Time Irreversibility Problem and Functional Formulation of Classical Mechanics

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Abstract

The time irreversibility problem is the dichotomy of the reversible microscopic dynamics and the irreversible macroscopic physics. This problem was considered by Boltzmann, Poincaré, Bogolyubov and many other authors and though some researchers claim that the problem is solved, it deserves a further study. In this paper an attempt is performed of the following solution of the irreversibility problem: a formulation of microscopic dynamics is suggested which is irreversible in time. In this way the contradiction between the reversibility of microscopic dynamics and irreversibility of macroscopic dynamics is avoided since both dynamics in the proposed approach are irreversible.

A widely used notion of microscopic state of the system at a given moment of time as a point in the phase space and also a notion of trajectory and microscopic equation of motion does not have an immediate physical meaning since arbitrary real numbers are non observable. In the approach presented in this paper the physical meaning is attributed not to an individual trajectory but only to a bunch of trajectories or to the distribution function on the phase space.

The fundamental equation of the microscopic dynamics in the proposed “functional” approach is not the Newton equation but the Liouville equation for the distribution function of the single particle. Solutions of the Liouville equation have the property of delocalization which accounts for irreversibility. It is shown that the Newton equation in this approach appears as an approximate equation describing the dynamics of the average values of the position and momenta for not too long time intervals. Corrections to the Newton equation are computed.
1 Introduction

The time irreversibility problem is the problem of how to explain the irreversible behaviour of macroscopic systems from the time-symmetric microscopic laws. The problem has been discussed by Boltzmann, Poincaré, Bogolyubov, Kolmogorov, von Neumann, Landau, Prigogine, Feynman and many other authors [1] - [19] and it deserves a further study.

In particular, in works by Poincaré [2], Landau and Lifshiz [5], Prigogine [10], Ginzburg [14], Feynman [16] it is stressed that the irreversibility problem is still an open problem. Poincaré [2] said that perhaps we will never solve the irreversibility problem. Landau and Lifshiz write about the principle of increasing entropy [5]: “Currently it is not clear whether the law of increasing entropy can be in principle derived from classical mechanics.” Landau speculated that to explain the second law of thermodynamics one has to use quantum mechanical measurement arguments.

From the other side Lebowitz [17], Goldstein [18] and Bricmont [19] state that the irreversibility problem was basically solved already by Boltzmann by using his notion of macroscopic entropy and the probabilistic approach.

The microscopic mechanical description of a system assumes that the state of the system at a given moment of time is represented by a point in the phase space with an invariant measure and the dynamics of the system is described by a trajectory in the phase space, see [5, 20, 21, 22, 23, 24]. It is assumed that the microscopic laws of motion are known (Newton or Schrodinger equations) and there is a problem of derivation from them the macroscopic (Boltzmann, Navier-Stokes,…) equations, see for example, [5, 8].

There are well known critical remarks by Loschmidt and Poincaré and Zermelo on the Boltzmann approach to the irreversibility problem and the \( H \)-theorem. Loschmidt remarked that from the symmetry of the Newton equations upon the reverse of time it follows that to every motion of the system on the trajectory towards the equilibrium state one can put into correspondence the motion out of the equilibrium state if we reverse the velocities at some time moment. Such a motion is in contradiction with the tendency of the system to go to the equilibrium state and with the law of increasing of entropy.

Then, there is the Poincaré recurrence theorem which says that a trajectory of a bounded isolated mechanical system will be many times come to a very small neighborhood of an initial point. This is also in contradiction with the motion to the equilibrium state. This is the Poincaré–Zermelo paradox.

Boltzmann [25] gave the following answer to the Loschmidt argument: “We do not have to assume a special type of initial condition in order to give a mechanical proof of the second law, if we are willing to accept a statistical viewpoint. While any individual non-uniform state (corresponding to low entropy) has the same probability as any individual uniform state (corresponding to high entropy), there are many more uniform states than non-uniform states. Consequently, if the initial state is chosen at random, the system is almost certain to evolve into a uniform state, and entropy is almost certain to increase.”

So, the answer by Boltzmann to the objection of Loschmidt was that, firstly, the probabilistic considerations has been involved, and secondly, he argued that with the overwhelming probability the evolution of the system will be occur in the direction of flow of time, corresponding to the increasing entropy, since there are many more uniform states than non-
uniform states. The answer by Boltzmann to the Poincaré–Zermelo objection was in the pointing out the extremely long Poincaré recurrence time.

These Boltzmann's responses are not very convincing, from our point of view, despite their vigorous support in recent works. Involvement of probability considerations alone does not clarify the issue of irreversibility, because if there is symmetry in relation to the direction of time, it remains unclear why the evolution in one direction is more likely than the other.

Then, the argument, that there are many more uniform states than non-uniform states does not clarify the issue of the dynamical evolution since the dynamics does depend on the form of the potential energy between particles and for many potentials the argument is simply wrong. Therefore this general Boltzmann's argument does not give a real insight to the irreversibility problem.

Actually, Boltzmann in [25] considered “a large but not infinite number of absolutely elastic spheres, which move in a closed container whose walls are completely rigid and likewise absolutely elastic. No external forces act on our spheres.” Even for this simple model it is very difficult to make the Boltzmann argument convincing, i.e. to get a mathematical result, see [21, 24].

Further, an indication to the extremely long Poincaré recurrence time does not remove the contradiction between microscopic reversibility and macroscopic irreversibility, and moreover no clear mechanism for relaxation to equilibrium is presented.

