The functional mechanics: evolution of the moments of distribution function and the Poincare recurrence theorem.

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1 Introduction.

The irreversibility problem, i.e. the problem correspondence between irreversible in time the equations of macroscopic dynamics (transport equations

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and etc.) and the fundamental reversible microscopic equations (Hamilton and Schrödinger equations) is one of the most profound problems of the physical theory. Since paradoxes of Loschmidt and Poincare-Zermelo finding contradiction between the picture of relaxation to thermodynamic balance and the fundamental properties of mechanical motion were formulated, became clear that the reductionism in the narrow sense, i.e. to deduce macroscopic equations only from the elements of mechanics, rather likely, impossible, and methodologically unacceptable. One of the manifestations of the above-mentioned controversy is the fact that the Poincare’s recurrence theorem implies the impossibility of entropy as a function of canonical variables, monotone increasing on the trajectories of the system. On the other hand, the validity of both mechanics equations and the equations of physical kinetics makes it necessary to construct procedure, to deduce of the macroscopic equations from some extra prescription, and within these prescription withdrawal must be unambiguous, and prescription themselves should be independent of the specific form of the Hamiltonian system. To date, approaches to solve the problem of irreversibility have been proposed, and, nevertheless, the problem is still not investigated to the end and requires additional study. Most modern approaches consider the properties of macroscopic dynamics of the attributes of the phase flow mechanics system as a whole, rather than a single isolated trajectory, substantially different in the implementation of this methodological principle. The most well-known approach of this kind is the method of Bogolyubov [1], being constructing the hierarchy Bogolyubov-Born - Green - Kirkwood - Yvon (BBGKY) by averaging the multiparticle Liouville equation. Another original method in statistical mechanics was developed by Prigogine [2]. This method also comes from the Liouville equation, but it offers quite a different interpretation based on an analogy between the Liouville equation and Schrödinger equation. Poisson bracket with Hamiltonian (Liouville operator) is considered as an analogue of the Hamiltonian acting in the space of states - distribution functions, as well as macroscopic quantities (primarily temperature and entropy) are the operators which do not commute with the Liouville operator. Recently, I.V. Volovich has offered another approach to classical mechanics the so called functional mechanics [3]. He suggested way to interpret the Liouville equation as the fundamental equations of mechanics [4], the distribution function is also considered as the system state, but the state is not of the macroscopic but microscopic system. In the functional mechanics one considers the mean value of the coordinate when includes corrections to the Newton trajectory. Since the functional
mechanics modifies the equations of classical microscopic dynamics, it is necessary to understand, to what observed effects such a modification can lead. In the first two articles (see [3][5]), devoted to the functional mechanics, it was assumed that the existence of deviations of functional mechanics mean from Newtonian trajectories and within the perturbation theory was shown by the example of the simplest nonlinear mechanical systems that such deviations occur.

In this paper the general formula for the corrections to Newtonian trajectories in the form expansion in the moments of the initial distribution and the calculation of the evolution of all moments of higher order will be displayed. The results will be used for proof of the destruction of the periodicity of the functional mechanics and of non-conservation classical invariants of movement in the functional mechanic trajectories. This paper, I hope, will elaborate further observable consequences of the functional mechanics.

2 Liouville equation and the evolution of the distribution function.

The Liouville equation determines the dynamics of the system in functional formulation of classical mechanics.

\[ \partial_t \rho + \partial_i (\rho v^i) = 0 \]  \hspace{1cm} (1)
\[ \rho(0, x) = \rho_0(x) \]  \hspace{1cm} (2)

Here, \( x \) belongs to the phase space, ie is a pair variables \( x = (p, q) \), where \( p, q \in \mathbb{R}^n \), and \( v^i, (i = 1, \ldots 2n) \) is a vector field of corresponding Hamiltonian system with Hamiltonian \( H(p, q) \).

\[ \mathbf{v} = \sum_{\mu=1}^{n} \left( \frac{\partial H}{\partial p_{\mu}} \partial_{q_{\mu}} - \frac{\partial H}{\partial q_{\mu}} \partial_{p_{\mu}} \right) \]  \hspace{1cm} (3)

State of the mechanical system is determined by the probability density \( \rho(t, x) \). It makes sense to draw parallels with quantum mechanics - probability density is an analogue of the density matrix and the linear functionals over state space are meaningful observables. If in the case of quantum mechanics, observables are determined self-adjoint operators and the average
value of the observable $\langle \hat{O} \rangle = Tr \hat{O} \hat{\rho}$, in the case of the functional mechanics the observables are c-integrable numerical\(^1\) over measure $\rho$ functions and the average value of the observable $\langle O \rangle = \int O(x) \rho(x) dx$. Since the functional mechanics observables commute with each other, the problem of simultaneous measurement is absent—in particular, the momentum and coordinate can be measured simultaneously with any desired (but not absolute, that is essential) precision within defined properties of the instrument\(^2\), that is why the functional mechanics is classical.

