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Irreversibility in Thermodynamics

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The problem of irreversibility in thermodynamics is revisited and analyzed on the microscopic, stochastic, and macroscopic levels of description. It is demonstrated that Newtonian dynamics can be represented in the Reynolds form when each dynamical variable is decomposed into mean and fluctuation components. Additional equations coupling fluctuations and the mean values follow from the stabilization principle. The main idea of this principle is that the fluctuations must be selected from the condition that they suppress the original instability down to a neutral stability. Supplemented by the stabilization principle, the Hamiltonian or Lagrangian formalisms can describe the transition from fully reversible to irreversible motions as a result of the decomposition of chaotic motions (which are very likely to occur in many-body problems) into regular (macroscopic) motions and fluctuations. On the stochastic level of description, a new phenomenological force with non-Lipschitz properties is introduced. This force, as a resultant of a large number of collisions of a selected particle with other particles, has characteristics which are uniquely defined by the thermodynamic parameters of the process under consideration, and it represents a part of the mathematical formalism describing a random-walk-like process without invoking any probabilistic arguments. Additional non-Lipschitz thermodynamic forces are incorporated into macroscopic models of transport phenomena in order to introduce a time scale. These forces are effective only within a small domain around equilibria. Without causing any changes in other domains, they are responsible for the finite time of approaching equilibria. Such a property is very important for the interpretation of irreversibility on the macroscopic scale.

INTRODUCTION

Transport phenomena such as thermal conductivity and diffusion represent nonequilibrium thermodynamic processes which are described by parabolic partial differential equations of the following type:

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$$\frac{\partial u}{\partial t} = \mathfrak{D}_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j}, \qquad \mathfrak{D}_{ij} = \text{const} \tag{1}$$

It is known that equation (1) subject to the initial condition

$$u\big|_{t=0} = u_0(x) \tag{2}$$

has a unique bounded solution for $t > 0$.

However, for $t < 0$ the same problem is ill posed, and this expresses the fundamental property of irreversibility of thermal conductivity and diffusion. Actually this property directly follows from the second law of thermodynamics.

Although solutions to equation (1) are in sufficiently good agreement with experiments, there are still some logical difficulties in reconciling this macroscopic phenomenological model with the fully reversible Hamiltonian dynamics on the microscopic level, since the irreversible processes described by (1) are completely composed of reversible events; this is known as the irreversibility paradox. However, strictly speaking, the formal derivation of equation (1) from microscopic Hamiltonian mechanics requires some additional arguments of a probabilistic nature. But can these arguments be represented in terms of classical mechanics? Or, more precisely, can they be replaced by some equivalent mechanical forces on the microscopic level?

1. NON-LIPSCHITZ MECHANICS

Turning to governing equations of classical dynamics

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} = \frac{\partial L}{\partial q_i} - \frac{\partial R}{\partial \dot{q}_i}, \qquad i = 1, 2, \ldots, n \tag{3}$$

where L is the Lagrangian, q_i, $\dot{q}_i$ are the generalized coordinates and velocities, and R is the dissipation function, one should recall that the structure of $R(\dot{q}_i, \ldots, \dot{q}_n)$ is not prescribed by Newton's laws: some additional assumptions need to be made in order to define it. The "natural" assumption (which has been never challenged) is that these functions can be expanded in Taylor series with respect to equilibrium states: $\dot{q}_i = 0$. Obviously this requires the existence of the derivative

$$\left|\frac{\partial^2 R}{\partial \dot{q}_i\, \partial \dot{q}_i}\right| < \infty \qquad \text{at} \quad \dot{q}_i \to 0$$

A departure from this condition was proposed in Zak (1992, 1993a,b), where the following dissipation function was introduced:

$$R = \frac{1}{k+1} \sum_i \alpha_i \left| \sum_j \frac{\partial r_i}{\partial q_j} \dot{q}_j \right|^{k+1} \tag{4}$$

in which

$$k = \frac{p}{p+2} < 1, \qquad p >> 1 \tag{5}$$

while p is a large, odd number.

By selecting large p, one can make k close to 1 so that (4) is almost identical to the classical condition (when $k = 1$) everywhere excluding a small neighborhood of the equilibrium point $\dot{q}_j = 0$, while at this point

$$\left| \frac{\partial^2 R}{\partial \dot{q}_i \partial \dot{q}_j} \right| \to \infty \qquad \text{at} \quad \dot{q}_j \to 0 \tag{6}$$

Hence, the Lipschitz condition is violated; the friction force $F_i = \dfrac{\partial R}{\partial \dot{q}_i}$ grows sharply at the equilibrium point, and then it gradually approaches its "classical" value. This effect can be interpreted as a mathematical representation of a jump from static to kinetic friction, when the dissipation force does not vanish with the velocity.

It appears that this "small" difference between the friction forces at $k = 1$ and $k < 1$ leads to fundamental changes in Newtonian dynamics. In order to demonstrate this, we will consider the relationship between the total energy E and the dissipation function R:

$$\frac{dE}{dt} = -\sum_i \dot{q}_i \frac{\partial R}{\partial \dot{q}_i} = -(k+1)R \tag{7}$$

Within the small neighborhood of an equilibrium state (where the potential energy can be set to zero) the energy E and the dissipation function R have the order, respectively,

$$E \sim \dot{q}_i^2, \qquad R \sim \dot{q}_i^{k+1} \qquad \text{at} \quad E \to 0 \tag{8}$$

Hence, the asymptotic form of (7) can be represented as

$$\frac{dE}{dt} = AE^{(k+1)/2} \qquad \text{at} \quad E \to 0, \quad A = \text{const} \tag{9}$$

If $A > 0$ and $k < 1$, the equilibrium state $E = 0$ is an attractor where the Lipschitz condition ($|d\dot{E}/dE| \to \infty$ at $E \to 0$) is violated. Such a terminal attractor (Zak, 1992) is approached by the solution originating at $E = \Delta E_0 > 0$, in finite time:

$$t_0 = \int_{\Delta E_0}^{0} \frac{dE}{AE^{(k+1)/2}} = \frac{2\Delta E_0^{(1-k)/2}}{(1-k)|A|} < \infty$$

Obviously, this integral diverges in the classical case $k \geq 1$, where $t_0 \to \infty$. The motion described by (9) has a singular solution $E \equiv 0$ and a regular solution

$$E = \left[\Delta E_0^{(1-k)/2} + \frac{1}{2} A(1 - k)t \right]^{2/(1-k)}$$

In a finite time the motion can reach equilibrium and switch to the singular solution $E \equiv 0$, and this switch is irreversible.

As is well known from the dynamics of nonconservative systems, dissipative forces can destabilize the motion when they feed external energy into the system (the transmission of energy from laminar to turbulent flow in fluid dynamics, or from rotations to oscillations in dynamics of flexible systems). In terms of (9) this would mean that $A > 0$, and the equilibrium state $E = 0$ becomes a terminal repeller (Zak, 1992).

If the initial condition is infinitely close to this repeller, the transient solution will escape it during a finite time period:

$$t_0 = \int_{\epsilon \to 0}^{\Delta E_0} \frac{dE}{AE^{(k+1)/2}} = \frac{2\Delta E_0^{(1-k)/2}}{(1 - k)A} < \infty$$

while for a regular repeller, the time would be infinite.

Expressing equation (9) in terms of velocity at $i = 1$, $\dot{q}_1 = v$,

$$\dot{v} = Bv^k, \qquad B = \text{const} > 0 \tag{10}$$

one arrives at the following solution:

$$v = \pm\{[B(1 - k)t]^{p+2}\}^{1/2} \tag{11}$$

As in the case of a terminal attractor, here the motion is also irreversible: the time-backward motion obtained by formal time inversion $t \to -t$ in equation (11) is imaginary, since p is an odd number [see equation (5)].

But in addition, terminal repellers possess even more surprising characteristics: the solution (11) becomes totally unpredictable. Indeed, two different motions described by the solution (11) are possible for "almost the same" ($v_0 = +\epsilon \to 0$ or $v_0 = -\epsilon \to 0$ at $t = \to 0$) initial conditions.

Thus, a terminal repeller represents a vanishingly short, but infinitely powerful "pulse of unpredictability" which is pumped into the system via terminal dissipative forces. Obviously, failure of the uniqueness of the solution here results from the violation of the Lipschitz condition at $v = 0$.

Hence, the non-Lipschitz forces $\partial R/\partial q_i$ in equation (3) following from equations (4) and (5) change the most fundamental property of Newtonian mechanics: its determinism. At the same time, these forces affect only the dissipation function, which is not prescribed by Newton's laws anyway.

Let us turn to stochastic processes which connect microscopic mechanics and thermodynamics. These processes are based upon some probabilistic arguments which cannot be formally derived from Newtonian mechanics. But can they be derived from a non-Lipschitzian version of Newtonian mechanics? Next, based on non-Lipschitz forces, we will introduce a purely mechanical model of a random walk—the simplest stochastic process—whose macroscopic interpretation leads to equation (1).

2. MECHANICAL MODEL OF RANDOM WALK

A random walk is a stochastic process where changes occur only at fixed times; it represents the position at time t_m of a particle taking a random "step" x_m independently of its previous steps.

In order to implement this process based only upon Newton's laws, consider a rectilinear motion of a particle of unit mass driven by a non-Lipschitz force:

$$\dot{v} = \nu v^{1/3} \sin \omega t, \qquad \nu = \text{const}, \qquad [\nu] = \frac{\text{m}^{1-k}}{\text{sec}^{2-k}} \tag{12}$$

$$\dot{x} = v \tag{13}$$

where v and x are the particle velocity and position, respectively.

