Basic Types of Coarse-Graining

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Summary. We consider two basic types of coarse-graining: the Ehrenfest's coarse-graining and its extension to a general principle of non-equilibrium thermodynamics, and the coarse-graining based on uncertainty of dynamical models and ε-motions (orbits). Non-technical discussion of basic notions and main coarse-graining theorems are presented: the theorem about entropy overproduction for the Ehrenfest's coarse-graining and its generalizations, both for conservative and for dissipative systems, and the theorems about stable properties and the Smale order for ε-motions of general dynamical systems including structurally unstable systems. A brief discussion of two other types, coarse-graining by rounding and by small noise, is also presented. Computational kinetic models of macroscopic dynamics are considered. We construct a theoretical basis for these kinetic models using generalizations of the Ehrenfest's coarse-graining.

1 Introduction

Almost a century ago Paul and Tanya Ehrenfest in their paper for scientific Encyclopedia [1] introduced a special operation, the coarse-graining. This operation transforms a probability density in phase space into a "coarse-grained" density, that is a piece-wise constant function, a result of density averaging in cells. The size of cells is assumed to be small, but finite, and does not tend to zero. The coarse-graining models uncontrollable impact of surrounding (of a thermostat, for example) onto ensemble of mechanical systems.

To understand reasons for introduction of this new notion, let us take a phase drop, that is, an ensemble of mechanical systems with constant probability density localized in a small domain of phase space. Let us watch evolution of this drop in time according to the Liouville equation. After a long time, the shape of the drop may be very complicated, but the density value remains the same, and this drop remains "oil in water." The ensemble can tend to the equilibrium in the weak sense only: average value of any continuous function tends to its equilibrium value, but the entropy of the distribution remains constant. Nevertheless, if we divide the phase space into cells and supplement

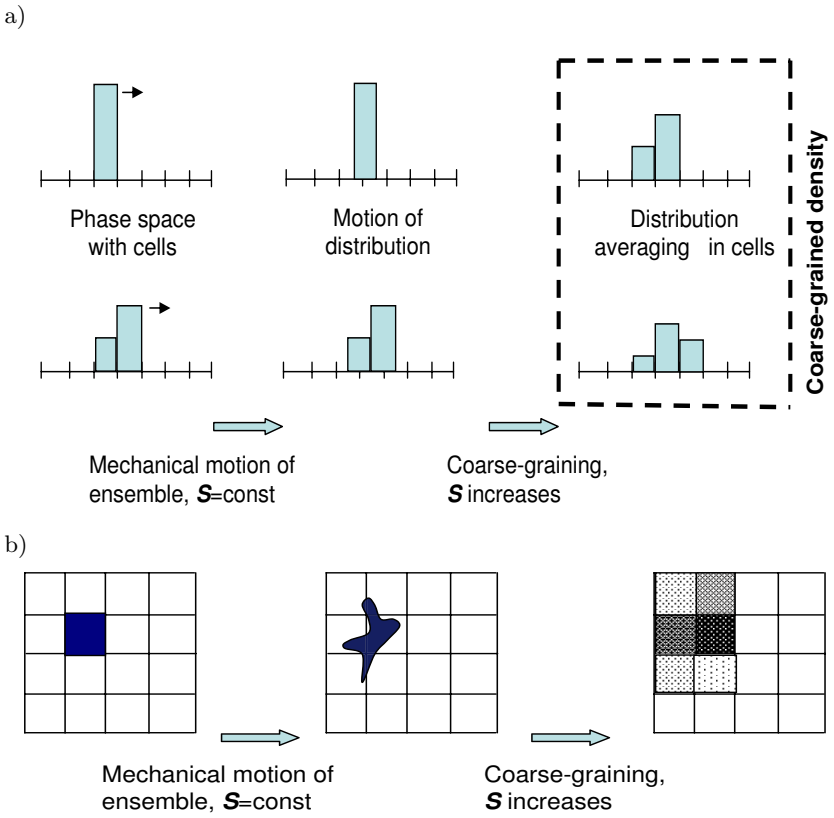

Fig. 1. The Ehrenfest's coarse-graining: two "motion – coarse-graining" cycles in 1D (a, values of probability density are presented by the height of the columns) and one such cycle in 2D (b, values of probability density are presented by hatching density).

the mechanical motion by the periodical averaging in cells (this is the Ehrenfest's idea of coarse-graining), then the entropy increases, and the distribution density tends uniformly to the equilibrium. This periodical coarse-graining is illustrated by Fig. 1 for one-dimensional (1D)[1] and two-dimensional (2D) phase spaces.

Recently, we can find the idea of coarse-graining everywhere in statistical physics (both equilibrium and non-equilibrium). For example, it is the central idea of the Kadanoff transformation, and can be considered as a background of the Wilson renormalization group [6] and modern renormalisation

[1] Of course, there is no mechanical system with one-dimensional phase space, but dynamics with conservation of volume is possible in 1D case too: it is a motion with constant velocity.

group approach to dissipative systems [7, 8]. [2] It gave a simplest realization of the projection operators technique [2] long before this technic was developed. In the method of invariant manifold [3, 4] the generalized Ehrenfest's coarse-graining allows to find slow dynamics without a slow manifold construction. It is also present in the background of the so-called equation-free methods [9]. Applications of the Ehrenfest's coarse-graining outside statistical physics include simple, but effective filtering [10]. The Gaussian filtering of hydrodynamic equations that leads to the Smagorinsky equations [13] is, in its essence, again a version of the Ehrenfest's coarse-graining. In the first part of this paper we elaborate in details the Ehrenfest's coarse-graining for dynamical systems.

The central idea of the Ehrenfest's coarse-graining remains the same in most generalizations: we combine the genuine motion with the periodic *partial equlibration*. The result is the Ehrenfest's chain. After that, we can find the macroscopic equation that does not depend on an initial distribution and describes the Ehrenfest's chains as results of continuous autonomous motion [5, 11]. Alternatively, we can just create a computational procedure without explicit equations [9]. In the sense of entropy production, the resulting macroscopic motion is "more dissipative" than initial (microscopic) one. It is the theorem about entropy overproduction. In its general form it was proven in [12].

Kinetic models of fluid dynamics become very popular during the last decade. Usual way of model simplification leads from kinetics to fluid dynamics, it is a sort of dimension reduction. But kinetic models go back, and it is the simplification also. Some of kinetic equations are very simple and even exactly solvable. The simplest and most popular example is the free flight kinetics, $\partial f(\boldsymbol{x}, \boldsymbol{v}, t)/\partial t = -\sum_i v_i \partial f(\boldsymbol{x}, \boldsymbol{v}, t)/\partial x_i$, where $f(\boldsymbol{x}, \boldsymbol{v}, t)$ is one-particle distribution function, $\boldsymbol{x}$ is the space vector, $\boldsymbol{v}$ is velocity. We can "lift" a continuum equation to kinetic model, and than approximate the solution by a chain, each link of which is a kinetic curve with a jump from the end of this curve to the beginning of the next link. In this paper, we describe how to construct these curves, chains, links and jumps on the base of Ehrenfest's idea. Sometimes simplification can be reached by dimension increase.

In practice, kinetic models in the form of lattice Boltzmann models are in use [14]. The Ehrenfest's coarse-graining provides theoretical basis for kinetic models. First of all, it is possible to replace projecting (partial equilibration) by involution (i.e. reflection with respect to the partial equilibrium). This *entropic involution* was developed for the lattice Boltzmann methods in [77]. In the original Ehrenfest's chains, "motion–partial equilibration–motion–...," dissipation is coupled with time step, but the chains "motion–involution–motion–..." are conservative. The family of chains between conservative (with entropic involution) and maximally dissipative (with projection) ones give us a

[2] See also the paper of A. Degenhard and J. Javier Rodriguez-Laguna in this volume.

possibility to model hydrodynamic systems with various dissipation (viscosity) coefficients that are decoupled with time steps.

Several other notions of coarse-graining were introduced and studied for dynamical systems during last hundred years. In this paper, we shall consider one of them, the coarse-graining by ε-motions (ε-orbits, or pseudo orbits) and briefly mention two other types: coarse-graining by rounding and by small random noise.

ε-motions describe dynamics of models with uncertainty. We never know our models exactly, we never deal with isolated systems, and the surrounding always uncontrollably affect dynamics of the system. This dynamics can be presented as a usual phase flow supplemented by a periodical *ε-fattening*: after time τ, we add a ε-ball to each point, hence, points are transformed into sets. This periodical fattening expands all attractors: for the system with fattening they are larger than for original dynamics.

Interest to the dynamics of ε-motions was stimulated by the famous work of S. Smale [16]. This paper destroyed many naive dreams and expectations. For generic 2D system the phase portrait is the structure of attractors (sinks), repellers (sources), and saddles. For generic 2D systems all these attractors are either fixed point or closed orbits. Generic 2D systems are structurally stable. It means that they do not change qualitatively after small perturbations. Our dream was to find a similar stable structure in generic systems for higher dimensions, but S. Smale showed it is impossible: Structurally stable systems are not dense! Unfortunately, in higher dimensions there are regions of dynamical systems that can change qualitatively under arbitrary small perturbations.

One of the reasons to study ε-motions (flow with fattening) and systems with sustained perturbations was the hope that even small errors coarsen the picture and can wipe some of the thin peculiarities off. And this hope was realistic, at least, partially [17–19]. The thin peculiarities that are responsible for appearance of regions of structurally unstable systems vanish after the coarse-graining via arbitrary small periodical fattening. All the models have some uncertainty, hence, the features of dynamics that are unstable under arbitrary small coarse-graining are unobservable.

Rounding is a sort of coarse-graining that appears automatically in computer simulations. It is very natural that in era of intensive computer simulation of complex dynamics the coarse-graining by rounding attracted special attention [20–26]. According to a very idealized popular dynamic model, rounding might be represented as restriction of shift in given time τ onto ε-net in phase space. Of courses, the restriction includes some perturbation of dynamics (Fig. 2). The formal definition of rounding action includes a tiling: around any point of the ε-net there is a cell, these cells form a tiling of the phase space, and rounding maps a cell into corresponding point of the ε-net. These cells have equal volumes if there are no special reasons to make their volumes different. If this volume is dynamically invariant then, for sufficiently large time of motion between rounding steps, all the mixing dynamical sys-

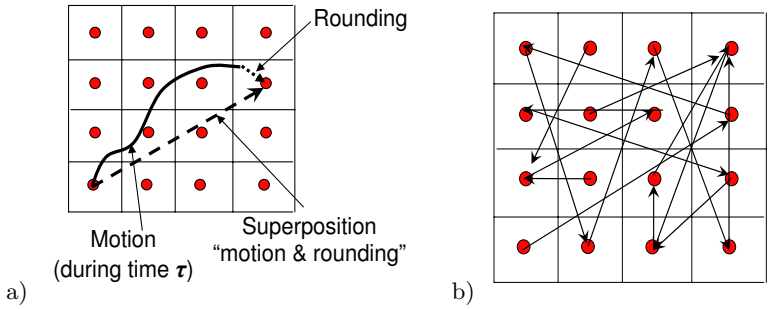

Fig. 2. Motion, rounding and "motion with rounding" for a dynamical system (a), and the universal result of motion with rounding: a random dynamical system (b).

tems with rounding can be described by an universal object. This is a random dynamical system, the random map of a finite set: any point of the ε-net can be the image of a given point with probability $1/m$ (where m is the number of points in the ε-net). The combinatorial theory of such *random graphs* is well–developed [27].

After rounding, some unexpected properties of dynamics appear. For example, even for transitive systems with strong mixing significant part of points of the ε-net becomes transient after rounding. Initially, attractor of such a continuous system is the whole phase space, but after rounding attractor of discrete dynamical system on the ε-net includes, roughly speaking, a half of its points (or, more precisely, the expectation of the number of transient points is $m(\mathrm{e}-1)/\mathrm{e}$, where m is number of points, $\mathrm{e}=2.7...$). In some circumstances, complicated dynamics has a tendency to collapse to trivial and degenerate behaviour as a result of discretizations [23]. For systems without conservation of volume, the number of periodic points after discretization is linked to the dimension of the attractor d. The simple estimates based on the random map analysis, and numerical experiments with chaotic attractors give $\sim \varepsilon^{-d}$ for the number of periodic points, and $\sim \varepsilon^{-d/2}$ for the scale of the expected period [22, 26]. The first of them is just the number of points in ε-net in d-dimensional compact, the second becomes clear after the following remark. Let us imagine a random walk in a finite set with m elements (a ε-net). When the length of the trajectory is of order $\sqrt{m}$ then the next step returns the point to the trajectory with probability $\sim 1/\sqrt{m}$, and a loop appears with expected period $\sim \sqrt{m}$ (a half of the trajectory length). After $\sim \sqrt{m}$ steps the probability of a loop appearance is near 1, hence, for the whole system the expected period is $\sim \sqrt{m} \sim \varepsilon^{-d/2}$.

