Mechanism of irreversibility in a many-body systems

V.M. Somsikov

Laboratory of Physics of the geoheliocosmic relation,
Institute of Ionosphere, Almaty, 480020, Kazakhstan
E-mail: nes@kaznet.kz

Abstract

The mechanism of irreversible dynamics in the mixing systems is constructed in the frames of the classical mechanics laws. The offered mechanism can be found only within the framework of the generalized Hamilton’s formalism. The generalized formalism is created by expansion of the canonical Hamilton’s formalism to the open systems. A formula, which expresses the entropy through the work of subsystems interaction forces was obtained. The essential link between thermodynamics and classical mechanics was established.

1 Introduction

Irreversibility is a main difficulty in aspiration of linking classical mechanics with thermodynamics [1-4]. A first attempt to overcome this difficulty has been done by Boltzmann. He found that many-body systems should be equilibrated. But for obtaining this result, Boltzmann had used probabilistic principles. Therefore the difficulty was not overcome. Since Boltzmann and till now the attempts to overcome irreversibility problem do not stop. For this purpose practically all areas of physics are used: statistical physics, kinetics, classical and quantum mechanics, nonequilibrium dynamics and so on.

In a basis of statistical physics and kinetics probabilistic laws are used. They allow to describe effectively collective properties of systems, having refused from an inconceivable task of calculation of dynamics of each element. So, for example, the method of Gibbs’ microcanonical ensembles consists in splitting equilibrium system to subsystems and studying them, basing on probabilistic laws in the assumption of ergodicity hypotheses performance [2, 4-6]. The statistical theory of equilibrium systems was created having excluded with the help of ergodicity hypotheses the interaction of subsystems and dependences of their statistical distribution from the entry conditions [2]. But a similar sort of a hypotheses and probabilistic principles for a substantiation of irreversibility is unacceptable.

Near ten years ago the method of non-extensive thermodynamics, applicable for the analysis of stationary nonequilibrium systems has been arisen [7]. It allows to determine function of distribution of nonequilibrium systems and to study connection between parameters of thermodynamic and mechanic [8]. The certain successes in studying nonequilibrium systems within the framework of the statistical theory of open systems have been achieved [9]. The feature of the offered approach is taking into consideration the structure of the continuous environment at all levels of the description. But this method is inapplicable for the solving of irreversibility problem because it is also based on probabilistic laws.
Attempts to prove thermodynamics on the basis of strict methods of classical mechanics were undertaken also. It has been proved by Liouville, that only those systems of many bodies, which can be split into systems with one degree of freedom by transformations of independent variables, are integrable [10, 11]. I.e., the system is integrable, when it is possible to exclude interactions between its elements. Poincare also has proved the theorem, according to which the dynamic systems in most cases are not integrable because of impossibility of exception of forces acting between subsystems [10]. But if potentiality of the forces between elements means potentiality of forces between systems of these elements, as it follows from a formalism of Hamilton [12], the problem will be reduced to independent integrable systems with one degree of freedom. The contradiction is obviously. On the one hand, it is proved, that the class of integrable systems is very narrow. On the other hand, potentiality of interacting forces should provide an opportunity to transform the natural systems to the integrable systems [12].

The discovering of the deterministic chaos was the reason of creating of the stochastic dynamics. Stochastic dynamics is constructed on the basis of laws and principles of classical mechanics [13-15]. Basing on the methods of stochastic dynamics, the connection between entropy and Lyapunov’s exponents was established. Performance of the mixing property for dynamic systems was proved. Mixing provides a randomness of dynamics and decay correlations. Basing on the mixing properties the modern mechanism of irreversibility has been offered [1, 10, 13-15]. But this mechanism has an insuperable barrier. It is explanation of the nature of "coarse-grain" of the phase-space. But Poincare has proved impossibility of its explanation within the framework of canonical formalism of classical mechanics. Thus the irreversibility problem was reduced to the problem of "coarse-grain" of the phase-space [13-15].

I. Prigogine has guessed that difficulties of the solution of a problem of irreversibility may be connected with limitation of a canonical formalism of classical mechanics for the description of real systems. Indeed, this formalism is applicable to conservative systems while irreversibility is caused by their openess [10]. This assumption has defined our approach to researches of a problem of irreversibility.

The goal of this work is investigation about how the mixing creates irreversibility and what is the nature of the link between classical mechanics and thermodynamics. We will do it by extending Hamilton’s formalism so that it will be applicable to analyzing of the open systems.

Our investigation is based on the following method. A conservative system of hard disks and potentially interacting elements, which is not in equilibrium, is prepared. This system is then split into small subsystems that are accepted as being in equilibrium. The subsystem dynamics under condition of their interactions is analyzed on the basis of classical mechanical laws. It allows us to reduce a problem of the description of dynamics of systems elements to a problem of the dynamics of interacting equilibrium subsystems.

The researches were constructed in the following way [16-18, 20, 21]. The generalized Liouville equations was obtained. These equations are applicable either for the description of systems of hard disks, and of open systems. Based on the generalized Liouville equation the necessary condition for occurrence of irreversible dynamics has been obtained, and an opportunity of existence of irreversibly dynamics in a disk system has been proved.

The dynamics of a hard-disks system was studied. The equation of motion for them has been obtained. Based on this equation the non-potentiality of the interaction forces of disks and their subsystems was established.

The mechanism of irreversibility of hard disks has been generalized to the systems consisting of potentially interacting elements. It has been made basing on the equation for energy exchange between interacting subsystems. This equation has been obtained from the law of conservation of energy. The non-potentiality of forces acting between the subsystems which consists of the
potentially interacting elements has been established.

The connection between classical mechanics and the first thermodynamics law was found. The formula for entropy production has been obtained.

2 The general Liouville equation

The approach to the solution of a problem of irreversibility offered here is based on the generalized Liouville equation. Let us to find out than this equation is differs from the canonical Liouville equation, which lay in the bases of canonical Hamilton’s formalism?

