists the limit,

$$\lim_{\tau\to\infty} T_\tau(f^*_{M_{-\tau}}) = q_M \ ,$$

The flow T_τ conserves the entropy, hence, the difference of the values of the quasiequilibrium entropy, $S(M) - S(M_{-\tau}) = \Delta S_\tau$, 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 $S(M) - S(M_1) > \Delta S_\infty(M)$. Thus, possible fixed points of the equation (12.44), regardless of their obvious interest, likely demonstrate some exotic possibilities.

12.5.4 The Failure of the Simplest Galerkin-Type Approximations for Conservative Systems

Usually, the simplest approach to the problem is the projection approximation: one considers a projection of the vector field, $J(f)$, onto the manifold in question and investigates the obtained equations of motion. However, it is not difficult to see sure that such an approach is unfruitful in the present case of conservative systems. If the orthogonal with respect the entropic scalar product projection is taken, then only the quasiequilibrium approximations with increased number of moments could be obtained.

For the dissipative systems, in contrast, such a projection approximations leads to quite satisfactory results. For example, if for the Boltzmann equation and the hydrodynamic moments the approximate invariant manifold is to be searched in the form $f^\#_M = f^*_M + a(M)\Delta_{f^*_M}$, where f^*_M is local Maxwellian, then we obtain the Navier–Stokes equations with the viscosity and heat conductivity calculated within the first Sonine polynomials approximation. Using another scalar product simply leads to unphysical results.

In order to highlight the pitfall in the conservative case, let us give an example with a linear field, $J(f) = Af$, and a quadratic entropy, $S(f) = (1/2)\langle f|f\rangle$. The conservativity of J means that for each f it holds

$$\langle f|Af\rangle = 0 \ . \tag{12.61}$$

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. For the defect of invariance $\Delta_{f^*_M}$ we obtain:

$$\Delta_{f^*_M} = (A - \pi A)f^*_M \ . \tag{12.62}$$

Under the simplest projection approximation we write

$$q_{M,\tau} = f^*_M + a(M,\tau)\Delta_{f^*_M} \ . \tag{12.63}$$

Projector on $\Delta_{f^*_M}$ is

$$\frac{|\Delta_{f^*_M}\rangle\langle\Delta_{f^*_M}|}{\langle\Delta_{f^*_M}|\Delta_{f^*_M}\rangle} \ . \tag{12.64}$$

Thus, we pass from the equation of motion of the film (12.44) to the Galerkin-type approximation for $a(M,\tau)$.

$$\begin{aligned}\dot{a} = 1 + a\frac{\langle\Delta_{f^*_M}|A\Delta_{f^*_M}\rangle}{\langle\Delta_{f^*_M}|\Delta_{f^*_M}\rangle} - a\frac{\langle\Delta_{f^*_M}|A\pi A\Delta_{f^*_M}\rangle}{\langle\Delta_{f^*_M}|\Delta_{f^*_M}\rangle} \\ -a^2\frac{\langle\Delta_{f^*_M}|A\pi A\Delta_{f^*_M}\rangle}{\langle\Delta_{f^*_M}|\Delta_{f^*_M}\rangle} - (D_M a)m\frac{Af^*_M + aA\Delta_{f^*_M}}{\langle\Delta_{f^*_M}|\Delta_{f^*_M}\rangle} \ .\end{aligned} \tag{12.65}$$

One can try to find 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

$$\langle\Delta_{f^*_M}|A\Delta_{f^*_M}\rangle = 0 \ , \tag{12.66}$$

$$\langle\Delta_{f^*_M}|A\pi A\Delta_{f^*_M}\rangle = -\langle\pi A\Delta_{f^*_M}|(\pi A^2 - (\pi A)^2)\Delta_{f^*_M}\rangle \ . \tag{12.67}$$

On the other hand, for the dissipative systems the form (12.66) is negatively definite, and it is this form that determines the Navier–Stokes equations (in the first Sonine's polynomials approximation) in the derivation of these equations from the Boltzmann equation. For the conservative equations this main part vanishes, while the second term in equation (12.65), generally speaking, is sign-indefinite.