It is easy to demonstrate the difference between coarse-graining by fattening and coarse-graining by rounding. Let us consider a trivial dynamics on a connected phase space: let the shift in time be identical transformation. For coarse-graining by fattening the ε-motion of any point tends to cover the

whole phase space for any positive ε and time $t \to \infty$: periodical ε-fattening with trivial dynamics transforms, after time $n\tau$, a point into the sum of n ε-balls. For coarse-graining by rounding this trivial dynamical system generates the same trivial dynamical system on ε-net: nothing moves.

Coarse-graining by small noise seems to be very natural. We add small random term to the right hand side of differential equations that describe dynamics. Instead of the Liouville equation for probability density the Fokker–Planck equation appears. There is no fundamental difference between various types of coarse graining, and the coarse-graining by ε-fattening includes major results about the coarse-graining by small noise that are insensitive to most details of noise distribution. But the knowledge of noise distribution gives us additional tools. The *action functional* is such a tool for the description of fluctuations [97]. Let $X^\varepsilon(t)$ be a random process "dynamics with ε-small fluctuation" on the time interval $[0,T]$. It is possible to introduce such a functional $\mathbf{S}[\varphi]$ on functions $x = \varphi(t)$ $(t \in [0,T])$ that for sufficiently small $\varepsilon, \delta > 0$

$$\mathbf{P}\{\|X^\varepsilon - \varphi\| < \delta\} \approx \exp(-\mathbf{S}[\varphi]/\varepsilon^2).$$

Action functional is constructed for various types of random perturbations [97]. Introduction to the general theory of random dynamical systems with invariant measure is presented in [98].

In following sections, we consider two types of coarse-graining: the Ehrenfest's coarse-graining and its extension to a general principle of non-equilibrium thermodynamics, and the coarse-graining based on the uncertainty of dynamical models and ε-motions.

2 The Ehrenfest's Coarse-graining

2.1 Kinetic equation and entropy

Entropy conservation in systems with conservation of phase volume

The Erenfest's coarse-graining was originally defined for conservative systems. Usually, Hamiltonian systems are considered as conservative ones, but in all constructions only one property of Hamiltonian systems is in use, namely, conservation of the phase volume $\mathrm{d}\Gamma$ (the Liouville theorem). Let X be phase space, $v(x)$ be a vector field, $\mathrm{d}\Gamma = \mathrm{d}^n x$ be the differential of phase volume. The flow,

$$\frac{\mathrm{d}x}{\mathrm{d}t} = v(x), \tag{1}$$

conserves the phase volume, if $\mathrm{div} v(x) = 0$. The continuity equation,

$$\frac{\partial f}{\partial t} = -\sum_i \frac{\partial (f v_i(x))}{\partial x_i}, \tag{2}$$

describes induced dynamics of probability density $f(x,t)$ on the phase space. For incompressible flow (conservation of volume), the continuity equation can be rewritten in the form

$$\frac{\partial f}{\partial t} = -\sum_i v_i(x)\frac{\partial f}{\partial x_i}. \tag{3}$$

It means that the probability density is constant along the flow: $f(t+\mathrm{d}t,x) = f(t,x-v(x)\mathrm{d}t)$. Hence, for any continuous function $h(f)$ the integral

$$H(f) = \int_X h(f(x))\,\mathrm{d}\Gamma(x) \tag{4}$$

does not change in time, provided the probability density satisfies the continuity equation (2) and the flow $v(x)$ conserves the phase volume. For $h(f) = -f\ln f$ integral (4) gives the classical Boltzmann–Gibbs–Shannon entropy functional:

$$S(f) = -\int_X f(x)\ln(f(x))\,\mathrm{d}\Gamma(x). \tag{5}$$

For flows with conservation of volume entropy is conserved: $\mathrm{d}S/\mathrm{d}t \equiv 0$.

Kullback entropy conservation in systems with regular invariant distribution

Let the phase volume be not invariant with respect to flow (1), but a regular invariant density $f^*(x)$ (equilibrium) exists:

$$\sum_i \frac{\partial(f^*(x)v_i(x))}{\partial x_i} = 0. \tag{6}$$

In this case, instead of invariant phase volume $\mathrm{d}\Gamma$, we have invariant volume $f^*(x)\,\mathrm{d}\Gamma$. We can use (6) instead of incompressibility condition and rewrite (2):

$$\frac{\partial(f(x,t)/f^*(x))}{\partial t} = -\sum_i v_i(x)\frac{\partial(f(x,t)/f^*(x))}{\partial x_i}. \tag{7}$$

The function $f(x,t)/f^*(x)$ is constant along the flow, the measure $f^*(x)\,\mathrm{d}\Gamma(x)$ is invariant, hence, for any continuous function $h(f)$ integral

$$H(f) = \int_X h(f(x,t)/f^*(x))f^*(x)\,\mathrm{d}\Gamma(x) \tag{8}$$

does not change in time, if the probability density satisfies the continuity equation. For $h(f) = -f\ln f$ integral (8) gives the Kullback entropy functional [32]:

$$S_K(f) = -\int_X f(x)\ln\left(\frac{f(x)}{f^*(x)}\right)\mathrm{d}\Gamma(x). \tag{9}$$

This situation does not differ significantly from the entropy conservation in systems with conservation of volume. It is just a kind of change of variables.

General entropy production formula

Let us consider the general case without assumptions about phase volume invariance and about existence of a regular invariant density (6). In this case, let a probability density $f(x,t)$ be a solution of the continuity equation (2). For the Boltzmann–Gibbs–Shannon entropy functional (5)

$$\frac{\mathrm{d}S(f)}{\mathrm{d}t} = \int_X f(x,t)\mathrm{div}v(x)\,\mathrm{d}\Gamma(x), \tag{10}$$

if the left hand side exists. This *entropy production formula* can be easily proven for small phase drops with constant density, then for finite sums of such distributions with positive coefficients. After that, we obtain formula (10) by limit transition.

For a regular invariant density $f^*(x)$ (equilibrium) entropy $S(f^*)$ exists, and for this distribution $\mathrm{d}S(f)/\mathrm{d}t = 0$, hence,

$$\int_X f^*(x)\mathrm{div}v(x)\,\mathrm{d}\Gamma(x) = 0. \tag{11}$$

Entropy production in systems without regular equilibrium

If there is no regular equilibrium (6), then the entropy behaviour changes drastically. If volume of phase drops tends to zero, then the BGS entropy (5) and any Kullback entropy (9) increases to infinity. The simplest example clarifies the situation. Let all the solutions converge to unique exponentially stable fixed point $x = 0$. In linear approximation $\mathrm{d}x/\mathrm{d}t = Ax$ and $S(t) = S(0) + t\,\mathrm{tr}A$. Entropy decreases linearly in time with the rate $\mathrm{tr}A$ ($\mathrm{tr}A = \mathrm{div}v(x)$, $\mathrm{tr}A < 0$), time derivative of entropy is $\mathrm{tr}A$ and does not change in time, and the probability distribution goes to δ-function $\delta(x)$. Entropy of this distribution does not exist (it is "minus infinity"), and it has no limit when $f(x,t) \to \delta(x)$.

Nevertheless, time derivative of entropy is well defined and constant, it is $\mathrm{tr}A$. For more complicated singular limit distributions the essence remains the same: according to (10) time derivative of entropy tends to the average value of $\mathrm{div}v(x)$ in this limit distribution, and entropy goes linearly to minus infinity (if this average in not zero, of course). The order in the system increases. This behaviour could sometimes be interpreted as follows: the system is open and produces entropy in its surrounding even in a steady–state. Much more details are in review [31].[3]

[3] Applications of this formalism are mainly related to Hamiltonian systems in so-called force thermostat, or, in particular, isokinetic thermostat. These thermostats were invented in computational molecular dynamics for acceleration of computations, as a technical trick. From the physical point of view, this theory can be considered as a theory about a friction of particles on the space, the "ether friction." For isokinetic thermostats, for example, this "friction" decelerates some of particles, accelerates others, and keeps the kinetic energy constant.

Starting point: a kinetic equation

For formalization of the Ehrenfest's idea of coarse-graining we start from a formal kinetic equation

$$\frac{\mathrm{d}f}{\mathrm{d}t} = J(f) \tag{12}$$

with concave entropy functional $S(f)$ that does not increase in time. This equation is defined in a convex subset U of a vector space E.

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.

We recall that, for an operator $A : E_1 \to E_2$, the adjoint operator, $A^T : E_1^T \to E_2^T$ is defined by the following relation: for any $l \in E_2^T$ and $\varphi \in E_1$, $l(A\varphi) = (A^T l)(\varphi)$.

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

$$S(f+\varphi) = S(f) + D_f S(f)(\varphi) + \frac{1}{2} D_f^2 S(f)(\varphi, \varphi) + o(\|\varphi\|^2). \tag{13}$$

We keep the same notation for the corresponding symmetric bilinear form, $D_f^2 S(f)(\varphi, \psi)$, and also for the linear operator, $D_f^2 S(f) : E \to E^T$, defined by the formula $(D_f^2 S(f)\varphi)(\psi) = D_f^2 S(f)(\varphi, \psi)$. In this formula, on the left hand side $D_f^2 S(f)$ is the operator, on the right hand side it is the bilinear form. Operator $D_f^2 S(f)$ is symmetric on E, $D_f^2 S(f)^T = D_f^2 S(f)$.

In finite dimensions the functional $D_f S(f)$ can be presented simply as a row vector of partial derivatives of S, and the operator $D_f^2 S(f)$ is a matrix of second partial derivatives. For infinite–dimensional spaces some complications exist because $S(f)$ is defined only for classical densities and not for all distributions. In this paper we do not pay attention to these details.

We assume strict concavity of S, $D_f^2 S(f)(\varphi, \varphi) < 0$ if $\varphi \neq 0$. It means that for any f the positive definite quadratic form $-D_f^2 S(f)(\varphi, \varphi)$ defines a scalar product

$$\langle \varphi \mid \psi \rangle_f = -(D_f^2 S)(\varphi, \psi). \tag{14}$$

This *entropic scalar product* is an important part of thermodynamic formalism.

The most important assumption about kinetic equation (12) is: entropy does not decrease in time:

$$\frac{\mathrm{d}S}{\mathrm{d}t} = D_f S(f)(J(f)) \geq 0. \tag{15}$$

A particular case of this assumption is: the system (12) is conservative and entropy is constant. The main example of such conservative equations is the

Liouville equation with linear vector field $J(f) = -Lf = \{H, f\}$, where $\{H, f\}$ is the Poisson bracket with Hamiltonian H.

For the following consideration of the Ehrenfest's coarse-graining the underlying mechanical motion is not crucial, and it is possible to start from the formal kinetic equation (12) without any mechanical interpretation of vectors f. We develop below the coarse-graining procedure for general kinetic equation (12) with non-decreasing entropy (15). After coarse-graining the entropy production increases: conservative systems become dissipative ones, and dissipative systems become "more dissipative."

2.2 Conditional equilibrium instead of averaging in cells

Microdescription, macrodescription and quasi-equilibrium state

Averaging in cells is a particular case of entropy maximization. Let the phase space be divided into cells. For the ith cell the population M_i is

$$M_i = m_i(f) = \int_{\mathrm{cell}_i} f(x)\,\mathrm{d}\Gamma(x).$$

The averaging in cells for a given vector of populations $M = (M_i)$ produces the solution of the optimization problem for the BGS entropy:

$$S(f) \to \max,\ m(f) = M, \tag{16}$$

where $m(f)$ is vector $(m_i(f))$. The maximizer is a function $f^*_M(x)$ defined by the vector of averages M.

This operation has a well-known generalization. In the more general statement, vector f is a microscopic description of the system, vector M gives a macroscopic description, and a linear operator m transforms a microscopic description into a macroscopic one: $M = m(f)$. The standard example is the transformation of the microscopic density into the hydrodynamic fields (density–velocity–kinetic temperature) with local Maxwellian distributions as entropy maximizers (see, for example, [4]).