The canonical Liouville equation is convenient for systems under conditions of short enough times when it is possible to neglect an exchange of energy between subsystems [2, 3]. Moreover, it is applicable for the description of only potentially interacting systems. But in the nonequilibrium hard disks system, the interaction forces of subsystems are non-potentially [17]. Thus, the description of dynamics of nonequilibrium hard disks systems within the framework of the canonical equation with these restrictions is impossible. These restrictions for the generalized Liouville equation are absent.

The generalized Liouville equation for subsystems was obtained by the next way [17, 18]. We took a closed nonequilibrium system, which consist of \( N \) elements. Divide this system into \( R \) equilibrium subsystems. Then we select one of subsystem, which we call \( m \)-subsystems. With the help of D’Alambert equation, basing on variational method, the generalizing Lagrange, Hamilton equations were obtained for \( m \)-subsystem. Basing on these equations, the generalized Liouville equation was obtained within the framework of laws of classical mechanics. This equation can be written so [16]:

\[
\frac{df_m}{dt} = -f_m \sum_{k=1}^{L} \frac{\partial}{\partial \vec{p}_k} F^m_k
\]  

Here \( f_m = f_m(\vec{r}_k, \vec{p}_k, t) \) is a normalized distribution function of subsystem disks; \( F^m_k \) is external force acting on \( k \) -disks of \( m \)-subsystem from outside, \( F^m_k = \sum_{s=1}^{N-L} F^m_{ks} \); \( k = 1, 2,...L \) are disks of \( m \)-subsystem; the \( s = 1, 2, 3, ..., N - L \) are external disk acting on \( k \)-disk of \( m \)-subsystem; \( m = 1, 2, 3, ..., R \); \( \vec{p}_k \) and \( \vec{r}_k \) are momentous and coordinates for \( m \)-subsystem disks consequently; \( t \) is a time.

The right hand side of the eq. (1) plays the role of the collisions integral. It is equal to zero, when the forces are potential, and when the system is in equilibrium state. The right hand side can be found from the equations of motion for elements of system.

The important step on the way to the generalize Liouville equation were failure from a requirement of potentiality of forces between subsystems. Therefore this equation is fair for anyone opens and nonholonomic systems. It does applicable this equation for the study of irreversibility [12, 18].

Let us remark, that the similar form of the generalized Liouville equation can be obtained if accepted forces is dissipative [19]. But in this case the generality of the obtained equation will be lost. It will be so because the presence of the dissipative forces is equivalent to irreversibility. Moreover, acceptance of condition dissipative forces essentially narrows area of applicability of this equation. Indeed, forces of interaction of disks though are non-potential, but they and nondissipative [12]. Let us call further the forces between subsystems as ”generalized forces”.

Let us consider the important properties of dynamics that directly follow from generalized Liouville equation. These properties can be obtained by the analysis of character of interrelation
of dynamics of selected subsystems with dynamics of system as a whole. They are caused by preservation of phase-space for the full system [18].

As the equality, \( \sum_{m=1}^{R} \sum_{k=1}^{L} F_{m}^k = \sum_{m=1}^{R} F_{m} = 0 \), is carried out, the next equation for the full system Lagrangian, \( L_R \), will have a place: \( \frac{d}{dt} \frac{\partial L_R}{\partial \dot{r}_k} - \frac{\partial L_R}{\partial r_k} = 0 \) and the appropriate Liouville equation:

\[
\frac{\partial f_R}{\partial t} + v_k \frac{\partial f_R}{\partial r_k} + \dot{p}_k \frac{\partial f_R}{\partial p_k} = 0.
\]

Here \( f_R \) is a distribution function corresponds to the full system; \( v_k \) is a velocity of \( k \)-disk. The full system is conservative. Therefore, we have:

\[
\sum_{m=1}^{R} \text{div} J_m = 0.
\]

Here, \( J_m = (\dot{r}_k, \dot{p}_k) \) is a generalized current vector of the \( m \)-subsystem in a phase space. This expression is equivalent to the next equality:

\[
\frac{d}{dt} \left( \prod_{m=1}^{R} f_m \right) = 0. \quad \text{So, } \prod_{m=1}^{R} f_m = \text{const}.
\]

Because the equality \( \sum_{m=1}^{R} F_{m} = 0 \) is fulfilled during all time, we have that equality, \( \prod_{m=1}^{R} f_m = f_R \), is a motion integral. It is in agreement with Liouville theorem about conservation of phase space.

So, only in two cases the Liouville equation for the whole non-equilibrium system is in agreement with the general Liouville equation for selected subsystems: if the condition \( \int_{0}^{t} (\sum_{m=1}^{R} \frac{\partial}{\partial p_k} F_{m}^k) dt \rightarrow \text{const} \) is satisfied when \( t \rightarrow \infty \), or when, \( (\sum_{m=1}^{R} \frac{\partial}{\partial p_k} F_{m}^k) \), is a periodic function of time. The first case corresponds to the irreversible dynamics, and the second case corresponds to reversible dynamics.

Thus the irreversible dynamics is possible under condition of redistribution of phase-space volume between subsystems when full volume is invariant. Reversibility exists, when the system is placed near to equilibrium or in a point of invariant set of phase-space. In the latter case a periodic change of phase-space volume of subsystems have a place under condition of system phase-space volume preservation as a whole.

Thus, generalized Liouville equation allows describing dynamics of nonequilibrium systems within the framework of classical mechanics. According to this equation both reversible and irreversible dynamics have a place. Irreversibility is possible only at presence of subsystems motions and dependence of the generalized forces from subsystems velocities. Presence of such dependence eliminate an interdiction on irreversibility, which dictated by the Poincare’s theorem of reversibility. Therefore first of all for the proof of existence of irreversibility it is necessary to show presence of the relative motion of subsystems in nonequilibrium systems.