Lebowitz advanced [17], following to Boltzmann, the following arguments to explain irreversibility: a) the great disparity between microscopic and macroscopic scales, b) a low entropy state of the early universe, and c) the fact that what we observe is the behaviour of systems coming from such an initial state – not all possible systems.

From our viewpoint these arguments do not lead to explanation of irreversibility even though it is said in [17] that “common alternative explanations, such as those based on the ergodic or mixing properties of probability distribution ... are either unnecessary, misguided or misleading”.

Boltzmann proposed that we and our observed low-entropy world are a random fluctuation in a higher-entropy universe. These cosmological considerations of the early universe might be entertaining but they should be related with the modern Friedmann gravitational picture of the Big Bang and, what is most important, there is no evidence that the irreversible behaviour of gas in a box is related somehow with conditions in the early universe 14 billions years ago.

Notice that in [28] it is shown that the Hawking black hole information paradox is a special case of the irreversibility problem.

Goldstein said in [18]: “The most famous criticisms of Boltzmann’s later works on the subject have little merit. Most twentieth century innovations – such as the identification of the state of a physical system with a probability distribution \( \rho \) on its phase space, of its thermodynamic entropy with the Gibbs entropy of \( \rho \), and the invocation of the notions of ergodicity and mixing for the justification of the foundations of statistical mechanics – are thoroughly misguided.”

And then: “This use of ergodicity is thoroughly misguided. Boltzmann’s key insight was that, given the energy of a system, the overwhelming majority of its phase points on the
corresponding energy surface are equilibrium points, all of which look macroscopically more or less the same.”

The Boltzmann argument about “the overwhelming majority” (i.e. “many more uniform states”) was discussed above. Moreover, the main point of the current paper is that we shall use the probability distribution and the Liouville equation not only in statistical mechanics but also in classical mechanics, even for a single particle in empty space.

A powerful method for obtaining kinetic equations from the Newton – Liouville equations was developed by Bogolyubov [3]. He has considered infinite number of particles in infinite volume and postulated the condition of weakening of initial correlations between particles in the distant past, through which the irreversibility entered into the equation for the distribution functions, as well as using a formal expansion in powers of density, which leads to divergences.

Poincaré considered the model of free motion of gas particles in a box with reflecting walls and showed that for solutions of the Liouville equation in this model there is, in some sense, an irreversible diffusion [29]. This result of Poincaré was introduced to modern scientific literature by Kozlov, see [11], where the result of Poincaré was significantly strengthened and consolidated. In the works of Kozlov a method of the weak limit in the nonequilibrium statistical mechanics has been developed, and, in particular, it was proved that for some models the system in the sense of weak convergence tends to one and the same limit in the past and in the future [11, 12]. The method of the weak limit of [11, 12] had a significant influence to the formulation of the approach to the problem of irreversibility through functional formulation of classical mechanics.

Note that the stochastic limit [13] gives a systematic method for investigation of irreversible processes.

Questions about the increase of the fine and coarse entropies are discussed in [30, 5, 6, 7, 8, 31, 12].

In this paper we attempt to suggest the following approach to the irreversibility problem and to paradoxes of Loschmidt and Poincaré – Zermelo: we propose a formulation of microscopic dynamics which is irreversible in time. Thus the contradiction between microscopic reversibility and macroscopic irreversibility of the dynamics disappears, since both microscopic and macroscopic dynamics in the proposed approach are irreversible.

Note that the conventional widely used concept of the microscopic state of the system at some moment in time as the point in phase space, as well as the notion of trajectory and the microscopic equations of motion have no direct physical meaning, since arbitrary real numbers not observable (observable physical quantities are only presented by rational numbers, cf. the discussion of concepts of space and time in [33, 34, 35, 36, 37, 38, 39, 40]).

In the proposed “functional” approach, the physical meaning is attached not to a single trajectory, but only to a “beam” of trajectories, or the distribution function on phase space. Individual trajectories are not observable, they could be considered as “hidden variables”, if one uses the quantum mechanical notions, see [41, 42].

The fundamental equation of the microscopic dynamics of the proposed functional probabilistic approach is not Newton’s equation, but a Liouville equation for distribution function. It is well known that the Liouville equation is used in statistical mechanics for the description of the motions of gas. Let us stress that we shall use the Liouville equation for the
description of a single particle in the empty space.

Although the Liouville equation is symmetric in relation to the reversion of time, but his solutions have the property of delocalization, that, generally speaking, can be interpreted as a manifestation of irreversibility. It is understood that if at some moment in time the distribution function describes a particle, localized to a certain extent, then over time the degree of localization decreases, there is the spreading of distribution function. Delocalization takes place even for a free particle in infinite space, where there is no ergodicity and mixing.

In the functional approach to classical mechanics we do not derive the statistical or chaotic properties of deterministic dynamics, but we suggest that the Laplace’s determinism at the fundamental level is absent not only in quantum, but also in classical mechanics.

We show that Newton’s equation in the proposed approach appears as an approximate equation describing the dynamics of the average values of coordinates and momenta for not too long time. We calculate corrections to Newton’s equation.

In the next section the fundamentals of the functional formulation of classical mechanics are presented. Sections 3 and 4 deal with the free movement of particles and Newton’s equation for the average coordinates. Comparison with quantum mechanics is discussed in Section 5. General comments on the Liouville and Newton equations are contained in section 6. Corrections to the Newton equation for a nonlinear system are calculated in Section 7. Reversibility of motion in classical mechanics and irreversibility in the functional approach to the mechanics discussed in section 8. The dynamics of the classical and quantum particle in a box and their interrelationships are summarized in section 9.