For any macroscopic description M, let us define the correspondent f^*_M as a solution to optimization problem (16) with an appropriate entropy functional $S(f)$ (Fig. 3). This f^*_M has many names in the literature: MaxEnt distribution, reference distribution (reference of the macroscopic description to the microscopic one), generalized canonical ensemble, conditional equilibrium, or *quasi-equilibrium*. We shall use here the last term.

Following [4] let us mention that most of the works on nonequilibrium thermodynamics deal with quasi-equilibrium approximations and corrections to them, or with applications of these approximations (with or without corrections). This viewpoint is not the only possible but it proves very efficient for the construction of a variety of useful models, approximations and equations, as well as methods to solve them.

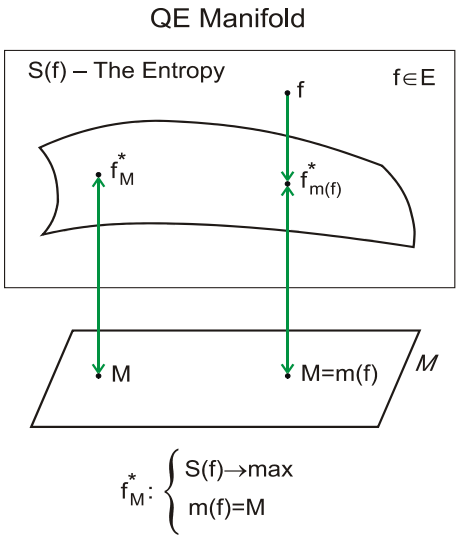

Fig. 3. Relations between a microscopic state f, a corresponding macroscopic state $M = m(f)$, and a quasi-equilibrium state f^*_M.

From time to time it is discussed in the literature, who was the first to introduce the quasi-equilibrium approximations, and how to interpret them. At least a part of the discussion is due to a different role the quasi-equilibrium plays in the entropy-conserving and in the dissipative dynamics. The very first use of the entropy maximization dates back to the classical work of G. W. Gibbs [37], but it was first claimed for a principle of informational statistical thermodynamics by E. T. Jaynes [38]. Probably, the first explicit and systematic use of quasiequilibria on the way from entropy-conserving dynamics to dissipative kinetics was undertaken by D. N. Zubarev. Recent detailed exposition of his approach is given in [39].

For dissipative systems, the use of the quasi-equilibrium to reduce description can be traced to the works of H. Grad on the Boltzmann equation [40]. A review of the informational statistical thermodynamics was presented in [41]. The connection between entropy maximization and (nonlinear) Onsager relations was also studied [42, 43]. Our viewpoint was influenced by the papers by L. I. Rozonoer and co-workers, in particular, [44–46]. A detailed exposition of the quasi-equilibrium approximation for Markov chains is given in the book [28] (Chap. 3, *Quasi-equilibrium and entropy maximum*, pp. 92-122), and for the BBGKY hierarchy in the paper [47].

The maximum entropy principle was applied to the description the universal dependence the three-particle distribution function F_3 on the two-particle distribution function F_2 in classical systems with binary interactions [48]. For a discussion of the quasi-equilibrium moment closure hierarchies for the Boltzmann equation [45] see the papers [49–51]. A very general discussion of the

maximum entropy principle with applications to dissipative kinetics is given in the review [52]. Recently, the quasi-equilibrium approximation with some further correction was applied to the description of rheology of polymer solutions [54, 55] and of ferrofluids [56, 57]. Quasi-equilibrium approximations for quantum systems in the Wigner representation [60, 61] was discussed very recently [53].

We shall now introduce the quasi-equilibrium approximation in the most general setting. The coarse-graining procedure will be developed after that as a method for enhancement of the quasi-equilibrium approximation [5].

Quasi-equilibrium manifold, projector and approximation

A *quasi-equilibrium manifold* is a set of quasi-equilibrium states f^*_M parameterized by macroscopic variables M. For microscopic states f the correspondent quasi-equilibrium states are defined as $f^*_{m(f)}$. Relations between f, M, f^*_M, and $f^*_{m(f)}$ are presented in Fig. 3.

A *quasi-equilibrium approximation* for the kinetic equation (12) is an equation for $M(t)$:

$$\frac{\mathrm{d}M}{\mathrm{d}t} = m(J(f^*_M)). \tag{17}$$

To define $\dot{M}$ in the quasi-equilibrium approximation for given M, we find the correspondent quasi-equilibrium state f^*_M and the time derivative of f in this state $J(f^*_M)$, and then return to the macroscopic variables by the operator m. If $M(t)$ satisfies (17) then $f^*_{M(t)}$ satisfies the following equation

$$\frac{\mathrm{d}f^*_M}{\mathrm{d}t} = D_M f^*_M \left(\frac{\mathrm{d}M}{\mathrm{d}t}\right) = D_M f^*_M(m(J(f^*_M))). \tag{18}$$

The right hand side of (18) is the projection of vector field $J(f)$ onto the tangent space of the quasi-equilibrium manifold at the point $f = f^*_M$. After calculating the differential $D_M f^*_M$ from the definition of quasi-equilibrium (16), we obtain $\mathrm{d}f^*_M/\mathrm{d}t = \pi_{f^*_M} J(f^*_M)$, where $\pi_{f^*_M}$ is the *quasi-equilibrium projector*:

$$\pi_{f^*_M} = (D_M f^*_M)_M\, m = \left(D^2_f S\right)^{-1}_{f^*_M} m^T \left(m \left(D^2_f S\right)^{-1}_{f^*_M} m^T\right)^{-1} m. \tag{19}$$

It is straightforward to check the equality $\pi^2_{f^*_M} = \pi_{f^*_M}$, and the self-adjointness of $_{f^*_M}$ with respect to entropic scalar product (14). In this scalar product, the quasi-equilibrium projector is the orthogonal projector onto the tangent space to the quasi-equilibrium manifold. The quasi-equilibrium projector for a quasi-equilibrium approximation was first constructed by B. Robertson [58].

Thus, we have introduced the basic constructions: quasi-equilibrium manifold, entropic scalar product, and quasi-equilibrium projector (Fig. 4).

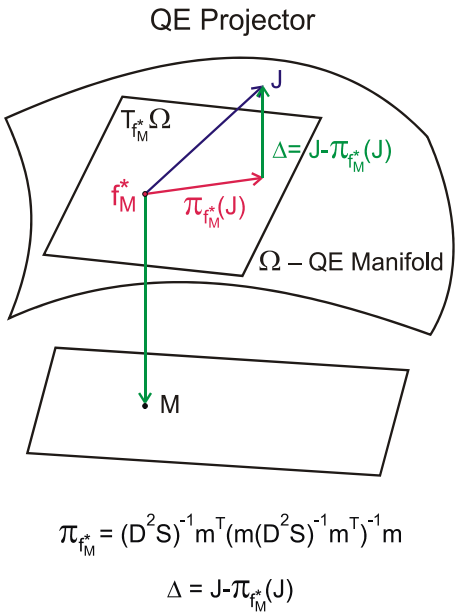

Fig. 4. Quasi-equilibrium manifold Ω, tangent space $T_{f_M^*}\Omega$, quasi-equilibrium projector $\pi_{f_M^*}$, and defect of invariance, $\Delta = \Delta_{f_M^*} = J - \pi_{f_M^*}(J)$.

Preservation of dissipation

For the quasi-equilibrium approximation the entropy is $S(M) = S(f_M^*)$. For this entropy,

$$\frac{\mathrm{d}S(M)}{\mathrm{d}t} = \left(\frac{\mathrm{d}S(f)}{\mathrm{d}t}\right)_{f=f_M^*}, \tag{20}$$

Here, in the left hand side stands the macroscopic entropy production for the quasi-equilibrium approximation (17), and the right hand side is the microscopic entropy production calculated for the initial kinetic equation (12). This equality implies *preservation of the type of dynamics* [28, 29]:

- If for the initial kinetics (12) the dissipativity inequality (15) holds then the same inequality is true for the quasi-equilibrium approximation (17);
- If the initial kinetics (12) is conservative then the quasi-equilibrium approximation (17) is conservative also.

For example, let the initial kinetic equation be the Liouville equation for a system of many identical particles with binary interaction. If we choose as macroscopic variables the one-particle distribution function, then the quasi-equilibrium approximation is the Vlasov equation. If we choose as macroscopic variables the hydrodynamic fields, then the quasi-equilibrium approximation

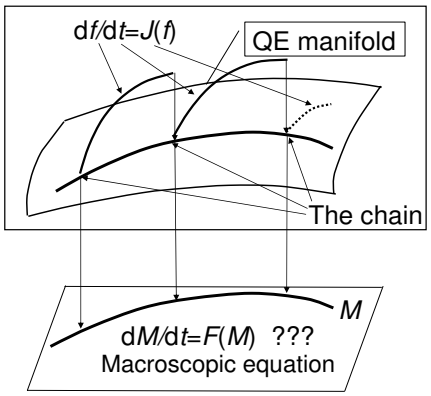

Fig. 5. The Ehrenfest's chain.

is the compressible Euler equation with self–interaction of liquid. Both of these equations are conservative and turn out to be even Hamiltonian systems [59].

Measurement of accuracy

Accuracy of the quasi-equilibrium approximation near a given M can be measured by the *defect of invariance* (Fig. 4):

$$\Delta_{f^*_M} = J(f^*_M) - \pi_{f^*_M} J(f^*_M). \tag{21}$$

A dimensionless criterion of accuracy is the ratio $\|\Delta_{f^*_M}\|/\|J(f^*_M)\|$ (a "sine" of the angle between J and tangent space). If $\Delta_{f^*_M} \equiv 0$ then the quasi-equilibrium manifold is an invariant manifold, and the quasi-equilibrium approximation is exact. In applications, the quasi-equilibrium approximation is usually not exact.

2.3 The Ehrenfest's Chain, Macroscopic Equations and Entropy production

The Ehrenfest's Chain and entropy growth

Let Θ_t be the time shift transformation for the initial kinetic equation (12):

$$\Theta_t(f(0)) = f(t).$$

The Ehrenfest's chain (Fig. 5) is defined for a given macroscopic variables $M = m(f)$ and a fixed time of coarse-graining τ. It is a chain of quasi-equilibrium states $f_0, f_1, \ldots$:

$$f_{i+1} = f^*_{m(\Theta_\tau(f_i))}. \tag{22}$$

To get the next point of the chain, f_{i+1}, we take f_i, move it by the time shift Θ_τ, calculate the corresponding macroscopic state $M_{i+1} = m(\Theta_\tau(f_i))$, and find the quasi-equilibrium state $f^*_{M_{i+1}} = f_{i+1}$.

If the point $\Theta_\tau(f_i)$ is not a quasi-equilibrium state, then $S(\Theta_\tau(f_i)) < S(f^*_{m(\Theta_\tau(f_i))})$ because of quasi-equilibrium definition (16) and strict concavity of entropy. Hence, if the motion between f_i and $\Theta_\tau(f_i)$ does not belong to the quasi-equilibrium manifold, then $S(f_{i+1}) > S(f_i)$, entropy in the Ehrenfest's chain grows. The entropy gain consists of two parts: the gain in the motion (from f_i to $\Theta_\tau(f_i)$), and the gain in the projection (from $\Theta_\tau(f_i)$ to $f_{i+1} = f^*_{m(\Theta_\tau(f_i))}$). Both parts are non-negative. For conservative systems the first part is zero. The second part is strictly positive if the motion leaves the quasi-equilibrium manifold. Hence, we observe some sort of duality between entropy production in the Ehrenfest's chain and invariance of the quasi-equilibrium manifold.

For conservative systems some authors [67,68] call entropy $S(f)$ the Gibbs entropy, and introduce a notion of the "Boltzmann entropy". Boltzmann defined the entropy of a macroscopic system in a macrostate M as the log of the volume of phase space (number of microstates) corresponding to M. In the proposed level of generality [28,29], the Boltzmann entropy of the state f can be defined as $S_{\rm B}(f) = S(f^*_{m(f)})$. It is entropy of the projection of f onto quasi-equilibrium manifold (the "shadow" entropy). For conservative systems the Gibbs entropy is constant, but the Boltzmann entropy increases [29] (during some time, at least) for motions that start on the quasi-equilibrium manifold, but not belong to this manifold. The motions that build the Ehrenfest's chain restart periodically from the quasi-equilibrium manifold and the entropy growth along this chain is similar to the Boltzmann entropy growth.

