

Irreversibility of Kinetic Equations and Locality of Interactions

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Abstract

The relationship between classical and quantum statistical mechanics is considered in the issue of the irreversibility of evolutionary processes described using the formalism of wave functions, Wigner functions, and distribution functions, which are solutions of kinetic equations. It is shown that the dynamics of multiparticle systems with increasing entropy is significantly related to the assumptions of locality of interactions.

Keywords

Lagrange Geometry, Scalar Potential, Weyl Manifold

1. Introduction

The time-irreversibility of physicochemical processes, associated with the interaction of particles at the microlevel, significantly distinguishes them from mechanical processes and interactions of macroscopic bodies. Newton's laws of mechanics are invariant with respect to the direction of the "arrow of time", and therefore their possible application to the description of, say, kinetic processes in transport theory should lead to corresponding results: the trajectories of particles should be time-reversible, which, in particular, means the possibility of the aforementioned processes occurring with the formal replacement of $t \rightarrow -t$. However, this contradicts the "zeroth law" of thermodynamics (the one-way heat transfer from a hotter body to a cooler one). Therefore, kinetic processes belong to the class of nonequilibrium processes, and the dynamic evolution of the systems in which they occur cannot be directly described using the formalism of the laws of macroscopic mechanics without appropriate corrections.

Understanding this "paradox" and the possible modification of the mathematical apparatus of microphysics have been the subject of an extremely large number

of works, since the 19th century, currently considered fundamental and classical. However, with the emergence of quantum mechanics, the problem of understanding the structure of nonequilibrium transport and interaction of particles has resurfaced, with new urgency and clarity. Indeed, as it turns out, the equations for the evolution of quantum objects (Schroedinger, Heisenberg, Dirac, etc.) are again time-reversible. Accordingly, the transitivity of the correspondence principle is “threatened” upon the transition to classical kinetic equations, and an explanation for the time covariance of quantum kinetic equations is also required.

This paper does not claim to provide a comprehensive coverage or detailed analysis of existing approaches to the problem described above. This would require a considerable amount of space (a simple list of publications devoted to the properties of classical and quantum-statistical irreversibility would take tens, if not hundreds, of pages). Nevertheless, it seems appropriate to mention some works that can be used to build a fairly comprehensive and in-depth understanding of the subject under discussion. In particular, the papers [1]-[10] present the fundamentals of the theory of nonequilibrium statistical physics and provide an exhaustive analysis of the concept of “irreversibility” for Boltzmann-type kinetic equations, as well as the relationship of this concept to the structure of the BBGKY chain; in the works [11]-[20] the connection between the irreversibility of transport processes and the mathematical apparatus used in topology, differential geometry, and the general theory of algebras was revealed; in the works [21]-[30] issues of irreversibility at the quantum-mechanical level were considered.

The subject of this work is the development of the simplest (in the authors’ opinion) method for analyzing the connection between the time irreversibility of kinetic equations and the evolution equations of dynamical systems in symplectic geometry.

2. Basic Aspects of Classical Dynamics of Structureless Particles

Consider a system of N classical particles in \mathbb{R}^3 space with coordinates $\mathbf{x}^i \in \mathbb{R}^3$, masses m_i , and momenta $\mathbf{p}_i \in \mathbb{R}^3$ ($i = \overline{1, N}$), interacting via the potential $V: \mathbb{R}^3 \rightarrow \mathbb{R}^1$; Let us denote $\mathfrak{B} = \mathbb{R}^3 \times \mathbb{X}_p^3$ the μ -space of this system. A point of μ -space (of the cotangent bundle over the configuration space, see point 4) $(\mathbf{X}, \mathbf{P}) = (x^1, \dots, x^N; p_1, \dots, p_N)$, where $\mathbf{x}^k = (x^{k,1}, x^{k,2}, x^{k,3})$, $k = \overline{1, N}$ (and similarly for \mathbf{p}_k), characterizes the state of the system and observables (quantities) of the system (*i.e.*, its macrocharacteristics). The Hamiltonian of the system is of the form

$$H(\mathbf{X}, \mathbf{P}) = \sum_{i=1}^N \frac{\mathbf{P}_i^2}{2m_i} + V(\mathbf{X}), \quad V(\mathbf{X}) = \sum_{i < j} V(|\mathbf{x}^i - \mathbf{x}^j|). \quad (1)$$

Equations of motion of the system’s points:

$$\frac{d\mathbf{x}^i}{dt} = \frac{\partial H(\mathbf{X}, \mathbf{P})}{\partial \mathbf{p}_i}, \quad \frac{d\mathbf{p}_i}{dt} = -\frac{\partial H(\mathbf{X}, \mathbf{P})}{\partial \mathbf{x}^i}, \quad i = \overline{1, N}. \quad (2)$$

Given that $\mathbf{p}_i = m_i \cdot (\mathbf{dx}^i / dt)$, the last system yields Newton's equations: $m_i \cdot (d(\mathbf{x}^i)^2 / dt^2) = -\partial V(\mathbf{X}) / \partial \mathbf{x}^i$. If the potential V is stationary (or, in a more general formulation of the problem, the Hamiltonian H does not depend on time), then one can define a stationary energy hypersurface or energy, which is for a classical system a topologically simply connected section of a hypercylinder—in contrast to the quantum case, when the energy of the system can decompose into a discrete spectral sequence of topologically separated manifolds,—in μ -space: $E = H(\mathbf{X}(0), \mathbf{P}(0)) = H(\mathbf{X}(t), \mathbf{P}(t)) \quad (\forall t > 0)$.