3 The relative motion of subsystems

The proof of existence of relative motion of subsystems in nonequilibrium systems is following from [2] (see, §10). In agreement with [2] the entropy \( S \) for system can be writing as:

\[
S = \sum_{m=1}^{R} S_m(E_m - T_m^{tr})
\]

(2)

Here, \( S_m \) is entropy for \( m \)-subsystem; \( E_m \) is full energy of the \( m \)-subsystem; \( T_m^{tr} = P_m^2 / 2M_m \) is a kinetic energy of motion of \( m \)-subsystem; \( M_m \) is a subsystems mass; \( P_m \) is a momentum. The argument in \( S_m \) is internal energy of \( m \)-subsystem.
As the system is closed, we have: \[ \sum_{m=1}^{R} P_m = \text{const}, \quad \sum_{m=1}^{R} [r_m P_m] = \text{const}. \] Here \( r_m \) is a position vector of \( m \)-subsystem.

The entropy in equilibrium state as a function of momentum of subsystems has a maximum. Using a method of uncertain Lagrange multipliers, it is possible to determine necessary conditions of a maximum if to equate to zero the derivatives with respect to momentum from the following expression:

\[
\sum_{m=1}^{R} \{ S_m + a P_m + b [r_m P_m] \},
\]

where \( a, b \) are constant multipliers.

Differentiating \( S_m \) with respect \( P_m \), taking into account definition of temperature, we shall obtain:

\[
\frac{\partial}{\partial P_m} S_m (E_m - T_M r_m) = -P_m / (m T) = -v_m / (m T) = -v_m / T.
\]

Hence, differentiating eq. (3) with respect \( P_m \), we shall have:

\[
v_m = u + \Omega [r_m] (a),
\]

where \( \Omega = b T, \quad u = a T, \quad T \) is a temperature. From here follows, that the entropy has a maximum, when velocities of all subsystems are determined by the formula (a). According to this formula in equilibrium all subsystems should to move with identical translational velocities and to rotate with identical angular velocity. It means, that a closed system in equilibrium state can only move and rotate as the whole; any relative motions of subsystems are impossible.

As it follows from the formula (2), the rate of systems deviation from equilibrium is determined by value \( T_M r_m \). This energy can be selected by dividing the system on equilibrium subsystems. At such splitting all energy of system strictly equals the sum of two types of energy. The first type of energy is the sum of internal energy of subsystems. The second type of energy is \( T_M r_m \). In connection with eq. (2), the process of equilibration is caused by transformation of energy, \( T_M r_m \) in internal energy of systems.

Thus, equilibrium is characterized by a condition, \( T_M r_m = 0 \), which have a place at any splitting of the equilibrium system into subsystems. Otherwise a subsystems will have the relative motion. Therefore a subsystems in nonequilibrium system will have relative motion. If the system goes to equilibrium, the energy \( T_M r_m \) should aspire to zero also.

Below, using a method of splitting into subsystems, and basing on generalized Liouville equation, we shall view the closed nonequilibrium a hard-disk system. We shall show, that in such system the energy, \( T_M r_m \), is transformed by irreversible way into internal energy as a result of the generalized forces work [18].

### 4 Irreversibility for a hard-disks system

The equation of motion for hard disks is deduced on the basis of a matrix of collision from laws of conservation of energy and a momentum. This equation can be written so [20]:

\[
\ddot{V}_k = \Phi_{kj} \delta(\psi_{kj}(t)) \Delta_{kj}
\]

where \( \Phi_{kj} = i(l_{kj} \Delta_{kj})/(l_{kj} \Delta_{kj}) \); \( \psi_{kj} = [1 - l_{kj} ||l_{kj}] ||\Delta_{kj}] \); \( \delta(\psi_{kj}) \)-delta function; \( l_{kj}(t) = z_{kj}^0 + t \int_0^t \Delta_{kj} dt \) are distances between centers of colliding disks; \( z_{kj}^0 = z_k^0 - z_j^0 \); \( z_k^0 \) and \( z_j^0 \) - are initial values of disks coordinates; \( k \) and \( j \) are numbers of colliding disks; \( i \) is an imaginary unit; \( t \) is a time; \( z_{kj}^0 = z_k^0 - z_j^0 \) are initial value of disks coordinates; \( \Delta_{kj} = V_k - V_j \) are relative disks velocities; \( D \) is a diameter of disks. The collisions are considered to be central, and friction is neglected. Masses and diameters of disks are accepted to be equal to 1. The moments of
collisions \( k \) and \( j \) disks are determined by equality \( \psi_{kj} = 0 \). The collisions are considered to be central, and friction is neglected. Masses and diameters of disks are accepted to be equal to 1.

The eq. (4) is a non-Newtonian equation because the forces depend on relative disks velocities. As the disks are absolutely rigid, the internal degrees of freedom in them do not exist. Therefore introduction of potential energy is contradicting the condition of rigidity of disks. But potential energy can be used formally if determined it by delta of function. The eq. (4) is shown, that the disks dynamics is determine by the redistribution of kinetic energy without its transformation to potential energy. As the force of interaction of the disks depends on their relative velocities, the generalized subsystems forces will depend also on subsystems velocities.

Now let us consider the question, how equilibrium is established by the mixing. Let us take the nonequilibrium system of disks consisting from two equilibrium subsystems: \( L \) and \( K \) consequently. Let us \( L \)- subsystem will fly on \( K \)- subsystem. Let’s assume that all disks collide simultaneously through equal, short enough intervals of time \( \tau \). Such assumption does not influence qualitative characteristics of evolution. Then the equation of motion of disks (4) will become [17]:

\[
\dot{V}_n^k = \Phi_{kj}^n \Delta_{kj}^{n-1}
\]

Here \( k \) is a disks from \( L \)-subsystem. To each \( k \) and the moment of time \( t = n\tau \) there corresponds number \( j; k \neq j \).