The natural projector and macroscopic dynamics

How to use the Ehrenfest's chains? First of all, we can try to define the *macroscopic kinetic equations* for $M(t)$ by the requirement that for any initial point of the chain f_0 the solution of these macroscopic equations with initial conditions $M(0) = m(f_0)$ goes through all the points $m(f_i)$: $M(n\tau) = m(f_n)$ $(n = 1, 2, \ldots)$ (Fig. 5) [5] (see also [4]). Another way is an "equation–free approach" [9] to the direct computation of the Ehrenfest's chain with a combination of microscopic simulation and macroscopic stepping.

For the definition of the macroscopic equations only the first link of the Ehrenfest's chain is necessary. In general form, for an ansatz manifold Ω, projector $\pi : U \to \Omega$ of the vicinity of Ω onto Ω, phase flow of the initial kinetic equation Θ_t, and macroscopic phase flow $\tilde{\Theta}_t$ on Ω the matching condition is (Fig. 6):

$$\pi(\Theta_\tau(f)) = \tilde{\Theta}_\tau(f) \text{ for any } f \in \Omega. \tag{23}$$

We call this projector of the flow Θ onto an ansatz manifold Ω by fragments of trajectories of given duration τ the *natural projector* in order to distinguish it from the standard infinitesimal projector of vector fields on tangent spaces.

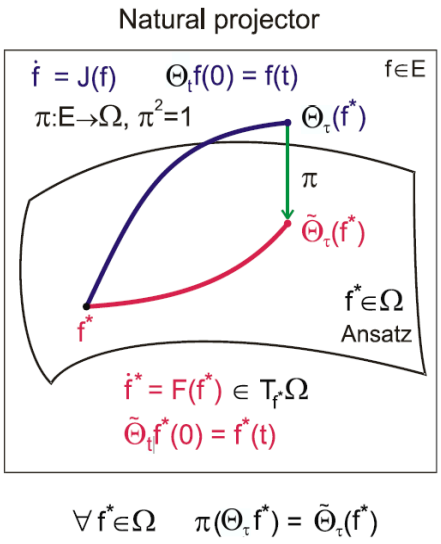

Fig. 6. Projection of segments of trajectories: The microscopic motion above the manifold Ω and the macroscopic motion on this manifold. If these motions begin in the same point on Ω, then, after time τ, projection of the microscopic state onto Ω should coincide with the result of the macroscopic motion on Ω. For quasi-equilibrium Ω, projector $\pi : E \to \Omega$ acts as $\pi(f) = f^*_{m(f)}$.

Let us look for the macroscopic equations of the form

$$\frac{\mathrm{d}M}{\mathrm{d}t} = \Psi(M) \tag{24}$$

with the phase flow Φ_t: $M(t) = \Phi_t M(0)$. For the quasi-equilibrium manifold and projector the matching condition (23) gives

$$m(\Theta_\tau(f^*_M)) = \Phi_\tau(M) \text{ for any macroscopic state } M. \tag{25}$$

This condition is the equation for the macroscopic vector field $\Psi(M)$. Solution of this equation is a function of τ: $\Psi = \Psi(M, \tau)$. For sufficiently smooth microscopic vector field $J(f)$ and entropy $S(f)$ it is easy to find the Taylor expansion of $\Psi(M, \tau)$ in powers of τ. It is a straightforward exercise in differential calculus. Let us find the first two terms: $\Psi(M, \tau) = \Psi_0(M) + \tau\Psi_1(M) + o(\tau)$. Up to the second order in τ the matching condition (25) is

$$\begin{aligned} &m(J(f^*_M))\tau + m((D_f J(f))_{f=f^*_M}(J(f^*_M)))\frac{\tau^2}{2} \\ &= \Psi_0(M)\tau + \Psi_1(M)\tau^2 + (D_M\Psi_0(M))(\Psi_0(M))\frac{\tau^2}{2}. \end{aligned} \tag{26}$$

From this condition immediately follows:

$$\Psi_0(M) = m(J(f^*_M)); \tag{27}$$
$$\Psi_1(M) = \frac{1}{2}m[(D_f J(f))_{f=f^*_M}(J(f^*_M)) - (D_M J(f^*_M))(m(J(f^*_M)))]$$
$$= m[(D_f J(f))_{f=f^*_M} \Delta_{f^*_M}]$$

where $\Delta_{f^*_M}$ is the defect of invariance (21). The macroscopic equation in the first approximation is:

$$\frac{\mathrm{d}M}{\mathrm{d}t} = m(J(f^*_M)) + \frac{\tau}{2}m[(D_f J(f))_{f=f^*_M} \Delta_{f^*_M}]. \tag{28}$$

The first term $m(J(f^*_M))$ gives the quasi-equilibrium approximation, the second term increases dissipation. The formula for entropy production follows from (30) [11]. If the initial microscopic kinetic (12) is conservative, then for macroscopic equation (28) we obtain:

$$\frac{\mathrm{d}S(M)}{\mathrm{d}t} = \frac{\tau}{2}\langle \Delta_{f^*_M}, \Delta_{f^*_M} \rangle_{f^*_M}, \tag{29}$$

where $\langle \bullet, \bullet \rangle_f$ is the entropic scalar product (14). From this formula we see again a duality between the invariance of the quasi-equilibrium manifold and the dissipativity: entropy production is proportional to the square of the defect of invariance of the quasi-equilibrium manifold.

For linear microscopic equations ($J(f) = Lf$) the form of the macroscopic equations is

$$\frac{\mathrm{d}M}{\mathrm{d}t} = mL\left[1 + \frac{\tau}{2}(1 - \pi_{f^*_M})L\right] f^*_M, \tag{30}$$

where $\pi_{f^*_M}$ is the quasi-equilibrium projector (19).

The Navier–Stokes equation from the free flight dynamics

The free flight equation describes dynamics of one-particle distribution function $f(\boldsymbol{x}, \boldsymbol{v})$ due to the free flight:

$$\frac{\partial f(\boldsymbol{x}, \boldsymbol{v}, t)}{\partial t} = -\sum_i v_i \frac{\partial f(\boldsymbol{x}, \boldsymbol{v}, t)}{\partial x_i}. \tag{31}$$

The difference from the continuity equation (2) is that there is no velocity field $\boldsymbol{v}(\boldsymbol{x})$, but the velocity vector $\boldsymbol{v}$ is an independent variable. Equation (31) is conservative and has an explicit general solution

$$f(\boldsymbol{x}, \boldsymbol{v}, t) = f_0(\boldsymbol{x} - \boldsymbol{v}t, \boldsymbol{v}). \tag{32}$$

The coarse-graining procedure for (31) serves for modeling kinetics with an unknown dissipative term $I(f)$

$$\frac{\partial f(\boldsymbol{x}, \boldsymbol{v}, t)}{\partial t} = -\sum_i v_i \frac{\partial f(\boldsymbol{x}, \boldsymbol{v}, t)}{\partial x_i} + I(f). \tag{33}$$

The Ehrenfest's chain realizes a splitting method for (33): first, the free flight step during time τ, than the complete relaxation to a quasi-equilibrium distribution due to dissipative term $I(f)$, then again the free flight, and so on. In this approximation the specific form of $I(f)$ is not in use, and the only parameter is time τ. It is important that this hypothetical $I(f)$ preserves all the standard conservation laws (number of particles, momentum, and energy) and has no additional conservation laws: everything else relaxes. Following this assumption, the macroscopic variables are: $M_0 = n(\boldsymbol{x}, t) = \int f \mathrm{d}\boldsymbol{v}$, $M_i = nu_i = \int v_i f \mathrm{d}\boldsymbol{v}$ $(i = 1, 2, 3)$, $M_4 = \frac{3k_\mathrm{B}T}{m} + u^2 = \int v^2 f \mathrm{d}\boldsymbol{v}$. The zero-order (quasi-equilibrium) approximation (17) gives the classical Euler equation for compressible non-isothermal gas. In the first approximation (28) we obtain the Navier–Stokes equations:

$$\begin{aligned}
\frac{\partial n}{\partial t} &= -\sum_i \frac{\partial (nu_i)}{\partial x_i}, \\
\frac{\partial (nu_k)}{\partial t} &= -\sum_i \frac{\partial (nu_k u_i)}{\partial x_i} - \frac{1}{m}\frac{\partial P}{\partial x_k} \\
&\quad + \underline{\frac{\tau}{2}\frac{1}{m}\sum_i \frac{\partial}{\partial x_i}\left[P\left(\frac{\partial u_k}{\partial x_i} + \frac{\partial u_i}{\partial x_k} - \frac{2}{3}\delta_{ki}\mathrm{div} u\right)\right]}, \\
\frac{\partial \varepsilon}{\partial t} &= -\sum_i \frac{\partial (\varepsilon u_i)}{\partial x_i} - \frac{1}{m}\sum_i \frac{\partial (Pu_i)}{\partial x_i} + \underline{\frac{\tau}{2}\frac{5k_\mathrm{B}}{2m^2}\sum_i \frac{\partial}{\partial x_i}\left(P\frac{\partial T}{\partial x_i}\right)},
\end{aligned} \tag{34}$$

where $P = nk_\mathrm{B}T$ is the ideal gas pressure, $\varepsilon = \frac{1}{2}\int v^2 f \,\mathrm{d}\boldsymbol{v} = \frac{3nk_\mathrm{B}T}{2m} + \frac{1}{2}u^2$ is the energy density per unite mass ($P = \frac{2m}{3}\varepsilon - \frac{m}{3}u^2$, $T = \frac{2m}{3nk_\mathrm{B}}\varepsilon - \frac{m}{3nk_\mathrm{B}}u^2$), and the underlined terms are results of the coarse-graining additional to the quasi-equilibrium approximation.

The dynamic viscosity in (34) is $\mu = \frac{\tau}{2}nk_\mathrm{B}T$. It is useful to compare this formula to the mean–free–path theory that gives $\mu = \tau_\mathrm{col}nk_\mathrm{B}T = \tau_\mathrm{col}P$, where τ_col is the collision time (the time for the mean–free–path). According to these formulas, we get the following interpretation of the coarse-graining time τ for this example: $\tau = 2\tau_\mathrm{col}$.

The equations obtained (34) coincide with the first–order terms of the Chapman–Enskog expansion applied to the Bhatnagar–Gross–Krook (BGK) equations with $\tau_\mathrm{col} = \tau/2$ and meet the same problem: the Prandtl number (i.e., the dimensionless ratio of viscosity and thermal conductivity) is $\mathrm{Pr} = 1$ instead of the value $\mathrm{Pr} = \frac{2}{3}$ verified by experiments with perfect gases and by more detailed theory [69] (recent discussion of this problem for the BGK equation with some ways for its solution is presented in [70]).

In the next order in τ we obtain the stable post–Navier–Stokes equations instead of the unstable Burnett equations that appear in the Chapman–Enskog expansion [11, 66].

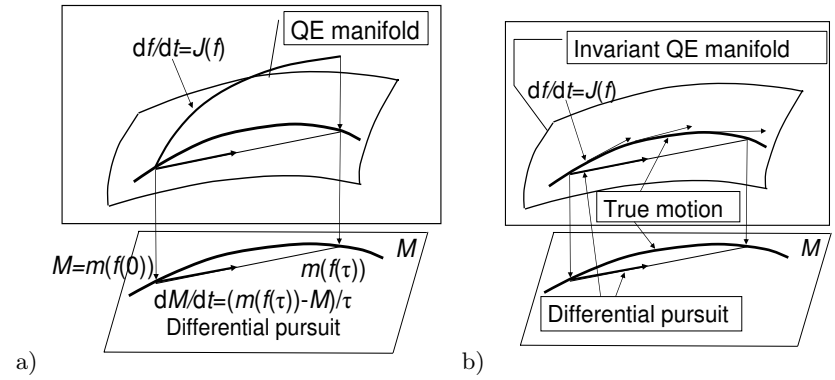

Fig. 7. Differential pursuit of the projection point (a). The mistake of differential pursuit (b): invariant manifold should preserve its invariance, but it does not!