On a given hypersurface (*i.e.*, when the system's conservation law is satisfied), for any observable $\varpi : \mathfrak{P} \rightarrow \mathbb{R}^1$ (defined on a $6N$ -dimensional μ -system with values on the real axis), the evolution along a classical trajectory $\varpi[t] = \varpi(\mathbf{X}(t), \mathbf{P}(t))$ is given by the linear operator equation

$$\frac{d\varpi[t]}{dt} = \hat{L}[H]\varpi[t], \tag{3}$$

where the formulation of the corresponding Cauchy problem is ensured by the presence of initial data in the form $\varpi[t = 0] \equiv \varpi(\mathbf{X}(0), \mathbf{P}(0))$. The linear operator of shift along trajectories $\hat{L}[H]$ is defined on the vector space of observables by Poisson brackets:

$$\hat{L}[H](\dots) = \frac{\partial H(\mathbf{X}, \mathbf{P})}{\partial \mathbf{P}} \frac{\partial}{\partial \mathbf{X}}(\dots) - \frac{\partial H(\mathbf{X}, \mathbf{P})}{\partial \mathbf{X}} \frac{\partial}{\partial \mathbf{P}}(\dots) \equiv -\{H, \dots\}. \tag{4}$$

We introduce the Lebesgue measure on \mathfrak{P} in the usual way: $d\mu_{\mathfrak{P}} = \prod_{i=1}^N \prod_{j=1}^3 dx^{i,j} \prod_{k=1}^3 dx^{i,k}$. The operator $\hat{L}[H]$ is anti-self-adjoint in the Hilbert space $\mathfrak{H}_{cl} = L^2(\mathfrak{P}, d\mu)$ (*i.e.*, $(\hat{L}[H])^* = -\hat{L}[H]$), and its continuous spectrum $C\sigma(\hat{L}[H])$ lies on the imaginary axis in the complex λ -plane (it has no discrete or residual spectrum). It should be noted that the spectrum of the composition of the Fourier transform (with respect to the variable X) and the operator $\hat{L}[H]$, by virtue of G. Weyl's theorem on functions of the essential spectrum, will coincide with the spectrum of $C\sigma(\hat{L}[H])$; for simplicity, we take the one-dimensional case without interaction and external forces:

$$\sigma(ikp) = \sigma(p \cdot \partial / \partial x). \text{ This fact will be used below.}$$

The formal solution of the evolution equation of the observable (3) is of the form:

$$\varpi(\mathbf{X}(t), \mathbf{P}(t)) = \exp(t\hat{L}[H])\varpi(\mathbf{X}(0), \mathbf{P}(0)), \tag{5}$$

and the operator semigroup $\varphi[t] \equiv \exp(t\hat{L}[H])$ is unitary in $L^2(\mathfrak{P}, d\mu)$. In other words, the condition of conservation of phase volume (Liouville's theorem) is satisfied:

$$\frac{\partial(\mathbf{X}(t), \mathbf{P}(t))}{\partial(\mathbf{X}(0), \mathbf{P}(0))} = 1.$$

Based on this theorem, we can introduce the Liouville equation for the phase density $D_N(\mathbf{X}, \mathbf{P}, t)$ of a $6N$ -dimensional system in \mathfrak{P} :

$$\frac{\partial D_N}{\partial t} + \hat{L}[H](D_N) \equiv \frac{\partial D_N}{\partial t} + \sum_{i=1}^N \left(\frac{\partial H}{\partial p_i} \frac{\partial D_N}{\partial x^i} - \frac{\partial H}{\partial x^i} \frac{\partial D_N}{\partial p_i} \right) = 0. \tag{6}$$

This equation will be used in Section 4.

Now let us turn directly to the concept of time (ir)reversibility. Following [31], we note that “changing the direction of time” is not experimentally feasible. If we formally replace $t \rightarrow -t$, then the canonical variables corresponding to the new “direction of time” are transformed as follows: $x^i(t) \rightarrow x^i(-t)$, $p_i(t) \rightarrow -p_i(-t)$. In other words, it is possible to define a time reversal operator \hat{T} on the variables of μ -space:

$$\hat{T}(x^i, p_i) = (\hat{T}x^i, \hat{T}p_i) = (x^i, -p_i).$$

With its help, one can easily describe the dynamics of the “reversed” motion (we will denote it by the symbol \dots^\dagger) of the system under study; Let’s take the following initial data for it: $(x^i)^\dagger(0) = x^i(0)$, $p_i^\dagger(0) = -p_i(0)$ ($i = \overline{1, N}$). The motion of points is reversible, if $(x^i)^\dagger(t) = x^i(-t)$, $p_i^\dagger(t) = -p_i(-t)$. If we assume that the Hamiltonian of the system is quadratic in the momenta, then

$$\hat{T}H(x^i, p_i) = H(\hat{T}x^i, \hat{T}p_i) = H(x^i, -p_i) = H(x^i, p_i),$$

that is, such a Hamiltonian has time symmetry (invariance under time reversal).