2 States and Observables in
Functional Classical Mechanics

Usually in classical mechanics the motion of a point body is described by the trajectory in the phase space, i.e. the values of the coordinates and momenta as functions of time, which are solutions of the equations of Newton or Hamilton.

Note, however, that this mathematical model is an idealization of the physical process, rather far separated from reality. The physical body always has the spatial dimensions, so a mathematical point gives only an approximate description of the physical body. The mathematical notion of a trajectory does not have direct physical meaning, since it uses arbitrary real numbers, i.e. infinite decimal expansions, while the observation is only possible, in the best case, of rational numbers, and even them only with some error. Therefore, in the proposed “functional” approach to classical mechanics, we are not starting from Newton’s equation, but with the Liouville equation.

Consider the motion of a classical particle along a straight line in the potential field. The general case of many particles in the 3-dimensional space is discussed below. Let \((q, p)\) be co-ordinates on the plane \(\mathbb{R}^2\) (phase space), \(t \in \mathbb{R}\) is time. The state of a classical particle at time \(t\) will be described by the function \(\rho = \rho(q, p, t)\), it is the density of the probability that the particle at time \(t\) has the coordinate \(q\) and momentum \(p\).

Note that the description of a mechanical system with the help of probability distribution function \(\rho = \rho(q, p, t)\) does not necessarily mean that we are dealing with a set of identically
prepared ensemble of particles. Usually in probability theory one considers an ensemble of events and a sample space \[55, 56, 57\]. But we can use the description with the function \( \rho = \rho(q, p, t) \) also for individual bodies, such as planets in astronomy (the phase space in this case the 6-dimensional). In this case one can think on the “ensemble” of different astronomers which observe the planet, or on the “ensemble” of different models of behaviour of a given object. Actually, it is implicitly always dealt with the function \( \rho = \rho(q, p, t) \) which takes into account the inherent uncertainty in the coordinates and momentum of the body.

An application of these remarks to quantum mechanics will be discussed in a separate work.

The specific type of function \( \rho \) depends on the method of preparation of the state of a classical particle at the initial time and the type of potential field. When \( \rho = \rho(q, p, t) \) has sharp peaks at \( q = q_0 \) and \( p = p_0 \), we say that the particle has the approximate values of coordinate and momentum \( q_0 \) and \( p_0 \).

Emphasize that the exact derivation of the coordinate and momentum can not be done, not only in quantum mechanics, where there is the Heisenberg uncertainty relation, but also in classical mechanics. Always there are some errors in setting the coordinates and momenta. The concept of arbitrary real numbers, given by the infinite decimal series, is a mathematical idealization, such numbers can not be measured in the experiment.

Therefore, in the functional approach to classical mechanics the concept of precise trajectory of a particle is absent, the fundamental concept is a distribution function \( \rho = \rho(q, p, t) \) and \( \delta \)-function as a distribution function is not allowed.

We assume that the continuously differentiable and integrable function \( \rho = \rho(q, p, t) \) satisfies the conditions:

\[
\rho \geq 0, \quad \int_{\mathbb{R}^2} \rho(q, p, t)dqdp = 1, \quad t \in \mathbb{R}.
\] (1)

The formulation of classical mechanics in the language of states and observables is considered in \[33, 14, 15\]. The functional approach to classical mechanics differs in the following respects. Because the exact trajectory of a particle in the functional approach does not exist, then the function \( \rho = \rho(q, p, t) \) can not be an arbitrary generalized function, it is the usual function of class \( L^1(\mathbb{R}^2) \), or even continuously differentiable and integrable function.

In addition, the motion of particles in the functional approach is not described directly by the Newton (Hamilton) equation. Newton’s equation in the functional approach is an approximate equation for the average coordinates of the particles, and for non-linear dynamics there are corrections to the Newton equations.

As is known, the mathematical description of a moving fluid or gas is given by means of the density distribution functions \( \rho(q, t) \), as well as the velocity \( v(q, t) \) and pressure \( p(q, t) \), see, for example, \[46\]. Let the function \( \rho(q, p, t) \) describes a particle, as proposed in the functional formulation of classical mechanics, and we set \( \rho_c(q, t) = \int \rho(q, p, t)dp \). We could ask the question can we determine by the form of functions \( \rho(q, t) \) and \( \rho_c(q, t) \) whether we are dealing with a continuous medium or with a particle? The general answer is the following: functions \( \rho(q, t) \) and \( \rho_c(q, t) \) satisfy different equations (the Navier-Stokes or Liouville equation) and different conditions of normalization.

Note, however, that if an error in determining the coordinates and momentum of particles is large enough, it really is not so easy to determine, we have a case of, say, a fast-moving particle in a box with reflecting walls, either a gas of particles.
If $f = f(q,p)$ is a function on phase space, the average value of $f$ at time $t$ is given by the integral

$$\bar{f}(t) = \int f(q,p)\rho(q,p,t)dqdp.$$  \hspace{1cm} (2)

In a sense we are dealing with a random process $\xi(t)$ with values in the phase space. Motion of a point body along a straight line in the potential field will be described by the equation

$$\frac{\partial \rho}{\partial t} = -\frac{p}{m} \frac{\partial \rho}{\partial q} + \frac{\partial V(q)}{\partial q} \frac{\partial \rho}{\partial p}.$$  \hspace{1cm} (3)

Here $V(q)$ is the potential field and mass $m > 0$.