Persistence of invariance and mistake of differential pursuit

L.M. Lewis called a generalization of the Ehernfest's approach a "unifying principle in statistical mechanics," but he created other macroscopic equations: he produced the differential pursuit (Fig. 7a)

$$\frac{\mathrm{d}M}{\mathrm{d}t} = \frac{m(\Theta_\tau(f^*_M)) - M}{\tau} \tag{35}$$

from the full matching condition (23). This means that the macroscopic motion was taken in the first-order Tailor approximation, while for the microscopic motion the complete shift in time (without the Taylor expansion) was used. The basic idea of this approach is a non-differential time separation: the infinitesimal shift in macroscopic time is always such a significant shift for microscopic time that no Taylor approximation for microscopic motion may be in use. This sort of non-standard analysis deserves serious attention, but its realization in the form of the differential pursuit (35) does not work properly in many cases. If the quasi-equilibrium manifold is invariant, then the quasi-equilibrium approximation is exact and the Ehrenfest's chain (Fig. 5) just follows the quasi-equilibrium trajectory. But the differential pursuit does not follow the trajectory (Fig. 7b); this motion leaves the invariant quasi-equilibrium manifolds, and the differential pursuit does not approximate the Ehrenfest's chain, even qualitatively.

Ehrenfest's coarse-graining as a method for model reduction

The problem of model reduction in dissipative kinetics is recognized as a problem of time separation and construction of slow invariant manifolds. One obstacle on this way is that the slow invariant manifold is the thing that many people would like to find, but nobody knows exactly what it is. There

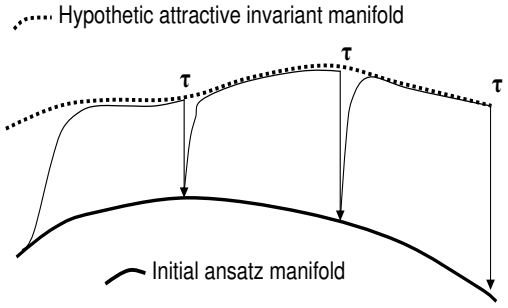

Fig. 8. Natural projector and attractive invariant manifolds. For large τ, the natural projector gives the approximation of projection of the genuine motion from the attractive invariant manifold onto the initial ansatz manifold Ω.

is no conventional definition of *slow* invariant manifold without explicit small parameter that tends to zero. It seems now that the most reasonable way for such a definition is the analysis of induced dynamics of manifolds immersed into phase space. Fixed points of this dynamics are invariant manifolds, and asymptotically stable (stable and attracting) fixed points are slow invariant manifolds. This concept was explicitly developed very recently [3, 4, 72], but the basic idea was used in earlier applied works [29, 73].

The coarse-graining procedure was developed for *erasing* some details of the dynamics in order to provide entropy growth and uniform tendency to equilibrium. In this sense, the coarse-graining is opposite to the model reduction, because for the model reduction we try to find slow invariant manifolds as exactly, as we can. But unexpectedly the coarse-graining becomes a tool for model reduction without any "erasing."

Let us assume that for dissipative dynamics with entropy growth there exists an attractive invariant manifold. Let us apply the Ehrenfest's coarse graining to this system for sufficiently large coarse-graining time τ. For the most part of time τ the system will spend in a small vicinity of the attractive invariant manifold. Hence, the macroscopic projection will describe the projection of dynamics from the attractive invariant manifold onto ansatz manifold Ω. As a result, we shall find a shadow of the proper slow dynamics without looking for the slow invariant manifold. Of course, the results obtained by the Taylor expansion (26–28) are not applicable for the case of large coarse-graining time τ, at least, directly. Some attempts to utilize the idea of large τ asymptotic are presented in [4] (Ch. 12).

One can find a source of this idea in the first work of D. Hilbert about the Boltzmann equation solution [30] (a recent exposition and development of the Hilbert method is presented in [74] with many examples of applications). In the Hilbert method, we start from the local Maxwellian manifold (that is, quasi-equilibrium one) and iteratively look for "normal solutions." The nor-

mal solutions $f_{\rm H}(\boldsymbol{v},\, n(\boldsymbol{x},t),\, \boldsymbol{u}(\boldsymbol{x},t),\, T(\boldsymbol{x},t))$ are solutions to the Boltzmann equation that depend on space and time only through five hydrodynamic fields. In the Hilbert method no final macroscopic equation arises. The next attempt to utilize this idea without macroscopic equations is the "equation free" approach [9, 75].

The Ehrenfest's coarse graining as a tool for extraction of exact macroscopic dynamics was tested on exactly solvable problems [63]. It gives also a new approach to the fluctuation–dissipation theorems [62].

2.4 Kinetic models, entropic involution, and the second–order "Euler method"

Time-step – dissipation decoupling problem

Sometimes, the kinetic equation is much simpler than the coarse-grained dynamics. For example, the free flight kinetics (31) has the obvious exact analytical solution (32), but the Euler or the Navier–Stokes equations (34) seem to be very far from being exactly solvable. In this sense, the Ehrenfest's chain (22) (Fig. 5) gives a stepwise approximation to a solution of the coarse-grained (macroscopic) equations by the chain of solutions of the kinetic equations.

If we use the second-order approximation in the coarse graining procedure (26), then the Ehrenfest's chain with step τ is the second–order (in time step τ) approximation to the solution of macroscopic equation (28). It is very attractive for hydrodynamics: the second–order in time method with approximation just by broken line built from intervals of simple free–flight solutions. But if we use the Ehrenfest's chain for approximate solution, then the strong connection between the time step τ and the coefficient in equations (28) (see also the entropy production formula (29)) is strange. Rate of dissipation is proportional to τ, and it seems to be too restrictive for computational applications: decoupling of time step and dissipation rate is necessary. This decoupling problem leads us to a question that is strange from the Ehrenfest's coarse-graining point of view: *how to construct an analogue to the Ehrenfest's coarse-graining chain, but without dissipation?* The *entropic involution* is a tool for this construction.

Entropic involution

The entropic involution was invented for improvement of the lattice–Boltzmann method [77]. We need to construct a chain with zero macroscopic entropy production and second order of accuracy in time step τ. The chain consists of intervals of solution of kinetic equation (12) that is conservative. The time shift for this equation is Θ_t. The macroscopic variables $M = m(f)$ are chosen, and the time shift for corresponding quasi-equilibrium equation is (in this section) $\widetilde{\Theta}_t$. The standard example is: the free flight kinetics (31,32) as a microscopic conservative kinetics, hydrodynamic fields (density–velocity–kinetic temperature) as macroscopic variables, and the Euler equations as a

macroscopic quasi-equilibrium equations for conservative case (see (34), not underlined terms).

Let us start from construction of one link of a chain and take a point $f_{1/2}$ on the quasi-equilibrium manifold. (It is not an initial point of the link, f_0, but a "middle" one.) The correspondent value of M is $M_{1/2} = m(f_{1/2})$. Let us define $M_0 = m(\Theta_{-\tau/2}(f_{1/2}))$, $M_1 = m(\Theta_{\tau/2}(f_{1/2}))$. The dissipative term in macroscopic equations (28) is linear in τ, hence, there is a symmetry between forward and backward motion from any quasiequilibrium initial condition with the second-order accuracy in the time of this motion (it became clear long ago [29]). Dissipative terms in the shift from M_0 to $M_{1/2}$ (that decrease macroscopic entropy $S(M)$) annihilate with dissipative terms in the shift from $M_{1/2}$ to M_1 (that increase macroscopic entropy $S(M)$). As the result of this symmetry, M_1 coincides with $\widetilde{\Theta}_\tau(M_0)$ with the second-order accuracy. (It is easy to check this statement by direct calculation too.)

It is necessary to stress that the second-order accuracy is achieved on the ends of the time interval only: $\widetilde{\Theta}_\tau(M_0)$ coincides with $M_1 = m(\Theta_\tau(f_0))$ in the second order in τ

$$m(\Theta_\tau(f_0)) - \widetilde{\Theta}_\tau(M_0) = o(\tau^2).$$

On the way $\widetilde{\Theta}_t(M_0)$ from M_0 to $\widetilde{\Theta}_\tau(M_0)$ for $0 < t < \tau$ we can guarantee the first-order accuracy only (even for the middle point). It is essentially the same situation as we had for the Ehrenfest's chain: the second order accuracy of the matching condition (25) is postulated for the moment τ, and for $0 < t < \tau$ the projection of the $m(\Theta_t(f_0))$ follows a solution of the macroscopic equation (28) with the first order accuracy only. In that sense, the method is quite different from the usual second–order methods with intermediate points, for example, from the Crank–Nicolson schemes. By the way, the middle quasi-equilibrium point, $f_{1/2}$ appears for the initiation step only. After that, we work with the end points of links.

The link is constructed. For the initiation step, we used the middle point $f_{1/2}$ on the quasi-equilibrium manifold. The end points of the link, $f_0 = \Theta_{-\tau/2}(f_{1/2})$ and $f_1 = \Theta_{\tau/2}(f_{1/2})$ don't belong to the quasi-equilibrium manifold, unless it is invariant. Where are they located? They belong a surface that we call a *film of non-equilibrium states* [4,64,65]. It is a trajectory of the quasi-equilibrium manifold due to initial microscopic kinetics. In [4,64,65] we studied mainly the positive semi-trajectory (for positive time). Here we need shifts in both directions.

A point f on the film of non-equilibrium states is naturally parameterized by M, τ: $f = q_{M,\tau}$, where $M = m(f)$ is the value of the macroscopic variables, and $\tau(f)$ is the time of shift from a quasi-equilibrium state: $\Theta_{-\tau}(f)$ is a quasi-equilibrium state. For each M and positive s from some interval $]0, \varsigma[$ there exist two such $\tau_\pm(M,s)$ ($\tau_+(M,s) > 0$, $\tau_-(M,s) < 0$) that

$$S(q_{M,\tau_\pm(M,s)}) = S(M) - s. \tag{36}$$

Up to the second order in $\tau_\pm$

$$s = \frac{\tau_\pm^2}{2}\langle \Delta_{f_M^*}, \Delta_{f_M^*}\rangle_{f_M^*} + o(\tau_\pm^2) \tag{37}$$

(compare to (29)), and

$$\tau_+ = -\tau_- + o(\tau_-);\ |\tau_\pm| = \sqrt{\frac{s}{\langle \Delta_{f_M^*}, \Delta_{f_M^*}\rangle_{f_M^*}}}(1 + o(1)). \tag{38}$$

Equation (36) describes connection between entropy change s and time coordinate τ on the film of non-equilibrium states, and (37) presents the first non-trivial term of the Taylor expansion of (36).

The *entropic involution* I_S is the transformation of the film of non-equilibrium states:

$$I_S(q_{M,\tau_\pm}) = q_{M,\tau_\mp}. \tag{39}$$

This involution transforms τ_+ into τ_-, and back. For a given macroscopic state M, the entropic involution I_S transforms the curve of non-equilibrium states $q_{M,\tau}$ into itself.

In the first order in τ it is just reflection $q_{M,\tau} \to q_{M,-\tau}$. A partial linearization is also in use. For this approximation, we define nonlinear involutions of straight lines parameterized by α, not of curves:

$$I_S^0(f) = f^*_{m(f)} - \alpha(f - f^*_{m(f)}),\ \alpha > 0, \tag{40}$$

with condition of entropy conservation

$$S(I_S^0(f)) = S(f). \tag{41}$$

The last condition serves as equation for α. The positive solution is unique and exists for f from some vicinity of the quasi-equilibrium manifold. It follows from the strong concavity of entropy. The transformation I_S^0 (41) is defined not only on the film of non-equilibrium states, but on all distributions (microscopic) f that are sufficiently closed to the quasi-equilibrium manifold.

