Mixing and irreversibility in classical mechanics

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Abstract

The mechanism of irreversible dynamics in the systems with mixing is analyzed. The procedure of splitting of system on equilibrium subsystems and studying of dynamics of one of them under condition of its interaction with other subsystems in the basis of the approach to the analysis of dynamics of nonequilibrium systems is used. The problem of "coarse-grain" of the phase space in this method is eliminated. The formula, which expresses the entropy through the work of forces between systems, is submitted. The essential link between thermodynamics and classical mechanics was found.

1 Introduction

Irreversibility is an essential part of the second law of thermodynamics in fundamental physics. According to this law there is function $\prime S\prime$ named entropy, which can only grow for isolated systems, achieving a maximum at a state of equilibrium. But this is in contradiction with reversibility of the Newton equation and potentiality of the fundamental forces [1, 2]. The great importance of the irreversibility problem for fundamental physics explains its big popularity among the physicists. The history of its solution was very extensive and sometimes, dramatic. Therefore, let us reference only few those works, which precisely enough gives a clear picture of the state in the problem of irreversibility [1, 3, 8, 17].

A first attempt to resolve this contradiction has been done by Boltzmann. From the $H$-theorem it follows that many-body systems should equilibrate. But for obtaining this result, Boltzmann had used principles of probability. Therefore the contradiction was not overcome. For overcoming this problem, it was suggested to try to create an expanded formalism of open systems within the framework of classical mechanics laws [9]. It turned out that such formalism appears in the process of solving the problem of irreversibility [12-15].

The substantiation of the mechanism of equilibration for non-dissipative hard-disks system was based on the dependence of force of disks interaction on their relative velocities, and on the necessary condition for irreversibility [12]. The dependence of the
force of disks interaction on the velocities followed from their equation of motion. The existence of irreversibility condition followed from the general Liouville equation. But in natural systems the forces of interacting of the elementary particles are potential [2] and therefore the equation of motion is reversible. Thus there is a key question on a way of a substantiation of thermodynamics: is it possible to connect the fact of the potentiality of interaction elements in the system with irreversibility which in real systems exists? The search of the answer on this question is the purpose of this work.

The investigation is based on the next method. A conservative system of 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.

The work was carried out in the following way. First of all, based on the equation of motion for disks, we will show that the forces between the selected subsystems, which we called the generalized forces, are dependent on the velocities. This result has led us to the key point that on the base of usual canonical Hamilton and Liouville equations, the fundamental problem of irreversibility cannot be solved. Instead we have used so-called generalized Hamilton and Liouville equations [12]. Based on this, we discover the condition of irreversible dynamics. This condition follows from the generalized Liouville equation.

Then the dynamics of the systems constructed from potentially interaction elements is analyzed. The equation for the energy exchange between subsystems is obtained. Based on this equation we answer the question of why and how the velocity dependence of generalized forces between subsystems appears when the forces between the elements are potential. Then the essential link between thermodynamics and classical mechanics is analyzed. A formula, which expresses the entropy through the work of generalized forces, is obtained. This formula is determined by the fact that the energy of subsystem interaction is transformed into internal energy as a result of the work done by the generalized forces in an irreversible way.

2 Irreversibility in a hard-disks system

The study of a hard-disk system is based on the equation of motion for disks. This equation is deduced with help of the matrix of pair collisions. In the complex plane this matrix is given [11]:

\[ S_{kj} = \begin{pmatrix} a & -ib \\ -ib & a \end{pmatrix} \]

where \( a = d_{kj} \exp(i\vartheta_{kj}) \); \( b = \beta \exp(i\vartheta_{kj}) \); \( d_{kj} = \cos\vartheta_{kj} \); \( \beta = \sin\vartheta_{kj} \); \( i \) is the imaginary unit; \( k \) and \( j \) numbers of colliding disks; \( d_{kj} \) is the impact parameter (IP), determined by the distance between the centers of colliding disks in a Cartesian plane system of coordinates with axes of \( x \) and \( y \), in which the \( k \)-disk swoops on the lying \( j \)- disk along the \( x \)-axis. The scattering angle \( \vartheta_{kj} \) varies from 0 to \( \pi \). In consequence of collision the transformation of disks velocities can be presented in such form: \( V_{kj}^+ = S_{kj}V_{kj}^- \) (a), where \( V_{kj}^- \) and \( V_{kj}^+ \) are bivectors of velocities of \( k \) and \( j \) - disks before \(-\), and after \(+\) collisions, correspondingly; \( V_{kj} = \{V_k, V_j\}, V_j = V_{jx} + iV_{jy} \) - are complex velocities of
the incident disk and the disk - target with corresponding components to the x- and y-axes. The collisions are considered to be central, and friction is neglected. Masses and diameters of disks, "d", are accepted to be equal to 1. Boundary conditions are given as either periodical or in form of hard walls. From (a) we can obtain equations for the change of velocities of colliding disks:

\[
\begin{pmatrix}
\delta V_k \\
\delta V_j
\end{pmatrix} = \varphi_{kj} \begin{pmatrix}
\Delta^+_{kj} \\
-\Delta^-_{kj}
\end{pmatrix}.
\]

Here, \(\Delta_{kj} = V_k - V_j\) are relative velocities, \(\delta V_k = V_k^+ - V_k^-\), and \(\delta V_j = V_j^+ - V_j^-\) - are changes of disks velocities in consequence of collisions, \(\varphi_{kj} = i\beta e^{i\theta_{kj}}\).

That is, Eq. (1) can be presented in the differential form:

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

where \(\psi_{kj} = [1 - |l_{kj}|]/|\Delta_{kj}|\); \(\delta(\psi_{kj})\)-delta function; \(l_{kj}(t) = z^0_{kj} + \int_0^t \Delta_{kj} dt\) are distances between centers of colliding disks; \(z^0_{kj} = z^0_k - z^0_j\), \(z^0_k\) and \(z^0_j\) - are initial values of disks coordinates; \(\Phi_{kj} = i(l_{kj}\Delta_{kj})/(|l_{kj}||\Delta_{kj}|)\).

The Eq. (2) determines a redistribution of kinetic energy between the colliding disks. It is not a Newtonian equation because the forces between the colliding disks depend on their relative velocities. Hence, for the analysis of systems of disks it is impossible to use the canonical Hamilton equation [4]. So, we get the generalized Hamilton equation to be applied for studying the subsystem dynamics [12]:

\[
\frac{\partial H_p}{\partial r_k} = -\dot{p}_k + F^p_k
\]

\[
\frac{\partial H_p}{\partial p_k} = V_k
\]

These are the general Hamilton equations for the selected \(p\)-subsystem. The external forces, which acted on \(k\) disks belong to the \(p\)-subsystem, presented in a right-hand side on Eq. (3). These forces are not potential.

Using Eqs. (3,4), we can find the Liouville equation for \(p\)-subsystem. For this purpose, let us take a generalized current vector \(J_p = (\dot{r}_k, \dot{p}_k)\) of the \(p\)-subsystem in a phase space. From Eqs. (3,4), we find [12, 13]]:

\[
\frac{df_p}{dt} = -f_p \sum_{k=1}^T \frac{\partial}{\partial p_k} F^p_k
\]

Eq. (5) is a Liouville equation for the \(p\)-subsystem. We can rewrite it in differential form as:

\[
\frac{df_p}{dt} + f_p \text{div}_p \vec{F} = 0, \text{ where } \vec{p} = \{p_k\}; \vec{F} = \{F^p_k\}, k = 1, 2...T.
\]

The Liouville equation has the formal solution: \(f_p = \text{const} \cdot \exp [- \int_0^t \left( \sum_{k=1}^T \frac{\partial}{\partial p_k} F^p_k \right) dt]\).

The Eq. (5) is obtained from the common reasons. Therefore it is suitable for any interaction forces of subsystems, as dissipative, as non-dissipative. For a hard-disks system the energy dissipation does not exist. There is only a redistribution of kinetic energy
between colliding disks. Thus, Eq. (5) is applicable to analyze any open nonequilibrium systems, because it takes into account the energy exchange between subsystems. Therefore it can be used also for the explanation of irreversibility in a frames of the classical mechanics laws.

The right side of Eq. (5), $f_p \sum_{k=1}^{T} \frac{\partial}{\partial p_k} F^p_k$, is a similar to the integral of collisions. It can be obtained using the subsystems motions equations. For a hard disks system it can be found with the help of Eq. (2).

In the non-equilibrium system the right term of Eq. (5) is not zero, because generalized forces are dependent on velocities. Therefore the relative subsystems velocities are distinguish from zero. This conclusion is in agreement with the fact, that subsystems velocities in the non-equilibrium systems are non-zero [5]. This can mean only, that when the system goes to equilibrium state, the relative velocities of subsystems go to zero.