Equation (3) looks like the Liouville equation which is used in statistical physics to describe a gas of particles but here we use it to describe a single particle.

If the distribution $\rho_0(q,p)$ for $t = 0$ is known, we can consider the Cauchy problem for the equation (3):

$$\rho|_{t=0} = \rho_0(q,p).$$  \hspace{1cm} (4)

Let us discuss the case when the initial distribution has the Gaussian form:

$$\rho_0(q,p) = \frac{1}{\pi ab} e^{-\frac{(q-q_0)^2}{a^2}} e^{-\frac{(p-p_0)^2}{b^2}}.$$  \hspace{1cm} (5)

At sufficiently small values of the parameters $a > 0$ and $b > 0$ the particle has coordinate and momentum close to the $q_0$ and $p_0$. For this distribution the average value of the coordinates and momentum are:

$$\bar{q} = \int q \rho_0(q,p)dqdp = q_0, \quad \bar{p} = \int p \rho_0(q,p)dqdp = p_0,$$  \hspace{1cm} (6)

and dispersion

$$\Delta q^2 = (q - \bar{q})^2 = \frac{1}{2}a^2, \quad \Delta p^2 = (p - \bar{p})^2 = \frac{1}{2}b^2.$$  \hspace{1cm} (7)

3 Free Motion

Consider first the case of the free motion of the particle when $V = 0$. In this case the equation (3) has the form

$$\frac{\partial \rho}{\partial t} = -\frac{p}{m} \frac{\partial \rho}{\partial q}$$  \hspace{1cm} (8)

and the solution of the Cauchy problem is

$$\rho(q,p,t) = \rho_0(q - \frac{p}{m}t, p).$$  \hspace{1cm} (9)

Using expressions (5), (9),

$$\rho(q,p,t) = \frac{1}{\pi ab} \exp\left\{-\frac{(q - q_0 - \frac{p}{m}t)^2}{a^2} - \frac{(p - p_0)^2}{b^2}\right\},$$  \hspace{1cm} (10)
we get the time dependent distribution of coordinates:

\[
\rho_c(q,t) = \int \rho(q,p,t) dp = \frac{1}{\sqrt{\pi} \sqrt{a^2 + \frac{b^2 t^2}{m^2}}} \exp\left\{ -\frac{(q - q_0 - \frac{p_0 t}{m})^2}{(a^2 + \frac{b^2 t^2}{m^2})} \right\},
\]

while the distribution of momenta is

\[
\rho_m(p,t) = \int \rho(q,p,t) dq = \frac{1}{\sqrt{\pi} b} e^{-\frac{(p - p_0)^2}{b^2}}.
\]

Thus, for the free particle the distribution of the particle momentum with the passage of time does not change, and the distribution of the coordinates change. There is, as one says in quantum mechanics, the spreading of the wave packet. From (11) it follows that the dispersion \(\Delta q^2\) increases with time:

\[
\Delta q^2(t) = \frac{1}{2} \left( a^2 + \frac{b^2 t^2}{m^2} \right).
\]

Even if the particle was arbitrarily well localized \((a^2\) is arbitrarily small) at \(t = 0\), then at sufficiently large times \(t\) the localization of the particle becomes meaningless, there is a delocalization of the particle.

### 4 Newton’s Equation for the Average Coordinate

In the functional approach to classical mechanics there is no ordinary picture of an individual trajectory of a particle. The starting equation is the dynamic equation for the distribution function, rather than the Newton equation.

What role can play the Newton equation in the functional approach? We show that the average coordinate for the free particle in the functional approach satisfies the Newton equation. Indeed, the average coordinate and momentum for the free particles have the form

\[
\bar{q}(t) = \int q \rho_c(q,t) dq = q_0 + \frac{p_0}{m} t, \quad \bar{p}(t) = \int p \rho_m(p,t) dp = p_0.
\]

Hence we get

\[
\frac{d^2}{dt^2} \bar{q}(t) = 0,
\]

i.e. we have Newton’s equation for the average coordinates.

We also have Hamilton’s equations for the average values of the coordinate and momentum:

\[
\dot{\bar{q}} = \frac{\partial H}{\partial \bar{p}}, \quad \dot{\bar{p}} = -\frac{\partial H}{\partial \bar{q}},
\]

where the Hamiltonian \(H = H(\bar{q}, \bar{p})\) for the free particle has the form

\[
H = \frac{\bar{p}^2}{2m}.
\]
Note that in the functional mechanics the Newton equation for the average coordinates is obtained only for the free particle or for quadratic Hamiltonians with a Gaussian initial distribution function. For a more general case there are corrections to Newton’s equations, as discussed below.

We discussed the spreading of Gaussian distribution functions. Similar results are obtained for the distribution functions of other forms, if they describe in some sense localized coordinates and momenta at the initial time.

5 Comparison with Quantum Mechanics

Compare the evolutions of Gaussian distribution functions in functional classical mechanics and in quantum mechanics for the motion of particles along a straight line. The scene of work for the functional classical mechanics is $L^2(\mathbb{R}^2)$ (or $L^1(\mathbb{R}^2)$), and for quantum mechanics - $L^2(\mathbb{R}^1)$.