In order to avoid stepwise accumulation of errors in entropy production, we can choose a constant step in a conservative chain not in time, but in entropy. Let an initial point in macro-variables M_0 be given, and some $s > 0$ be fixed. We start from the point $f_0 = q_{M,\tau_-(M_0,s)}$. At this point, for $t = 0$, $S(m(\Theta_0(f_0)))) - s = S((\Theta_0(f_0)))$ ($\Theta_0 = \mathrm{id}$). Let the motion $\Theta_t(f_0)$ evolve until the equality $S(m(\Theta_t(f_0))) - s = S(\Theta_t(f_0))$ is satisfied next time. This time will be the time step τ, and the next point of the chain is:

$$f_1 = I_S(\Theta_\tau(f_0)). \tag{42}$$

We can present this construction geometrically (Fig. 9a. The quasi-equilibrium manifold, $\mathbf{M}^* = \{q_{M,0}\}$, is accompanied by two other manifolds, $\mathbf{M}^*_\pm(\mathbf{s}) = \{q_{M,\tau_\pm(M,s)}\}$. These manifolds are connected by the entropic involution: $I_S\mathbf{M}^*_\pm(\mathbf{s}) = \mathbf{M}^*_\mp(\mathbf{s})$. For all points $f \in \mathbf{M}^*_\pm(\mathbf{s})$

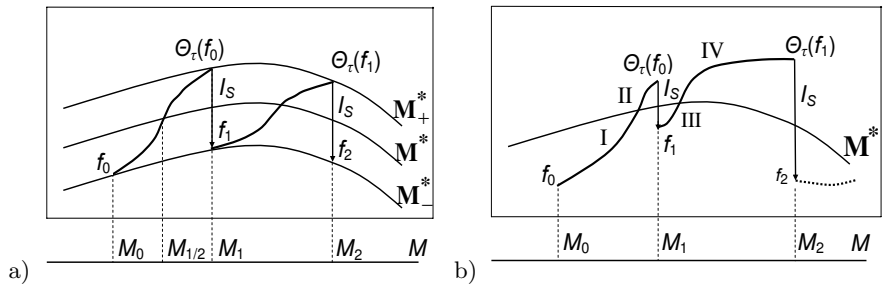

Fig. 9. The regular (a) and irregular (b) conservative chain. Dissipative terms for the regular chain give zero balance inside each step. For the irregular chain, dissipative term of part I (the first step) annihilates with dissipative term of part IV (the second step), as well, as annihilate dissipartive terms for parts II and III.

$$S(f) = S(f^*_{m(f)}) - s.$$

The conservative chain starts at a point on $f_0 \in \mathbf{M}^*_-(\mathbf{s})$, than the solution of initial kinetic equations, $\Theta_t(f_0)$, goes to its intersection with $\mathbf{M}^*_+(\mathbf{s})$, the moment of intersection is τ. After that, the entropic involution transfers $\Theta_\tau(f_0)$ into a second point of the chain, $f_1 = I_S(\Theta_\tau(f_0)) \in \mathbf{M}^*_-(\mathbf{s})$.

Irregular conservative chain

The regular geometric picture is nice, but for some generalizations we need less rigid structure. Let us combine two operations: the shift in time Θ_τ and the entropic involution I_S. Suppose, the motions starts on a point f_0 on the film of non-equilibrium states, and

$$f_{n+1} = I_S(\Theta_\tau(f_n)). \tag{43}$$

This chain we call an *irregular conservative chain*, and the chain that moves from $\mathbf{M}^*_-(\mathbf{s})$ to $\mathbf{M}^*_+(\mathbf{s})$ and back, the regular one. For the regular chain the dissipative term is zero (in the main order in τ) already for one link because this link is symmetric, and the macroscopic entropy ($S(M)$) loose for a motion from $\mathbf{M}^*_-(\mathbf{s})$ to $\mathbf{M}^*$ compensate the macroscopic entropy production on a way from $\mathbf{M}^*$ to $\mathbf{M}^*_+(\mathbf{s})$. For the irregular chain (43) with given τ such a compensation occurs in two successive links (Fig. 9b) in main order in τ.

Kinetic modeling for non-zero dissipation. 1. Extension of regular chains

The conservative chain of kinetic curves approximates the quasi-equilibrium dynamics. A typical example of quasi-equilibrium equations (17) is the Euler equation in fluid dynamics. Now, we combine conservative chains construction with the idea of the dissipative Ehrenfest's chain in order to create a method for kinetic modeling of dissipative hydrodynamics ("macrodynamics") (28) with arbitrary kinetic coefficient that is decoupled from the chain step τ:

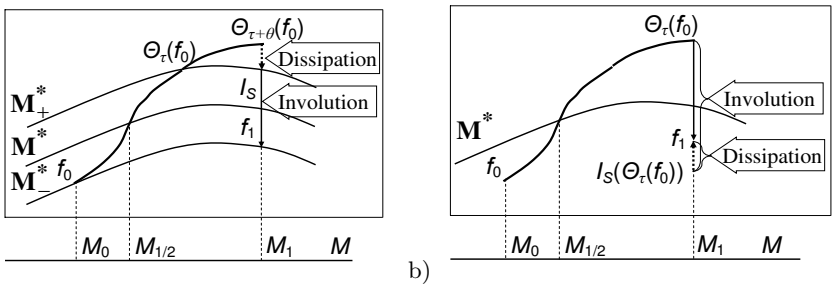

Fig. 10. Realization of dissipative chain by the extra time ϑ on the base of a regular conservative chain (a), and by the incomplete involution on the base of an irregular conservative chain (b).

$$\frac{\mathrm{d}M}{\mathrm{d}t} = m(J(f^*_M)) + \kappa(M)m[(D_f J(f))_{f=f^*_M}\Delta_{f^*_M}]. \tag{44}$$

Here, a kinetic coefficient $\kappa(M) \geq 0$ is a non-negative function of M. The entropy production for (10) is:

$$\frac{\mathrm{d}S(M)}{\mathrm{d}t} = \kappa(M)\langle\Delta_{f^*_M}, \Delta_{f^*_M}\rangle_{f^*_M}. \tag{45}$$

Let us start from a regular conservative chain and deform it. A chain that approximates solutions of (44) can be constructed as follows (Fig. 10a). The motion starts from $f_0 \in \mathbf{M}^*_-(\mathbf{s})$, goes by a kinetic curve to intersection with $\mathbf{M}^*_+(\mathbf{s})$, as for a regular conservative chain, and, after that, follows the same kinetic curve an extra time ϑ. This motion stops at the moment $\tau + \vartheta$ at the point $\Theta_{\tau+\vartheta}(f_0)$ (Fig. 10a). The second point of the chain, f_1 is the unique solution of equation

$$m(f_1) = m(\Theta_{\tau+\vartheta}(f_0)),\ f_1 \in \mathbf{M}^*_-(\mathbf{s}). \tag{46}$$

The time step is linked with the kinetic coefficient:

$$\kappa = \frac{\vartheta}{2} + o(\tau + \vartheta). \tag{47}$$

For entropy production we obtain the analogue of (29)

$$\frac{\mathrm{d}S(M)}{\mathrm{d}t} = \frac{\vartheta}{2}\langle\Delta_{f^*_M}, \Delta_{f^*_M}\rangle_{f^*_M} + o(\tau + \vartheta). \tag{48}$$

All these formulas follow from the first–order picture. In the first order of the time step,

$$\begin{aligned} q_{M,\tau} &= f^*_M + \tau\Delta_{f^*_M};\\ I_S(f^*_M + \tau\Delta_{f^*_M}) &= f^*_M - \tau\Delta_{f^*_M};\\ f_0 &= f^*_{M_0} - \frac{\tau}{2}\Delta_{f^*_{M_0}};\\ \Theta_t(f_0) &= f^*_{M(t)} + \left(t - \frac{\tau}{2}\right)\Delta_{f^*_{M_0}}, \end{aligned} \tag{49}$$

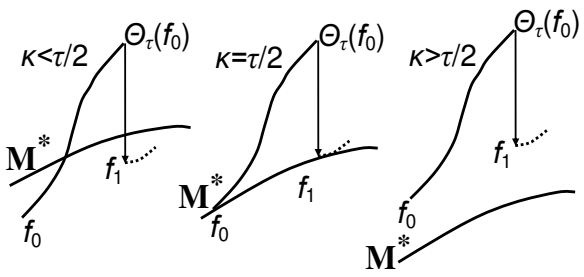

Fig. 11. The Ehrenfest's limit of dissipation: three possible links of a dissipative chain: overrelaxation, $\kappa(M) < \frac{\tau}{2}$ ($\langle\sigma\rangle = s_\tau - 2\sqrt{s_\tau\langle s_0\rangle}$), Ehrenfest's chain, $\kappa(M) = \frac{\tau}{2}$ ($\sigma = s_\tau$), and underrelaxation, $\kappa(M) > \frac{\tau}{2}$ ($\langle\sigma\rangle = s_\tau + 2\sqrt{s_\tau\langle s_0\rangle}$).

and up to the second order of accuracy (that is, again, the first non-trivial term)

$$S(q_{M,\tau}) = S(M) + \frac{\tau^2}{2}\langle\Delta_{f^*_M}, \Delta_{f^*_M}\rangle_{f^*_M}. \tag{50}$$

For a regular conservative chains, in the first order

$$f_1 = f^*_{M(\tau)} - \frac{\tau}{2}\Delta_{f^*_{M_0}}. \tag{51}$$

For chains (46), in the first order

$$f_1 = f^*_{M(\tau+\vartheta)} - \frac{\tau}{2}\Delta_{f^*_{M_0}}. \tag{52}$$

Kinetic modeling for non-zero dissipation. 2. Deformed involution in irregular chains

For irregular chains, we introduce dissipation without change of the time step τ. Let us, after entropic involution, shift the point to the quasi-equilibrium state (Fig. 10) with some entropy increase $\sigma(M)$. Because of entropy production formula (45),

$$\sigma(M) = \tau\kappa(M)\langle\Delta_{f^*_M}, \Delta_{f^*_M}\rangle_{f^*_M}. \tag{53}$$

This formula works, if there is sufficient amount of non-equilibrium entropy, the difference $S(M_n) - S(f_n)$ should not be too small. In average, for several (two) successive steps it should not be less than $\sigma(M)$. The Ehrenfest's chain gives a limit for possible value of $\kappa(M)$ that we can realize using irregular chains with overrelaxation:

$$\kappa(M) < \frac{\tau}{2}. \tag{54}$$

Let us call the value $\kappa(M) = \frac{\tau}{2}$ the *Ehrenfest's limit*. Formally, it is possible to realize a chain of kinetic curves with time step τ for $\kappa(M) > \frac{\tau}{2}$ on the other side of the Ehrenfest's limit, without overrelaxation (Fig. 11).

Let us choose the following notation for non-equilibrium entropy: $s_0 = S(M_0) - S(f_0)$, $s_1 = S(M_1) - S(f_1)$, $s_\tau(M) = \frac{\tau^2}{2}\langle \Delta_{f^*_M}, \Delta_{f^*_M}\rangle_{f^*_M}$. For the three versions of steps (Fig. 11) the entropy gain $\sigma = s(f_1) - S(I_S(\Theta_\tau(f_0)))$ in the main order in τ is:

- For overrelaxation ($\kappa(M) < \frac{\tau}{2}$) $\sigma = s_\tau + s_0 - s_1 - 2\sqrt{s_\tau s_0}$;
- For the Ehrenfest's chain (full relaxation, $\kappa(M) = \frac{\tau}{2}$) $s_0 = s_1 = 0$ and $\sigma = s_\tau$;
- For underrelaxation ($\kappa(M) > \frac{\tau}{2}$) $\sigma = s_\tau + s_0 - s_1 + 2\sqrt{s_\tau s_0}$.

After averaging in successive steps, the term $s_0 - s_1$ tends to zero, and we can write the estimate of the average entropy gain $\langle\sigma\rangle$: for overrelaxation $\langle\sigma\rangle = s_\tau - 2\sqrt{s_\tau\langle s_0\rangle}$ and for underelaxation $\langle\sigma\rangle = s_\tau + 2\sqrt{s_\tau\langle s_0\rangle}$.

In the really interesting physical problems the kinetic coefficient $\kappa(M)$ is non-constant in space. Macroscopic variables M are functions of space, $\kappa(M)$ is also a function, and it is natural to take a space-dependent step of macroscopic entropy production $\sigma(M)$. It is possible to organize the involution (incomplete involution) step at different points with different density of entropy production step σ.

Which entropy rules the kinetic model?

For linear kinetic equations, for example, for the free flight equation (31) there exist many concave Lyapunov functionals (for dissipative systems) or integrals of motion (for conservative systems), see, for example, (4).

There are two reasonable conditions for entropy choice: additivity with respect to joining of independent systems, and trace form (sum or integral of some function $h(f, f^*)$). These conditions select a one-parametric family [33, 34], a linear combination of the classical Boltzmann–Gibbs–Shannon entropy with $h(f) = -f\ln f$ and the Burg Entropy with $h(f) = \ln f$, both in the Kullback form:

$$S_\alpha = -\alpha\int f\ln\frac{f}{f^*}\,\mathrm{d}\Gamma(x) + (1-\alpha)\int f^*\ln\frac{f}{f^*}\,\mathrm{d}\Gamma(x),$$

where $1 \geq \alpha \geq 0$, and $f^*\mathrm{d}\Gamma$ is invariant measure. Singularity of the Burg term for $f \to 0$ provides the positivity preservation in all entropic involutions.