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

$$\dot{a} = 1 + a\frac{\langle\Delta_{f^*_M}|A\Delta_{f^*_M}\rangle}{\langle\Delta_{f^*_M}|\Delta_{f^*_M}\rangle} \ . \tag{12.68}$$

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

$$a = -\frac{\langle\Delta_{f^*_M}|\Delta_{f^*_M}\rangle}{\langle\Delta_{f^*_M}|A\Delta_{f^*_M}\rangle} > 0 \ . \tag{12.69}$$

This fixed point is "the leading order term" in the solution of the invariance equation, $\dot{a} = 0$ (12.65).

However, for the conservative systems $\dot{a} = 1$. This result was expected from the entropy production formula (12.24), and

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

12.5.5 Second Order Kepler Models of the Film

In the problems of the dissipative kinetics (namely, in the problem of the initial layer for the Boltzmann equation) it was found efficient 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 the entropy increases. Further, the procedure was repeated from the obtained point (for details see [26, 27] and Sect. 9.3).

Unfortunately, in the problem of the initial layer for the conservative systems there are no termination points during the motion along a straight line (more precisely, the beginning of the motion itself can be considered as a termination point because under the linear approximation the relation (12.66) 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 should be arcs of ellipses (in linear space), or the constant entropy lines, rather than straight lines. In the film problem the simplest "good" model is a general conic section. A simple example: $J(f) = Af$, A is generator of rotation around the axis with the direction $\boldsymbol{r} = \boldsymbol{e}_x + \alpha\boldsymbol{e}_y$, $M = x$, the film is the lateral surface of the cone, obtained by rotation of the quasiequilibrium manifold, the axis $\{x\boldsymbol{e}_x\}$, around the axis $\{\varphi\boldsymbol{r}\}$. For $\alpha < 1$ the curve $q_{M,\tau}$ is an ellipse, for $\alpha > 1$ it is a hyperbole, for $\alpha = 1$ it is a parabola.

The curve $q_{M,\tau}$ is an intersection of two manifolds: one of them is the result of the motion of the quasiequilibrium manifold along the vector field $J(f)$, other 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 $e^{A\tau}$, the unknown curve is the section:

$$(f_M^* + \ker m) \bigcap e^{AR_+} (\ker m)^\perp \,, \tag{12.70}$$

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

Thus, 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-order 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. 12.5):

$$r = q_0 - \ddot{q}\frac{\langle \dot{q}_\perp | \dot{q}_\perp \rangle}{\langle \dddot{q} \, | \dot{q}_\perp \rangle} \,, \tag{12.71}$$

where q_0 is the initial point where all the derivatives are taken. The force is:

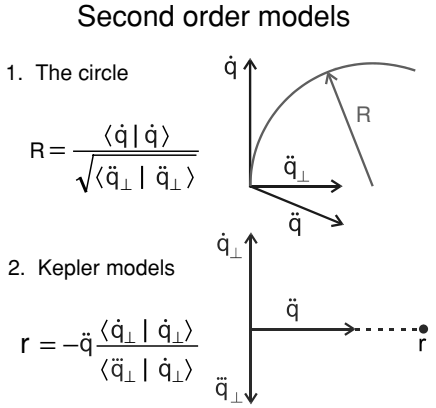

Fig. 12.5. The definition of the second-order models

$$F = \alpha \frac{r-q}{\langle r-q|r-q\rangle^{3/2}} \; ;$$
$$\alpha^2 = \langle \ddot{q}|\ddot{q}\rangle \langle r-q|r-q\rangle^2 = \langle \ddot{q}|\dot{q}\rangle^3 \frac{\langle \ddot{q}_\perp|\ddot{q}_\perp\rangle^4}{\langle \dddot{q}\ |\dot{q}_\perp\rangle^4} \; ; \tag{12.72}$$

$$\begin{array}{lll} \alpha > 0 & \text{(attraction)} & \text{if} \quad \langle \dddot{q}\ |\dot{q}_\perp\rangle < 0 \; ; \\ \alpha < 0 & \text{(repulsion)} & \text{if} \quad \langle \dddot{q}\ |\dot{q}_\perp\rangle > 0 \; . \end{array} \tag{12.73}$$