The Schrodinger equation for a free quantum particle on a line reads:

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}. \tag{18}$$

Here $\psi = \psi(x,t)$ is the wave function and $\hbar$ is the Planck constant. The density of the distribution function for the Gaussian wave function has the form (see, for example [47])

$$\rho_q(x,t) = |\psi(x,t)|^2 = \frac{1}{\sqrt{\pi} \sqrt{a^2 + \frac{\hbar^2}{a^2 m^2}}} \exp\left\{ -\frac{(x - x_0 - \frac{p_0}{m} t)^2}{(a^2 + \frac{\hbar^2}{a^2 m^2})} \right\}. \tag{19}$$

We find that the distribution functions in functional classical and in quantum mechanics (11) and (19) coincide, if we set

$$a^2 \hbar^2 = \hbar^2. \tag{20}$$

If the condition (20) is satisfied then the Wigner function $W(q,p,t)$ [48] for $\psi$ corresponds to the classical distribution function (10), $W(q,p,t) = \rho(q,p,t)$.

The problem of spreading of the quantum wave packet in dealing with the potential barrier is considered in [49].

Gaussian wave functions on the line are coherent or compressed states. The compressed states on the interval are considered in [50].

6 Liouville Equation and the Newton Equation

In the functional classical mechanics the motion of a particle along the straight line is described by the Liouville equation (3). A more general Liouville equation on the manifold $\Gamma$ with coordinates $x = (x^1, ..., x^k)$ has the form

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{k} \frac{\partial}{\partial x^i}(\rho v^i) = 0. \tag{21}$$
Here $\rho = \rho(x, t)$ is the density function and $v = v(x) = (v^1, ..., v^k)$ - vector field on $\Gamma$. The solution of the Cauchy problem for the equation (21) with initial data
\[ \rho|_{t=0} = \rho_0(x) \] (22)
might be written in the form
\[ \rho(x, t) = \rho_0(\varphi_t(x)) . \] (23)
Here $\varphi_t(x)$ is a phase flow along the solutions of the characteristic equation
\[ \dot{x} = v(x) . \] (24)
In particular, if $k = 2n$, and $M = M^n$ is a smooth manifold, the phase space $\Gamma = T^*M$ is a cotangent bundle, $H = H(q, p)$ is a Hamiltonian function on $\Gamma$, then the Liouville equation has the form
\[ \frac{\partial \rho}{\partial t} + \sum_{i=1}^{n} \left( \frac{\partial H}{\partial p_i^\alpha} \frac{\partial \rho}{\partial q_i^\alpha} - \frac{\partial H}{\partial q_i^\alpha} \frac{\partial \rho}{\partial p_i^\alpha} \right) = 0 . \] (25)
The Liouville measure $d\mu = dq dp$ is invariant under the phase flow $\varphi_t$.

Classical dynamical system in the functional approach to mechanics is a stochastic process $\xi(t) = \xi(t; q, p) = \varphi_t(q, p)$ which takes values in $\Gamma$ and with the probabilistic measure $dP(q, p) = \rho_0(q, p)dq dp$. Correlation functions have the form
\[ < \xi_{i_1}(t_1) ... \xi_{i_s}(t_s) > = \int \xi_{i_1}(t_1; q, p)...\xi_{i_s}(t_s; q, p)\rho_0(q, p)dq dp . \] (26)
Here $i_1, ..., i_s = 1, ..., k$.

It is assumed usually that the energy surfaces $\{ H = \text{const} \}$ are compact.

A system from $N$ particles in the 3-dimensional space has the phase space $\mathbb{R}^{6N}$ with coordinates $q = (q_1, ..., q_N)$, $p = (p_1, ..., p_N)$, $q_i = (q^1_i, q^2_i, q^3_i)$, $p_i = (p^1_i, p^2_i, p^3_i)$, $i = 1, ..., N$ and it is described by the Liouville equation for the function $\rho = \rho(q, p, t)$
\[ \frac{\partial \rho}{\partial t} = \sum_{i, \alpha} \left( \frac{\partial V(q)}{\partial q_i^\alpha} \frac{\partial \rho}{\partial p_i^\alpha} - \frac{p_i^\alpha}{m_i} \frac{\partial \rho}{\partial q_i^\alpha} \right) . \] (27)
Here summation goes on $i = 1, ..., N$, $\alpha = 1, 2, 3$. The characteristics equations for (27) are Hamilton’s equations
\[ q_i^\alpha = \frac{\partial H}{\partial p_i^\alpha} , \quad p_i^\alpha = -\frac{\partial H}{\partial q_i^\alpha} , \] (28)
where the Hamiltonian is
\[ H = \sum_i \frac{p_i^2}{2m_i} + V(q) . \] (29)
Emphasize here again that the Hamilton equations (28) in the current functional approach to the mechanics do not describe directly the motion of particles, and they are only the characteristic equations for the Liouville equation (27) which has a physical meaning. The Liouville equation (27) can be written as
\[ \frac{\partial \rho}{\partial t} = \{ H, \rho \} , \] (30)
where the Poisson bracket
\[ \{H, \rho\} = \sum_{i, \alpha} \left( \frac{\partial H}{\partial q_i^\alpha} \frac{\partial \rho}{\partial p_i^\alpha} - \frac{\partial H}{\partial p_i^\alpha} \frac{\partial \rho}{\partial q_i^\alpha} \right). \] (31)

Criteria for essential self-adjointness of the Liouville operator in the Hilbert space \( L^2(\mathbb{R}^{6N}) \) are given in [51].