If we weaken these conditions and require that there exists such a monotonic (nonlinear) transformation of entropy scale that in one scale entropy is additive, and in transformed one it has a trace form, then we get additionally a family of Renyi–Tsallis entropies with $h(f) = \frac{1-f^q}{1-q}$ [34] (these entropies and their applications are discussed in details in [35]).

Both the Renyi–Tsallis entropy and the Burge entropy are in use in the entropic lattice Boltzmann methods from the very beginning [36, 77]. The connection of this entropy choice with Galilei invariance is demonstrated in [36].

In this section, we presented the theoretical backgrounds of kinetic modelling. These problems were discussed previously for development of lattice Boltzmann methods in computational fluid dynamics. The "overrelaxation" appeared in [76]. In papers [78, 79] the overrelaxation based method for the Navier–Stokes equations was further developed, and the entropic involution was invented in [77]. Due to historical reasons, we propose to call it the *Karlin–Succi* involution. The problem of computational stability of entropic lattice Boltzmann methods was systematically analyzed in [81,82]. H-theorem for lattice Boltzmann schemes was presented with details and applications in [80]. For further discussion and references we address to [14].

3 Errors of Models, ε-trajectories and Stable Properties of Structurally Unstable Systems

3.1 Phase flow, attractors and repellers

Phase flow

In this section, we return from kinetic systems to general dynamical systems, and lose such specific tools as entropy and quasi-equilibrium. Topological dynamics gives us a natural language for general discussion of limit behaviour and relaxation of general dynamical systems [83]. We discuss a general dynamical system as a semigroup of homeomorphisms (phase flow transformations): $\Theta(t, x)$ is the result of shifting point x in time t.

Let the phase space X be a compact metric space with the metrics ρ,

$$\Theta : [0, \infty[\times X \to X \tag{55}$$

be a continuous mapping for any $t \geq 0$; let mapping $\Theta(t, \cdot) : X \to X$ be homeomorphism of X into subset of X and let these homeomorphisms form monoparametric semigroup:

$$\Theta(0, \cdot) = \mathrm{id},\ \Theta(t, \Theta(t', x)) = \Theta(t + t', x) \tag{56}$$

for any $t, t' \geq 0, x \in X$.

Below we call the semigroup of mappings $\Theta(t, \cdot)$ a *semiflow of homeomorphisms* (or, for short, semiflow), or simply system (55). We assume that the continuous map $\Theta(t, x)$ is continued to negative time t as far as it is possible with preservation of the semigroup property (56). For phase flow we use also notations Θ_t and $\Theta_t(x)$. For any given $x \in X$, *x-motion* is a function of time $\Theta(t, x)$, x-motion is the *whole motion* if the function is defined on the whole axis $t \in]-\infty, \infty[$. The image of x-motion is the *x-trajectory*.

Attractors and repellers

First of all, for the description of limit behaviour we need a notion of an ω-limit set.

A point $p \in X$ is called ω- (α-)*-limit point* of the x-motion (correspondingly of the whole x-motion), if there is such a sequence $t_n \to \infty$ ($t_n \to -\infty$) that $\Theta(t_n, x) \to p$ as $n \to \infty$. The totality of all ω- (α-)-limit points of x-motion is called its ω- (α-)*-limit set* and is denoted by $\omega(x)$ ($\alpha(x)$).

A set $W \subset X$ is called *invariant* set, if, for any $x \in W$, the x-motion is whole and the whole x-trajectory belongs to W.

The sets $\omega(x)$, $\alpha(x)$ (the last in the case when x-motion is whole) are nonempty, closed, connected, and invariant.

The set of all ω-limit points of the system $\omega_\Theta = \bigcup_{x \in X} \omega(x)$ is nonempty and invariant, but may be disconnected and not closed. The sets $\omega(x)$ might be considered as attractors, and the sets $\alpha(x)$ as repellers (attractors for $t \to -\infty$). The system of these sets represents all limit behaviours of the phase flow.

Perhaps, the most constructive idea of attractor definition combines pure topological (metric) and measure points of view. A *weak attractor* [87] is a closed (invariant) set A such that the set $At(A) = \{x \mid \omega(x) \subset A\}$ has strictly positive measure. A *Milnor attractor* [86] is such a weak attractor that there is no strictly smaller closed $A' \subsetneqq A$ so that $At(A)$ coincides with $At(A')$ up to a set of measure zero. If A is a Milnor attractor and for any closed invariant proper subset $A' \subsetneqq A$ the set $At(A')$ has zero measure, then we say that A is a *minimal Milnor attractor.*

Below in this section we follow a purely topological (metric) point of view, but keep in mind that its combination with measure–based ideas create a richer theory.

The dream of applied dynamics

Now we can formulate the "dream of applied dynamics." There is such a finite number of invariant sets $A_1, \dots A_n$ that:

- Any attractor or repeller is one of the A_i;
- The following relation between sets $A_1, \dots A_n$ is acyclic: $A_i \succeq A_j$ if there exists such x that $\alpha(x) = A_i$ and $\omega(x) = A_j$;
- The system $A_1, \dots A_n$ with the preorder $A_i \succeq A_j$ does not change qualitatively under sufficiently small perturbations of the dynamical system: all the picture can be restored by a map that is close to id.

For generic two-dimensional systems this dream is the reality: there is a finite number of fixed points and closed orbits such that any motion goes to one of them at $t \to \infty$, and to another one at $t \to -\infty$ for a whole motion.

The multidimensional analogues of generic two-dimensional systems are the Morse–Smale systems. For them all attractors and repellers are fixed points or closed orbits. The relation $A_i \succeq A_j$ for them is the *Smale order.*

But the class of the Morse–Smale systems is too narrow: there are many systems with more complicated attractors, and some of these systems are structurally stable and do not change qualitatively after sufficiently small perturbations.[4] It is necessary to take into account that typically some of motions have smaller attractors (for example, in A_i exists a dense set of closed orbits), and $\omega(x) = A_j$ not for all, but for almost all x. Finally, the "dream of applied dynamics" was destroyed by S. Smale [16]. He demonstrated that "structurally stable systems are not dense." It means that even the last item of this dream contradicts the multidimensional reality.

3.2 Metric coarse-graining by ε-motions

ε-motions

The observable picture must be structurally stable. Any real system exists under the permanent perturbing influence of the external world. It is hardly possible to construct a model taking into account all such perturbations. Besides that, the model describes the internal properties of the system only approximately. The discrepancy between the real system and the model arising from these two circumstances is different for different models. So, for the systems of celestial mechanics it can be done very small. Quite the contrary, for chemical engineering this discrepancy can be if not too large but not such small to be neglected. Structurally unstable features or phase portrait should be destroyed by such an unpredictable divergence of the model and reality. The perturbations "conceal" some fine details of dynamics, therefore these details become irrelevant to analysis of real systems.

There are two traditional approaches to the consideration of perturbed motions. One of them is to investigate the motion in the presence of small sustained perturbations [93,94,96], the other is the study of fluctuations under the influence of small stochastic perturbations [97,98]. In this section, we join mainly the first direction.

A small unpredictable discrepancy between the real system and the dynamical model can be simulated by periodical "fattening." For a set $A \subset X$ its ε-fattening is the set

$$A_\varepsilon = \{x \mid \rho(x, y) < \varepsilon \text{ for all } y \in A\}. \tag{57}$$

Instead of one x-motion we consider motion of a set, $A(t) = \Theta_t A$, and combine this motion with periodical ε-fattening for a given period τ. For superposition of Θ_τ with ε-fattening we use the notation $\mathbf{\Theta}_\tau^\varepsilon$:

$$\mathbf{\Theta}_\tau^\varepsilon A = (\Theta_\tau . A)_\varepsilon \tag{58}$$

For $t \in [n\tau, (n+1)\tau[$ We need to generalize this definition for $t \in [n\tau, (n+1)\tau[$:

[4] Review of modern dynamics is presented in [84, 85]

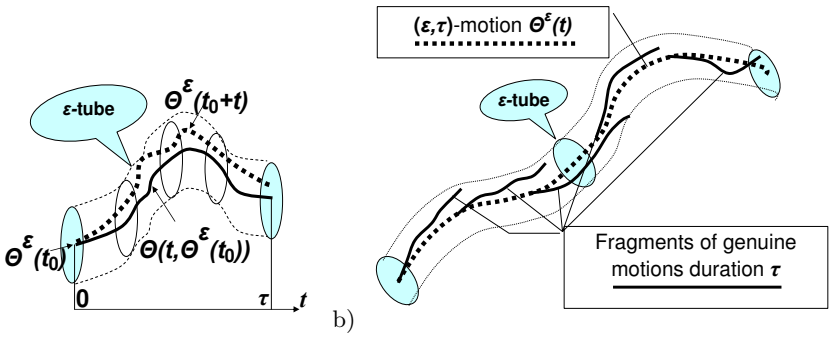

Fig. 12. An (ε,τ)-motion $\Theta^\varepsilon(t_0+t)$ $(t\in[0,\tau])$ in the ε-tube near a genuine motion $\Theta(t,\Theta^\varepsilon(t_0))$ $(t\in[0,\tau])$ duration τ (a), and an (ε,τ)-motion $\Theta^\varepsilon(t)$ with fragments of genuine motions duration τ in the ε-tube near $\Theta^\varepsilon(t)$ (b).

$$\mathbf{\Theta}^\varepsilon_t A = \Theta_{t-n\tau}((\mathbf{\Theta}^\varepsilon_\tau)^n A). \tag{59}$$

Analysis of these motions of sets gives us the information about dynamics with ε-uncertainty in model. Single-point sets are natural initial conditions for such motions.

One can call this coarse-graining the *metric coarse-graining*, and the Erenfest's coarse-graining for dynamics of distribution function might be called the *measure coarse-graining*. The concept of *metric–measure spaces* (*mm*-spaces [99]) gives the natural framework for analysis of various sorts of coarse-graining.

It is convenient to introduce individual ε-motions. A function of time $\Theta^\varepsilon(t)$ with values in X, defined at $t\geq 0$, is called (ε,x)-motion $(\varepsilon>0)$, if $\Theta^\varepsilon(0)=x$ and for any $t_0\geq 0$, $t\in[0,\tau]$ the inequality $\rho(\Theta^\varepsilon(t_0+t),\Theta(t,\Theta^\varepsilon(t_0)))<\varepsilon$ holds. In other words, if for an arbitrary point $\Theta^\varepsilon(t_0)$ one considers its motion due to phase flow of dynamical system, this motion will diverge $\Theta^\varepsilon(t_0+t)$ from no more than at ε for $t\in[0,\tau]$. Here $[0,\tau]$ is a certain interval of time, its length τ is not very important (it is important that it is fixed), because later we shall consider the case $\varepsilon\to 0$. For a given τ we shall call the (ε,x)-motion (ε,x,τ)-motion when reference to τ is necessary. On any interval $[t_0,t_0+\tau]$ an (ε,x,τ)-motion deviates from a genuine motion not further than on distance ε if these motions coincide at time moment t_0 (Fig. 12a). If a genuine motion starts from a point of an (ε,x,τ)-trajectory, it remains in the ε-tube near that (ε,τ)-motion during time τ (Fig. 12b).

Limit sets of ε-motions

Let us study the limit behaviour of the coarse-grained trajectories $\mathbf{\Theta}^\varepsilon_t A$, and than take the limit $\varepsilon\to 0$. For systems with complicated dynamics, this limit may differ significantly from the limit behaviour of the original system for $\varepsilon=0$. This effect of the perturbation influence in the zero limit is a "smile of

a Cheshire cat:" the cat tends to disappear, leaving only its smile hanging in the air.

For any $\Theta^\varepsilon(t)$ the ω-limit set $\omega(\Theta^\varepsilon)$ is the set of all limit points of $\Theta^\varepsilon(t)$ at $t \to \infty$. For any $x \in X$ a set $\omega^\varepsilon(x)$ is a totality of all ω-limit points of all (ε, x)-motions:

$$\omega^\varepsilon(x) = \bigcup_{\Theta^\varepsilon(0)=x} \omega(\Theta^\varepsilon).$$

For $\varepsilon \to 0$ we obtain the set

$$\omega^0(x) = \bigcap_{\varepsilon>0} \omega^\varepsilon(x).$$

Firstly, it is necessary to notice that $\omega^\varepsilon(x)$ does not always tend to $\omega(x)$ as $\varepsilon \to 0$: the set $\omega^0(x)$ may not coincide with $\omega(x,k)$.

The sets $\omega^0(x)$ are closed and invariant. Let $x \in \omega^0(x)$. Then for any $\varepsilon > 0$ there exists periodical (ε, x)-motion (This is a version of Anosov's C^0-closing lemma [85, 88]).