It is necessary to point out 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 model motion finite? The answer is simple in terms of the Kepler problem [182]:

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

or

$$\frac{\|\dot{q}\|^2 |\langle \dot{q}_\perp|\ \dddot{q}\rangle|}{2\|\dot{q}_\perp\|^2 \|\ddot{q}\|^2} < 1 \; . \tag{12.74}$$

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

12.5.6 The Finite Models: Termination at the Horizon Points

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

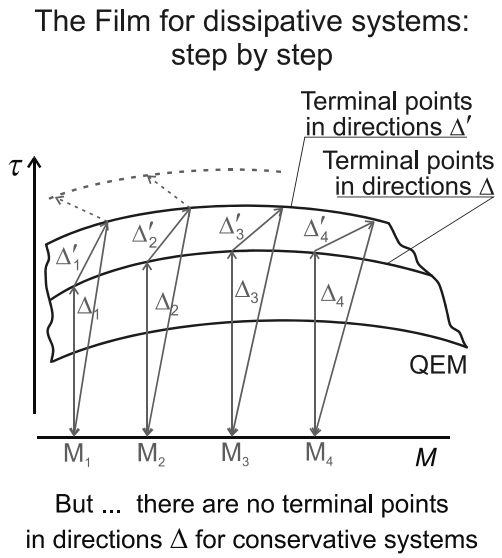

Fig. 12.6. The stepwise construction of the film for dissipative system. First-order models: The motion along the defect of invariance

If the motion $q_{M,\tau}$ is taken along the straight line (dissipative systems), the direction of the step is $\dot{q}_{M,\tau_0}$ (let us remind that $\dot{q}_{M,\tau_0}$ is the defect of the invariance of the manifold $q_M = q_{M,\tau_0}$ at fixed $\tau = \tau_0$), and the size of the step should be adjusted in such a way as to reach a stable point, that is, the point where the direction $\dot{q}_{M,\tau}$ becomes orthogonal to the initial one, $\dot{q}_{M,\tau_0}$ (Fig. 12.6). The current direction of $\dot{q}_{M,\tau}$ is calculated with the help of (12.44), where the projector is frozen ($D_M q_{M,\tau_0} m$ 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 termination of motion. 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 the motion becomes orthogonal to the initial one.

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 the condition for the transition to the next model is

$$\left\langle \dot{q}_{M,\tau_0} \middle| \frac{\mathrm{d}\tilde{q}_{M,\tau_0+\theta}}{\mathrm{d}\theta} \right\rangle = 0 \tag{12.75}$$

(in the entropic scalar product).

Let us call *the horizon points* such points, $q_{M,\tau_0+\theta_0}$, where the scalar product (12.75) for the first time becomes equal to 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

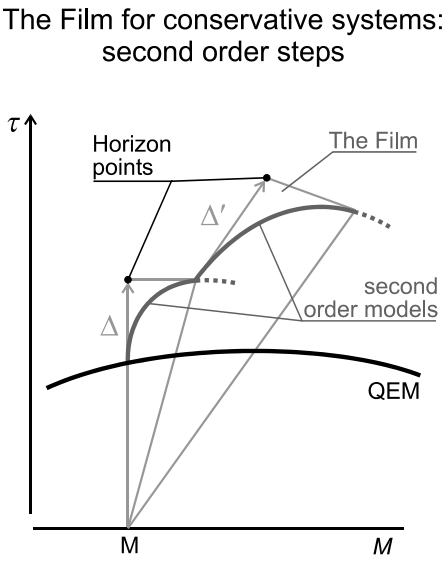

Fig. 12.7. The stepwise construction of the film for conservative system. Finite second-order models: The motion starts in the direction of the defect of invariance, and stops when the direction of motion becomes orthogonal to the defect of invariance

horizon", and its orthogonal projection on the line parallel to $\dot{q}_{M,\tau_0}$ starts to move back passing the same points for the second time.