The solution of the Cauchy problem \(^1\) - \(^2\) for the Liouville equation can be written as

$$\rho(t, x) = \rho_0(u(-t, x))$$  \hspace{1cm} (4)

where $u(-t, x)$-phase flow along the solutions of the equations of the characteristics, i.e. the family of Cauchy problem for equations of a dynamical system with all possible initial data

$$\dot{u}(t, x) = v(u)$$  \hspace{1cm} (5)
$$u(0, x) = x$$  \hspace{1cm} (6)

We will consider not only the Hamiltonian system, but also a wider class of dynamical systems which preserves the phase volume flow of $\det(\frac{\partial u_i}{\partial x_j}) = 1$ for which functional reformulation dynamics is reasonable due to the equality

$$\int f(x) \rho_0(u(-t, x)) dx = \int f(u(t, x)) \rho_0(x) dx$$  \hspace{1cm} (7)

Here $f$ is a function on the phase space. Formally, the solution of the problem \(^5\) - \(^6\) can be represented by an exponential function of a vector field

\(^1\)It would be natural to assume that the observables and the state are square integrable, but in the original paper on the functional mechanics formulation of the amendments to the Newtonian trajectory is designed to enhance the state space to a space of generalized functions, which in turn would narrow the class of observables. Although in our calculation of the corrections we shall not resort to the apparatus of generalized functions, it should be noted that the question of the class of state functions needs further clarification.

\(^2\)Note that the quantum mechanical analogue of the axiom of measurement in the functional mechanics had not yet formulated, we can only say that, as in quantum mechanics, the measurement is a reduction of the density function (see \(^3\)), but the specific form of the density after a measurement and its relation to the properties of the device requires additional discussion.
\[ u(t, x) = e^{tv^i x} \tag{8} \]

where the exponent is the sum of series

\[ e^{tv^i} \equiv 1 + tv^i \partial_i + \frac{1}{2} t^2 v^k \partial_k v^i \partial_i + \ldots = \sum_{n=0}^{\infty} \frac{t^n}{n!} (v^i \partial_i)^n \tag{9} \]

The exact solution is not necessarily obtained by summing the series, it can be obtained in any other way - by the summation perturbation series, or explicitly in some special cases - all subsequent arguments we will build on the assumption that the exact solution is known.

As it is known from the theory of ordinary differential equations function \( u(t, x) \) is continuously differentiable as many times as \( v \), in particular, if \( v \) is analytic and that \( u(t, x) \) analytic (see eg [7] to «local» theorem and [8] for «global») on some time interval, so we can expand this solution in a number of Taylor on the coordinate \( \xi = x - x_0 \) in the vicinity of some point \( x_0 = \int \rho(x)dx \), chosen so that it coincided with the expectation of the coordinates on the initial distribution.

\[ u(t, x_0 + \xi) = \sum_{\alpha \in \mathbb{N}_0^D} \frac{1}{\alpha!} \xi^\alpha \partial^\alpha u(t, x_0) \equiv \sum_{\alpha} \xi^\alpha u_\alpha \tag{10} \]

We have used the compact notation of the Taylor series through multi-index \( \alpha \in \mathbb{N}_0^D \) - vector non-negative integer components, for which in addition to operations of linear algebra operations are defined the modulus \( |\alpha| = \sum_{i=1}^{2n} \alpha_i \), componentwise multiplication \( \alpha \beta = \{\alpha_i \beta_i\} \), the factorial of \( \alpha! = \prod_{i=1}^{2n} \alpha_i! \), as well as the erection of a vector in the degree \( x^\alpha = \prod_{i=1}^{2n} x_i^{\alpha_i} \), and the taking of partial derivative \( \partial^\alpha = \prod_{i=1}^{2n} \partial_i^{\alpha_i} \) order \( \alpha \). Taylor series coefficients, ie the partial derivative order \( \alpha \), with appropriate weight, we have denoted as \( u_\alpha = u_\alpha(t) = \partial^\alpha u/\alpha! \).