7 Corrections to Newton’s Equations

In section 4, it was noted that for the free particle in the functional approach to classical mechanics the averages coordinates and momenta satisfy the Newton equations. However, when there is a nonlinear interaction, then in functional approach corrections to the Newton’s equations appear.

Consider the motion of a particle along the line in the functional mechanics. Average value \( \overline{f} \) of the function on the phase space \( f = f(q,p) \) at time \( t \) is given by the integral
\[ \overline{f}(t) = \langle f(t) \rangle = \int f(q,p)\rho(q,p,t)dqdp. \] (32)

Here \( \rho(q,p,t) \) has the form
\[ \rho(q,p,t) = \rho_0(\varphi_t(q,p)). \] (33)

By making the replacement of variables, subject to the invariance of the Liouville measure, we get
\[ \langle f(t) \rangle = \int f(q,p)\rho(q,p,t)dqdp = \int f(\varphi_t(q,p))\rho_0(q,p)dqdp. \] (34)

Let us take
\[ \rho_0(q,p) = \delta_\epsilon(q - q_0)\delta_\epsilon(p - p_0), \] (35)

where
\[ \delta_\epsilon(q) = \frac{1}{\sqrt{\pi \epsilon}} e^{-q^2/\epsilon^2}, \] (36)

\( q \in \mathbb{R}, \epsilon > 0. \)

Let us show that in the limit \( \epsilon \to 0 \) we obtain the Newton (Hamilton) equations:
\[ \lim_{\epsilon \to 0} \langle f(t) \rangle = f(\varphi_t(q_0,p_0)). \] (37)

**Proposition 1.** Let the function \( f(q,p) \) in the expression \( \overline{f}(t) \) be continuous and integrable, and \( \rho_0 \) has the form \( \delta_\epsilon \). Then
\[ \lim_{\epsilon \to 0} \int f(q,p)\rho(q,p,t)dqdp = f(\varphi_t(q_0,p_0)). \] (38)
**Proof.** Functions $\delta_\epsilon(q)$ form a $\delta$-sequence in $D'(\mathbb{R})$ \cite{52}. Hence we obtain

$$\lim_{\epsilon \to 0} \int f((q,p))\rho(q,p,t)dqdp = \lim_{\epsilon \to 0} \int f(\varphi(t,q,p))\delta_\epsilon(q-q_0)\delta_\epsilon(p-p_0) = f(\varphi(t,q_0,p_0)), \quad (39)$$

that was required to prove.

Now calculate the corrections to the solution of the equation of Newton. In functional mechanics consider the equation, see (3),

$$\frac{\partial \rho}{\partial t} = -p\frac{\partial \rho}{\partial q} + \lambda q^2 \frac{\partial \rho}{\partial p}. \quad (40)$$

Here $\lambda$ is a small parameter and we set the mass $m = 1$. The characteristic equations have the form of the following Hamilton (Newton) equations:

$$\dot{p}(t) + \lambda q(t)^2 = 0, \quad \dot{q}(t) = p(t). \quad (41)$$

Solution of these equations with the initial data

$$q(0) = q, \quad \dot{q}(0) = p \quad (42)$$

for small $t$ has the form

$$(q(t),p(t)) = \varphi_t(q,p) = (q + pt - \frac{\lambda}{2}q^2t^2 + ..., \quad p - \lambda q^2t + ...) \quad (43)$$

Use the asymptotic expansion $\delta_\epsilon(q)$ in $D'(\mathbb{R})$ for $\epsilon \to 0$, compare \cite{13 53}:

$$\delta_\epsilon(q) = \delta(q) + \frac{\epsilon^2}{4}\delta''(q) + ..., \quad (44)$$

then for $\epsilon \to 0$ we obtain corrections to the Newton dynamics:

$$<q(t)> = \int (q + pt - \frac{\lambda}{2}q^2t^2 + ...)\left[\delta(q-q_0) + \frac{\epsilon^2}{4}\delta''(q-q_0) + ...ight] \quad (45)$$

$$\cdot \delta(p-p_0) + \frac{\epsilon^2}{4}\delta''(p-p_0) + ...]dqdp = q_0 + p_0t - \frac{\lambda}{2}q_0^2t^2 - \frac{\lambda\epsilon^2t^2}{4}.$$

Denoting the Newton solution

$$q_{\text{Newton}}(t) = q_0 + p_0t - \frac{\lambda}{2}q_0^2t^2,$$

we obtain for small $\epsilon, t$ and $\lambda$:

$$<q(t)> = q_{\text{Newton}}(t) - \frac{\lambda}{4}\epsilon^2t^2. \quad (46)$$

Here $-\frac{\lambda}{4}\epsilon^2t^2$ is the correction to the Newton solution received within the functional approach to classical mechanics with the initial Gaussian distribution function. If we choose a different initial distribution we get correction of another form.
We have proved

**Proposition 2.** *In the functional approach to mechanics the first correction at $\epsilon$ to the Newton dynamics for small $t$ and $\lambda$ for equation (41) has the form (46).*

Note that in the functional approach to mechanics instead of the usual Newton equation

$$m\frac{d^2}{dt^2}q(t) = F(q), \quad (47)$$

where $F(q)$ is a force, we obtain

$$m\frac{d^2}{dt^2} <q(t)> = <F(q)(t)>. \quad (48)$$

Indeed, multiplying the equation

$$\frac{\partial \rho}{\partial t} = -\frac{p}{m}\frac{\partial \rho}{\partial q} - F(q)\frac{\partial \rho}{\partial p}. \quad (49)$$

by $q$ and making integration over $p$ and $q$ and then integrating by parts, we get

$$\frac{d}{dt} <q(t)> = \frac{<p(t)>}{m}. \quad (50)$$

Similarly, multiplying the equation (49) by $p$ and integrating on $p$ and $q$ and then integrating by parts, we get

$$\frac{d}{dt} <p(t)> = <F(q)(t)>, \quad (51)$$

which gives (48).