The evolution of the subsystem is determined by the vector-column \( \vec{V}_L \), which components is a velocities of disks of the \( L \)- subsystem; \( \vec{V}_L = \{V_k\}, k = 1, 2, 3, ...L \). Some of the evolution’s properties of this subsystem will be determined by behavior with the time of the sum its components. Let us designate this sum as \( V_L \). Carrying out the summation in (5) on all disks of the subsystem, we shall obtain [17]:

\[
\dot{V}_L^n = \sum_{k=1}^{L} \Phi_{ks}^n \Delta_{ks}^{n-1}
\]

Here we taken into account, that the contribution to the right hand side of eq. (6) gives collisions of disks \( L \)-subsystem with external \( s \)- disks. This equation is written down in approach of pair collisions.

The eq. (6) describes change of a total momentum, effecting onto the \( L \)-subsystem as a result of collisions at the moment \( n\tau \). The aspiration of a total momentum to zero is equivalent to aspiration to zero of force, acting on the part of external disks. Thus the eq. (6) is determining the relative subsystems velocities.

When \( L \to \infty \), from a condition of mixing the uniformity of distribution of impact parameters of disks follow. Really, according to definition of mixing, for system of disks fairly a condition [14]: \( \mu(\delta)/\mu(d) = \delta/d \) (b). Here, \( \mu(\delta) \) is a measure, corresponding to the total value of impact parameter "\( d \)"; \( \delta \) is an arbitrary interval of impact parameters and, \( \mu(\delta) \), is a corresponding measure. The fulfillment of the (b) condition means the proportionality between the number of collisions of disks, falling at the interval, \( \delta \), and the disk diameter-\( d \). i.e. the distribution of impact parameters is homogeneous.

At performance (b) the condition of decay correlations is fair. Therefore from eq. (6) follows:

\[
< \Phi_{ks}^n \Delta_{ks}^{n-1} > = < \Phi_{ks}^n > < \Delta_{ks}^{n-1} >
\]

As the first multiplier depends on impact parameters, and the second depends on relative velocities, the condition of decay of correlations is equivalent to a condition of independence of coordinates and momentums [3, 14, 15]. i.e., when \( L \to \infty \), it is possible to pass from summation to integration phase of the multiplier \( \phi = < \Phi_{ks}^n > \) on impact parameter. Then we will have [17]:

\[
\phi = \frac{1}{L} \lim_{L \to \infty} \sum_{k=1}^{L} \Phi_{ks}^n = \frac{1}{\pi} \int_0^{\frac{\pi}{2}} \Phi_{ks}^n \cos(\vartheta) = -\frac{2}{3},
\]

where \( G = 2 \) is normalization factor; \( \cos(\vartheta) = d \) is impact parameters.
As their velocities of the center of mass at determine relative velocities of subsystems, we shall have: \( V_L^n = \langle \Delta^{n-1}_{k_s} \rangle \). Therefore, we have: \( V_L^n = -\frac{2}{3} V_L^{n-1} \).

Thus, the velocity of a subsystem is decrease. The rate of decreasing is determined by factor 2/3. In a result the system is equilibrates. In our case the sense of replacement of summation on integration on impact parameters will consist only in transition from the discrete description to continuous one. It has allowed estimating the rate of an establishment of an equilibrium state. It will be clear from below, this summation has no relation to the process of the irreversibility proving, as in "coarse-grain" case it have a place [17].

Let us designate the equilibrium point as \( Z_0 \). As it followed from eq. (6), this point is asymptotically steady [17]. Stability is provided with occurrence of returning force \( F_L \) (right hand side of the eq. (6)) acting on \( L \)-subsystem at a deviation of it from an equilibrium point. Therefore the stability of equilibrium state leads to limitation of permissible amplitudes of fluctuations of the system parameters. Really, any nonequilibrium condition is characterized by force \( F_L \). So we have: \( \dot{V}_L = F_L \). As a result of mixing this force should decrease. Time of decrease of force is determined from a condition \( t = \int \frac{dV_L}{F_L} \). Hence, if the system in the artificial way appeared in a nonequilibrium point, through characteristic time, \( t_{din} \sim \frac{1}{F_L} \), this system will come to balance. Hence, the rate of nonequilibrium is determined by the value \( F_L \). So, are possible only those fluctuations, for which condition, \( t_{fluct} < t_{din} \) is satisfied. The time \( t_{fluct} \) is determined probabilistic laws. According to the formula Smoluhovsky [15], for a case ergodic of systems average resetting time, \( t_p \), or Poincare’s cycle times is equal \( \tau = t_p(1 - P_0)/(P_0 - P_1) \), were \( P_1 \) -is a probability of reversibility during the time \( t_p \); \( P_0 \) is a probability of initial phase region. So, the originating of forces \( F_L \) at spontaneous deviation of a system from equilibrium, leads to limitation of permissible amplitudes of fluctuations. Only such spontaneous fluctuations are possible, which one does not contradict a condition \( t_{din} > \tau \).

Thus, spontaneous motion of system from equilibrium point is possible only into such points of phase-space, for which the characteristic time of return, determined to corresponding these points by a field of forces, more than the characteristic time necessary for a spontaneous deviation. From here follows, that framework of applicability probabilistic descriptions of dynamics of systems, and, also, the rate of possible fluctuations, are determined by a condition \( t_{prob} < t_{din} \) [17].

Though the mechanism of irreversibility offered here bases on property of mixing, the coarse-grain problem is eliminated in it. Really, in a basis of this mechanism the dependence of the generalized force on velocities of elements is lays. Evolution of such systems is described by the generalized Liouville equation. The generalized Liouville equation, as against the canonical prototype, does not forbid the existence of irreversible dynamics.

For a hard disks system we have the following explanation of the mechanism of irreversibility [18, 21]. Subsystems of disks in nonequilibrium systems possess relative motion. As a result of their interaction, because of mixing property of phase-space, the chaotic state of disks velocities is increases. It is lead to transformation of energy \( T_{tr} \) into internal energy, reduction of the relative subsystems velocities and their interaction forces. The process of increasing of the relative velocities of subsystems is forbidden due to the law of preservation of a momentum (it will be discussed below more carefully). Therefore the system equilibrates.