Subject to the zero initial condition

$$v = 0 \qquad \text{at} \quad t = 0 \tag{14}$$

equation (10) has a singular solution

$$v \equiv 0 \tag{15}$$

and a regular solution

$$v = \pm\left(\frac{4\nu}{3\omega} \sin^2 \frac{\omega}{2}\, t\right)^{3/2} \tag{16}$$

These two solutions coexist at $t = 0$, and this is possible because at this point the Lipschitz condition fails:

$$\left|\frac{\partial \dot{v}}{\partial v}\right|_{t\to 0} = k\nu v^{k-1} \sin \omega t\big|_{t\to 0} \to \infty \tag{17}$$

Since

$$\frac{\partial \dot{v}}{\partial v} > 0 \qquad \text{at} \quad |v| \neq 0, \quad t > 0 \tag{18}$$

the singular solution (15) is unstable, and the particle departs from rest following the solution (16). This solution has two (positive and negative) branches [since the power in (16) includes the square root], and each branch can be chosen with the same probability 1/2. It should be noticed that as a result of (17), the motion of the particle can be initiated by infinitesimal disturbances (which never can occur when the Lipschitz condition holds: an infinitesimal initial disturbance cannot become finite in finite time).

Strictly speaking, the solution (16) is valid only in the time interval

$$0 \le t \le \frac{2\pi}{\omega} \tag{19}$$

and at $t = 2\pi/\omega$ it coincides with the singular solution (15).

For $t > 2\pi/\omega$, equation (15) becomes unstable, and the motion repeats itself to the accuracy of the sign in equation (16).

Hence, the particle velocity v performs oscillations with respect to its zero value in such a way that the positive and negative branches of the solution (16) alternate randomly after each period equal to $2\pi/\omega$.

Turning to equation (13), one obtains the distance between two adjacent equilibrium positions of the particle:

$$x_i - x_{i-1} = \pm \int_0^{2\pi/\omega} \left(\frac{4\nu}{3\omega} \sin \frac{\omega}{2} t \right)^{3/2} dt = 64(3\omega)^{-5/2}\nu^{3/2} = \pm h \qquad (20), (21)$$

Thus, the equilibrium positions of the particle are

$$x_0 = 0, \qquad x_1 = \pm h, \qquad x_2 = \pm h \pm h \ldots \tag{22}$$

while the signs randomly alternate with equal probability 1/2.

Obviously, the particle performs an unrestricted symmetric random walk: after each time period

$$\tau = \frac{2\pi}{\omega} \tag{23}$$

it changes its value on $\pm h$ [see equation (22)].

The probability density $u(x, t)$ is governed by the following difference equation:

$$u(x, t + \tau) = \frac{1}{2} u(x - h, t) + \frac{1}{2} u(x + h, t) \tag{24}$$

while

$$\int_{-\infty}^{\infty} u(x, t)\, dx = 1 \tag{25}$$

3. PHENOMENOLOGICAL FORCE

Thus, as demonstrated above, a non-Lipschitz force

$$F = m\nu v^{1/3} \sin \omega t = \pm\gamma\left(\frac{4\nu}{3\omega}\right)^{1/2} \sin \frac{\omega}{2} t \sin \omega t \tag{26}$$

applied to a particle of mass m leads to a classical random walk.

It should be stressed that the governing equations (12), (13) are fully deterministic: they are based upon Newton's laws. The stochasticity here is generated by the alternating stability and instability effects due to failure of the Lipschitz conditions at equilibria.

Let us analyze the properties of the force (28).

First of all, the time average of this force is zero,

$$\tilde{F} = 0 \tag{27}$$

since, as follows from equation (26), the signs + and − have equal probability.

For the same reason, the ensemble average of F is also zero:

$$\langle F \rangle = 0 \tag{28}$$

The work done by the force (26) during one step is zero:

$$A = \int_0^{2\pi/\omega} Fv \,\mathrm{dt} = \pm\nu\left(\frac{4\nu}{3\omega}\right)^2 \int_0^{2\pi/\omega} \sin^4 \frac{\omega}{2} t \sin \omega t \, dt = 0 \tag{29}$$

Since the time average of the particle's kinetic energy can be expressed via the temperature, one obtains

$$\tilde{v}^2 = \left(\frac{4\nu}{3\omega}\right)^3 \int_0^{2\pi/\omega} \sin^6 \frac{\omega}{2} t \, dt = \frac{5\pi}{8\omega}\left(\frac{4\nu}{3\omega}\right)^3 = \frac{KT}{m} \tag{30}$$

Then the only unspecified parameter ν in equation (26) is expressed via the temperature:

$$\nu = \frac{3\omega}{4}\left(\frac{8\omega KT}{5\pi m}\right)^{1/3} \tag{31}$$

Here T is the absolute temperature and K is Boltzmann's constant.

The parameter ω^{-1} is of the order of the time period between collisions of the particle:

$$\omega \sim \frac{1}{\tau} \sim 10^{14} \frac{1}{\sec} \tag{32}$$

On the macroscale this is a very large number, and one can consider a continuous approximation assuming that

$$\omega \to \infty \tag{33}$$

Then, as follows from equations (20), (23), and (31),

$$\tau \to 0, \qquad h \to 0, \qquad \text{and} \qquad \frac{h^2}{\tau} \to 0.19\,\frac{KT}{m} = 2\mathfrak{D} \tag{34}$$

and therefore equation (24) can be replaced by the Fokker–Planck equation, i.e., by a one-dimensional version of equation (1). It is interesting to emphasize that the diffusion coefficient $\mathfrak{D}$ is defined by the amplitude ν of the non-Lipschitz force (26).

Now the following question can be asked: does the force (26) exist in the sense that it can be detected by direct measurements on the microscopic level? Probably not. Indeed, on that level, this force is a resultant of a large number of collisions with other particles. However, on the stochastic level as an intermediate between the micro- and macrolevels, the phenomenological force (26) represents a part of the mathematical formalism, and it can be accepted.

As follows from equation (26), on a microscale of time

$$t \sim \tau \tag{35}$$

the system (12), (13) is not conservative, and the motion is irreversible. Moreover, each time the particle arrives at an equilibrium point, it totally "forgets" its past.

On the contrary, on a macroscale of time when

$$t >> \tau \tag{36}$$

the system (12), (13) can be treated as conservative based upon equations (28) and (29), and therefore it is fully reversible. This means that the particle whose motion is described by equations (12) and (13) can return to its original position passing through all of its previous steps backward; however, the probability of such an event will be vanishingly small (but not zero!), or, in other words, the period of time t_0 during which this event can occur is very large (but finite!):

$$\tau << t_0 < \infty \tag{37}$$

4. NON-LIPSCHITZ MACROSCOPIC EFFECTS

Turning back to the macroscopic equation (1), one can notice its inconsistency with the results discussed in the last section, and in particular with the condition (37). Indeed, equation (1) does not have any time scale which would allow one to implement the condition (37): the time of approaching a thermodynamic equilibrium is unbounded, and therefore (1) excludes any reversible solutions even if $t_0 \to \infty$. The only logical way out of this situation is to introduce a time scale into equation (1) so that the time of approaching an equilibrium would be finite. Then one can argue that this time is not large enough to include reversible solutions. In order to do that, let us turn to equation (1), and, for the sake of concreteness, treat it as an equation for thermal conductivity. Then the relationship between the heat flow q and the temperature u can be sought in the following form:

$$q = q(\nabla u) \tag{38}$$

It should be emphasized that the function (38) is not prescribed by any macroscopic laws, and therefore it must be found from experiments. The basic mathematical assumption about equation (38) is its expandability in Taylor series. Then, for small gradients

$$q = -\chi \nabla u + \cdots \tag{39}$$

where χ is the thermal conductivity, and this leads to equation (1). But even if higher order gradients of u are taken into account, the time of approaching equilibria would still remain unbounded.

However, there is another possibility of representing equation (38) if one relaxes the Lipschitz condition at $\nabla u = 0$. Indeed, instead of (39) one can write

$$q = -\chi \left(\frac{\nabla u}{\epsilon_0} \right)^{k-1} \nabla u + \cdots \tag{40}$$

where k has the form (5), and ϵ_0 has the dimensionality of ∇u, i.e.,

$$[\epsilon_0] = [\nabla u] \tag{41}$$

Equation (40) is different from equation (39) only within an infinitesimally small neighborhood of the equilibrium states where

$$\nabla u \to 0 \tag{42}$$

Otherwise

$$\left(\frac{\nabla u}{\epsilon_0} \right)^{k-1} \simeq 1 \tag{43}$$

One can verify that the Lipschitz condition for the function (40) at $\nabla u \to 0$ is violated:

$$\left|\frac{\partial q}{\partial \nabla u}\right| \to \infty \qquad \text{at} \quad \nabla u \to 0 \tag{44}$$

The mathematical consequences of this property will be discussed below.

Turning to equation (40), one can write the following equation instead of (1):

$$\frac{\partial u}{\partial t} = \mathcal{D} \frac{\partial}{\partial x}\left[\left(\frac{\partial u}{\partial x}\right)^k\right], \qquad \mathcal{D} = \frac{\chi \epsilon_0^{1-k}}{\rho c} = \text{const} > 0 \tag{45}$$

where χ, c, and ρ are the coefficients of thermal conductivity, specific heat, and density, respectively. Equation (45) reduces to the classical diffusion equation:

$$\frac{\partial u}{\partial t} = \mathcal{D} \frac{\partial^2 u}{\partial x^2} \tag{46}$$

if $k = 1$.