Now, averaging (10) on the initial distribution, it is easy to calculate the average values of coordinates (11) and deviations of averages of Newtonian trajectories (12) through centered moments of the initial distribution of \( M^\alpha \).
defined by (13), where \( \langle u(t, x) \rangle = \int u(t, x) \rho_0(x) dx \)

\[
\langle u(t, x) \rangle = \sum_{\alpha} M^\alpha u_\alpha 
\]

(11)

\[
\langle u(t, x) \rangle - u(t, x_0) = \sum_{|\alpha|>1} M^\alpha u_\alpha 
\]

(12)

\[
M^\alpha = \langle \prod_{i=1}^{D} (x^i - x_0^i)^{\alpha_i} \rangle = \int \prod_{i=1}^{D} (x^i - x_0^i)^{\alpha_i} \rho_0(x) dx = \int \prod_{i=1}^{D} (\xi^i)^{\alpha_i} \rho_0(x_0 + \xi) d\xi 
\]

(13)

Thus, the functional mechanical corrections to the classical Newtonian trajectories are given a countable set of time functions \( U_\alpha \) - all the partial trajectory classical motion of the initial data, which were calculated on the classical trajectory itself. Therefore, to calculate the deviations from well-known classical trajectory it is not necessary to find solution for all initial data - enough to know the behavior trajectories in the vicinity of the known one, or build a chain of variational equations (see [8]), which defines the evolution Partial solutions of differential equations parameters - in this case the initial data. After desired set of functions is found, it remains only to sum its pre-defined and time-varying weights - moments of the initial distribution. We see that the trajectory of the average values of coordinates is defined by all moments of the distribution function at the initial moment of time, therefore there is no differential equation with a finite number of parameters that would be effect the trajectory averages, since the solution of this equation is uniquely determined by initial conditions and parameters, while the trajectory mean values depend on the moments of the initial distribution, which can be chosen rather arbitrarily. Then naturally arises the problem of tracing the evolution centered moments of all orders. This requires in the original definition of (13) to make the substitution \( x \mapsto u(t, x) \) and input a series of (11) into a new definition of a centered moment of order \( \alpha \), and then to rearrange the multiplication and summation. We carry out this tedious calculations in three stages. At first, we transform the definition of centered moments with the

\[ M^\alpha(0) = M^\alpha \] due to the fact that \( u(0, x) = x \)
Then we calculate the average degree of any monomial coordinates at a certain time by

\[\langle u^{\alpha-\beta}(t, x) \rangle = \sum_{\gamma} \langle \xi^\gamma u_\gamma \rangle^{\alpha-\beta} = \sum_{\gamma} \langle \xi^{(\alpha-\beta)\gamma} \rangle u_\gamma^{\alpha-\beta} = \sum_{\gamma} M^{(\alpha-\beta)\gamma} u_\gamma^{\alpha-\beta} \tag{15}\]

Here the lower multi-index is the order of the derivative, and the upper is the power of its components. Finally it remains to convert the power of mean coordinates by selecting the coefficients of the products of the moments, for which we use the computation

\[\langle u(t, x) \rangle^\beta = \prod_{i=1}^{D} \left( \sum_{\delta_i} M^\delta u_\delta^i \right)^{\beta_i} = \sum_{\delta_i; \delta_k \leq \delta_{k+1} \forall k} \prod_{\text{permutations}} \sum_{\delta_k \leq \delta_{k+1} \forall k; \, \delta_k \leq \delta_{k+1} \forall k} \prod_{k=1}^{\beta} \prod_{k=1}^{\beta} M^\delta \tag{16}\]

In (16) summation in the coefficient of ordered product of the moment is made in such a way as to take all possible permutations of an integer index \(i\) so that the index \(i\)-th component appeared no more than \(\beta_i\) times.

Now we can construct an algorithm for to compute every moment of the distribution, given the initial moments.

\[M^\alpha(t) = \sum_{\delta_i; \delta_k \leq \delta_{k+1} \forall k} \sum_{\beta \leq \alpha} \prod_{\text{permutations}} \sum_{1 \leq i_k \leq D} \prod_{k=1}^{\beta} \sum_{\delta_k \leq \delta_{k+1} \forall k} \prod_{k=1}^{\beta} M^\delta \tag{17}\]

Note that if the distribution has the form \(\rho(x) = \frac{1}{\varepsilon^{D}} \phi\left(\frac{x}{\varepsilon}\right)\), then for the moments the following estimate on the order of \(M^\alpha \sim \varepsilon^{\mid\alpha\mid}\) is valid, so using (17) in the numerical calculation, we can retain only a finite number of terms, while maintaining an acceptable accuracy in studying the dynamics of average values of canonical variables on time scales comparable to the period.
As an example, we calculate the matrix of second moments of the distribution, given the initial moments \( B_{ij}(t) = \langle u^i(t, x) - \langle u^i(t, x) \rangle \rangle \) =

\[
= \langle u^i(t, x)u^j(t, x) \rangle - \langle u^i(t, x) \rangle \langle u^j(t, x) \rangle = \sum_{\alpha, \beta} u^j_{\alpha} \bar{u}_{\beta}(M^{\alpha+\beta} - M^{\alpha}M^{\beta})
\]