Thus, the proof of existence of irreversible dynamics of hard disks is based on the dependence of forces of interaction of disks on their velocities. But all forces in the nature are potential [22]. And according to the eq. (1) for existence of irreversibility in systems of potentially interacting elements, the presence of dependence of the generalized forces from velocities of motion of subsystems is necessary. It will be shown below, that such dependence takes place in nonequilibrium systems of potentially interacting elements.
5 The subsystems dynamics

In this section presence of dependence of the generalized forces from velocities in nonequilibrium systems of potentially interacting elements will be shown. With this purpose we shall obtain the equation, describing an energy exchange between subsystems. Basing on it we shall find an analytical form of the generalized forces.

Let us take the system consisting from \( N \) elements. Masses of elements are accepted to 1. We shall present energy of the system as the sum of kinetic energy of the motion of system as the whole-\( T_\text{tr}^N \); the kinetic energy of the motion of its elements concerning the center of mass-\( \tilde{T}_\text{ins}^N \); and their potential energy-\( \tilde{U}_\text{ins}^N \). The energy, \( E_\text{ins}^N = \tilde{T}_\text{ins}^N + \tilde{U}_\text{ins}^N \), is internal energy of the system. It is the sum of the kinetic energy of the relative motion of elements and the energy of the potential interaction. Relative elements velocities and distances between them determine the internal energy.

The energy, \( T_\text{tr}^N \) is determined by the velocity, \( V_N \) of the center of mass. This energy is depended on the rate of regularity of the particles velocities because \( V_N = \frac{1}{N} \sum_{i=1}^{N} v_i \).

When the external forces are absent, the energies, \( T_\text{tr}^N \) and \( E_\text{ins}^N \) are constants. It is because in connection with the momentum preservation law these energies are the motion integrals.

The full energy of the closed system of potentially interacting elements in homogeneous space can be presented so: \( E_N = T_N + U_N = \text{const} \), where \( T_N = \frac{1}{2} \sum_{i=1}^{N} v_i^2 \) is a kinetic energy; \( U_N(r_{ij}) \) is potential energy; \( r_{ij} = r_i - r_j \) is the distance between \( i \) and \( j \) elements.

The equation of motion for elements of system can be obtained differentiating the expression of energy systems with respect to time [7, 12, and 19]. We will have: \( \dot{v}_i = - \sum_{i=1,j\neq i}^{N} \frac{\partial}{\partial r_{ij}} U (c) \).

The eq. (c) generally is nonlinear. Let us consider the nature of this nonlinearity on the example of two-body system. In the laboratory system of coordinates the kinetic energy of particles can be divided into energy of motion of the center of mass of system, \( T_\text{tr} \), and energy of the particles motion relative to the center of mass, \( T_\text{ins}^i \), where \( i \) is a number of subsystems (in this case "i" is number of elements, \( i = 1, 2 \)). Eventually the redistribution character of these types of energies between particles is various. So, the change of energy \( T_\text{ins}^i \) connected with it transformation into the particles potential energy. The energy, \( T_\text{tr} = T_\text{tr}^1 + T_\text{tr}^2 = \text{const} \) is redistributed between particles by nonlinear way without its transformation to potential energy. By transition to the system of coordinates of the center of mass, the nonlinearity and non-potentiality for two-body system are eliminated because this operation is excludes kinetic energy of motion of the center of mass. In a result the task becomes integrable. For the systems of three and more bodies the excluding of nonlinearity by this way in general case is impossible. Therefore these systems are not integrable.

From here becomes clear why it is necessary to divide system into the equilibrium subsystems. By such splitting the nonlinearity of dynamics caused by relative motion of microsystems inside subsystems is excluded. If the subsystem is in equilibrium, it does not matter how we divide it on the microsystems. In any case these microsystems will be motionless relative to each other and nonlinearity of dynamics is absent. Owing to splitting of nonequilibrium system into equilibrium subsystems, the question about irreversibility nature is reduced to a problem about character of subsystems energy exchange. To emphasize the absence of the energy relative motion of the microsystems in internal energy of an equilibrium subsystem, we shall name internal energy of equilibrium subsystem as "bound energy".

Let us to take the system consisting of two interacting equilibrium subsystems. It is \( L \), and
The number of elements in $L$-subsystem is equal to $L$, and the number of elements in $K$-subsystem is equal to $K$. Let us equalities, $L + K = N$ and $LV_L + KV_K = 0$, have a place, i.e. the center of mass of system is motionless.

It is obvious, if the interaction of subsystems will strong enough; these subsystems can be broken on the different number of smaller equilibrium microsystems. It will complicate the analysis though will not bring in qualitative changes to process of evolution. Therefore we shall accept that interaction of subsystems is weak enough. It will allow accepting that the subsystems are in equilibrium during all process of interaction.

The equations for energy exchange between subsystems can be obtained, by differentiating system energy with respect of time, grouping together the terms, which corresponds to elements different subsystems. Having executed necessary transformations and having allocated the terms corresponding to the different two types of energy: the bound energy and energy of motion of subsystems, the next equations we shall obtain [21]:

$$LV_L \dot{V}_L + \sum_{i=1}^{L} \sum_{j=i+1}^{L-1} \left\{ v_{ij} \left[ \frac{\partial v_{ij}}{L} + \frac{\partial U}{\partial r_{ij}} \right] \right\} = - \sum_{j=1}^{K} \sum_{i=1}^{L} v_{iL} \frac{\partial U}{\partial r_{iLJK}} \tag{7}$$

$$KV_K \dot{V}_K + \sum_{i=1}^{K} \sum_{j=1}^{K} \left\{ v_{ij} \left[ \frac{\partial v_{ij}}{K} + \frac{\partial U}{\partial r_{ij}} \right] \right\} = - \sum_{j=1}^{K} \sum_{i=1}^{L} v_{jK} \frac{\partial U}{\partial r_{iLJK}} \tag{8}$$

Here, $v_{ij} = v_i - v_j$ are the relative velocities. The subindexes, $L, K$, denote to which subsystems some elements belong.