Let us compare the solutions to equations (45) and (46) subject to the same initial and boundary conditions. Introducing the function

$$\theta = \int \left(\frac{\partial u}{\partial x}\right)^{k-1} dx \tag{47}$$

one obtains

$$\frac{d\theta}{dt} = (k+1)\int \left(\frac{\partial u}{\partial x}\right)^k \frac{\partial^2 u}{\partial x \partial t}\, dx = (k+1)\mathcal{D} \int \left(\frac{\partial u}{\partial x}\right)^k \frac{\partial^2}{\partial x^2}\left[\left(\frac{\partial u}{\partial x}\right)\right]^k dx$$

Assuming separation of the variables

$$u(x, t) = u_1(t) u_2(x) \tag{48}$$

one arrives at the following ordinary differential equation:

$$\dot{u}_1 = -A u_1^k \tag{49}$$

where

$$A = \mathcal{D} \int \left(\frac{\partial u_2}{\partial x}\right)^k \frac{\partial^2}{\partial x^2}\left[\left(\frac{\partial u}{\partial x}\right)^k\right] dx = \text{const} \tag{50}$$

For $k = 1$ [see equation (46)]

$$u_1 = \mathring{u}_1 e^{-At}, \qquad u_1^2 \to 0 \qquad \text{at} \quad t \to \infty \tag{51}$$

For $k < 1$ [see equation (45)]

$$u_1 = [(\mathring{u}_1)^{1-k} - A(1 - k)t]^{1/(1-k)} \tag{52}$$

Here

$$\mathring{u}_1 = u_1 \qquad \text{at} \quad t = 0 \tag{53}$$

Thus, as follows from equation (51), the solution to the classical equation (46) approaches the equilibrium state in infinite time, while the solution to the "scaled" equation (45) approaches the same equilibrium state in a finite time [see equation (52)]

$$t_0 = \frac{(\mathring{u}_1)^{1-k}}{(1 - k)A} < \infty \qquad \text{if} \quad k < 1 \tag{54}$$

One can notice that although equation (46) can be obtained from equation (45) as a limit at $k \to 1$, the solution (51) cannot be obtained as the same limit of equation (52). However, the quantitative difference between these solutions can be detected only within a very small neighborhood of the equilibrium when

$$\left|\frac{\partial u}{\partial x}\right| \sim \epsilon_0 \tag{55}$$

The period t_0 in equation (54) represents the macroscopic time scale

$$0 < \tau << t_0 << t_{00} < \infty \tag{56}$$

where

$$t_{00} \sim \tau n! \tag{57}$$

and

$$n \sim \frac{u_0}{\epsilon_0(\mathcal{D}\tau)^{1/2}} \tag{58}$$

Here $\tau \sim 10^{-10}$ is the relaxation time, u_0/ϵ_0 is a macroscopic representative length, and $(\mathcal{D}\tau)^{1/2}$ is of the order of the distance between two adjacent collisions.

Two new constants, k and ϵ_0, in equation (45) can be found from a simple experiment: turning to equation (54) and recording the time t_0 of approaching the state of equilibrium for different initial conditions, one can calculate k and A, and therefore ϵ_0 [see equations (45) and (50)].

Equation (45) possesses many other interesting properties such as non-uniqueness and non-Lipschitz instability with respect to infinitesimal disturbances at equilibrium. These properties and their relevance to the onset of turbulence [in the case of the fluid dynamic interpretation of equation (45)] are discussed in Zak (1992).

5. MICROSCOPIC VIEW

In the previous sections, the problem of irreversibility in thermodynamics was discussed on the stochastic and macroscopic levels of description. This and the next sections will be devoted to the same problem, but from the viewpoint of the microscopic level of description. On that level, the microscopic state of a system may be specified in terms of positions and momenta of a constituent set of particles: the atoms and molecules. Within the Born–Oppenheimer approximation, it is possible to express the Hamiltonian (or the Lagrangian) of a system as a function of nuclear variables, the (rapid) motions of electrons having been averaged out. Making the additional approximation that a classical description is adequate, one can write the Lagrange equations which govern the microscopic motion of the system:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i} - \frac{\partial L}{\partial q_i} = 0, \qquad i = 1, 2, \ldots, n, \quad L = W + \Pi \tag{59}$$

Here q_i and $\dot{q}_i$ are the generalized coordinates and velocities characterizing the system, W is the kinetic energy including translational components (as well as rotational components if polyatomic molecules are considered), and Π is the potential energy representing the effects of an external field (including, for example, the container walls), the particle interactions, and elastic collisions.

All the solutions to equation (59) are fully deterministic and reversible if the initial conditions are known exactly. But since the last requirement is physically unrealistic, small errors in initial conditions will grow exponentially in the case of instability of equation (59). (Such an instability may have the same origin as the instability in the famous three-body problem.) As a result, the solution to equation (59) acquires stochastic features, i.e., becomes chaotic, and therefore it loses its determinism and reversibility. The connection between chaotic instability and the problem of irreversibility in thermodynamics was stressed by Progogine (1980): "The structure of the equations of motion with randomness on the microscopic level then emerges as irreversibility on the macroscopic level." Based upon the same ideas as those introduced by Prigogine, we will propose a different mathematical framework for their implementation. This framework exploits the stabilization principle introduced and discussed in Zak (1994). As will be shown below, this principle imposes some additional constraints upon the motion, and that makes the solutions to (59) irreversible.

6. ORBITAL INSTABILITY IN HAMILTONIAN MECHANICS

Most dynamical processes are so complex that a universal theory which would capture all the details during all time periods is unthinkable. That is why the art of mathematical modeling is to extract only the fundamental aspects of the process and to neglect its insignificant features, without losing the core of information. But "insignificant features" is not a simple concept. In many cases even vanishingly small forces can cause large changes in the dynamical system parameters, and such situations are intuitively associated with the concept of instability. Obviously the destabilizing forces cannot be considered as "insignificant features," and therefore they cannot be ignored. But since it may not be possible for us to distinguish them at the very beginning, there is no way to incorporate them into the model. This simply means that the model is not adequate for quantitative description of the corresponding dynamical process: it must be changed or modified.

However, the instability yields important qualitative information: it shows the boundaries of applicability of the original model.

We will distinguish short- and long-term instabilities. A short-term instability occurs when the system has alternative stable states. For dissipative systems such states can be represented by static or periodic attractors. At the very beginning of the postinstability transition period, the unstable motion cannot be traced quantitatively, but it becomes more and more deterministic as it approaches the attractor. Hence, a short-term instability does not necessarily require a modification of the model. Usually this type of instability is associated with a bounded deviation of position coordinates whose changes affect the energy of the system. Indeed, if the growth of a position coordinate persists, the energy of the system would become unbounded.

Long-term instability occurs when the system does not have an alternative stable state. Such a type of instability can be associated only with ignorable coordinates since these coordinates do not affect the energy of the system. Long-term instability is the main cause of chaos. It can occur in the form of orbital instability, Hadamard's instability, Reynolds instability, etc. We will illustrate the concept of long-term instability by orbital instability.

First we recall that a coordinate q_α is called ignorable if it does not enter the Lagrangian function L and the corresponding nonconservative generalized force Q_α is zero:

$$\frac{\partial L}{\partial q_\alpha} = 0, \qquad Q_\alpha = 0 \tag{60}$$

Therefore,

$$\frac{\partial L}{\partial \dot{q}_\alpha} = P_\alpha = \text{const} \tag{61}$$

i.e., the generalized ignorable impulse P_α is constant.

As follows from equation (61), there exist such states of dynamical systems (called stationary motions) that all the position (i.e., nonignorable) coordinates retain a constant value while the ignorable coordinates vary in accordance with a linear law. For example, a regular precession of a heavy symmetric gyroscope is a stationary motion characterized by

$$\Theta = \text{const}, \qquad \dot{\psi} = \text{const}, \qquad \dot{\phi} = \text{const} \tag{62}$$

where the angle of precession ψ and the angle of pure rotation ϕ are ignorable coordinates, while the angle of nutation Θ—the angle formed by the axis of the gyroscope and the vertical—is a position coordinate.

Obviously, stationary motions are not stable with respect to ignorable velocities: a small change in $\dot{q}_\alpha$ at $t = 0$ yields, as time progresses, an arbitrarily large change in the ignorable coordinates themselves. However, since this change increases linearly (but not exponentially), the motion is still considered as predictable. In particular, the Lyapunov exponents for stationary motions are zero:

$$\sigma = \lim_{d(0)\to 0, t\to\infty} \left(\frac{1}{t}\right) \ln \frac{d(0)t}{d(0)} = 0 \tag{63}$$

However, in case of nonstationary motions, the ignorable coordinate can exhibit more sophisticated behavior. In order to demonstrate this, let us consider an inertial motion of a particle M of unit mass on a smooth pseudosphere S having a constant negative curvature:

$$G_0 = \text{const} < 0 \tag{64}$$

Remembering that trajectories of inertial motions must be geodesics of S, we will compare two different trajectories assuming that initially they are parallel and that the distance between them ϵ_0 is very small.

As shown in differential geometry, the distance between such geodesics will exponentially increase:

$$\epsilon = \epsilon_0 \exp[(-G_0)^{1/2} t], \qquad G_0 < 0 \tag{65}$$

Hence, no matter how small the initial distance ϵ_0, the current distance ϵ tends to infinity.