The convention about the change of the model in the horizon points seems quite natural. The following sequence of calculations becomes self-explaining (Fig. 12.7):

1. we seed the film with the quasiequilibrium manifold, $q_{M,0} = f^*_M$;
2. we calculate $\dot{q}_{M,0}$, $\ddot{q}_{M,0}$, ... in accordance with equation (12.44);
3. we construct the (finite) second order models, $q_{M,\theta}$;
4. we find the horizon points, $q_{M,\theta_0(M)}$, from (12.75);
5. then we take the manifold of the horizon points as a new initial manifold, and dio the next iteration.

At a 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 thus it 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 model curve does not coincide with the proper time, τ. More precisely, it coincides only within the second order. However, now global, not local approximation are constructed. Therefore, global corrections to the time, or ways to circumvent these corrections, are required.

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

12.5.7 The Transversal Restart Lemma

Let $q_{M,\tau}$ ($\tau \in [0;+\infty)$) be the solution to (12.44) under initial condition (12.45) (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 $0 \le \theta(M) \le t < \infty$.

Let *the transversality condition* be satisfied. Namely, for every bounded domain that does not include equilibrium there exists $\varepsilon > 0$ such that in this patch

$$\frac{\|J(q_{M,\theta(M)}) - D_M q_{M,\theta(M)} m J(q_{M,\theta(M)})\|}{\|J(q_{M,\theta(M)})\|} > \varepsilon \tag{12.76}$$

in an appropriate norm. Let $\tilde{q}_{M,\tau}$ be the solution to (12.44) under the initial condition $\tilde{q}_{M,0} = q_{M,\theta(M)}$. Then the following *transverse restart lemma* is valid:

$$q_{M,[0;+\infty)} = q_{M,[0;\theta(M)]} \bigcup \tilde{q}_{M,[0;+\infty)} \,. \tag{12.77}$$

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

The transversality condition (12.76) can be understood as a condition of an "uniform noninvariance". As we already know, fixed points of the film equations are irrelevant.

The transversal restart lemma is the statement about the correctness of the film. One way to derive the film is to seed it at the quasiequilibrium edge and to evolve in τ to $+\infty$ along the film equation (12.44). Another way is to evolve it to some transverse section, not obligatory uniformly in time, and then continue growing the film from this new edge. The result will be the same.

In order to "prove"[4] this lemma, we notice that it is equivalent to the following statement. For every $\widetilde{M}$ the segment of the trajectory, $T_{\widetilde{\tau}} f^*_{\widetilde{M}}$ ($\widetilde{\tau} \in [0;t]$), 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 $\widetilde{M}$ and $\widetilde{\tau}$: $q = T_{\widetilde{\tau}} f^*_{\widetilde{M}}$. In these coordinates the transversality condition excludes folds on $q_{M,\theta(M)}$.

In order to demonstrate the existence of the crossing point, q^*, of the segment $T_{\widetilde{\tau}} f^*_{\widetilde{M}}$ ($\widetilde{\tau} \in [0;t]$) with the section manifold $q_{M,\theta(M)}$, we define in the neighborhood of the point $f^*_{\widetilde{M}}$ on the quasiequilibrium manifold the mapping into the neighborhood of this section point. Image of the point $f^*_{\widetilde{M}}$ is section of the trajectory $T_{\widetilde{\tau}} f^*_{\widetilde{M}}$ ($\widetilde{\tau} \in [0;t]$) with the manifold $q_{M,\theta(M)}$ in the neighborhood of q^*. Due to the transversality condition, it performs an isomorphism

[4] Let us remind that within the degree of generality used here there are no proofs to the theorems of existence and uniqueness.

of the neighborhoods. Therefore, the set of $\widetilde{M}$ 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.