A dynamical system Υ defined by the above set of rules for the evolution of particles in μ -space with time (including the presence of a semigroup $\varphi[t]$ with an action described by formula (5) and the topology of the state space of the system $\mathfrak{H}_{cl}(\mathfrak{P}, d\mu)$. Following [32], we define the evolution of the dynamical system Υ as irreversible if there exists a real-valued function $\wp \in \mathfrak{H}_{cl}(\mathfrak{P}, d\mu)$ such that $\wp(\varphi[t]\varpi)$ decreases monotonically with increasing t , possibly with the exception of some subset $\Pi_0 \subset \mathfrak{P}$, where the function being defined remains constant. Thus, if $\varpi[t_1]$ and $\varpi[t_2]$ are the system’s states (observable) at times of t_1 and $t_2 (> t_1)$, respectively, then $\varpi[t_1] \geq \varpi[t_2]$; the set Π_0 is an attractor of the system: a set of fixed points, periodic orbits, or a set of chaotization of the particle trajectory dynamics (a “strange” attractor).

The accepted definition of irreversibility of processes in a dynamic system is entirely consistent with its thermodynamic empirical definition: the space \mathfrak{H}_{cl} (membership of observables) should be understood as the set of thermodynamic states of the system, and the function \wp , respectively, H is the Boltzmann function (*i.e.*, the entropy of the system, taken with the minus sign).

3. Dynamics of a Quantum System

Let us briefly consider the properties of quantum particle systems. In a sense, they follow from the properties of classical particles discussed below, naturally, with certain modifications that are determined by the known quantization rules:

- 1) the μ -space of the dynamical system \mathfrak{P} is replaced by the Hilbert space/HP $\mathfrak{H} = L^2(\mathbb{R})^{3N}$ with the scalar product $\langle h_1 | h_2 \rangle$ ($h_{1,2} \in \mathfrak{H}$), and the (pure) state of the system is characterized by the unit vector $\psi(x)$ from this HP

(unique up to a phase factor) or a complex-valued normalized wave function.

2) The observable systems are defined by self-adjoint linear operators on the GP \mathfrak{H} , obtained from their classical analogs: in particular, $\mathbf{p}_i \rightarrow -i\hbar \cdot \partial(\dots)/\partial \mathbf{x}^i$, $\mathbf{x}^i \rightarrow (\dots) \cdot \mathbf{x}^i$ ($i = \overline{1, N}$), and the Hamiltonian becomes a Hermitian operator of the form

$$\hat{H} = \sum_{i=1}^N (-\hbar^2/2m_i) \nabla_i^2 + \hat{V}(\mathbf{x}^1, \dots, \mathbf{x}^N). \tag{7}$$

For the general form of observables, which in the classical case were previously denoted as $\varpi(\mathbf{x}, \mathbf{p}): \mathbb{R}^6 \rightarrow \mathbb{R}^1$ (taking $N = 1$), we have a quantum analog in the form of the Weyl transform of the wave function $\varpi \rightarrow \varpi_\psi$:

$$(\varpi_\psi)(\mathbf{x}) \equiv \frac{1}{(2\pi\hbar)^3} \int \varpi\left(\frac{\mathbf{x} + \mathbf{x}'}{2}, \mathbf{p}\right) \exp\left(i \frac{(\mathbf{x} - \mathbf{x}') \cdot \mathbf{p}}{\hbar}\right) \psi(\mathbf{x}') d\mathbf{x}' d\mathbf{p}. \tag{8}$$

In fact, we have here a Wigner function integrated over momenta; it corresponds not to pure states, but to mixed states of a (quantum) system: it simultaneously involves both configuration and momentum variables.

3) The result of measuring an observable ϖ for a quantum-mechanical system characterized by a wave function $\psi \in \mathfrak{H}$ is the number $\epsilon_\sigma \in \mathbb{R}^1$, which belongs to the spectrum $\sigma(\hat{\varpi})$ of the self-adjoint operator $\hat{\varpi}$. The probability of finding an eigenvalue ϵ_σ in the interval $(\epsilon_\sigma^1; \epsilon_\sigma^2]$ is $\|\hat{P}_\sigma((\epsilon_\sigma^1; \epsilon_\sigma^2])\psi\|^2$, where $\hat{P}_\sigma(\zeta)$ is the spectral projection of the operator $\hat{\varpi}$ onto the interval $\zeta \subset \mathbb{R}^1$.

4) The time evolution of the system is determined by the Hamiltonian operator \hat{H} (the observable energy of the system). To describe the evolution of the observables of the system, we use a direct generalization of the Equation (3) for the classical observable $\varpi(t)$, taking into account the replacement of the Poisson brackets $\{.,.\}$ with the quantum commutator $[.,.]/(i\hbar)$:

$$\frac{d\hat{\varpi}(t)}{dt} = -\frac{1}{i\hbar} [\hat{H}, \hat{\varpi}(t)], \quad \hat{\varpi}(0) = \hat{\varpi}_0. \tag{9}$$

This is the so-called Heisenberg equation for the non-stationary operator of the observable $\hat{\varpi}(t)$ (depending, in addition to time, only on configuration variables) in the space of Hermitian operators over the GP \mathfrak{H} . It is equivalent to the Schrodinger equation using a time-dependent wave function:

$$i\hbar \frac{d\psi(t)}{dt} = \hat{H}\psi(t), \quad \psi(0) = \psi_0. \tag{10}$$

Accordingly, a unitary evolution semigroup $\hat{U}(t) = \exp(i\hat{H}t/(i\hbar))$ is defined such that the following properties are satisfied:

$$\psi(t) = \hat{U}(t)\psi_0, \quad \hat{\varpi}(t) = (\hat{U}(t))^* \hat{\varpi}(0) \hat{U}(t). \tag{11}$$