Let us assume now that the accuracy to which the initial conditions are known is characterized by L. This means that any two trajectories cannot be distinguished if the distance between them is less than L, i.e., if

$$\epsilon < L \tag{66}$$

The period during which the inequality (66) holds is of the order

$$\Delta t \sim \frac{1}{|(-G_0)^{1/2}|} \ln \frac{L}{\epsilon_0} \tag{67}$$

However, for

$$t >> \Delta t \tag{68}$$

these two trajectories diverge such that they can be distinguished and must be considered as two different trajectories. Moreover, the distance between them tends to infinity even if ϵ_0 is small (but not infinitesimal). That is why the motion, once recorded, cannot be reproduced again (unless the initial conditions are known exactly), and consequently, it acquires stochastic features. The Lyapunov exponent for this motion is positive and constant:

$$\sigma = \lim_{t\to\infty, d(0)\to 0} \left(\frac{1}{t}\right) \ln \frac{\epsilon_0 \exp[-G_0)^{1/2}t]}{\epsilon_0} = (-G_0)^{1/2} = \text{const} > 0 \tag{69}$$

Let us introduce a system of coordinates at the surface S: the coordinate q_1 along the geodesic meridians, and the coordinate q_2 along the parallels. In differential geometry such a system is called semigeodesic. The square of the distance between adjacent point on the pseudosphere is

$$ds^2 = g_{11}\, dq_1^2 + 2g_{12}\, dq_1\, dq_2 + g_{22}\, dq_2^2 \tag{70}$$

where

$$g_{11} = 1, \qquad g_{12} = 0, \qquad g_{22} = -\frac{1}{G_0} \exp[-2(-G)^{1/2} q_1] \tag{71}$$

The Lagrangian for the inertial motion of the particle M on the pseudosphere is expressed via the coordinates and their temporal derivatives as

$$L = g_{ij} \dot{q}_i \dot{q}_j = \dot{q}_1^2 - \frac{1}{G_0} \{\exp[-2(-G)^{1/2} q_1]\} \dot{q}_2 \tag{72}$$

and, consequently,

$$\frac{\partial L}{\partial q_2} = 0 \tag{73}$$

while

$$\frac{\partial L}{\partial q_1} \neq 0 \qquad \text{if} \quad \dot{q}_2 \neq 0 \tag{74}$$

Hence, q_1 and q_2 play the roles of position and ignorable coordinates, respectively.

Therefore, an inertial motion of a particle on a pseudosphere is stable with respect to the position coordinate q_1, but it is unstable with respect to the ignorable coordinate. However, in contrast to the stationary motions considered above, here the instability is characterized by exponential growth of the ignorable coordinate, and that is why the motion becomes unpredictable. It can be shown that such a motion becomes stochastic (Arnold, 1988).

Instability with respect to ignorable coordinates can be associated with orbital instability. Indeed, turning to the last example, one can represent the particle velocity v as the product

$$v = |\mathbf{v}|\tau$$

In the course of the instability, the velocity magnitude $|\mathbf{v}|$ and consequently the total energy remain unchanged, while all the changes affect only τ, i.e., the direction of motion. In other words, orbital instability leads to redistribution of the total energy between the coordinates, and it is characterized by positive Lyapunov exponents.

The results described above were related to the inertial motions of a particle on a smooth surface. However, they can be easily generalized to motions of any finite-degree-of-freedom mechanical system by using the concept of configuration space. Indeed, if the mechanical system has N generalized coordinates q^1 $(i = 1, 2, \ldots, N)$ and is characterized by the kinetic energy

$$W = \alpha_{ij}\dot{q}^i\dot{q}^j \tag{75}$$

then the configuration space can be introduced as an N-dimensional space with the following metric tensor:

$$g_{ij} = a_{ij} \tag{76}$$

while the motion of the system is represented by the motion of the unit-mass particle in this configuration space.

In order to continue the analogy to the motion of a particle on a surface in actual space, we will consider only two-dimensional subspaces of the N-dimensional configuration space, without loss of generality. Indeed, a motion which is instable in any such subspace has to be qualified as unstable in the entire configuration space.

Now the Gaussian curvature of a two-dimensional configuration subspace (q^1, q^2) follows from the Gauss formula

$$G = \frac{1}{a_{11}a_{22} - a_{12}^2}\left(\frac{\partial^2 a_{12}}{\partial q^1 \partial q^2} - \frac{1}{2}\frac{\partial^2 a_{11}}{\partial q^2 \partial q^2} - \frac{1}{2}\frac{\partial^2 a_{22}}{\partial q^1 \partial q^1}\right) - \Gamma_{12}^{\gamma}\Gamma_{12}^{\delta}a_{\gamma\delta} - \Gamma_{11}^{\alpha}\Gamma_{22}^{\beta}a_{\alpha\beta} \tag{77}$$

where the connection coefficients Γ_{sk}^{l} are expressed via the Christoffel symbols:

$$\Gamma^l_{sk} = \frac{1}{2} a^{lp}\left(\frac{\partial a_{sp}}{\partial q^k} + \frac{\partial a_{kp}}{\partial q^s} - \frac{\partial a_{sk}}{\partial q^p}\right) \tag{78}$$

while

$$a^{\alpha\beta}a_{\beta\gamma} = a^\alpha_\gamma = \begin{cases} 0 & \text{if} \quad \alpha \neq \gamma \\ 1 & \text{if} \quad \alpha = \gamma \end{cases} \tag{79}$$

Thus, the Gaussian curvature of these subspaces depends only on the coefficients a_{ij}, i.e., it is fully determined by the kinematic structure of the system [see equation (75)]. In the case of inertial motions, the trajectories of the representative particle must be geodesics of the configuration space. Indeed, as follows from (74),

$$\frac{d\tau}{dt} = \frac{d\tau}{ds}\dot{s} = 0 \qquad \text{if} \quad \dot{v} = 0, \qquad \text{and} \qquad |\dot{v}| = |\dot{s}| = \text{const} \neq 0 \tag{80}$$

where s is the arc coordinate along the particle trajectory:

$$ds = a_{ij}dq^i dq^j \tag{81}$$

But then

$$\frac{d\tau}{ds} = 0 \tag{82}$$

which is the condition that the trajectory is geodesic.

If the Gaussian curvature (77) which is uniquely defined by the parameters of the dynamical system a_{ij} is negative

$$G < 0 \tag{83}$$

then the trajectories of inertial motions of the system that originated at close, but different points of the configuration space diverge exponentially from each other, and the motion becomes unpredictable and stochastic. Some examples of orbital instability in inertial, potential, and general motions as well as other types of instability are discussed by Zak (1994).

Returning to the motion of the particle M on a smooth pseudosphere, let us depart from inertial motions and introduce a force F acting on this particle. For noninertial motions ($F \neq 0$) the trajectories of the particle will not be geodesics, while the rate of their deviation from geodesics is characterized by the geodesic curvature χ. It is obvious that this curvature must depend on the forces F:

$$\chi = \chi(F) \tag{84}$$

Synge (1926) has shown that if the force F is potential,

$$F = -\nabla\Pi \tag{85}$$

where Π is the potential energy, then the condition (83) is replaced by

$$G_0 + 3\chi^2 + \frac{1}{W}\left(\frac{\partial^2\Pi}{\partial q^i \partial q^j} - \Gamma^k_{ij}\frac{\partial\Pi}{\partial q^k}\right)n^i n^j < 0; \qquad i, j = 1, 2 \tag{86}$$

Here Γ^k_{ij} are defined by equation (78), and n^i are the contravariant components of the unit normal $\mathbf{n}$ to the trajectory.

The geodesic curvature χ in (86) can be expressed via the potential force $\mathbf{F}$:

$$\chi = \frac{\mathbf{F}\cdot\mathbf{n}}{2W} = -\frac{\nabla\Pi\cdot\mathbf{n}}{2W} \tag{87}$$

It follows from (86) and (87) that the condition (86) reduces to (83) if $F = 0$.

Suppose, for example, that the elastic force

$$F = -\alpha^2\epsilon, \qquad \alpha^2 = \text{const} \tag{88}$$

proportional to the normal deviation ϵ from the geodesic trajectory is applied to the particle M moving on the smooth pseudosphere. If the initial velocity is directed along one of the meridians (which are all geodesics), the unperturbed motion will be inertial, and its trajectory will coincide with this meridian since there $\epsilon = 0$, and therefore $F = 0$. In order to verify the orbital stability of this motion, let us turn to the criterion (38). Since

$$\chi = 0 \qquad \text{and} \qquad \frac{\partial\Pi}{\partial q^k} = F^k = 0 \tag{89}$$

for the unperturbed motion, one obtains the condition for orbital stability:

$$G_0 + \frac{\alpha^2}{2W} > 0, \qquad \text{i.e.,} \quad \alpha^2 < -2WG, \quad G < 0 \tag{90a}$$

where

$$W = \frac{1}{2}mv_0^2 \tag{90b}$$

As in the case of inertial motions, the inequality

$$\alpha^2 < -2WG_0 \tag{91}$$

leads to unpredictable (stochastic) motions which are characterized by

$$\sigma = \left(G_0 - \frac{\alpha^2}{2W}\right)^{1/2} = \text{const} > 0 \tag{92}$$

For pure inertial motions ($\alpha = 0$), equation (92) reduces to equation (64).

Following discovery of chaos, the stochastic motions which are generated by the instability and are characterized by positive Lyapunov exponents are called chaotic. Hence, the inequalities (83) and (86) can be associated with criteria of chaos: if the left-hand part in (86) is bounded away from zero by a negative number $-B$ in all the configuration space where the motion can occur, then the motion will be chaotic, and its positive Lyapunov exponent will be

$$\sigma \geq B^2 \tag{93}$$

Unfortunately, this criterion is too strong to be of practical significance: it is sufficient, but not necessary. Indeed, this criterion assumes that not only global, but also the local Lyapunov exponents are positive at any point of the configuration space. At the same time, for many chaotic motions, local Lyapunov exponents in certain domains of the configuration space are all negative or zero, although some of the global exponents are still positive.

Following Synge (1926), the results for the orbital instability of inertial and potential motions for a system of material points can be generalized to arbitrary motions (Zak, 1994).

Thus, there are some domains of dynamical parameters where the motion cannot be predicted because of instability of the solutions to the corresponding governing equations. How can this be interpreted? Does this mean that Newton's laws are not adequate? Or is there something wrong with our mathematical models? In order to answer these questions, we will discuss some general aspects of the concept of instability, and in particular the degree to which it is an invariant of motion. We will demonstrate that instability is an attribute of a mathematical model rather than a physical phenomenon, that it depends upon the frame of reference, upon the class of functions in which the motion is described, and upon the way in which the distances between the basic and perturbed solutions are defined.