The function $\omega^0(x)$ is *upper semicontinuous*. It means that for any sequence $x_i \to x$ all limit points of all sequences $y_i \in \omega^0(x_i)$ belong to $\omega^0(x)$.

In order to study the limit behaviour for all initial conditions, let us join all $\omega^0(x)$:

$$\omega^0 = \bigcup_{x\in X} \omega^0(x) = \bigcup_{x\in X} \bigcap_{\varepsilon>0} \omega^\varepsilon(x) = \bigcap_{\varepsilon>0} \bigcup_{x\in X} \omega^\varepsilon(x). \tag{60}$$

The set ω^0 is closed and invariant. If $y \in \omega^0$ then $y \in \omega^0(y)$. If $Q \subset \omega^0$ and Q is connected, then $Q \subset \omega^0(y)$ for any $y \in Q$.[5]

The ε-motions were studied earlier in differential dynamics, in connection with the theory of Anosov about ε-trajectories and its applications [88–92]. For systems with hyperbolic attractors an important *ε-motion shadowing property* was discovered: for a given $\eta > 0$ and sufficiently small $\varepsilon > 0$ for any ε-motion $\Theta^\varepsilon(t)$ there exists a motion of the non-perturbed system $\Theta(t, x)$ that belongs to η - neighborhood of $\Theta^\varepsilon(t)$:

$$\rho(\Theta^\varepsilon(\phi(t)), \Theta(t, x)) < \eta,$$

for $t > 0$ and some monotonous transformation of time $\phi(t)$ $(t - \phi(t) = O(\varepsilon t))$. The sufficiently small coarse-graining changes nothing in dynamics of systems with this shadowing property, because any ε-motion could be approximated uniformly by genuine motions on the whole semiaxis $t \in [0, \infty[$.

Preorder and equivalence generated by dynamics

Let $x_1, x_2 \in X$. Let us say $x_1 \succsim_\Theta x_2$ if for any $\varepsilon > 0$ there exists such a (ε, x_1)-motion $\Theta^\varepsilon(t)$ $(\Theta^\varepsilon(0) = x_1)$ that $\Theta^\varepsilon(t_0) = x_2$ for some $t_0 \geq 0$.

[5] For all proofs here and below in this section we address to [18, 19].

Let $x_1, x_2 \in X$. Say that points x_1 and x_2 are Θ-*equivalent* (denotation $x_1 \sim_\Theta x_2$), if $x_1 \succsim_\Theta x_2$ and $x_2 \succsim_\Theta x_1$.

The relation $\succsim_\Theta$ is a closed Θ-invariant preorder relation on X:

- It is reflexive: $x \succsim_\Theta x$ for all $x \in X$;
- It is transitive: $x_1 \succsim_\Theta x_2$ and $x_2 \succsim_\Theta x_3$ implies $x_1 \succsim_\Theta x_3$;
- The set of pairs (x_1, x_2), for which $x_1 \sim_\Theta x_2$ is closed in X;
- If $x_1 \succsim_\Theta x_2$ then $\Theta(t, x_1) \succsim_\Theta \Theta(t, x_2)$ for any $t > 0$.

The necessary and sufficient conditions for the preorder $\succsim_\Theta$ relation are as follows: $x_1 \succsim_\Theta x_2$ if and only if either $x_2 \in \omega^0(x_1)$ or $x_2 = \Theta(t, x_1)$ for some $t \geq 0$. Therefore,

$$\omega^0(x) = \{y \in \omega^0 \mid x \succsim_\Theta y\} \tag{61}$$

The relation $\sim_\Theta$ is a closed Θ-invariant equivalence relation:

- The set of pairs (x_1, x_2), for which $x_1 \sim_\Theta x_2$ is closed in X;
- If $x_1 \sim x_2$ and $x_1 \neq x_2$, then x_1- and x_2-motions are whole and $\sim_\Theta \Theta(t, x_2)$ for any $t \in]-\infty, \infty[$ $\Theta(t, x_1)$.

If $x_1 \neq x_2$, then $x_1 \sim_\Theta x_2$ if and only if $\omega^0(x_1) = \omega^0(x_2)$, $x_1 \in \omega^0(x_1)$, and $x_2 \in \omega^0(x_2)$.

Compare with [97], where analogous theorems are proved for relations defined by action functional for randomly perturbed dynamics.

The coarsened phase portrait

We present the results about the coarsened phase portrait as a series of theorems.

Let us remind, that topological space is called *totally disconnected* if there exist a base of topology, consisting of sets which are simultaneously open and closed. Simple examples of such spaces are discrete space and Cantor's discontinuum. In a totally disconnected space all subsets with more than one element are disconnected. Due to the following theorem, in the coarsened phase portrait we have a totally disconnected space instead of finite set of attractors mentioned in the naive dream of applied dynamics.

Theorem 1. *The quotient space $\omega^0/\sim_\Theta$ is compact and totally disconnected.*

The space $\omega^0/\sim_\Theta$ with the factor-relation $\succsim_\Theta$ on it is the *generalized Smale diagram* with the *generalized Smale order* on it [18, 19].

Attractors and basins of attraction are the most important parts of a phase portrait. Because of (61), all attractors are *saturated downwards*. The set $Y \subset \omega^0$ is saturated downwards, if for any $y \in Y$,

$$\{x \in \omega^0 \mid y \succsim_\Theta x\} \subset Y.$$

Every saturated downwards subset in ω^0 is saturated also for the equivalence relation $\sim_\Theta$ and includes with any x all equivalent points. The following theorem states that coarsened attractors Y (open in ω^0 saturated downwards subsets of ω^0) have open coarsened basins of attraction $At^0(Y)$.

Theorem 2. *Let $Y \subset \omega^0$ be open (in ω^0) saturated downwards set. Then the set $At^0(Y) = \{x \in X \mid \omega^0(x) \subset Y\}$ is open in X.*

There is a natural expectation that ω-limit sets can change by jumps on boundaries of basins of attraction only. For the coarsened phase portrait it is true.

Theorem 3. *The set B of all points of discontinuity of the function $\omega^0(x)$ is the subset of first category in X.*[6] *If $x \in B$ then $\Theta(t, x) \in B$ for all t when $\Theta(t, x)$ is defined.*

Theorem 4. *Let $x \in X$ be a point of discontinuity of the function $\omega^0(x)$. Then there is such open in ω^0 saturated downwards set W that $x \in \partial At^0(W)$.*

The function $\omega^0(x)$ is upper semicontinuous, hence, in any point x^* of its discontinuity the *lower semicontinuity* is broken: there exist a point $y^* \in \omega^0(x^*)$, a number $\eta > 0$, and a sequence $x_i \to x^*$ such that

$$\rho(y^*, y) > \eta \text{ for any } y \in \omega^0(x_i) \text{ and all } i.$$

The classical Smale order for hyperbolic systems was defined on a finite totality $A_1, \dots A_n$ of basic sets that are closed, invariant, and transitive (i.e. containing a dense orbit). $A_i \succ A_j$ if there exists such $x \in X$ that x-trajectory is whole, $\alpha(x) \subset A_i$, $\omega(x) \subset A_j$. Such special trajectories exist in the general case of coarsened dynamical system also.

Theorem 5. *Let X be connected, ω^0 be disconnected. Then there is such $x \in X$ that x-motion is whole and $x \notin \omega^0$. There is also such partition of ω^0 that*

$$\omega^0 = W_1 \cup W_2,\ W \cap W_2 = \varnothing,\ \alpha_f(x) \subset W_1,\ \omega^0(x) \subset W_2,$$

and $W_{1,2}$ are open and, at the same time, closed subsets of ω^0 (it means that $W_{1,2}$ are preimages of open–closed subsets of the quotient space $\omega^0 / \sim_\Theta$).

This theorem can be applied, by descent, to connected closures of coarsened basins of attraction $At^0(Y)$ (see Theorem 2).

Theorems 1–5 give us the picture of coarsened phase portrait of a general dynamical system, and this portrait is qualitatively close to phase portraits of structurally stable systems: rough 2D systems, the Morse–Smale systems and the hyperbolic Smale systems. For proofs and some applications we address to [18, 19].

[6] A set of first category, or a meagre set is a countable union of nowhere dense sets. In a complete metric space a complement of a meagre set is dense (the Baire theorem).

Stability of the coarsened phase portrait under smooth perturbations of vector fields

In order to analyze stability of this picture under the perturbation of the vector field (or the diffeomorphism, for discrete time dynamics) it is necessary to introduce C^k ε-fattening in the space of smooth vector fields instead of periodic ε-fattening of phase points. We shall discuss a C^k-smooth dynamical system Θ on a compact C^m-manifold $M (0 \le k \le m)$. Let Θ_t be the semigroup of phase flow transformations (shifts in time $t \ge 0$) and $U_\varepsilon(\Theta)$ be the set of phase flows that corresponds to a closed ε-neighborhood of system Θ_t in the C^k-norm topology of vector fields. The positive semi-trajectory of phase point x is a set $\Theta(x) = \{\Theta_t(x) : t \ge 0\}$. The C^k ε-fattened semi-trajectory is $\Theta^\varepsilon(x) = \bigcup_{\Phi \in U_\varepsilon(\Theta)} \Phi(x)$. Let us take this set with all limits for $t \to \infty$. It is the closure $\overline{\Theta^\varepsilon(x)}$. After that, let us take the limit $\varepsilon \to 0$: $P_x = \bigcap_{\varepsilon > 0} \overline{\Theta^\varepsilon(x)}$ (it is an analogue of $\Theta(x) \cup \omega_0(x)$ from our previous consideration for general dynamical systems). Following [17] let us call this set P_x a *prolongation* of the semi-trajectory $\Theta(x)$.

A trajectory of a dynamical system is said to be *stable under C^k constantly-acting perturbations* if its prolongation is equal to its closure: $P_x = \overline{\Theta(x)}$

For a given dynamical system let $L(\Theta)$ denote the union of all trajectories that are stable in the above sense and let $\mathbb{L}_1$ be the set of all dynamical systems Θ for which $L(\Theta)$ is dense in phase space: $\overline{L(\Theta)} = M$. All structurally stable systems belong to $\mathbb{L}_1$. The main result of [17] is as follows:

Theorem 6. *The set $\mathbb{L}_1$ is a dense $\mathbb{G}_\delta$ in the space of C^k dynamical systems with the C^k norm.*[7]

So, for almost all smooth dynamical systems almost all trajectories are stable under smooth constantly-acting perturbations: this type of stability is typical.

4 Conclusion

Two basic ideas of coarse-graining are presented. In the Ehrenfest's inspired approach the dynamics of distributions with averaging is studied. In the metric approach the starting point of analysis is dynamics of sets with periodical ε-fattening.

The main question of the Ehrenfest's coarse-graining is: where should we take the coarse-graining time τ? There are two limit cases: $\tau \to 0$ and $\tau \to \infty$ (physically, ∞ here means the time that exceeds all microscopic time scales). The first limit, $\tau \to 0$, returns us to the quasi-equilibrium approximation. The

[7] In a topological space a $\mathbb{G}_\delta$ set is a countable intersection of open sets. A complement of a dense $\mathbb{G}_\delta$ set is a countable union of nowhere dense sets. It is a set of first category, or a meagre set.

second limit is, in some sense, exact (if it exists). Some preliminary steps in the study of this limit are made in [4,64,65]. On this way, the question about proper values of the Prandtl number, as well, as many other similar questions about kinetic coefficients, has to be solved.

The constructed family of chains between conservative (with the Karlin–Succi involution) and maximally dissipative (with Ehrenfest's projection) ones give us a possibility to model hydrodynamic systems with various dissipation (viscosity) coefficients that are decoupled with time steps. The *collision integral* is successfully substituted by combinations of the involution and projection.

The metric coarse-graining by ε-motions in the limit $\varepsilon \to 0$ gives the stable picture with the totally disconnected totality of basic sets that form sources and sinks structure in the phase space. Everything looks nice, but now we need algorithms for effective computation and representation of the coarsened phase portrait even in modest dimensions 3-5 (for discrete time systems in dimensions 2-4).

It is necessary to build a bridge between theoretical topological picture and applied computations. In some sense, it is the main problem of modern theory of dynamical system to develop language and tools for constructive analysis of arbitrary dynamics. Of course, the pure topological view is unsufficient, and we need an interplay between measure and topology of dynamical systems, perhaps, with inclusion of some physical and probabilistic ideas.

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