The task of calculating the corrections at $\epsilon$ for Newton’s equation for mean values is similar to the problem of calculating semiclassical corrections in quantum mechanics [54, 44, 50].

8 Time Reversal

8.1 Reversibility in classical mechanics

Let us present a famous discourse which proves reversibility of the dynamics in classical mechanics. From the symmetry of Newton’s equations upon the replacement the time $t$ for $-t$ it follows that if in the system there exists some motion, then it is possible also the reverse motion, i.e. such motion, in which the system passes same states in the phase space in the reverse order. Indeed, let the function $x(t)$ satisfies the Newton equation

$$\ddot{x}(t) = F(x(t)) \quad (52)$$

with initial data

$$x(0) = x_0, \quad \dot{x}(0) = v_0. \quad (53)$$
We denote the corresponding solution by

\[ x(t) = \Phi(t; x_0, v_0). \]

We fix \( T > 0 \) and let us reverse the motion of the particle at some moment in time \( T \) by reversing its velocity, i.e. let us consider the solution \( y(t) \) of the Newton equation

\[ \ddot{y}(t) = F(y(t)) \] (54)

with the following initial data:

\[ y(0) = x(T), \quad \dot{y}(0) = -\dot{x}(T). \] (55)

Then it is easy to see that at the time moment \( T \) we get

\[ y(T) = x_0, \quad \dot{y}(T) = -v_0, \] (56)

i.e. the particle comes back to the initial point with the inverse velocity. To prove the relation (56) it is enough to note that the solution of equation (54) with initial data (55) has the form

\[ y(t) = \Phi(T - t; x_0, v_0) \]

and use the relations (53).

Let us notice that these arguments about reversibility of motion in the classical mechanics used not only symmetry of the Newton equation concerning time reversibility, but also the fact that a state of the particle in the classical mechanics at some instant of time is completely characterized by two parameters - co-ordinate \( x \) and speed \( v \). Reversibility of the motion in classical mechanics means reversibility of the motion along a given trajectory.

As it was discussed above, the notion of an individual trajectory of a particle has no physical sense. In reality we deal with a bunch of trajectories or probability distribution. In the functional classical mechanics the state of the particle is characterized not by the two numerical parameters, but the distribution function \( \rho = \rho(q, p, t) \). In the following subsection it will be shown, how it leads to delocalization and irreversibility.

### 8.2 Irreversibility in the functional mechanics

The considered reversibility of motion in classical mechanics deals with the individual trajectory. In the functional mechanics the concept of the individual trajectory of the particle has no direct physical sense. Instead, the state of the particle is described by the distribution function \( \rho = \rho(q, p, t) \) which satisfies the Liouville equation (53)

\[ \frac{\partial \rho}{\partial t} = -\frac{p}{m} \frac{\partial \rho}{\partial q} + \frac{\partial V(q)}{\partial q} \frac{\partial \rho}{\partial p}. \] (57)

The Liouville equation is invariant under the replacement \( t \) to \(-t\): if \( \rho = \rho(q, p, t) \) is the solution of the equation (57), then \( \sigma(q, p, t) = \rho(q, -p, -t) \) - also its solution. However this symmetry does not mean reversibility of the motion of a particle in the functional approach
to mechanics, since the state of the particle is described there by the distribution function and the phenomenon of delocalization takes place.

In this way we obtain an answer to the arguments of Loschmidt and Poincaré - Zermelo. Indeed, to reverse the particle motion at the time moment $t = T$ as it is proposed in the Loschmidt argument, it is necessary make the co-ordinate and momentum measurement. But it will change the distribution $\rho(q,p,T)$. Further, it is necessary to prepare such condition of the particle that its evolution back in time would lead to the initial distribution $\rho_0$ that is difficult since the delocalization takes place. We will need something even better than Maxwell’s demon.

For free particle the delocalization leads to the increasing of dispersion $\Delta q^2$ with time ($13$):

$$\Delta q^2(t) = \frac{1}{2}(a^2 + b^2t^2/m^2).$$

(58)

Notice that the similar phenomena takes place for the Brownian motion $B(t)$ which has dispersion $t$ [55, 56].

Concerning the Zermelo argument related with the Poincaré recurrence theorem we note that this argument can not be applied to the functional mechanics because this argument is based on the notion of individual trajectory. In the functional mechanics the state of the system is characterized by the distribution function and here the mean values might irreversibly tend to some limits without contradiction with the Poincaré theorem as it will be shown in the next section.

The Poincaré theorem is not applicable to the bunch of trajectories or even to two trajectories as it follows from the Lyapunov theory: if two points are situated in some small region of the phase space then they are not necessary come back to this region by moving along their trajectories.