Let us turn to orbital instability discussed above. The metric of configuration space where the finite-degree-of-freedom dynamical system with N generalized coordinates q^i ($i = 1, 2, \ldots, N$) is represented by a unit-mass particle was defined by (75) and (76). Now there are at least two possible ways to define the distance between the basic and disturbed trajectories. Following Synge (1926), we will consider the distance in kinematic and in kinematico-static senses. In the first case the corresponding points on the trajectories are those for which time t has the same value. In the second case the correspondence between points on the basic trajectory C and a disturbed trajectory C^*

is established by the condition that P (a point on C) should be the base of the geodesic perpendicular let fall from P^* (a point on C^*) on C, i.e., here every point of the disturbed curve is adjacent to the undisturbed curve (regardless of the position of the moving particle at the instant t). As shown by Synge, both definitions of stability are invariant with respect to coordinate transformations, and in both cases the stability implies that the corresponding distance between the curves C and C^* remains permanently small.

It is obvious that stability in the kinematic sense implies stability in the kinematicostatic sense, but the converse is not true. Indeed, consider the motion of a particle of unit mass on a plane under the influence of a force system derivable from a potential

$$\Pi = -x + \frac{1}{2} y^2 \tag{94}$$

Writing the equations of motion and solving them, we get

$$x = \frac{1}{2} t^2 + At + B \tag{95}$$

$$y = c \sin(t + \alpha) \tag{96}$$

where A, B, C, and D are constants of integration.

Let the undisturbed motion be

$$x = \frac{1}{2} t^2 + t \tag{97}$$

$$y = 0 \tag{98}$$

The motion is clearly unstable in the kinematic sense. However, from the viewpoint of stability in the kinematicostatic sense, the distance between corresponding points is

$$PP^* = y = C \sin(t + D) \tag{99}$$

remains permanently small if C is small. Hence, there is stability in the kinematicostatic sense.

Thus, the same motion can be stable in one sense and unstable in another, depending upon the way in which the distance between the trajectories is defined.

It should be noticed that in both cases the metric of configuration space was the same [see equations (75) and (76)]. However, as shown by Synge (1926), for conservative systems, one can introduce a configuration space with another metric,

$$g_{mn} = (E - \Pi)\alpha_{mn} \tag{100}$$

where α_{mn} are expressed by (75), and E is the total energy.

The system of motion trajectories here consists of all the geodesics of the manifold. The correspondence between points on the trajectories is fixed by the condition that the arc O^*P^* should be equal to the arc OP, where O and O^* are arbitrarily selected origins on the basic trajectory and any disturbed one, respectively.

As shown by Synge, the problem of stability here (which is called stability in the action sense) is that of the convergence of geodesics in Riemannian space. If two geodesics pass through adjacent points in nearly parallel directions, the distance between points on the geodesics equidistant from the respective initial points is either permanently small or not. If not, there is instability. It appears that stability in the action sense may not be equivalent to stability in the kinematicostatic sense for distances which change the total energy E.

Turning to the example, equation (94), let us take the initial point O at the origin of coordinates and the initial point O^* on the y axis. Then, since the disturbance is infinitesimal, the (action) distance between corresponding points is

$$P^* = (E - \Pi)^{1/2} y = 2^{-1/2}(t + 1)C \sin(t + D) \tag{101}$$

Hence, the motion is unstable in the action sense.

Dynamical instability depends not only upon the metric in which the distances between trajectories are defined, but also upon the frame of reference in which the motion is described.

For instance, as noticed by Arnold (1988), an inviscid stationary flow with a smooth velocity field (in Eulerian representation)

$$v_x = A \sin z + C \cos y$$

$$v_y = B \sin x + A \cos z$$

$$v_z = C \sin y + B \cos x \tag{102}$$

has chaotic trajectories $x(t)$, $y(t)$, $z(t)$ of fluid particles (Lagrangian turbulence) due to negative curvature of the configuration space, which is obtained as a finite-dimensional approximation of a continuum. Thus, the same motion is stable in the Eulerian representation, but is unstable in the Lagrangian one.

In order to demonstrate the instability dependence upon the class of functions in which the motion is considered, start with the example of a vertical, ideally flexible, inextensible string with a free lower end suspended in a gravity field. The governing equation for small transverse motion of the string is

$$\frac{\partial^2 x}{\partial t^2} + \frac{T}{\rho}\frac{\partial^2 x}{\partial \psi^2} = 0 \tag{103}$$

It has the following characteristic speeds of transverse wave propagation:

$$\mu = \pm\left(\frac{T}{\rho}\right)^{1/2} \tag{104}$$

Since the tension of the string T vanishes at the free end,

$$T = 0 \qquad \text{at} \quad S = l \tag{105}$$

where l is the length of the string, the characteristic speeds (104) vanish, too, at $S = l$, and therefore equation (103) degenerates from hyperbolic into parabolic type at the very end of the string.

Suppose that an isolated transverse wave of small amplitude is generated at the point of suspension. The speed of propagation of the leading front of the transverse wave will be smaller than the speed of the trailing front because the tension decreases from the point of suspension to the free end. Hence, the length of the above wave will be decreasing and in some cases will tend to zero. Then, according to the law of conservation of energy, the specific kinetic energy per unit of length will tend to infinity, producing a snap (snap of a whip).

As shown in Zak (1994), a formal mathematical solution to equation (103) is stable in the open interval (which does not include the end)

$$0 \leq x < l$$

but it is unstable in the closed interval

$$0 \leq x \leq l$$

However, the stable solution does not describe the snap of the whip, while the unstable solution does!

Thus, the properties of solutions to differential equations such as existence, uniqueness, and stability have a mathematical meaning only if they are referred to a certain class of functions. Most of the results concerning the properties of solutions to differential equations require differentiability (up to a certain order) of the functions describing the solutions. However, the mathematical restrictions imposed upon the class of functions which guarantee the existence of a unique and stable solution do not necessarily lead to the best representation of the corresponding physical phenomenon. Indeed, turning again to equation (103), one notices that the unique and stable solution does not describe a cumulative effect (a snap of a whip) which is well pronounced in experiments. At the same time, an unstable solution in a closed interval gives a qualitative description of this effect. Hence, purely mathematical restrictions imposed upon the solutions are not always consistent; the long-term instability in classical dynamics discussed above can be interpreted as a discrepancy between these mathematical restrictions and physical reality. This means that unpredictability in classical dynamics is the price to be paid for mathematical "convenience" in dealing with dynamical models. Therefore, the concept of unpredictability in dynamics should be stated as unpredictability in a selected class of functions, or in a selected metric of configuration space, or in a selected frame of reference.

In this connection one should notice that the governing equations of classical dynamics, and in particular of continuous systems, in addition to Newton's laws, are based upon a purely mathematical assumption that all the functions describing the system motions must be differentiable "as many times as necessary." But since this assumption is not always consistent with the physical nature of motions, such an inconsistency leads to instability (in the class of smooth functions) of the governing equations (Zak, 1994).

Hence, the occurrence of chaos or turbulence in the description of mechanical motions means only that these motions cannot be properly described by smooth functions if the scale of observations is limited. These arguments can be linked to Gödel's (1931) incompleteness theorem and Richardson's (1968) proof that the theory of elementary functions in classical analysis is undecidable.

Thus, since instability is not an invariant of motions, the following question can be posed: is it possible to find such a new (enlarged) class of functions, or a new metric of configuration space, or a new frame of reference in order to eliminate instability? Actually such a possibility would lead to different representative parameters describing the same motion in such a way that small uncertainties in external forces cause small changes of these parameters. For example, in turbulent and chaotic motions, mean velocities, Reynolds stresses, and power spectra represent "stable" parameters, although classical governing equations neither are explicitly expressed via these parameters nor uniquely define them.

The first step toward enlarging the class of functions for modeling turbulence was made by Reynolds (1895), who decomposed the velocity field into mean and pulsating components and actually introduced a multivalued velocity field. However, this decomposition brought new unknowns without additional governing equations, and that created a "closure" problem. In Zak (1994) it is shown that the Reynolds equations can be obtained by referring the Navier–Stokes equations to a rapidly oscillating frame of reference, while the Reynolds stresses represent the contribution of inertia forces. From this viewpoint the "closure" has the same status as the "proof" of Euclid's parallel postulate, since the motion of the frame of reference can be chosen arbitrarily. In other words, the "closure" of the Reynolds equations represents a case of undecidability in classical mechanics. However, based upon the interpretation of the Reynolds stresses as inertia forces, it is reasonable to choose the motion of the frame of reference such that the inertia forces eliminate the original instability. In other words, the enlarged class of functions should be selected such that the solution to the original problem in that class of functions will not possess an exponential sensitivity to changes in initial conditions. This stabilization principle has been formulated and applied to chaotic and turbulent motions in Zak (1994). As shown there, the motions which are chaotic (or turbulent) in the original frame of reference can be represented as a sum of the "mean" motion and rapid fluctuations, while both components are uniquely defined. It is worth emphasizing that the amplitude of the velocity fluctuation is proportional to the degree of the original instability, and therefore the rapid fluctuations can be associated with the measure of the uncertainty in the description of the motion. It should be noticed that both "mean" and "fluctuation" components representing the originally chaotic motion are stable, i.e., they are not sensitive to changes of initial conditions, and are fully reproducible.