To discuss the property of reversibility in a quantum system, we will focus on an operator-algebraic approach to its evolution. We will consider only bounded observables, which correspond to bounded self-adjoint operators in the Hilbert

space \mathfrak{H} (the generalization to unbounded operators is trivial). We introduce the set $\tilde{\mathfrak{K}}$ of all such operators in the specified Hilbert space; $\tilde{\mathfrak{K}}$ is an $*$ -algebra, since this set is closed under the operations of binary addition (commutative and associative), multiplication (associative and non-commutative), multiplication by an element $\kappa \in \mathbb{C}$ (with the distributive property under addition), and the mapping of elements to conjugate $K \rightarrow K^*$, where $(K^*)^* = K$ and $(K_1 K_2)^* = K_2^* K_1^*$. Moreover, the set $\tilde{\mathfrak{K}}$ is a Banach space with an operator norm and the property $\|K^* K\| \equiv \|K\|^2$. Based on all of the above, we can assume that $\tilde{\mathfrak{K}} \subset C^*$ is an algebra (a Naimark algebra).

We introduce the quantum time reversal operator \hat{T} , defined as follows. If we have a nonstationary Schrodinger equation $i\hbar \cdot \partial\psi/\partial t = \hat{H}\psi$ (the Hamiltonian operator is given by the formula (7)), then the equation $-i\hbar \cdot \partial\bar{\psi}/\partial t = \hat{H}\bar{\psi}$ (where the bar over the wave function denotes complex conjugation) corresponds to the dynamics of a system with inverse momenta, *i.e.*, to reversed time ($t \rightarrow -t$). Thus, we define the operator \hat{T} as an action on the wave function that transforms it into its complex conjugate: $\hat{T}\psi = \bar{\psi}$ ($\forall \psi \in \mathfrak{H}$). Next, we define the operation $\hat{\tau}$ on $\tilde{\mathfrak{K}}$: $\hat{\tau}K = \hat{T}K^*\hat{T}$ ($\forall K \in \tilde{\mathfrak{K}}$), which, by the definition of the algebra under consideration, has the antiautomorphism property (with $\hat{\tau}^2 = \hat{I}$). Its action on the coordinate, momentum, and Hamiltonian operators is: $\hat{\tau}\hat{x} = \hat{x}$, $\hat{\tau}\hat{p} = -\hat{p}$, $\hat{\tau}\hat{H} = \hat{H}$. Applying this operation to $\hat{U}(t)K$, we obtain: $\hat{\tau}\hat{U}(t)K = \hat{U}(-t)\hat{\tau}K$ ($K \in \tilde{\mathfrak{K}}$, $t \in \mathbb{R}^1$); In other words, the operation $\hat{\tau}$ corresponds to time reversal. The last equality can (due to the arbitrariness of the algebra element K) be rewritten as $\hat{\tau}\hat{U}(t) = \hat{U}(-t)\hat{\tau}$ for any $t > 0$.

Therefore, the system of quantum particles under study has the following property: the reversal of all momenta after the system's evolution from the initial instant to time t is equivalent to the system's evolution in reversed time (the principle of microscopic reversibility).

Thus, we see that, despite the differences in the mathematical apparatus used to describe classical and quantum dynamical systems, both are time-reversible.

But this contradicts, as already indicated, phenomenological theories. Therefore, we need to understand how the evolution of particle systems, understood as a set of physical points (in classical mechanics) or a set of wave functions (in quantum mechanics), will differ from statistical systems, whose evolution is described using time-irreversible equations.

4. Irreversibility as a Consequence of the Properties of Operators, Associated with Kinetic Equations

The question of the fundamental difference between the “kinetic” approach and the dynamic (quasi)deterministic consists of several aspects. First, we must clarify what assumptions are made in the transition to a statistical description of multiparticle systems that lead to new effects; in particular, whether the dynamics of these multiparticle systems can be reduced to the dynamics of a set of local subsystems (down to a single particle); Second, we need to establish what properties

kinetic equations have, and whether the mathematical formalism used in their theory can explain time irreversibility.

Let's consider the first aspect in more detail.

We have already constructed a preliminary model of some many-body dynamics (see section 1): In \mathbb{R}^{3N} with points $\mathbf{X} = (\mathbf{x}^1, \mathbf{x}^2, \dots, \mathbf{x}^N)$, a curve $\mathbf{X}(t)$ is defined, where $t \in \mathbb{R}^1$ is a parameter, that is, the functions $\mathbf{x}^i = \mathbf{x}^i(t)$, $i = 1, \dots, N$ are defined. The tangent vector "at time t " is the vector $\dot{\mathbf{x}} = (\dot{\mathbf{x}}^1, \dot{\mathbf{x}}^2, \dots, \dot{\mathbf{x}}^N)$.

The phase space $\mathfrak{P} \equiv \mathfrak{P}_{(2N)}$ is, generally speaking, the space of points

$$\mathbf{Z} \equiv (\mathbf{X}, \dot{\mathbf{X}}) = (\mathbf{x}^1, \dots, \mathbf{x}^N; \dot{\mathbf{x}}^1, \dots, \dot{\mathbf{x}}^N), \quad \mathbf{X} \in X^{(N)}, \quad \dot{\mathbf{X}} \in X^{(N)}.$$