12.5.8 The Time Replacement, and the Invariance of the Projector

Let the film of nonequilibrium states be constructed as $\tilde{q}_{M,\theta}$, where relation between θ and τ is implicit; $\tau = \tau(M,\theta)$, $\theta = \theta(M,\tau)$. In order to determine these functions one needs to solve equation obtained from (12.44) with substitution $q_{M,\tau} = \tilde{q}_{M,\theta(M,\tau)}$ (and projection, because $\tilde{q}$ is only an approximation). The calculation itself presents no difficulties. However, is it possible to avoid the inversion in replacing of time for a derivation of the kinetic equations? In another words, could we use the constructed geometrical object, the film, without an exact reconstruction of the time, τ, on it?

For a positive answer to this question it is sufficient to demonstrate that the equations of motion, constructed with the projector (12.51–12.53), describe the same motion on the film after the time replacement.

This property of the π_{A} is evident: while deriving equations (12.51–12.53), we did not use that τ is the "true time" from the equation (12.44), and made the local replacement of variables, passing from ΔM, $\Delta\tau$ to ΔM, ΔS.

Thus, the projector π_{A} is invariant with respect to the time replacement, and, when constructing equations of motion, it is not necessary to restore the "true time".

Results of this and previous subsections allow to apply the sequence of operations suggested in Subsect. 12.5.6.

12.5.9 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 $q_{M,\tau}$ (not just for its initial segment, as it was for the finite models). Naturally, there arises a problem of correction to this approximation, and, in general, construction of a step-by-step computational procedure.

The projector π_{A} on the film is defined (12.50). Correspondingly, the invariance defect of the film is determined too

$$\begin{aligned}\Delta q_{M,\theta} &= (1-\pi_{\mathrm{A}}|_{q_{M,\theta}})J(q_{M,\theta}) \\ &= \left[1-\left(1-\frac{D_\theta q_{M,\theta} D_f S|_{q_{M,\theta}}}{D_f S|_{q_{M,\theta}} D_\theta q_{M,\theta}}\right) D_M q_{M,\theta} m\right] J(q_{M,\theta}) \quad (12.78)\end{aligned}$$

It is easy to verify, that if $q_{M,\theta}$ is a solution to (12.44), then $\Delta q_{M,\theta} \equiv 0$.

Subsequently we calculate the corrections to $q_{M,\tau}$ using an iterative method for the manifold correction (see Chaps. 6 and 9).

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

12.5.10 The Film, and the Macroscopic Equations

Let the film of nonequilibrium states be constructed. What next? There are two routes.

1. Investigation of the conservative dynamics of "$N + 1$" variables, where "N" is moments for the moments M, and "+1" is for the coordinate τ on the film;
2. Derivation of the macroscopic equations for M.

Actually, the second route is more desirable, it leads to familiar classes of kinetic 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 essentially the same as suggested by us [29], [30–33] following Ehrenfests [15], and Zubarev [195]. That is,

– One chooses a time T.
– For arbitrary M_0 one solves the problem of the motion on the film (12.51), (12.53) under initial conditions $M(0) = M_0$, $\tau(0) = \tau_0$ on the segment $t \in [0; T]$. The solution is $M(t, M_0)$.
– For the mapping $M_0 \to M(T)$ the system $\mathrm{d}M/\mathrm{d}t = F(M)$ is constructed. It has the property that for its phase flow, $\theta_t(M)$, the identity

$$\theta_T(M_0) \equiv M(T, M_0) \tag{12.79}$$

is satisfied. This is the method of natural projector once again (see (12.22) and Chap. 11).