7. CHAOS IN RAPIDLY OSCILLATING FRAME OF REFERENCE

Formally, chaos is caused by the instability of trajectories (orbital instability). If the velocity of a particle is decomposed as $\mathbf{v} = \nu\boldsymbol{\tau}$ ($\boldsymbol{\tau}$ is the unit vector along the trajectory), then orbital instabilities are identified with instabilities of $\boldsymbol{\tau}$. In other words, the orbital instability leads only to redistributions of the energy between different coordinates, and it can be associated with an ignorable variable which does not contribute to kinetic energy. Therefore, an unlimited growth of this variable does not violate the boundedness of energy. That is why the orbital instability may not lead to classical attractors and chaos can emerge. In dissipative systems the persisting instability can be "balanced" by dissipative forces in the sense that exponentially diverging trajectories are locked within a contracting phase-space volume, and this leads to chaotic attractors. In both conservative and dissipative systems, exponential divergence of trajectories within a constant or a contracting volume causes their mixing, so that the motion cannot be traced unless the initial conditions are known to infinite accuracy. This means that in configuration space, two different trajectories which may be initially indistinguishable (because of the finite scale of observation) diverge exponentially, so that a "real" trajectory can fill up all the spacing between these exponentially diverging trajectories. In other words, in the domain of exponential instability, each trajectory "multiplies," and therefore the predicted trajectory becomes multivalued, so the velocities can be considered as random variables:

$$\dot{q}^i = \dot{q}^i(t, \epsilon), \qquad 0 \leq \epsilon \leq 1 \tag{106}$$

where $\dot{q}$ and ϵ for a fixed t are a function and a point on a probability space, respectively. Let us refer the original equations of motion to a noninertial frame of reference which rapidly oscillates with respect to the original inertial frame of reference. Then the absolute velocity q can be decomposed into the relative velocity $\dot{q}_1$ and the transport velocity $\dot{q}_2 = 2\dot{q}_{2(0)}$:

$$\dot{q} = \dot{q}_1 + 2\dot{q}_{2(0)} \cos \omega t, \qquad \omega \to \infty \tag{107}$$

where $\dot{q}_1$ and $\dot{q}_{2(0)}$ are "slow" functions of time in the sense that

$$\omega >> 1/\tau \tag{108}$$

where τ is the time scale upon which the changes q_1 and $\dot{q}_{2(0)}$ can be ignored.

Then for the mean $\bar{q}$

$$q \cong q_1 \quad \text{since} \quad \int_0^{t>>\tau} \dot{q}_{2(0)} \cos \omega t \, dt \simeq \frac{1}{\omega} \dot{q}_{2(0)} \sin \omega t \to 0 \quad \text{if} \quad \omega \to \infty \tag{109}$$

In other words, a rapidly oscillating velocity practically does not change the displacements.

Taking into account that

$$\frac{\omega}{2\pi} \int_0^{2\pi/\omega} \dot{q}_1 \, dt \simeq \dot{q}_1$$

$$\int_0^{2\pi/\omega} \dot{q}_{2(0)} \sin \omega t \, dt = 0$$

$$\int_0^{2\pi/\omega} \ddot{q}_{2(0)} \cos \omega t \, dt = 0$$

$$\int_0^{2\pi/\omega} \dot{q}_{2(0)}^2 \cos^2 \omega t \, dt = \frac{1}{2} \dot{q}_{2(0)}^2 \tag{110}$$

one can transform the system

$$\dot{x}^i = a^i_j x^j + b^i_{jm} x^j x^m, \qquad i = 1, 2, \ldots, n \tag{111}$$

into the form

$$\dot{\bar{x}}_i = a^i_j \bar{x}^j + b^i_{jm} \bar{x}^j \bar{x}^m + b^i_{jm} \overline{x^j x^m}, \qquad i = 1, 2, \ldots, n \tag{112}$$

where $\bar{x}^i$ and $\overline{x^i x^j}$ are means and double correlations of x^i as random variables, respectively.

Actually the transition from (111) to (112) is identical to the Reynolds transformation: indeed, applied to the Navier–Stokes equations, it leads to the Reynolds equations, and therefore the last term in (112) (which is a contribution of inertial forces due to fast oscillations of the frame of reference) can be identified with the Reynolds stresses. From a mathematical viewpoint, this transformation is interpretable as an enlarging of the class of smooth functions to multivalued ones. Indeed, as follows from (108), for any arbitrarily small interval Δt, there always exists such a large frequency $\omega > \Delta t/2\pi$ that within this interval the velocity $\dot{q}$ runs through all its values, and actually the velocity field becomes multivalued.

The most significant advantage of the Reynolds-type equations (112) is that they are explicitly expressed via the physically reproducible parameters $\bar{x}^i$, $\overline{x^i x^j}$ which describe, for instance, a mean velocity profile in turbulent motions, or a power spectrum of chaotic attractors. However, as a price for that, these equations require closure, since the number of unknowns in them is larger than the number of equations. Actually the closure problem has existed for almost 100 years since the Reynolds equations were derived. In the next sections, based upon the stabilization principle introduced in Zak (1994), this problem will be discussed.

Some comments should be made concerning the Reynolds transformation of the Lagrange equation (59). Their explicit form

$$\ddot{q}^r + \Gamma^r_{mn}\dot{q}^m\dot{q}^n = Q^r, \qquad Q^r = -\frac{\partial \Pi}{\partial q^r} \tag{113}$$

in general is nonlinear with respect to both the coordinates q^r and the velocities $\dot{q}^r$, since

$$\Gamma^r_{mn} = \Gamma^r_{mn}(q_1, \ldots, q_n), \qquad \Pi = \Pi(q_1, \ldots, q_n) \tag{114}$$

However, as follows from equations (107), the fluctuations of the coordinates are much smaller than the fluctuations of the velocities:

$$q_{2(0)} \sim \frac{1}{\omega}\dot{q}_{2(0)}, \qquad \omega \to \infty \tag{115}$$

and therefore they can be ignored.

Consequently, after the Reynolds transformation, equation (113) is given in the form

$$\ddot{\bar{q}}^r + \Gamma^r_{mn}\bar{\dot{q}}^m\bar{\dot{q}}^n = Q^r + Q^r_{(i)}, \qquad Q^r_{(i)} = \Gamma^r_{mn}\overline{\dot{q}^m\dot{q}^n} \tag{116}$$

where $\bar{q}^r = q_1^r$ is the mean value of the coordinate q^r, and $\overline{\dot{q}^m \dot{q}^n}$ is the averaged product of the fluctuation velocities, and the Reynolds force $Q^r_{(i)}$ represents the contribution of inertia caused by the transport motion of the frame of reference.

Actually the transformation from (113) to (116) can be based upon the axiomatically introduced Reynolds conditions

$$\overline{a + b} = \bar{a} + \bar{b}, \qquad \overline{ab} = \bar{a}\bar{b} + \overline{a'b'} \qquad \text{if} \quad a = \bar{a} + a', \quad \text{etc.} \tag{117}$$

In the particular case

$$\Gamma^r_{mn} \equiv 0 \tag{118}$$

i.e., when the configuration space is Euclidean,

$$Q^r_{(i)} \equiv 0 \tag{119}$$

and the nonlinearities of the coordinates can no longer be ignored. Representing Q^r in the form

$$Q^r(\bar{q} + q') = Q^r(\bar{q}) + Q^r_{(i)}, \qquad Q^r_{(i)} = [Q^r(\bar{q} + q') - Q^r(\bar{q})] \tag{120}$$

one obtains instead of equation (116)

$$\ddot{\bar{q}}^r = Q^r(\bar{q}) + \bar{Q}^r_{(i)} \tag{121}$$

8. STABILIZATION PRINCIPLE

The main purpose of the transition from the form (111) to the form (112) is to change the representative parameters describing the motion in such a way that they become physically reproducible, i.e., mathematically stable. Hence, the next logical step is to utilize the extra variables, i.e., the Reynolds stresses, for elimination of the original instability. In other words, one can seek such additional relationships

$$\varphi(\overline{x^i x^j}, \bar{x}^i, \bar{x}^j, \ldots) = 0 \tag{122}$$

which make the system (112), (122) stable. Obviously, in this way of posing the problem, the solution to the system (112), (122) is not unique: the system can be overstabilized to any degree, while each of these stable solutions will have physical meaning. But for the best solution one has to minimize the uncertainties represented by the Reynolds stresses, and therefore the system should be brought to the boundary of instability. Since the orbital instability causing chaos is characterized by positive Lyapunov exponents λ_i^+, one should select the Reynolds stresses in (112) such that

$$\lambda_i^+ = 0 \tag{123}$$

while keeping the rest of the Lyapunov exponents without changes:

$$\lambda_i^0 = \tilde{\lambda}_i^0, \qquad \lambda_i^- = \tilde{\lambda}_i^- \tag{124}$$

where λ_i^0, λ_i^-, $\tilde{\lambda}_i^-$, and $\tilde{\lambda}_i^-$ are nonpositive Lyapunov exponents of the system (112), (122) and equation (111), respectively.

Clearly, those components of the Reynolds stresses which do not affect the Lyapunov exponents must be omitted. In general, the solution to equations (112), (123), (124) will eventually approach a set of periodic attractors which "replaces" the chaotic attractor of equation (111). However, one should consider these sets not as an approximation to the original chaotic attractor, but rather as a different way of mathematical representation of the same physical phenomenon. This representation is provided by a new frame of reference whose oscillations are coupled with the dynamical variables such that the inertia forces (i.e., the Reynolds stresses) generated by transport motion eliminate the original instability. In other words, the new frame of reference provides the best "view" of the motion.

The decomposition (112) applied to equation (111) generates not only pair correlations $\overline{x^i x^j}$, but also correlations of higher order, such as triple correlations $\overline{x^i x^j x^k}$, quadruple correlations $\overline{x^i x^j x^k x^m}$, etc. Indeed, multiplying equation (111) by x^k and averaging and combining the results, one obtains the governing equation for the pair correlations $\overline{x^i x^k}$,

$$\begin{aligned} \dot{\overline{x^i x^k}} = a_j^i \overline{x^j x^k} + a^k \overline{x^j x^i} + b_{jm}^i(\overline{x^k x^j x^m} + \overline{x^k x^j}\bar{x}^m + \overline{x^k x^m}\bar{x}^j) \\ + b_{jm}(\overline{x^i x^j x^m} + \overline{x^i x^j}\bar{x}^m + \overline{x^i x^m}\bar{x}^j) \end{aligned} \tag{125}$$

which contains nine additional triple correlations $\overline{x^i x^j x^k}$.