The left hand sides in the eqs. (7, 8) are determining the changes of the energies, $T^r_N$ and $E_N^{me}$, subsystems as a result of their interaction. The first term is set the change of kinetic energy of motion of subsystems as the whole. The second term describes transformation of the bound energy. The right hand sides of the eqs. (7, 8) describe the interaction of subsystems and determine the rate of an exchange of energy between subsystems.

Velocities of any particles of a subsystem can be presented, as the sum of velocities of the center of mass of a subsystem plus their velocities concerning the center of mass. I.e., $v_i = \bar{v}_i + \nabla$. Then, having grouped both parts of the eq. (5) in appropriate way, we shall obtain:

$$LV_L \dot{V}_L + \sum_{jK=1}^{K} \sum_{iL=1}^{L} \frac{\partial U}{\partial r_{iLJK}} \left\{ v_{L} \left[ \frac{\partial v_{ij}}{L} + \frac{\partial U}{\partial r_{ij}} \right] \right\} = - \sum_{jK=1}^{K} \sum_{iL=1}^{L} \frac{\partial U}{\partial r_{iLJK}} \bar{v}_{iL} \tag{9}$$

The eq. (9) determines the change of energy of the $L$-subsystem at interaction it with a $K$-subsystem. As it follows from the right hand side term of the eq. (9), the change of energy of $L$-subsystem as a result of its interaction with a $K$-subsystem is determined by velocities of motion of particles $L$-subsystem concerning its center of mass and potential interaction with particles of the $K$-subsystem.

The first term of the left hand side of eq. (9) determines the change of kinetic energy of motion of $L$-subsystem as a result of its motion in a field of $K$-subsystem. The second term determines the change of the bound energy of a subsystem as a result of motion of its particles in a field of $K$-subsystem particles.

When $\dot{V}_L = 0$, the energy of relative motion of subsystems is absent, and the right hand side of the eq. (9) is equal to zero. In this case the full system energy is equal to the sum of the bound subsystems energies.

If the forces of particles interaction inside subsystems will be infinity, the velocities of motion of particles inside subsystems can be neglected. It corresponds to equality to zero of the right
hand side of eq. (9). In this case the second term in the left hand side of eq.(9) is equal to zero, and this equation will transformed to the usual equation of Newton describing motion of two hard bodies.

6 Difference between particles and subsystems dynamics

The Newton equations (c) can be treated, as equation for the particles interaction forces. The work of these forces is determining transformation of kinetic energy of particles to their potential energy. This energy transformation occurs at transition of system from one point of configuration space into another [12]. Forces are set by a gradient of the potential energy of particles. Thus, the forces and potential energy of particles are completely determined by coordinates, and work of potential forces on the closed contour is equal to zero. It corresponds to reversible dynamics.

And now we shall consider the eq. (9). From it follows, that in nonequilibrium systems the kinetic energy of relative motion of subsystems is appeared. This energy is connected with the rate of regularity of particles motion of subsystems. The regularity is determined by deviation from equilibrium of the velocities distribution functions. As against Newton’s forces, the work of the generalized forces between subsystems will transform kinetic energy of motion of subsystem not only to the potential energy of a subsystem as the whole, but also into the bound energy. Because of such transformation, the work of the generalized forces on the closed contour in configuration space is distinct from zero.

Thus, transformation of kinetic energy of relative motion of subsystems into the bound energy is determined by the work of the generalized forces. As a result the kinetic energy of relative motion of subsystems disappears. But in this process the kinetic energy of particles is not obliged to change. Really, in the coordinates of the center of mass of system, it is possible to see that as a result of interaction of subsystems the orderliness of velocities of particles decreases. But in the coordinates of the centers of mass of each subsystem we will find a decreasing of energy of motion and relative velocities of subsystems, and increasing of their bound energy. This process is caused by the increasing of directions disordering of the velocities vectors of particles in a result of work of the subsystems interaction force. And the system is equilibrates.

The transition of the bound energy into kinetic energy of a subsystem is impossible. It is a cause of irreversibility. Really, this transition would be possible only under condition of spontaneous occurrence inside an equilibrium subsystem of the generalized forces. But their occurrence would mean infringement of spherical symmetry of function of distribution of velocities of elements of equilibrium subsystems concerning the center of mass. And it contradicts the law of preservation of a momentum.

Thus, the eq. (9) as against the Newton equation describes process of transformation of energy in the system, caused not only by transformation of the potential energy into kinetic energy, but also by change of function of distribution of velocities of particles due to increasing the rate of chaotic motion of the particles.

There is a question why the Newton equation fairly for the description of dynamics of particles, but, nevertheless, it does not determine system equilibration? Let us to offer the following answer. Dynamics of selected particles is unequivocally determined by the equation of Newton. A motion of any particle is reversible. But the collective parameters describing subsystem dynamics such as a bound energy, the generalized forces, ambiguously depend on the particles motion parameters. Such ambiguity leads to occurrence of new legitimacies of systems which are not proper for separate particles. Let us view, for example, velocity of a motion of centre of masses of system. It is maintained in the homogeneous space. This velocity is collective
parameter of system and is determined by the total of velocities of all particles of system that leads to lack biunique conformity between velocity of center of mass and particles velocities. The impossibility of magnification of energy of a motion of an equilibrium subsystem due to its bound energy is the collective legitimacy determining its dynamics. Therefore, despite of reversibility of dynamics of a separate particle, dynamics of their subsystems can be irreversible. Thus, irreversibility is a new property of systems which absent in dynamics of their selected particles. Occurrence of this property within the limits of laws of classical mechanics becomes possible, owing to ambiguous dependence of parameters of collective of particles on the parameters determining dynamics of selected particles.

Having excluded from the eq. (9) the potential interaction, we shall obtain the equation for the elastic disks. It means that both in systems of elastic disks, and in systems of potentially interacting elements, the nature of irreversibility are identical.