Let $\mathbf{Z} \in \mathfrak{P}$, for a given L , go to the point $\mathbf{Z}' = \mathbf{Z}(t)$ in time t ; this defines the transformation $\hat{L}[t](\mathfrak{P} \rightarrow \mathfrak{P}): \mathbf{Z} \rightarrow \mathbf{Z}(t) \equiv \hat{L}[t]\mathbf{Z}$. The set of all $\hat{L}[t](t \in \mathbb{R}^1)$ is the phase flow in \mathfrak{P} , the lines $\hat{L}[t](\mathbf{Z})$ themselves are particle trajectories in the phase space \mathfrak{P} . A mechanical system of N points consists of points in the topological sense (that is, zero-dimensional disconnected sets—since each point—the mathematical image of a physical particle—is surrounded by the empty set—in physical terms, the vacuum), then $\dim \mathbf{x}^i = 0$, $i = 1, \dots, N$; a "phase space point" $\mathfrak{P}_{(2N)}$, representing the state of the mechanical system at some initial moment of time (t_0) is determined by $6N$ parameters: a metric "image" characterizing—in the infinite-dimensional space of possible initial states \mathcal{I}_0 the structure of such a set, and it is assumed that \mathcal{I}_0 is separable with discrete topology; thus, it turns out that, according to the definition of topological dimension, $\dim \mathbf{Z}(t_0) = 0$. In other words, considering a system of N "mechanical points", we cannot obtain a $6N$ -dimensional statistical ensemble.

According to Brouwer's theorem, manifolds with different topological dimensions cannot be continuously transformed into each other. Thus, for a dynamical system consisting of N points interacting according to Newton's laws, the initial state of the system consists of N sets of point coordinates ($\mathbf{x}^i = \{x^{1,1}, x^{2,1}, x^{3,1}\}$) and N sets of point velocities ($\dot{\mathbf{x}}^i = \{\dot{x}^{1,1}, \dot{x}^{2,1}, \dot{x}^{3,1}\}$); for a statistical system (classical or quantum), at the initial instant, a certain distribution of coordinates and/or velocities is characteristic.

To transition to a statistical system, it is necessary to define a tangent bundle of the momentum-configuration space, linking the system of discrete points into a topological space with nonzero dimension.

The tangent vector $\mathbf{v} = \dot{\mathbf{x}}$ at $\mathbf{X} \in \mathcal{M} \subset \mathbb{R}_x^3$ is the equivalence class C^1 of curves $[\sigma]$ on \mathcal{M} , where the equivalence relation between curves is that they are tangent at \mathbf{v} . The tangent space $T_x\mathcal{M}$ to \mathcal{M} at $\mathbf{x} \in \mathcal{M}$ is the set of all tangent vectors \mathbf{v} at \mathbf{x} .

The tangent bundle $T\mathcal{M}$ is defined as

$$T\mathcal{M} := \bigcup_{\mathbf{x} \in \mathcal{M}} T_x\mathcal{M}. \tag{12}$$

The elements of the tangent space $\dot{\mathbf{x}}^i \equiv \mathbf{v}^i$ (which can be interpreted as all

possible values of the velocity vectors subtended by a given point \mathbf{x}^i) are defined not locally, but along the parameterized displacements $d\mathbf{x}^i$; thus, the union of the set of pairs of elements $(\mathbf{x}^i, \dot{\mathbf{x}}^i)$ is the topological product of the two corresponding subspaces. The components of the \mathbf{x}^i tangent bundle are elements of the space of possible values of the “centers of mass” of physical particles, which is a continuous (non-discrete) set of topological dimension, and $\dot{\mathbf{x}}^i$ are elements of a similar kinematic space.

The cotangent vector at $\mathbf{x} \in \mathcal{M}$ is a real-valued mapping $\mathbf{p}: T_x\mathcal{M} \rightarrow \mathbb{R}^1$. The value of \mathbf{p} on the tangent vector $\dot{\mathbf{x}} \in T_x\mathcal{M}$ is denoted by $\langle \mathbf{p}, \dot{\mathbf{x}} \rangle_x$.

The cotangent space in $\mathbf{x} \in \mathcal{M}$ is the set $T_x^*\mathcal{M}$ of all such linear mappings, that is, the dual of the vector space $T_x\mathcal{M}$; in this case,

$$\dim T_x^*\mathcal{M} = \dim T_x\mathcal{M} = \dim \mathcal{M}.$$

The cotangent bundle $T^*\mathcal{M}$ is the union of all cotangent spaces to the manifold \mathcal{M} at all its points:

$$T^*\mathcal{M} := \bigcup_{\mathbf{x} \in \mathcal{M}} T_x^*\mathcal{M}. \tag{13}$$

Thus, a point (covector) from $T^*\mathcal{M}$ is a 1-form on the tangent space to \mathcal{M} at some point $\mathbf{x} \in \mathcal{M}$:

$$\omega_x = \sum_{s=1}^N \omega_s(\mathbf{x})(d\mathbf{x}^s)_x, \tag{14}$$

where the components ω_s of the 1-form ω are functions defined on the coordinate chart by the relation $\omega_s := \left\langle \omega, \left(\frac{\partial}{\partial \mathbf{x}^s} \right)_\xi \right\rangle_\xi \forall \xi \in U \subset \mathcal{M}$. If \mathbf{x} is a set of N local coordinates of a point in \mathcal{M} , then this 1-form is determined by its N components \mathbf{p}_s (and, as already noted, together $2N$ numbers x, p make up the set of local coordinates of the point $T^*\mathcal{M}$).