### 8.3 Mixing and weak limit

The state $\rho_t = \rho_t(x)$ on the compact phase space $\Gamma$ is called mixing if its weak limit at $t \to \infty$ is a constant,

$$\lim_{t \to \infty} \rho_t(x) = \text{const}.$$ More precisely, a dynamical system $(\Gamma, \varphi_t, d\mu)$ has the mixing property [24, 32] if

$$\lim_{t \to \infty} <f, U_t g> = \int f d\mu \cdot \int g d\mu$$

(59)

for every $f, g \in L^2(\Gamma)$. Here $U_t g(x) = g(\varphi_t(x))$. For the mixing systems the bunch of trajectories is spreading over the phase space, hence in the functional mechanics we have irreversibility.

The method of the weak limit which generalizes the Poincaré results and which can be applied to a wide class of dynamical systems is developed in [11, 12].

Connection with the irreversibility problem can be explained on the following example. Let us consider the function of two real variables

$$F(t, p) = e^{i tp} f(p),$$
where \( f(p) \) is an integrable function. It is clear that the function \( F(t, p) \) is periodic in \( t \) if \( p \) is fixed and it has no limit as \( t \to \infty \). However, if we integrate the function \( F(t, p) \) over \( p \),

\[
F(t) = \int e^{itp} f(p) dp,
\]

then we get the function \( F(t) \) which already has the limit (by the Riemann - Lebesgue lemma):

\[
\lim_{t \to \infty} F(t) = 0.
\]

9 Dynamics of a Particle in a Box

Dynamics of collisionless continuous medium in a box with reflecting walls is considered in [29, 11, 12]. This studied asymptotics of solutions of Liouville equation. In functional approach to mechanics, we interpret the solution of the Liouville equation as described the dynamics of a single particle. Here we consider this model in the classical and also in the quantum version for the special case of Gaussian initial data.

9.1 Dynamics of a classical particle in a box

Consider the motion of a free particle on the interval with the reflective ends. Using the method of reflections [52], the solution of the Liouville equation (8)

\[
\frac{\partial \rho}{\partial t} = -\frac{p}{m} \frac{\partial \rho}{\partial q}
\]

on the interval \( 0 \leq q \leq 1 \) with the reflective ends we write as

\[
\rho(q, p, t) = \sum_{n=-\infty}^{\infty} \left[ \rho_0(q - \frac{p}{m} t + 2n, p) + \rho_0(-q + \frac{p}{m} t + 2n, -p) \right],
\]

(60)

where it is assumed that the function \( \rho_0 \) has the Gaussian form [5].

One can show that for the distribution for coordinates

\[
\rho_c(q, t) = \int \rho(q, p, t) dp
\]

(61)

one gets the uniform limiting distribution (pointwise limit):

\[
\lim_{t \to \infty} \rho_c(q, t) = 1.
\]

For the distribution of the absolute values of momenta \((p > 0)\)

\[
\rho_a(p, t) = \rho_m(p, t) + \rho_m(-p, t),
\]

where

\[
\rho_m(p, t) = \int_{0}^{1} \rho(q, p, t) dq,
\]

as \( t \to \infty \) we get the distribution of the Maxwell type (but not the Maxwell distribution):

\[
\lim_{t \to \infty} \rho_a(p, t) = \frac{1}{\sqrt{\pi b}} \left[ e^{-\frac{(p-p_0)^2}{b^2}} + e^{-\frac{(p+p_0)^2}{b^2}} \right].
\]
9.2 Dynamics of a quantum particle in a box

The Schrödinger equation for free quantum particle on the interval $0 \leq x \leq 1$ with reflecting ends has the form

$$i\hbar \frac{\partial \phi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \phi}{\partial x^2}$$

(62)

with the boundary conditions

$$\phi(0, t) = 0, \quad \phi(1, t) = 0, \quad t \in \mathbb{R}.$$ 

Solution of this boundary problem can be written as follows:

$$\phi(x, t) = \sum_{n=-\infty}^{\infty} [\psi(x + 2n, t) - \psi(-x + 2n, t)],$$

where $\psi(x, t)$ is some solution of the Schrödinger equation. If we choose the function $\psi(x, t)$ in the form, corresponding to the distribution (19), then one can show that in the semiclassical limit for the probability density $|\phi(x, t)|^2$ the leading term is the classical distribution $\rho_c(x, t)$ (61).

10 Conclusions

In this paper the functional formulation of classical mechanics is suggested which is based not on the notion of an individual trajectory of the particle but on the distribution function on the phase space.

The fundamental equation of the microscopic dynamics in the proposed functional approach is not the Newton equation but the Liouville equation for the distribution function of a single particle. Solutions of the Liouville equation have the property of delocalization which accounts for irreversibility. It is shown that the Newton equation in this approach appears as an approximate equation describing the dynamics of the average values of the positions and momenta for not too long time intervals. Corrections to the Newton equation are computed.

Interesting problems related with applications of the functional formulation of mechanics to statistical mechanics, to singularities in cosmology and black holes, and new interpretation of quantum mechanics we hope to consider in further works.

11 Acknowledgements

The author expresses his sincere thanks to G.A. Alexeev, I.Ya. Aref’eva, O.V. Groshev, B. Dragovich, E.A. Dynin, M.G. Ivanov, A.Yu. Khrennikov, V.V. Kozlov, Yu.I. Manin, E.V. Piskovsky, A.S. Trushechkin, V.A. Zagrebnov, E.I. Zelenov, and participants of the special seminar on the irreversibility problem NOC MIAN for fruitful discussions of the fundamental problems of mechanics. The work is partially supported by grants NS-3224.2008.1, RFBR 08-01-00727-a, AVTSP 3341 and the program OMN RAS.
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