7 Classical mechanics and thermodynamics

It is possible to come to thermodynamics with the help of the eqs. (7, 8). Really, the right hand side of these equations determines an exchange of energy between subsystems as a result of their interaction. The first term of the left hand side of each equation determines the change of the motion energy of subsystem as the whole. In thermodynamics it corresponds to mechanical work, which is carried out by external forces acting on subsystem on the part of an environment. The second term of the left hand side corresponds to increase in the bound energy of a subsystem due to energy of relative motion of subsystems. In thermodynamics this term corresponds to the change of thermal energy of system.

It is easy to see the relation between the eq. (7) and the basic equation of thermodynamics [2, 3]: \(dE = dQ - PdY\). Here, according to common terminology, \(E\) is internal energy of a subsystem; \(Q\) is thermal energy; \(P\) is pressure; \(Y\) is volume.

The energy change of the selected subsystem is due to the work made by external forces. Therefore, the change in full energy of a subsystem corresponds to \(dE\).

The change of kinetic energy of motion of a subsystem as the whole, \(dT^{tr}\), corresponds to the term \(PdY\). Really, \(dT^{tr} = VdV = V\dot{V}dt = \dot{V}dr = PdY\)

Let us determine, what term in eq. (11) corresponds to the change of the binding energy in a subsystem. As follows from virial theorem [6], if the potential energy is a homogeneous function of second order of the radiuses-vectors, then \(\bar{E}^{ins} = 2\bar{T}^{ins} = 2\bar{U}^{ins}\). The line denotes the time average. Earlier we obtained that the binding energy, \(E^{ins}\), increases due to contribution of energy, \(T^{tr}\). But the opposite process is impossible. Therefore the change of the term \(Q\) in the eq. (11) corresponds to the change of the binding energy \(E^{ins}\).

Let us consider the system near to equilibrium. If the subsystem consist of \(N_m\) elements, the average energy of each element becomes, \(\bar{E}^{ins} = E^{ins}/N_m = \kappa T_0^{ins}\). Now let the binding energy increases with \(dQ\). According to the virial theorem, keeping the terms of the first order, we have:

\[
dQ \approx T_0^{ins}[dE^{ins}/T_0^{ins}] = T_0^{ins}[dv/v_0],
\]

where \(v_0\) is the average velocity of an element, and \(dv\) is its change. For subsystems in equilibrium, we have \(dv/v_0 \sim d\Gamma_m/\Gamma_m\), where \(\Gamma_m\) is the phase volume of a subsystem, \(d\Gamma_m\) will increase due to increasing of the subsystem energy on the value, \(dQ\). By keeping the terms of the first order we get:

\[
dQ \approx T_0^{ins}d\Gamma_m/\Gamma_m = T_0^{ins}d\ln\Gamma_m.
\]

By definition \(d\ln\Gamma_m = dS^{ins}\), where \(S^{ins}\) is a subsystem entropy [2, 3]. So, near equilibrium we have \(dQ \approx T_0^{ins}dS^{ins}\).
8 Relation of the generalized forces with entropy

Let us consider the relation of the generalized forces with entropy. According with the formula (2) the entropy production in the non-equilibrium system is determined by transformation of the kinetic energy of subsystems motion into the bound energy. Eventually relative velocities of subsystems and the generalized forces go to zero. In result the energy of relative motion of subsystems completely transforms into the bound energy and the systems equilibrates. It means that energy of motion of a subsystem goes on increase of entropy. Therefore the deviation of entropy from equilibrium is determined by the next formula [21]:

\[ \Delta S = \sum_{l=1}^{R} \left\{ m_l \sum_{k=1}^{m_l} \int \sum_{s} \frac{F_{ks} m_l v_k}{E_{ml}} dt \right\} \] (10)

Here \( E_{ml} \) is the kinetic energy of subsystem; \( m_l \) is the number elements in subsystem "l"; \( R \) is the number of subsystems; \( s \) is number of the external disks which collided with internal disk \( k \); \( F_{ks} \) is a force, acted on disk \( k \)-disks; \( v_k \) - velocity of the \( k \)- disk.

The integral (10) is determining the work of the force, \( F_{ks} \) during the system relaxation to equilibrium. In equilibrium the energy of the relative motion of subsystems and generalized forces are equal to zero. I.e. the integral in eq. (10) is determined by the energy of relative motion of subsystems. It is corresponds to phenomenological formula Clauses for entropy [3]. So the eq. (10) will be in agreement with the eq. (5).

Really, if \( E_{lns}^{ins} \gg T_{tr}^{ins} \), than we have: \( dS = \sum_{l=1}^{R} \frac{\partial S_l}{\partial T_{l}^{tr}} dT_{l}^{tr} \). It is corresponds to eq. (10). Both in eq. (5) and in eq. (10) entropy increasing is determined by change the energy of the relative motion of subsystems.

Thus, the eq. (10) connects dynamic parameter - force acting on a subsystem, with entropy which is a thermodynamic parameter. I.e. eq.(10) establishes connection between parameters of classical mechanics and thermodynamic parameters. The deviation of system from equilibrium is characterized by the ratio between energy of relative motion of subsystems and full energy of system.

Thus the interrelation of Boltzmann’s entropy definition, which based on the measure of chaos, and definition of the Clauses entropy is cleared by eq. (10).

9 Discussion

At present time the problem of irreversibility was reduced to the problem of the nature of coarse-grain of the phase-space. All attempts to solve this problem within the framework of classical mechanics encountered to Poincaré’s theorem of reversibility. The proof of this theorem is based on a strict formalism of Hamilton, in particular, on canonical Liouville equation. The impossibility of "coarse-grain" follows from this equation. It seems that this fact deprives of any hopes for successful solving the problem of irreversibility [10, 23]. But nevertheless we found this solution by expansion of a canonical formalism to open systems. This solution is in the framework of the laws of classical mechanics but not in the framework of canonical Hamilton’s formalism.