A symplectic structure on a (even-dimensional) manifold $T^*\mathcal{M}$ ($\dim T^*\mathcal{M} = 2N$) is a closed nondegenerate differential 2-form ω^2 on $T^*\mathcal{M}$:

$$d\omega^2 = d\omega^1 = 0, \quad \forall \mathfrak{A}_1 \neq 0 \quad \exists \mathfrak{A}_2 : \omega^2(\mathfrak{A}_1, \mathfrak{A}_2) \neq 0 \quad (\mathfrak{A}_1, \mathfrak{A}_2 \in T_x\mathcal{M}).$$

The cotangent bundle $T^*\mathcal{M}$ of the configuration space (the phase space of the statistical system in the formalism under consideration), according to Darboux’s theorem, has a natural symplectic structure, locally symplectomorphic to $\omega^2 = d\mathbf{p} \wedge d\mathbf{x}$.

The flow of the vector field $\hat{L}[t]$ on a symplectic (even-dimensional) manifold preserves the symplectic structure ω if and only if this field is locally Hamiltonian (Darboux’s theorem holds); for statistical mechanics, it is especially important that a Hamiltonian flow preserves the Liouville measure $\omega^N = N! \sum_{j=1}^N d\mathbf{x}^j \wedge d\mathbf{p}_j$. The evolution of the phase density ($\sim \omega^N$) under the action of a Hamiltonian field is described by the Liouville equation, which implies the stationarity of the Gibbs distribution $\exp(-\beta H)\omega^N$. Consequently, we can find the average value of any physical observable characterizing a given system (for a quantum system, we have the Gibbs-von Neumann distribution with similar

results).

Thus, the transition from a dynamic “mechanical” (and even quantum-mechanical) system to a statistical one is accompanied by the need to average the observables in accordance with some distribution. If the state is nonstationary, then the canonical distribution is inapplicable here, and it is necessary to solve the kinetic equation.

This brings us to the second aspect.

As mentioned above, the Liouville equation is initially formulated for the phase density D_N (which globally characterizes the dynamics of all N particles in a statistical nonequilibrium system).

The solution of the equation for D_N is impossible in direct form due to the astronomical number of variables, therefore the phase density of the system is reduced to single-particle functions F :

$$V^{-1}F(\mathbf{Z}_n, t) = \int d\mathbf{Z}_1 d\mathbf{Z}_2 \cdots d\mathbf{Z}_N D_N(\mathbf{Z}_1, \dots, \mathbf{Z}_N, t), \quad \mathbf{Z}_n = (\mathbf{X}_n, \mathbf{P}_n), \quad n = 1, \dots, N, \quad (15)$$

where V is the volume of the system. Similarly, s -particle functions ($s = 2, 3, \dots, N-1$) are introduced, in particular, the 2-particle function:

$$\begin{aligned} V^{-2}F(\mathbf{Z}_n, (\mathbf{Z}_m, t)) \\ = \int d\mathbf{Z}_1 d\mathbf{Z}_2 \cdots d\mathbf{Z}_{m-1} d\mathbf{Z}_{m+1} \cdots d\mathbf{Z}_{n-1} d\mathbf{Z}_{n+1} \cdots d\mathbf{Z}_N D_N(\mathbf{Z}_1, \dots, \mathbf{Z}_N, t). \end{aligned} \quad (16)$$

These multiparticle functions contain information about the interdependent motion of particles in the system (the F functions differ from the standard f functions by their normalization: $F = N_p f$, where N_p is the number of particles in the system). The effect of such interdependence can be characterized using so-called correlation functions. As an example, let us again take the 2-particle function:

$$\frac{N^2}{V^2} F_2(\mathbf{Z}_\ell, \mathbf{Z}_n, t) = f(\mathbf{X}_\ell, \mathbf{P}_\ell, t) \cdot f(\mathbf{X}_n, \mathbf{P}_n, t) + g(\mathbf{X}_\ell, \mathbf{P}_\ell, \mathbf{X}_n, \mathbf{P}_n, t). \quad (17)$$

The Liouville equation can be transformed by reducing the resulting chain of “interlocking” equations for multiparticle functions to the Boltzmann equation for a single-particle function under the condition of “weakening correlations”, which consists in a priori assuming the existence of some effective maximum radius of interparticle interaction, beyond which the particles are assumed to be independent and non-interfering. Thus, the two-particle distribution function becomes multiplicative ($f_2 = f_1 f_1$), and the BBGKY chain can be terminated. The so-called “collision term” obtained from the term with the self-consistent field of the Liouville equation is thus a generator Markov processes, the essence of which is the loss of information about the previous states of the system during the interaction of each pair of particles. As is well known, the “H-theorem” holds for the Boltzmann equation, which describes the process of entropy increase in the system (entropy is stationary only at equilibrium solutions). In other words, the transport process described by the Boltzmann kinetic equation becomes irreversible. This fact is due to the fact that this equation (for simplicity, we take its sim-

plest form):

$$\frac{\partial f(\mathbf{x}, \mathbf{p}, t)}{\partial t} + \mathbf{v} \frac{\partial f}{\partial \mathbf{x}} = \int b(\theta, |\mathbf{v}_* - \mathbf{v}|) (f'_* f' - f_* f) d\phi d\mathbf{v}' d\theta \tag{18}$$

has already been written out a priori, taking into account the sequence of temporal relationships between the events it describes. Indeed, the form of the bilinear operator on the right-hand side is chosen in a special way—under the assumption that the collision has already occurred relative to the instant t included in the left-hand side (the operator of the substantial derivative). This is precisely why a very specific sequence of events is predetermined, leading to the identification of the direction of the processes.