(18)

The first nonvanishing term in (18) coincides with the expression for conversion of a second-rank tensor under a coordinates change \( x \rightarrow u(x) \).

\[
B_{ij}(0)(t) = \sum_{2 \leq |\alpha| + |\beta| \leq 1} u^j_{\alpha} \bar{u}_{\beta}M^{\alpha+\beta} = \partial u_i \partial x^k \partial u_j \partial x^l B^{kl}
\]

(19)

Next correction by \( \varepsilon \) to (19) is given by (20) and contains moments of higher order.

\[
B_{ij}(1)(t) = \sum_{3 \leq |\alpha| + |\beta| \leq 2} u_{\alpha}u_{\beta}(M^{\alpha+\beta} - M^{\alpha}M^{\beta}) =
\]

\[
= \frac{1}{2} \left( \partial^2 u^i \partial u^j \partial x^k \partial x^m + \partial u^i \partial^2 u^j \partial x^k \partial x^m \partial x^l \right) \left( B^{kml} + \frac{1}{4} \partial^2 u^i \partial u^j \partial x^k \partial x^m \partial x^l (B^{kml} - B^{km}B^{ln}) \right)
\]

(20)

For sufficiently small times, you can use the decomposition of exponent of a vector field into a row and to get

\[
B_{ij}(0)(t) = B_{ij} + t \left( \frac{\partial u^i}{\partial x^l} B^{lj} + \frac{\partial v^j}{\partial x^l} B^{ii} \right) +
\]

\[
+ \frac{t^2}{2} \left( \partial (v^k \partial x^l v^j) \partial x^l B^{ji} + \partial (v^k \partial x^l v^j) \partial x^l B^{ii} \right) + \frac{t^2}{4} \partial v^i \partial v^j \partial x^l \partial x^l B^{kl} + o(t^2)
\]

(21)

Expression (21) reproduces the phenomenon is similar to a spreading wave packet in quantum mechanics. The results obtained in this section allow us to monitor the process of «spreading» over formally arbitrarily long time - just enough to calculate the classical trajectory starting at the point of phase space corresponding to the expectation of state variables over the initial distribution, calculate the partial derivatives of the classical equations of motion for the initial data, and specify the initial distribution of all its moments - the formula (17) describes the evolution of the moments by all orders in «spreading» of the initial distribution when phase flow transferring its.
3 Conclusion.

Let’s discuss the applicability of the results. Our arguments based on two premises - the analyticity phase flow for a sufficiently long period of time, and existence of all finite moments of the distribution function. «Global» theorem of continuous differentiability of the solution of (5) from the initial data, which we have already referred to in the preceding part of the article [8], guarantees the preservation of smoothness noncontinuable solutions to some of its neighborhood, so it suffices to have the infinite extendability solutions of (5) in order to ensure that they are analytic for analytic right-hand side. However, if the motion is finite, i.e. trajectory that began in some domain \( G \) does not leave it, and the vector field defining right-hand side of (4) defined over the entire \( G \) and has no the singular points in \( G^1 \), then the solution of (5) with initial conditions in \( G \) is infinitely extendable. For Hamiltonian systems of the above conditions follow from the compactness constant energy surface, which neighborhood should be chosen as an area of \( G = \{ x \equiv (p,q) : h - \delta < H(p,q) < h + \delta \} \). Then the analyticity of the right side system (5) of \( G \) provides an infinite differentiability of noncontinuable solution of (5) on initial data, and analytic \( u(t,x) \) in some neighborhood \( X_0 \), and hence the expression (10), (11) and (17) will be applicable to an arbitrarily long time, as comparable to the period of return, predicted by the Poincare theorem and beyond this period as well. On the other hand, the existence of a weak limit distribution function (see [9]) leads to that any trajectory of the average values of the canonical variables ends in the average values of the coordinates of the limit distribution, and hence to an infinitely large time, when needed take into account all the terms of the formula (17) does not convenient, because it allows to outline the asymptotic behavior. Preservation of phase volume and finite motion are conditions of Poincare’s recurrence theorem, but the functional mechanics predicts the occurrence of deviations (22) averaged trajectories from the starting point for the period \( T(x_0) \)

\[
\left( \sum_{i=1}^{D} (u^i(T(x_0), x) - u^i(0, x))^2 \right) = \sum_{\alpha, \beta} M^{\alpha+\beta} \sum_{i=1}^{D} (u^i_{\alpha}(T(x_0), x)u^i_{\beta}(T(x_0), x)) (22)
\]