Let us consider the important interrelation between descriptions of dynamics of separate subsystems and dynamics of system as a whole. As the expression, $\sum_{p=1}^{R} \sum_{k=1}^{T} F^p_k = 0$, is carried out, the next equation for the full system Lagrangian, $L_R$, will have a place:

$$\frac{d}{dt} \frac{\partial L_R}{\partial V_k} - \frac{\partial L_R}{\partial r_k} = 0$$

and the appropriate Liouville equation: $\frac{\partial f_R}{\partial t} + V_k \frac{\partial f_R}{\partial r_k} + p_k \frac{\partial f_R}{\partial p_k} = 0$. The function, $f_R$, corresponds to the full system. The full system is conservative. Therefore, we have: $\sum_{p=1}^{R} divJ_p = 0$. This expression is equivalent to the next equality: $\frac{d}{dt}(\sum_{p=1}^{R} \ln f_p) = \frac{d}{dt}(\ln \prod_{p=1}^{R} f_p) = (\prod_{p=1}^{R} f_p) \frac{\partial}{\partial t} (\prod_{p=1}^{R} f_p) = 0$. So, $\prod_{p=1}^{R} f_p = const$. In an equilibrium state we have $\prod_{p=1}^{R} f_p = f_R$.

Because the equality $\sum_{p=1}^{R} F^p_p = 0$ is fulfilled during all time, we have that equality, $\prod_{p=1}^{R} f_p = f_R$, is a motion integral. It is in agreement with Liouville theorem about conservation of phase space [4].

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 $\int_{0}^{t} (\sum_{k=1}^{T} \frac{\partial}{\partial p_k} F^p_k) dt \rightarrow const$ (c) is satisfied when $t \rightarrow \infty$, or when, $(\sum_{k=1}^{T} \frac{\partial}{\partial p_k} F^p_k)$, is a periodic function of time. The first case corresponds to the irreversible dynamics, and the second case corresponds to reversible dynamics.

Because the generalized forces for a hard-disks system depended on velocities, the irreversible dynamics is possible.

Dynamics of strongly rarefied systems of potentially interacting elements is also described by the Eq. (2)[12]. Therefore for those systems, irreversibility is possible as well.

Thus, the generalized Liouville equation allows describing dynamics of nonequilibrium systems within the framework of laws of classical mechanics. According to this equation the reversible and irreversible dynamics have a place. Irreversibility is possible only at presence of dependence of the generalized forces from subsystems velocities. The
dependence of the generalized forces on velocities deletes the restriction on irreversibility, superimposed by the Poincare’s theorem about reversibility [17] because this theorem is applicable to the systems with the potential forces only.

We see that the dependence of generalized forces on velocities for subsystems interaction is a necessary condition for the irreversibility to occur. So, the question about irreversibility for Newtonian systems is reduced to that about dependence of the forces between subsystems on the velocity.

For a hard-disks system and for strongly rarefied system of potentially interacting elements the presence of irreversibility is predetermined by Eq. (2). In these systems the interaction forces between the elements are depending on velocities. Therefore it is clear that the generalized forces will depend on velocities as well. But the forces between elements for Newtonian systems are potential. Therefore it is necessary to answer the question: how does velocity dependence of generalized force between subsystems appear when forces between the elements are independent on velocities. The answer on this question is a purpose of the next part of the paper.

3 The subsystems equation of motion

Let us to analyze Newtonian systems. We take a system with energy: \( E_N = T_N + U_N = \text{const} \), 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; \( N \) is the number of elements. Masses of elements are accepted to 1.

The Newton equation of motion for elements is:
\[
\dot{v}_i = - \sum_{i=1,j\neq i}^{N} \frac{\partial}{\partial r_{ij}} U
\]  

(7)

This equation in generally is nonlinearly. For two-body system by transition into the system of coordinates of the center of mass, the nonlinearity can be eliminated, as kinetic energy of the system’s motion is excluded. In a result the system becomes integrated. For the systems of three and more bodies the excluding of the nonlinearity in generally is impossible. Therefore they are non-integrated. From here, by the way, the reason why the nonequilibrium system should be splitting into equilibrium subsystems, becomes clear. By such splitting we exclude nonlinearity of dynamics inside subsystems. If the system is equilibrium, that, as though we did not split her into subsystems, these subsystems will be motionless be relative each other [5]. To emphasize the absence of energy of relative motion of subsystems in the internal energy of equilibrium system, we shall name internal energy of equilibrium system as a binding energy.