Furthermore, there is another aspect of the theory of kinetic equations that cannot be ignored when considering the possibility of the emergence of the identification of the direction of time. It is generally assumed that the phase density function D_N “...is a symmetric function of the coordinates of the phase space of the system of particles” [33]. The a priori acceptance of symmetry is based on the assumption of the identity of the particles and their indistinguishability upon permutation. However, in the classical case of a Hamiltonian dynamical system, “identical” particles can be distinguished, in particular, by their position at time $t = 0$: Let’s take, for example, the case where $D_N(t = 0)$ for the statistical system under study can be defined as

$$D_N(t = 0) = \prod_{i=1}^N \alpha_i \exp(-\delta_i(x_i - x_i(0))) \cdot \phi(p_i). \tag{19}$$

This function is asymmetric with respect to permutations of any pair of configuration variables; only if the values of δ_i are sufficiently large (the variance of the initial distribution is large) can the function D_N be symmetric with respect to permutations of some or all coordinates.

If D_N is an asymmetric function, then it will generally lead to N different single-particle functions. The system as a whole will be described by the “global” function $D^{(1)} = \sum_{k=1}^N [^k]f$, where $[^k]f$ are additive local particle distribution functions. For them, evolution will no longer be described by single equations (like the Boltzmann equation for a symmetric distribution function), but by systems of equations:

$$\frac{\partial [^k]f}{\partial t} + \mathbf{v} \frac{\partial [^k]f}{\partial \mathbf{x}} = \sum_{j=1}^N \int B(V_{rel}, \theta) ([^k]f_* \cdot [^j]f_2^* - [^k]f \cdot [^j]f_2) d\mathbf{v}_2 d\theta d\varphi, k = 1, N. \tag{20}$$

If D_N is symmetric, then all additive functions will coincide, and then we have $D^{(1)} = N[^1]f = Nf$, that is, we arrive at Boltzmann’s statistical theory.

It should be noted that additive functions can be combined into groups/complexes, the behavior of which will determine the overall dynamics of the system; for example, to calculate a shock wave (bimodal approximation) or a boundary layer, it is sufficient to use only two groups combining “spiritually related” particles with somewhat similar additive distribution functions.

Let us present the form of the system (20) for the 2-group case (having first

nondimensionalized it and isolated the small parameters):

$$\begin{aligned} \frac{\partial^{[1]}f}{\partial t} + v \frac{\partial^{[1]}f}{\partial x} &= (\epsilon_{[11]})^{-1} \int B(V_{rel}, \theta) \left([^1]f^* \cdot [^1]f_2^* - [^1]f \cdot [^1]f_2 \right) dv_2 d\theta d\varphi \\ &\quad + (\epsilon_{[12]})^{-1} \int B(V_{rel}, \theta) \left([^1]f^* \cdot [^2]f_2^* - [^1]f \cdot [^1]f_2 \right) dv_2 d\theta d\varphi \quad (21) \\ &= \hat{\mathcal{J}}^{[11]}(f, f) + \hat{\mathcal{J}}^{[12]}(f, f), \end{aligned}$$

$$\begin{aligned} \frac{\partial^{[2]}f}{\partial t} + v \frac{\partial^{[2]}f}{\partial x} &= (\epsilon_{[12]})^{-1} \int B(V_{rel}, \theta) \left([^1]f^* \cdot [^2]f_2^* - [^1]f \cdot [^2]f_2 \right) dv_2 d\theta d\varphi \\ &\quad + (\epsilon_{[22]})^{-1} \int B(V_{rel}, \theta) \left([^2]f^* \cdot [^2]f_2^* - [^2]f \cdot [^2]f_2 \right) dv_2 d\theta d\varphi \quad (22) \\ &= \hat{\mathcal{J}}^{[12]}(f, f) + \hat{\mathcal{J}}^{[22]}(f, f), \end{aligned}$$

where $\epsilon_{[ij]}$ are the local Knudsen numbers, $i, j = 1, 2$.

To study the properties of the solutions of these equations, we consider their representations as Frechet-Taylor series expansions of the right-hand side. In this case, the linearization is performed accordingly: for Equation (21)—near the equilibrium solution $\omega_{n_1, \beta_1}^{[1]}$ of this equation under the assumption $R^{[12]} \equiv 0$ ($Kn^{[12]} \rightarrow \infty$), for Equation (22)—near the equilibrium solution $\omega_{n_2, \beta_2}^{[2]}$ of this equation under the same assumption ($\beta = 1/(kT)$, n is the particle density). Then, in particular, for the right-hand side of the first equation of the system under consideration, we obtain:

$$\begin{aligned} &\hat{\mathcal{J}}^{[11]}(f, f) + \hat{\mathcal{J}}^{[12]}(f, f) \\ &= (\epsilon_{[11]})^{-1} \left(\hat{\mathcal{L}}^{[11]}(\phi) + \hat{\mathcal{N}}^{[11]}(\phi, \phi) \right) + (\epsilon_{[12]})^{-1} \left(\hat{\mathcal{L}}^{[12]}(\phi) + \hat{\mathcal{N}}^{[12]}(\phi, \phi) \right), \quad (23) \end{aligned}$$

$$\begin{aligned} \hat{\mathcal{L}}^{[11]}(\phi) &\equiv \left. \frac{\partial \hat{\mathcal{J}}^{[11]}}{\partial f} \right|_{f=0} \left([^1]\phi \right) \\ &= \int B(V_{rel}, \theta) \omega_{n_1, \beta_1}(v_2) \left([^1]\phi(v_2^*) + [^1]\phi(v^*) \right) dv_2 d\theta d\varphi \quad (24) \\ &\quad - \int B(V_{rel}, \theta) [^1]\phi(v_2) \omega_{n_1, \beta_1}(v_2) dv_2 d\theta d\varphi - v [^1]\phi(v), \end{aligned}$$