This effect arises because depending on the period from the starting point\(^4\)

\(^4\)it is clear that for points in one orbit, the period is the same
— differentiating the periodicity condition $u(T(x), x) = u(0, x)$ along the coordinate,

$$
\partial^\alpha u(0, x) = \partial^\alpha u(T(x), x) = \prod_{i=1}^{D} \left( \partial_i^\alpha + \partial_i^\alpha T(x) \right)^\alpha u(t, x) \tag{23}
$$

we get the non-periodicity of higher derivatives $u_\alpha(T(x), x) \neq u_\alpha(0, x)$, while the global periodicity (the case $\partial_i^\alpha T(x) = 0$ for $\forall x$) in the functional mechanics is preserved.

The destruction of the periodicity of the functional mechanics leads to nonconservation of the trajectories of the average values of coordinates of the integrals of motion of classical system - using arguments similar to the calculation of the evolution moments, we can obtain an expression (24) for amendments to the evolution invariants of the classical system.

$$
\delta I = I(\langle u(t, x) \rangle) - I(u(t, x)) = \sum(|\alpha| \geq 1) \left( \sum u_\alpha M^\alpha \right)^\beta I_\beta =
$$

$$
= \sum I_\beta \sum_{1 \leq \alpha_k; \alpha_k \leq \alpha_{k+1}}^{\beta} \left( \sum_{\text{permutations}} \prod_{k=1}^{\beta} u_{\alpha_k}^{i_k} \right) \prod_{k=1; \alpha_k \leq \alpha_{k+1}}^{\beta} \prod_{\forall k} M^{\alpha_k} \tag{24}
$$

The first nonvanishing term in the expansion (24) is given by (25) and is proportional to the covariance matrix.

$$
\delta I^{(0)} = \frac{1}{2} B_{ij} \frac{\partial^2 u^k}{\partial x_i \partial x_j} \frac{\partial I}{\partial x_k} \tag{25}
$$

Thus the paradox arises — the functional mechanics average values of the invariants of motion, for example, the energy, are conserved, but as a function of average values of the coordinates of the invariants and, specifically, the Hamiltonian is not preserved. It seems natural to assumed the decrease of the Hamiltonian path functional mechanical means for Hamiltonian systems with compact and convex Hamiltonian (and hence convex surface of constant energy), due to conservation of the average value of the Hamiltonian in the transition to the limit distribution of $\int H(x)\bar{\rho}(x)dx = \int H(x)\rho_0(x)dx$ and Jensen’s inequality $H(\bar{p}, \bar{q}) \equiv H(\bar{x}) = H(\int x\bar{\rho}(x)dx) < \int H(x)\bar{\rho}(x)dx = \int H(x)\rho_0(x)dx$, where $(\bar{p}, \bar{q}) \equiv \bar{x} —$ time-averaged phase variables $(p(t), q(t))$. 

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and averaging over the weak limit $\bar{\rho}(x)$ a probability measure $\rho(u(-t, x))$ of both the observables and their time average are the same because (26), where we have used invariance of the weak limit of the phase flow:

$$\int \left( \lim_{T \to +\infty} \frac{1}{T} \int_0^T u(t, x)dt \right) \bar{\rho}(x)dx = \lim_{T \to +\infty} \frac{1}{T} \int_0^T \int u(t, x)\bar{\rho}(x)dxdt =$$

$$= \lim_{T \to +\infty} \frac{1}{T} \int_0^T \int x\bar{\rho}(u(-t, x))dxdt = \lim_{T \to +\infty} \frac{1}{T} \int_0^T \int x\bar{\rho}(x)dxdt = \int x\bar{\rho}(x)dx$$

(26)

The above means that the prediction of dynamics are dependent on what values are measured - the measurement of invariants allows to predict the state of the classical system at subsequent times much more accurately. The latter can be interpreted in two ways - one single measurement of invariant of dynamic system is equivalent to multiple measurement of state variables, or, equivalently, the invariants allow consistent measurement, while measurement of state variables must be parallel (simultaneously).

Thus, we have shown that the trajectories of functional mechanical averages are not periodic and do not maintain the invariant of motion using the formulas for evolution of the moments of the distribution derived in the previous section, ie the functional mechanics is free from the paradox of the Poincare-Zermelo and describes effective dissipation, what which takes place in real-world mechanical systems.

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