

Geometry of irreversibility: Film of nonequilibrium states

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

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

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

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

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

A general geometrical setting of nonequilibrium thermodynamics is developed. The approach is based on the notion of the natural projection which generalizes Ehrenfests' coarse-graining. It is demonstrated how derivations of irreversible macroscopic dynamics from the microscopic theories can be addressed through a study of stability of quasi-equilibrium manifolds.

To solve the problem of irreversibility we have introduced the notion of the macroscopically definable ensembles. They are result of evolution of ensembles from the quasi-equilibrium initial conditions (ensembles of conditional maximum of the entropy under fixed macro-variables).

The notion of the invariant film of non-equilibrium states, and the method of its approximate construction allow us to solve the problem of macro-kinetic in cases when there are no autonomous equations of macro-kinetic.

The goal of this paper is to discuss the (nonlinear) problem of irreversibility, and how the nonequilibrium thermodynamics attempts to solve it. This problem has been intensively discussed in the past, and nice accounts of these discussions can be found in the literature. Here, we intend to develop a more geometrical viewpoint on the subject. The paper consists of two parts. First, we discuss in an informal way the origin of the problem, and demonstrate how the basic constructions arise. Second, we give a consistent geometric formalization of these constructions. Our presentation is based on the notion of the natural projection. We discuss in detail the method of natural projector as the consistent formalization of Ehrenfest's ideas of coarse-graining.

A one-dimensional model of nonequilibrium states is introduced. In the background of many derivations of nonequilibrium kinetic equations there is present the following picture: Above each point of the quasi-equilibrium manifold there is located a huge subspace of nonequilibrium distributions with the same values of the macroscopic variables, as in the quasi-equilibrium point. It is as if the motion decomposes into two projections, above

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

the point on the quasi-equilibrium manifold, and in the projection on this manifold. The motion in each layer above the points is highly complicated, but fast, and everything quickly settles in this fast motion.

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

The novel approach allows to go beyond limitations of the short memory approximations through a study of stability of the quasi-equilibrium manifold.

The one-dimensional models of nonequilibrium states form a *film of nonequilibrium states* over the quasiequilibrium manifold. We present a collection of methods for the film construction. The notion of the invariant film of non-equilibrium states, and the method of its approximate construction allow us to solve the problem of macro-kinetic in cases when there are no autonomous equations of macro-kinetic.