Now the application of the stabilization principle will lead to the system (112), (125) which will define $\bar{x}^i$, $\overline{x^i x^j}$ and those components of triple correlations $\overline{x^i x^j x^m}$ which affect the Lyapunov exponents in equations (123) and (124). Hence, the solutions to the systems (112), (124) and (112), (124), (125) can be regarded as the first and the second approximations, respectively, to the problem. Theoretically speaking, by considering next-order approximations, a complete probabilistic structure of the solution to equation (111) can be reproduced.

Application of the stabilization principle is significantly simplified for those systems whose boundaries of instability can be formulated analytically. For some cases of conservative chaos and simple turbulent flows new representations of solutions are given in Zak (1994).

In the next section we will demonstrate the application of the stabilization principle to some dissipative chaotic systems by numerical elimination of positive local Lyapunov exponents.

9. APPLICATION OF THE STABILIZATION PRINCIPLE TO REPRESENTATION OF CHAOS

9.1. Inertial Motions

In order to clarify the main idea of the approach, let us return to the inertial motion of a particle M of unit mass in a smooth pseudosphere S having a constant negative curvature (64). As shown there, the orbital instability and therefore the chaotic behavior of the particle M can be eliminated by the elastic force (88),

$$F = -\alpha^2 \epsilon, \qquad \alpha^2 = \text{const} > -2WG, \qquad G < 0 \tag{126}$$

proportional to the normal deviation ϵ from the geodesic trajectory which is applied to the particle M. But such a force can appear as an inertial force if the motion of the particle M is referred to an appropriate noninertial system of coordinates.

Indeed, so far this motion has been referred to an inertial system of coordinates q_1, q_2, where q_1 is the coordinate along the geodesic meridians and q_2 is the coordinate along the parallels. Let us introduce a frame of reference which rotates about the axis of symmetry of the pseudosphere with the oscillatory transport velocity

$$\dot{\epsilon} = 2\dot{\epsilon}_0 \cos \omega t, \qquad \omega \to \infty \tag{127}$$

so that the components of the resultant velocity along the meridians and parallels are, respectively,

$$v_1 = \dot{q}_1, \qquad v_2 = \dot{q}_2 + 2\dot{\epsilon}_0 \cos \omega t \tag{128}$$

Since equation (128) has the same structure as equation (107), the Lagrangian of the motion of the particle M relative to the new (noninertial) frame of reference can be written in the following form [see equation (72)]:

$$L^* = \dot{q}_1^2 - \frac{1}{G_0} \{\exp[-2(-G_0)^{1/2} q_1]\}(\dot{q}_2^2 + \dot{\epsilon}_0^2) \tag{129}$$

The last term in equation (129) represents the contribution of the inertia forces in the new frame of reference.

So far the transport velocity $\dot{\epsilon}_0$ has not been specified, and therefore the Lagrangian (129) has the same element of arbitrariness as the governing equations (112) describing chaotic motions.

Now, based upon the stabilization principle, we are going to specify the transport motion in such a way that the original orbital instability of the inertial motion of the particle M is eliminated. Turning to the condition (90), one obtains

$$\frac{\partial^2 L}{\partial \epsilon^2} \geq -2WG_0 \tag{130}$$

where $W = \frac{1}{2}v_0^2$ is the kinetic energy of the particle. This condition can be satisfied if the transport velocity $\dot{\epsilon}_0$ is coupled with the normal deviation ϵ as follows:

$$-\frac{1}{G_0}\{\exp[-2(-G_0)^{1/2}q_1]\}\dot{\epsilon}_0^2 = -WG_0q_2^2 \tag{131}$$

It follows from equation (92) that in this limit case the Lyapunov exponent of the relative motion in the new (noninertial) frame of reference will be zero:

$$\sigma = \left(-G_0 - \frac{\alpha_2}{W}\right)^{1/2} = 0, \qquad \alpha_2 = \frac{\partial^2 L}{\partial \epsilon^2} \tag{132}$$

and the trajectories of perturbed motions do not diverge. The normal deviation from the trajectory of the relative motion (in the case of zero perturbed velocity $\dot{\epsilon}_0$) can be written in the form

$$q_2 = q_2^0 = \text{const}, \qquad q_2^0 = q_2(t = 0) \tag{133}$$

which means that in the new frame of reference an initial error ϵ_0 does not grow—it remains constant. The relative motion along the trajectory is described by the differential equation following from the Lagrangian (129), which takes the following form [after substituting equation (131)]:

$$L = \dot{q}_1^2 - \frac{1}{G_0}\{\exp[-2(-G_0)^{1/2}q_1]\}\dot{q}_2 - WG_0q_2^0 \tag{134}$$

i.e.,

$$\ddot{q}_1 - \frac{2(-G_0)^{1/2}}{G_0}\{\exp[-2(-G_0)^{1/2}q_1]\}\dot{q}_2 = 0 \tag{135}$$

But the original (unperturbed) motion was directed along the meridians, i.e., $\dot{q} \equiv 0$. Consequently,

$$\ddot{q}_1 = 0, \qquad \dot{q}_1 = \bar{v}_0 = \text{const} \tag{136}$$

i.e., the relative motion along the trajectory is constant.

However, this velocity is different from the original velocity v_0. Indeed, the total kinetic energy of the particle now consists of the kinetic energy of the motion along the trajectory and the kinetic energy of transverse fluctuations expressed by (131), i.e.,

$$\frac{v_0^2}{2} = \frac{\bar{v}_0^2}{2} + \frac{v_0^2}{2} (q_2^0)^2 |G_0| \tag{137}$$

whence

$$\bar{v}_0 = v_0[1 - (q_2^0)^2 |G_0|]^{1/2} < v_0 \tag{138}$$

Thus, the original unstable (chaotic) motion is decomposed into the mean motion along the trajectory q_2 = const with the constant velocity (138) and transverse fluctuations whose kinetic energy is proportional to the original error q_2^0 and to the degree of instability $|G_0|$. It is important to emphasize that both components of the motion are stable in the sense that the initial error in q_2 at $t = 0$ does not grow, and the initial error in q_1 at $t = 0$ grows linearly with time.

Obviously the mean or averaged motion represents a macroscopic view of the particle behavior extracted from the microscopic world, while the irreversibility of this motion is manifested by the loss of the initial kinetic energy to microscopic fluctuations.

It should be emphasized that the decomposition of the motion into regular and fluctuation components was enforced by the stabilization principle as a supplement to Newtonian mechanics [see equation (131)], while without this principle any theory where dynamical instability can occur is incomplete.

9.2. Potential Motions

Based upon equations (116), for potential motions, the governing equations can be written in the form

$$\ddot{q}^\alpha + \Gamma^\alpha_{\beta\delta}\dot{q}^\beta\dot{q}^\delta = -\frac{\partial \Pi}{\partial q^\alpha} + a^\alpha_{(i)} \tag{139}$$

$$\frac{\partial \Pi}{\partial q^\alpha} = -Q^\alpha \tag{140}$$

where Π is the potential energy of the dynamical system, and $Q^\alpha_{(i)}$ are the inertia forces (or the "Reynolds stresses") caused by the rapidly oscillating transport motion of the frame of reference.

For simplicity, we will confine ourselves to a two-dimensional dynamical system assuming that $\alpha = 1, 2$.

Following the same strategy as applied to inertial motions, let us couple the inertia forces with the parameters of the dynamical system in such a way that the original orbital instability (if it occurs) is eliminated. For that purpose, first we represent these forces in the form

$$Q^\alpha_{(i)} = -\frac{\partial \Pi_{(i)}}{\partial q^\alpha} \tag{141}$$

where $\Pi_{(i)}$ is a fictitious potential energy equivalent to the kinetic energy of the fluctuations. Then, turning to the criteria of local orbital stability (86), one finds this potential energy $\Pi_{(i)}$ and consequently the inertia forces $Q^{\alpha}_{(i)}$ from the condition that original local orbital instability is eliminated:

$$G + 3\left[\frac{\nabla(\Pi + \Pi_{(i)})\cdot\mathbf{n}}{2W}\right]^2 + \frac{1}{2W}\left[\frac{\partial^2(\Pi + \Pi_{(i)})}{\partial q^i \partial q^j} - \Gamma^k_{ij}\frac{\partial(\Pi + \Pi_{(i)})}{\partial q^k}\right]n^i n^j = 0, \qquad i, j = 1, 2 \quad (142)$$

Here W, G, and Γ^k_{ij} are defined by the parameters of the dynamical system (116) via equations (75), (77), and (78), respectively, and n_i are the contravariant components of the unit normal n to the trajectory of the basic function.

Equation (142) contains only one unknown $\Pi_{(i)}$, which can be found from it, and will define the inertia forces or the "Reynolds stresses" (141).

It should be noticed that unlike the case of the inertial motion of a particle on a pseudosphere, here the Gaussian curvature G, as well as the gradients of the potential energy Π, are not constants, and consequently the local Lyapunov exponents may be different from the global ones. This means that the condition (142) eliminates local positive exponents, and therefore the solution to (139) and (142) represents an overstabilized motion. Obviously, elimination of only global positive Lyapunov exponents would lead to solutions with less uncertainties, while some of local exponents in certain domains of the phase space may even remain positive. However, the strategy for elimination of global positive exponents is more sophisticated, and it can be implemented only numerically.