$$\begin{aligned} \hat{\mathcal{N}}^{[11]}([^1]\phi, [^1]\phi) &\equiv \left. \frac{\partial^2 \hat{\mathcal{J}}^{[11]}}{\partial f^2} \right|_{f=0} \left([^1]\phi, [^1]\phi \right) \quad (25) \\ &= \int B(V_{rel}, \theta) \omega_{n_1, \beta_1}(v_2) \left([^1]\phi(v_2^*) [^1]\phi(v^*) - [^1]\phi(v_2) [^1]\phi(v) \right) dv_2 d\theta d\varphi. \end{aligned}$$

$$\begin{aligned} \hat{\mathcal{L}}^{[12]}(\phi) &\equiv \left. \frac{\partial \hat{\mathcal{J}}^{[12]}}{\partial f} \right|_{f=0} \left([^1]\phi \right) \\ &= \int B(V_{rel}, \theta) \omega_{n_1, \beta_1}(v_2) \left([^1]\phi(v_2^*) + [^1]\phi(v^*) \right) dv_2 d\theta d\varphi \quad (26) \\ &\quad - \int B(V_{rel}, \theta) [^1]\phi(v_2) \omega_{n_1, \beta_1}(v_2) dv_2 d\varphi - v [^1]\phi(v), \\ [^1]f(t, x, v) &= \omega_{n_1, \beta_1}(v) \left(1 + [^1]\phi(t, x, v) \right). \end{aligned}$$

We thus obtain the problem of branching the solution of a stationary solution of an integrodifferential equation with a bilinear operator in the presence of a perturbation. Applying the Fourier transform with respect to the configuration vari-

able to the linearized equations, we obtain a spectral problem. It is known that the linear Boltzmann operator (which is a Fredholm operator with a 5-dimensional kernel in the general case; in the one-dimensional case, the kernel is 3-dimensional) has a spectrum of eigenvalues located in the left half-plane, and, due to its self-adjointness, all eigenvalues lie on the real axis. The presence of the perturbation $-ikv$ transforms this operator into a sectorial operator with a spectrum symmetric with respect to the real axis and located in a sector with a rotation angle $< \pi$. The cross term, considered as a perturbation, yields a symmetric splitting of the value $\lambda = 0$ into 5 perturbed eigenvalues; for the remaining $\lambda_n \in \mathfrak{L}^{[1]}$, we obtain a shift to the right (into the right half-plane of the spectral plane), which, at the physical level, indicates instability of the motion and the emergence of vortex motions corresponding to Hopf solutions (the eigenvalues are purely imaginary).

Applying the Lyapunov-Schmidt method to the equation under study (choosing an endomorphism onto the set of summation invariants as the projector), we obtain a pair of equations. The first of these is a Riccati-type differential-functional equation for the flow profile. Reducing it to a second-order equation, we obtain a bifurcation of the non-stationary solution (for a certain value of the Knudsen parameter). This allows us to conclude that there exist two attractive sets of solutions to the original non-stationary equation, which, in turn, indicates chaos arising in the system. Thus, the reversibility of motion in a system described using the local kinetic approach as a set of additive distribution functions is an obvious consequence of the structure of the equations used and follows directly from the fact that their solutions can branch.

Thus, it can be argued that when the kinetic equation for a multiparticle system takes into account the dependence on: 1) individual particle interactions, or 2) a specific set of data for the Cauchy equation, irreversibility of the system's dynamics is inevitable. Indeed, the first option is realized in the Boltzmann equation, in which the 2-particle correlation function g_2 is annulled everywhere except at the collision point (small region); the second option (such as a small variance of the initial distribution) necessitates the introduction of Lynden-Bell statistics and a "coarse-grained" partition of subsets of the system's phase space. A common factor in both cases is the isolation of a certain volume of configuration space, where the global structure of a reversible system (the indistinguishability of particles, the collective influence of the system on any impersonal particle) loses physical meaning. This fact should be interpreted as the emergence of a new local structure of the system, leading to the irreversibility of the dynamics of particles in it.

The situation is similar with kinetic quantum equations: the quantum equation for the Wigner function (or, as it is also called, the quantum Vlasov equation) is reversible (like its classical counterpart). However, if we introduce an effective interaction term, analogous to the collisional Boltzmann term, the evolution of the quantum system becomes irreversible; the situation does not change when Bose

and Fermi statistics are taken into account—the corresponding Uehling-Uhlenbeck equation has a trilinear collision operator and is also subject to branching of solutions when perturbations are taken into account, which leads to the irreversibility of the quantum transport processes it describes.

5. Conclusions

In this paper, we briefly considered the question of the irreversibility of the evolution of classical and quantum dynamical systems. It can be concluded that both Hamiltonian and Schroedinger (and Heisenberg) formalisms do not lead to irreversibility of processes in the systems under consideration (naturally, only for the quadratic form of Hamiltonians). However, the transition to a kinetic description of motion in systems makes it possible to obtain a phenomenologically adequate picture, although it requires assumptions that cannot be considered a priori obvious.

At the same time, the question arises about the validity of the applicability of non-dissipative reversible equations for the analysis of dynamical systems. Perhaps one of the paths of development in this direction will be the development of H. Moyal's phase space quantization apparatus.

In any case, we are beginning to understand that the irreversibility of processes is a consequence of the chaotization of the system's dynamics, which is not some specific exotic feature of its behavior, but an inherent attribute of the presence of many particles and the objective absence of determinism in the definition of their state.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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