Therefore, for the description of evolution of nonequilibrium system, it is necessary to obtain an equation for energy exchange between subsystems, which determines the generalized forces. For this purpose we will do the following. In laboratory system of coordinates we represent the total subsystem energy as the sum of the kinetic energy of subsystem motion as the whole, \( T_n^{tr} \), the kinetic energy of its elements concerning the center of mass, \( \tilde{T}_N^{ins} \), the potential energy of its elements inside the subsystem, \( \tilde{U}_N^{ins} \), and finally it is an energy of interaction with other subsystems.
The energy, \( E_{ins}^N = \tilde{T}_{ins}^N + \tilde{U}_{ins}^N \), is an internal energy. The internal energy is the sum of kinetic energy of relative motion of particles and their energy of potential interaction. Its value is equal to full energy of a system minus potential energy of its interaction with other systems and kinetic energy of motion of a system as the whole. The internal energy, \( E_{ins}^N \), is determined by relative velocity of the particles and distances between them. If a system is in equilibrium we will call internal energy as binding energy.

The energy, \( T_{tr}^N \), is determined by velocity of the center of mass of system. It depend on relative velocities of subsystems, which depend on the orderliness of motion of particles. Therefore the energy \( T_{tr}^N \) is determine the degree of orderliness of the system.

At absence of external forces, the energies, \( T_{tr}^N \), and \( E_{ins}^N \), according to the law of preservation of a momentum of all systems, are motion integrals.

Let us assume for simplification that the system is consist from two interacting subsystems, both of them is in equilibrium. The equations for the energy exchange for two subsystems have the forms [14, 15]:

\[
LV_L \dot{V}_L + \sum_{j=i+1}^{L} \sum_{i=1}^{L-1} \{ v_{ij} \left( \dot{v}_{ij} \frac{\partial U}{\partial r_{ij}} \right) \} = - \sum_{jK=1}^{K} \sum_{iL=1}^{L} v_{iL} \frac{\partial U}{\partial r_{iLjK}} \tag{8}
\]

\[
KV_K \dot{V}_K + \sum_{j=i+1}^{K} \sum_{i=L+1}^{K-1} \{ v_{ij} \left( \dot{v}_{ij} \frac{\partial U}{\partial r_{ij}} \right) \} = - \sum_{jK=1}^{K} \sum_{iL=1}^{L} v_{jK} \frac{\partial U}{\partial r_{iLjK}} \tag{9}
\]

Here we take \( LV_L + KV_K = 0 \), \( V_L \) and \( V_K \) are the velocities of the center of mass for the subsystems; \( L \) and \( K \) are the number of elements in the subsystems; \( v_{ij} \) are the relative velocities between the \( i \) and \( j \) elements; \( L + K = N \). Masses of elements are accepted to 1. The sub-indexes denote to which subsystems some elements belong.

The first term in the left side Eqs. (8, 9) respectively expresses the rate of change of kinetic energy for the subsystems, \( T_{tr}^N \). The second term is related to transformation of binding energy for the subsystems, \( E_{ins}^N \).

The right side in the Eqs. (8, 9) determine the energy of subsystems interaction. The interaction is a cause of the kinetic energy transformation of the subsystem motion, \( T_{tr}^N \), into the binding energy.

The particles velocities can be write as a sum of velocity of the center of mass of subsystem and velocity relation on it. So, \( v = V + \tilde{v} \). Then, we can write in case \( L = K \) from the Eq. (8):

\[
LV_L \dot{V}_L + \sum_{jK=1}^{K} \sum_{iL=1}^{L} \frac{\partial U}{\partial r_{iLjK}} \dot{V}_L + \sum_{j=i+1}^{L} \sum_{i=1}^{L-1} \{ v_{ij} \left( \dot{v}_{ij} \frac{\partial U}{\partial r_{ij}} \right) \} = - \sum_{jK=1}^{K} \sum_{iL=1}^{L} \frac{\partial U}{\partial r_{iLjK}} \tilde{v}_{iL} \tag{10}
\]

The first term in the left side Eqs. (10) respectively expresses the rate of change of energy for the subsystem as a whole. The second term is related to transformation of binding energy for the subsystem. So the Eq. (10) determines the \( L \) subsystem energy change in interaction with the \( K \) subsystem. This change is determined by the general force, which depend on not only on the coordinates but on the velocities as well.

Let us notice that in the laboratory system of coordinates, the internal energy of the system is equal to the sum of internals energies of subsystems. So the interaction of subsystems do not change they internal energies. But if we take the binding energy,
which is determined concerning to the center of weights subsystems, all is differently. The binding energy will increase due to increasing of randomness of velocities vectors of the particles. This increase will occur due to the energy of relative motion of subsystems, which as a matter of fact is a measure of the order of system.