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

$$\dot{M} = \varepsilon P(M, \tau)\ ; \quad \dot{\tau} = Q(M, \tau) \tag{12.80}$$

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 [183]. 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,

$$M_1(t, M_0) = M_0 + \varepsilon t \left(\frac{1}{T} \int_0^T P(M_0, \tau_1(\theta, M_0))\, \mathrm{d}\theta \right) \tag{12.81}$$

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

$$M_1(T, M_0) = M_0 + \varepsilon \int_0^T P(M_0, \tau(\theta, M_0))\, \mathrm{d}\theta \,, \tag{12.82}$$

correspondingly.

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

$$F_1(M) = \frac{1}{T}(\theta_T(M) - M) \,. \tag{12.83}$$

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

$$\dot{M} = F_1(M) = \frac{1}{T} \int_0^T m(J(q_{M,\tau(t,M)}))\, \mathrm{d}t \,, \tag{12.84}$$

where $\tau(t, M)$ is a solution to the equation (12.53) under fixed M (actually, $mJ(q_{M,\tau})$ should be substituted into (12.53) instead of $\dot{M}$).

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

In general, the sequence of the horizon points of the second order finite Kepler models and corresponding $\dot{q}_i$, $\ddot{q}_i$ determines the macroscopic kinetic equations. Only the values of the coefficients remain unknown. Let us start from linearized in layers system (12.17)

$$\dot{f} = J(f^*_{m(f)}) + L_{m(f)}(f - f^*_{m(f)}) \,, \tag{12.85}$$

where linear operator L_M parameterized by macroscopic variables $M = m(f)$. For the system (12.85) the second order finite Kepler models give the macroscopic equation

$$\dot{M} = m(J(f^*_M)) + \sum_i (\alpha_i m(L_M(\dot{q}_i)) + \beta_i m(L_M(\ddot{q}_i))) \,, \tag{12.86}$$

with $\alpha_i,\ \beta_i > 0$.

The final comment on the positivity of the "kinetic coefficients" α_i and β_i is important, and cannot be easily verified every time. However, in the case under consideration it is so by the following 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

$$q - q_0 = \alpha\dot{q} + \beta\ddot{q} \,; \quad \alpha, \beta > 0 \,, \tag{12.87}$$

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

This theorem follows from elementary theorems about analytical geometry of second-order curves: Let a chord in an ellipse is passing through a focus, and $l_{1,2}$ are the tangents to the ellipse at the ends of this chord. Then the angle between $l_{1,2}$ that is based on the chord is acute. The starting point q_0 is one of the ends of the chord, the vector of acceleration $\ddot{q}$ is the direction of the chord (from q_0 to the focus), the velocity vector $\dot{q}$ is the tangent direction at the point q_0. Following these elementary facts, the horizon point belongs to the arc on which the angle between $l_{1,2}$ is based, hence the positivity condition (12.87) holds.

For the model motion on the entropic circle, strictly speaking, this is not always the case. 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 (12.86) as compared to the short-memory approximation: (i) alteration of the kinetic constants (terms are not orthogonal to each other, therefore, new terms contribute to the previous processes), (ii) birth of new processes.

Motion on an infinite film can lead to stabilization of kinetic coefficients as the 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 (12.51), (12.53). For every kinetic coefficient, k, expression $\mathrm{d}k/\mathrm{d}t = \psi_k(\tau, M) = \varphi_k(k, M)$ is calculated in accordance with (12.51), (12.53). Substitution of variables $(\tau, M) \to (k, M)$ 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:

$$\dot{M} = m(J(f^*_M)) + \sum_j k_j F_j(M)\ ; \quad \dot{k}_j = \varphi_j(k_j, M)\ . \tag{12.88}$$

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

12.5.11 New in the Separation of the Relaxation Times

Originally, there are no dissipative possesses 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 the emergence of the dissipation. It can be described (in the first non-vanishing approximation) by equation (12.23). It is of special

importance that there is yet no separation into dissipation processes with various relaxation times and kinetic coefficients on that stage. This separation occurs at further stages: Various processes appear, their kinetic coefficients are determined (see, for example, (12.86)) (or, in certain cases, the dynamics of the kinetic coefficients is determined).