Already during solving a problem of three bodies doubts appeared concerning completeness of methods of classical mechanics. Somehow or other the difficulty of its solution is connected to a problem of the description of nonlinear process of an exchange of energy between bodies. In statistical physics this problem compelled to be limited to make researches of only equilibrium
systems for which it was possible to neglect an exchange of energy between subsystems. In kinetics the account of streams of energy, substance, etc. was based on phenomenological formulas [2-6]. By this way a problem of the description of character of energy exchanging between interacting systems within the framework of classical mechanics has been bypassed. But the knowledge of this mechanism is necessary for understanding of the equilibration process nature. From here follows that for solving a problem of irreversibility it is necessary to find a method of describing of process of energy exchange between interacting systems. It explains our aspiration to expand the Hamilton formalism so that it would be possible to describe dynamics of opens systems in its framework.

The expansion of the formalism and research of the mechanism of irreversibility were carried out by us simultaneously. As a models the nonequilibrium many-body system were used. The system was divided into the equilibrium subsystems. To describe character of an energy exchange, we found the equation in which the energy of system is represented as the sum of energies of subsystems motions, their bound energy and interaction energy. Such representation of energy has played a main role in disclosing of the irreversibility mechanism.

At the beginning of our investigation the colliding hard disks were studied [20]. Their interaction is determined by a matrix of collisions. With its help the equation of motion of hard disks has been obtained. This equation turned out to be non-Newtonian because during collisions of disks there is a redistribution of kinetic energy between them without it transformation into the potential energy. I.e. the use of concept of potential energy for the description of hard disks dynamics turned out to be superfluous. From here there was a necessity for searching such expansion of Hamilton formalism which will allow to describe not potentially of systems interacting. Such expansion was created in a framework of classical mechanics by variational methods basing on D’Alambert equation [16, 17]. Expansion is consisted in replacement of canonical Lagrange, Hamilton and Liouville equations to the corresponding generalized equations.

The generalized Liouville equation obtained by us is applicable for the description of any systems, as potentially interacting systems so non-potentially. From this equation follows that the dependence of subsystems interaction forces on velocities is necessary for existence of irreversibility. Taking into account the mixing property and presence of dependence of forces between disks from velocities with the help of generalized Liouville equation an opportunity of existence, both reversible and irreversible dynamics was proved. But studying of disks dynamics was a preliminary step on a way to understanding of the irreversibility nature. Really, non-Newtonian forces determine dynamics of disks, but in real systems fundamental forces are potential [21]. Therefore the generalization these results on systems of potentially interacting elements were required.

The disks researches have shown that the question about irreversibility is reduced to a problem of existence of subsystems velocities and dependence on velocities of their interacting forces. Presence of such dependence in non-equilibrium systems was proved in [2]. For equilibrium systems the subsystems motions are absent. Therefore it was necessary to know, whether irreversible transformation of kinetic energy of relative motions of potentially interacting elements subsystems to other types of energy is possible. The Newton equation did not suit for this purpose. Really, it describes only such transformations of energy, which are connected to reversible transition of kinetic energy into potential and on the contrary. On the other hand, the Newton equation is fairly convenient for the description of dynamics of elements of any systems in which energy is kept. Therefore we assumed that the Newton equation is not responsible for transformation subsystems relative motion energy. For checking it up, it was necessary to obtain the equation of an energy exchange between subsystems. We have obtained this equation
from the law of conservation of energy. From this equation the expression for the generalized force of interaction of subsystems has been found.

According to the equation of energy exchange between subsystems, energy of their relative motion will be transformed both in their potential and into the bound energy. And energy transformation to the bound energy occurs as a result of increase of particles motion randomness. Such transformation of energy conducts to irreversible decrease of energy of motion of a subsystem. Irreversibility is provided with the law of preservation of a momentum of subsystems. From here the next explanation of the mechanism of irreversible dynamics follows.

The rate of the systems nonequilibrium is determined by the organizing of motion of systems elements. Therefore if we divide nonequilibrium system into the equilibrium subsystems, the relative motion of subsystems should exist due to the organizing of elements. As a result of the work of the generalized forces the energy of relative motion of a subsystem decreases. This energy is transformed both into the potentially and into the bound energy of subsystems. The process of increase of the bound energy is going due to increasing of a randomness of vectors of subsystem elements velocities. The mixing is a cause of the increase of randomness. Process of reduction of subsystems relative motion energy is irreversible because of the impossibility of increasing of their relative velocities due to the bound energy. It is follows from the law of preservation of a momentum of subsystems. Equilibrium is established when the subsystems relative motion kinetic energy completely transformed into the bound energy.

Interaction of elements of systems with each other is essence for the offered mechanism of irreversibility occurrence. Therefore this mechanism is unsuitable for ideal gas or Brownian particles because for them the establishment of equilibrium is determined by interaction with external environment which set in the stochastic way [24, 25]. Probabilistic laws are describing the process of establishment of equilibrium state in these systems.

The offered mechanism of irreversibility cannot be obtained on the basis of the canonical formalism equations for closed systems, as these equations do not describe the work of non-potential forces of interaction of the subsystems reducing orderliness of particles motion. Though this mechanism is connected to property of mixing, the problem of coarse-grain phase-space here does not arise. Moreover the coarse graining of the phase-space is sequent from this mechanism because it corresponds to the system equilibration when integrated velocity of particles in any physically small volume should aspire to zero.

The mechanism of irreversibility submitted here determines the connection between classical mechanics and thermodynamics. Really, the first law of thermodynamics follows from the equation describing energy transformation of interacting subsystems. This equation is determined by presence of two qualitatively various types of energy: the bound energy and kinetic energy of relative motion of a subsystem as the whole. Irreversible transition of subsystems motion energy into their bound energy as a result of increase of randomness determines the contents of the second law of thermodynamics. Really, energy of subsystems motion as a result of chaos increase goes to entropy increase.

The further development of subsystems dynamics researches on the basis of the offered approach represents significant interest. These researches will help to prove thermodynamic laws. They are also perspective from the point of view of classical mechanics expanded formalism creation, allowing to study systems interactions processes and also opening systems.
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