Let’s compare the equation of Newton and the equation (7). The Newton equation can be treated, as the equation for potential forces. The work of these forces determines transformation of kinetic energy of elements to their potential energy. This transformation has a place at transition of system from one point of configuration space to another. Forces are determined by a gradient of potential energy of particles. Thus, the forces and the potential energy of particles are completely determined by coordinates. The work of potential forces on the closed contour is equal to zero. It corresponds to reversible dynamics.

Let us consider now the equation (10). From it follows, that in nonequilibrium systems the kinetic energy of relative motion of subsystems is exist. It is connected with the orderliness of motion of particles of subsystems. Therefore it’s determined by their function of distribution. As against potential forces, work of the generalized forces will transform kinetic energy of motion of a subsystem not only to the potential energy of a subsystem as the whole, but also into the binding energy. Because of such transformation of kinetic energy of motion of subsystems, the work of the generalized forces on the closed contour in configuration space differs from zero. Really, in the same point of the configuration space, at the same values of kinetic energy of motion of particles, the kinetic energy of motion of subsystems can be various because of a various degree of orderliness of motion of particles. Thus, in nonequilibrium systems there is a new type of a stream of energy. This energy is connected to relative motion of subsystems. It is determined by a degree of a deviation of velocities distribution function of particles from the equilibrium.

The eq. (10) is transformed into the Newton equation in three cases: in equilibrium state; if subsystems can be taken as a hard without internal degrees of freedom; if the subsystems are conservative.

There is a question, why for the closed system the Newton equation for particles fairly, but, nevertheless, it does not determine evolution of system to equilibrium? It is because the work of the generalized forces determines transformation of kinetic energy of relative motion of subsystems into the binding energy. This transformation occurs in a result of approach of the velocity distribution of function of the subsystems elements to the equilibrium. Thus kinetic energy of relative motion of subsystems disappears, though total kinetic energy of particles of system can be saved. Really, in the system of coordinates of the center of mass it is possible to find decreasing of the orderliness of the particles velocities in a result of interaction of subsystems. It leads to reduction of relative velocities and energy of motion of subsystems, and increase of the binding energy. In result the system becomes equilibrium. All this process occurs due to disordering of the vectors of velocities of particles. But the Newton equation determines only the transition of kinetic energy of particles to the potential energy. So, the Newton equation ”does not react” to such transformations of energy that do not change a ratio between kinetic and potential energy of the particles.

Irreversibility is caused by that the return of the binding energy to kinetic energy of
a subsystem is impossible. Really, this return would be possible only under condition of spontaneous occurrence of the generalized forces inside an equilibrium subsystem. But their occurrence would mean broken of spherical symmetry of the distribution function of velocities of elements. It is also in contradiction with the law of preservation of a momentum.

Thus, the equation (10), as against of the Newton equation, describes process of transformation of energy in the system, caused not only by the transformation of the potential energy to kinetic energy, but also change of the distribution function of velocity of particles. This change of function of distribution is caused by increase in a randomness of velocities of particles as a result of mixing of the phase trajectories.

It is not difficult to generalize the equation (7) on a case when forces of interactions of particles inside subsystems will be much more than forces of interaction between particles of different subsystems. This case corresponds, or to different types of potential interaction of particles of different subsystems, or big enough distance between subsystems. If interaction forces of particles inside subsystems are infinite, the right part (7) is equal to zero. Then the change of the binding energy of subsystems will be zero and the equation (7) will transformed to the usual equation of Newton for interacting hard body.

Having excluded from the equation (7) of the potential energy, we shall obtain the equation of motion of a hard disks. It means, that both, in systems of hard disks, and in systems of potentially interacting elements, the nature of irreversibility is identically. The irreversibility is determined by transformation of energy of relative motion of subsystems to their binding energy as a result of amplification of the disorder.

In equilibrium the relative velocities of subsystems and the energy flow between them are equal to zero for any splitting [5]. The equilibrium state is stable. From the physical point of view the stability of an equilibrium state for mixed systems is caused by aspiration to zero of the generalized forces arising at a deviation of system from equilibrium [10, 13]. Hence, the system, having come to equilibrium, never leaves this state.