Generalizing, we can distinguish three stages:

1. birth of dissipation;
2. branching of dissipation: appearance of various processes;
3. macroscopic relaxation.

It is important to notice in this scheme 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.

12.6 The Main Results

In order to solve the problem of irreversibility we have introduced the notion of the *macroscopically definable ensembles*. They result from the evolution of ensembles out of the quasiequilibrium initial conditions *under macroscopic control*.

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 casts 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? These those parameters are fixed until "all the rest" come into equilibrium. The quasiequilibrium states are obtained in such a way.

A further development of this direction should lead to investigation of the macro-dynamics 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 method of the natural projector allows us to construct an approximate dynamics of macro-variables. When the time of projection, τ, tends to infinity, these equations should tend to the actual equations of macrodynamics, if the latter exist. This hypothesis about their existence in the thermodynamic limit (first, the number of particles $N \to \infty$, and after that, the time of projection $\tau \to \infty$) is the basis of Zubarev's nonequlibrium statistical operator approach [195].

Here, we need to make a remark. Frequently, physicists use mathematical objects whose existence and uniqueness are not proven: solutions to the

equations of hydro- and gaso-dynamics, kinetic equations etc. Often, the failure to prove theorems of existence and uniqueness is viewed as a lack of an adequate mathematical statement of the problem (definition of spaces, etc.). For all this, it is assumed that essential obstacles either are absent, or can be sorted out separately, independently of the theorem proof in physically trivial situations. Existence (or non-existence) of the macroscopic dynamics is a problem of a different kind. The cases of non-existence can be found as frequently as the physically expected existence.

The notion of the invariant film of non-equilibrium states, and the method of its approximate construction allows us to solve the problem of macro-kinetics even when there are no autonomous equations of macro-kinetics. The existence of the film seems to be one of the physically trivial problems of existence and uniqueness of solutions. Further computations will show how productive the methods of film construction are.

The formula for *entropy production*,

$$\sigma \sim \frac{\text{defect of invariance}}{\text{curvature}}$$

clarifies the geometrical sense of the dissipation. Here, "defect of invariance" is the defect of invariance of the quasiequilibrium manifold, and "curvature" is the curvature of the film of nonequilibrium states in the direction of the defect of invariance of the quasiequilibrium manifold.

At least one essential problem remains unsolved. This is the *problem of indivisible events*: For a macroscopically small time, a small microscopic subsystems can go through "its 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 the macroscopic time *cannot* be written in the form

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

The evolution of the microscopic subsystems in a macroscopically small time Δt should be described as an *"ensemble of indivisible events"*. An excellent hint is given by the Boltzmann equation with its indivisible collisions, another good hint gives the chemical kinetics with indivisible events of elementary reactions. The useful formalism for a description such ensembles of indivisible events is well developed. It is the "quasi-chemical" representation (see Chap. 7). But the way from general system to such ensembles remains unclear and presents *the challenge* to the future works (see, however, section "Neurons and particles" in the paper [10]).

There is an important link between the theory of invariant film and the Hilbert method in the theory of the Boltzmann equation (see Chap. 2). The Hilbert method constructs the invariant film for the Boltzmann equation, and the initial manifold for this film is the local Maxwellian manifold (the local equilibrium manifold). The significant novelty of the theory of the invariant

film of non-equilibrium states is the splitting of the problem in two parts: the geometrical part (construction of the film) and the dynamical part (dynamics on the film). The first (geometrical) part is solved here by the method of "large stepping" instead of a Taylor series expansion as in the original Hilbert method.