It is worth noting that equation (142) is simplified to

$$G + \frac{1}{2W}\left[\frac{\partial^2(\Pi + \Pi_{(i)})}{\partial q^i \partial q^j}\right]n^i n^j = 0 \qquad (143)$$

if the basic motion is characterized by zero potential forces

$$\frac{\partial \Pi}{\partial q^i} = 0 \qquad (144)$$

This may occur, for instance, when the dynamical system is in relative equilibrium with respect to a moving frame.

Thus, as in the previous case of inertial motion of a particle, here the Lagrange equations (139) are supplemented by the additional constraint (142) following from the stabilization principle. It is important to emphasize that this constraint is effective only in the case of orbital instability of (139); otherwise it is satisfied automatically.

As an illustration of the case of a potential system, we will consider the motion of a charged particle (charge $-e$, mass m) in a uniform magnetic field B in the vicinity of a metallic sphere (radius a) biased to a potential $\mathbf{V}_0 > 0$:

$$m\dot{v} = -ev \times \mathrm{B} + e\nabla \mathbf{v} \tag{145}$$

where $v = d\hat{r}/dt$ is the velocity of the particle, and $V = V_0(a/p)$ is the electrical potential due to the sphere.

Equation (145) can be written in a dimensionless form:

$$\dot{v}_x = -\frac{\mathrm{x}}{\mathrm{r}^3}\, v_y, \qquad \dot{v}_y = -\frac{\mathrm{y}}{\mathrm{r}^3} + v_x, \qquad \dot{v}_z = -\frac{\mathrm{z}}{\mathrm{r}^3} \tag{146}$$

$$v_x = \dot{\mathrm{x}}, \qquad v_y = \dot{\mathrm{y}}, \qquad v_z = \dot{\mathrm{z}} \tag{147}$$

where

$$\dot{x} = \frac{dx}{d\tau}, \ldots, \qquad r^2 = x^2 + y^2 + z^2$$

$$r = \frac{\hat{r}}{\lambda}, \qquad \tau = \omega_e t, \qquad \lambda^3 = eV_0 a/m\omega_e^2, \qquad \omega = eB/m$$

As reported in Barone (1993), there are certain domains of initial conditions which lead to chaotic trajectories. The system is chaotic, for instance, at $x = 1.5$, $y = 0$, $z = 4.0$, $x_x = v_y = v_z = 0$ at $t = 0$. We have reproduced these results (see Fig. 1) by solving (146) and (147) numerically.

The implementation of the stabilization principle, i.e., simultaneous solution of equations (146) and (147) [after their Reynolds decomposition into the form (139)] and the constraint (142) were performed numerically. The numerical strategy was very simple: along with the basic solution, a perturbed solution was calculated and compared with the basic one after certain time steps; if the perturbed solution diverged faster than a prescribed time polynomial, then an appropriate Reynolds force was applied to suppress it; otherwise no actions were taken. The resulting trajectories in the same x, y, z phase space are plotted in Fig. 2. These trajectories represent an averaged or expected motion which is no longer chaotic. It is important to emphasize that this motion is stable in the sense that small changes of the initial conditions will cause small changes in the motion.

Actually this example elucidates the mechanism of transition from the Hamiltonian mechanics describing fully reversible mechanical processes on the microscopic level to irreversible macroscopic motions describing thermodynamic processes. By the same line of argumentation, the stabilization principle implements the preference to more probable states of the system over the less probable states.

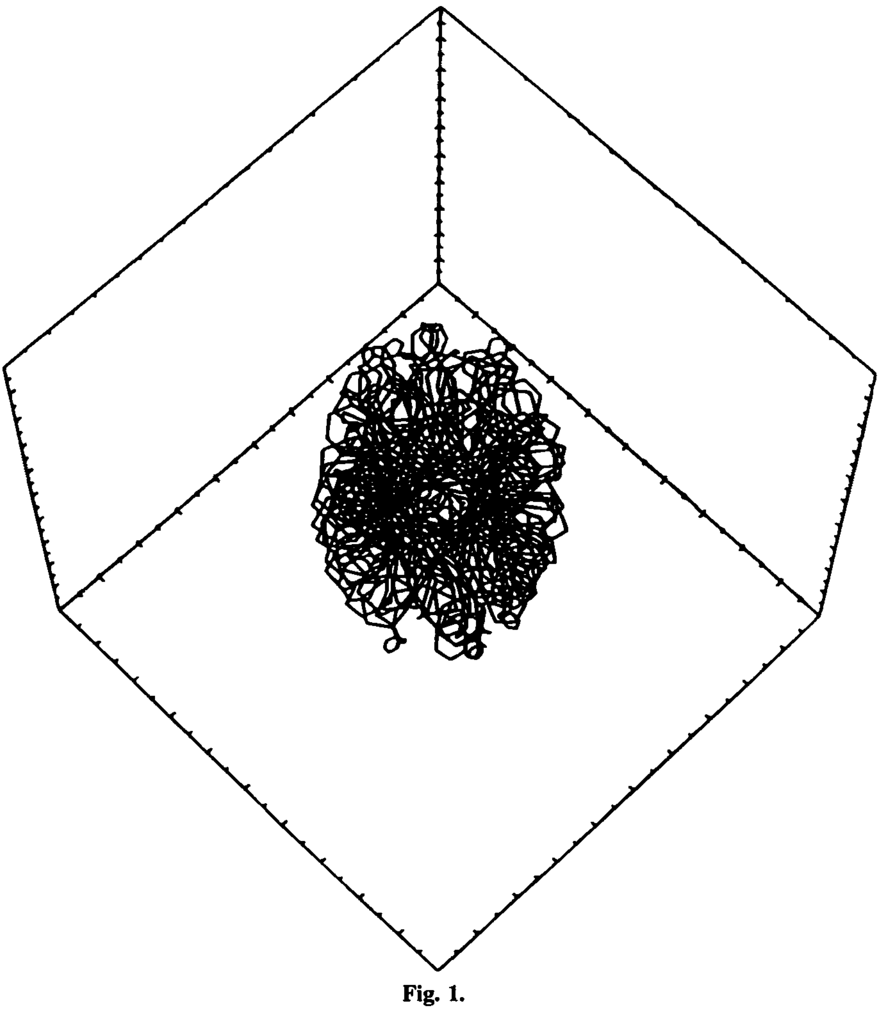

Fig. 1.

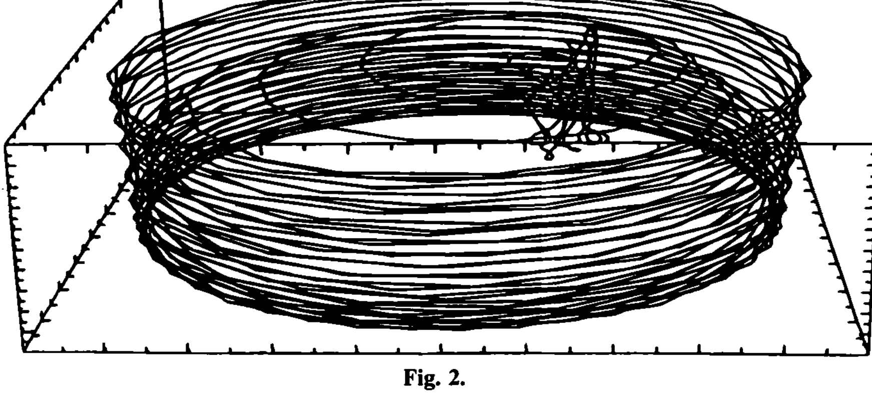

Fig. 2.

10. DISCUSSION AND CONCLUSION

The problem of irreversibility in thermodynamics was revisited and analyzed on the microscopic, stochastic, and macroscopic levels of description. It was demonstrated that Newtonian dynamics (as well as any dynamical theory where chaotic solutions are possible) can be represented in the Reynolds form when each dynamical variable is decomposed into mean and fluctuation components. Additional equations coupling fluctuations and the mean values follow from the stabilization principle formulated in Zak (1994) and briefly described in the previous sections. The main idea of this principle is that the fluctuations must be selected from the condition that they suppress the original instability down to a neutral stability. Supplemented by the stabilization principle, the Hamiltonian or Lagrangian formalisms can describe the transition from fully reversible to irreversible motions as a result of the decomposition of chaotic motions (which are very likely to occur in many-body problems) into regular (macroscopic) motions and fluctuations. Actually the stabilization principle implements the preference to more probable states of the system over the less probable states, and from that viewpoint it can be associated with the averaging procedure exploited in statistical mechanics. However, the averaging procedure was always considered as an "alien intrusion" into classical mechanics, and that led to many discussions about the problem of irreversibility on the macroscopic level. On the contrary, the stabilization principle is a part of Newtonian mechanics (as well as a part of any dynamical theory where chaotic motions can occur), and therefore it provides a formal mathematical explanation for the transition from fully reversible to irreversible processes.

On the stochastic level of description, a new phenomenological force with non-Lipschitz properties has been introduced. This force, as a resultant of a large number of collisions of a selected particle with other particles, has characteristics which are uniquely defined by the thermodynamic parameters of the process under consideration, and it represents a part of the mathematical formalism describing random-walk-like processes without invoking any probabilistic arguments.

Additional non-Lipschitz thermodynamic forces have been incorporated into macroscopic models of transport phenomena in order to introduce a time scale. These forces are effective only within a small domain around equilibria. Without causing any changes in other domains, they are responsible for the finite time of approaching equilibria. Such a property is very important for interpretation of irreversibility on the macroscopic scale. Indeed, there is always an extremely small (but nonzero) probability that a particle performing a random walk can return to its original position passing through all of its previous steps backward, and therefore this effect should not be excluded from the solutions to the macroscopic equations if they are observed during an infinitely large period of time. However, these practically unrealistic situations may be excluded from consideration in the case of the modified macroscopic equations since they are characterized by a limited time scale.

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