4 Thermodynamics and classical mechanics

With the help of the equations (8-10) it is possible to link classical mechanics with thermodynamics. Really, the right side of these equations determines an exchange of energy between subsystems as a result of their interaction. The first term of the left side of each equation determines change of energy of motion of the subsystem as the whole. In thermodynamics it corresponds to mechanical work done with subsystem by external influence. The second term of the left side corresponds to increase of the binding energy of a subsystem. In thermodynamics this term corresponds to change of thermal energy of system.

Let us now consider the essence link between thermodynamics and classical mechanics. It is easy to see the analogy between the Eqs. (8-10) and the basic equation of thermodynamics [10]:

\[ dE = dQ - PdY \] (11)

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, \( dT_{tr} = VdV = VVdt = Vdr = PdY \)

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:

\[
dQ \approx T_{0}^{ins} d\Gamma_m/\Gamma_m = T_{0}^{ins} d\ln \Gamma_m. \quad \text{By definition } d\ln \Gamma_m = dS^{ins}, \quad \text{where } S^{ins} \text{ is a subsystem entropy } [5, 10].\]

So, near equilibrium we have \( dQ \approx T_{0}^{ins} dS^{ins} \).

5 Relation between entropy and generalized forces

Let us consider the relation of the generalized field of forces with entropy. According to the results obtained here, and also in agreement with \([5]\) the equilibrium state of the system is characterized by absence of energy of relative motion, \( T_{tr}^{m} \), of subsystems. I.e. energy \( T_{tr}^{m} \), as a result of the work done by the generalized forces, will be redistributed between the subsystems into the binding energy. This causes an increase of entropy. When the relative velocities of the subsystems go to zero, the system goes to equilibrium. So, the entropy increasing, \( \Delta S \), can be determined as follows:

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

Here \( E_{m_l} \) 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 \( k \). The integral is determining the work of the force \( F_{k}^{m_l} \) during the relaxation to equilibrium. It is corresponds to phenomenological formula Clauses for entropy \([5, 10]\). So, Eq. (12) deduced entropy through the generalized force. Therefore we can use this equation for analyzing different kind of entropy \([3, 16]\).

Inherently Eq. (12) corresponds to the formula for entropy: \( S = \sum_{l=1}^{R} S_l(E_{l}^{ins} + T_{l}^{tr}) \),
In fact, if $E_i^{ns} \gg T_i^{tr}$, then $dS = \sum_{i=1}^{R} \frac{\partial S_i}{\partial T_i^{tr}} dT_i^{tr}$ which corresponds to Eq.(12).

Thus, the Eq. (12) connects the force acting on the system with entropy. I.e. this formula established the connection between parameters of classical mechanics and thermodynamic parameters. It determines a measure of a deviation of system from equilibrium. Moreover, it opens essence of interrelation of Boltzmann entropy definition, based on a measure of the chaos, and Clausen entropy, based on the energy measure.

6 Discussion

From the time of statement of a problem of irreversibility passed about 150 years. Up to now it was reduced to the problem of coarse-grain of the phase space. All attempts to solving this problem within the framework of classical mechanics were unsuccessful as they encountered Poincare’s theorem of reversibility. This theorem based on a strict of canonical formalism of Hamilton. All this, apparently, deprives us any hopes for the successful solution of a problem of irreversibility within the framework of classical mechanics [17]. Is it so?

Already at the solution of a problem of three bodies there were doubts concerning completeness of known methods of classical mechanics. Difficulty of its solution, anyhow, is connected with a problem of the description of the nonlinear process of an exchange of energy between bodies. The same problem forced scientists to be limited by researches only equilibrium systems when it is possible to neglect an exchange of energy between subsystems. In kinetic physics where energy flows, substances, etc. play a basic role, the phenomenological formulas basing on statistical laws were used for their calculation [7]. But the exchange of energy between particles and subsystems determines process of an establishment of equilibrium. From here we also came to the conclusion that it is impossible to solve a problem of irreversibility if not to find a way of the description of process of an exchange of energy inside systems within the framework of classical mechanics. It dictates desire to execute such expansion of a Hamilton formalism which will allow to describe dynamics of open systems.

Creation of the generalized formalism and studying of the mechanism of irreversibility was carried out by us in parallel [11-15]. With this purpose a conservative system of 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.

First of all the dynamics of hard-disk systems is analyzed. Here, based on the motion equation for disks [11], we showed that the non-dissipative forces between the selected subsystems are dependent on the velocities. This result has led us to the key point that on the base of usual canonical Liouville equation, the problem of irreversibility cannot be solved. Instead we have to use so-called generalized Liouville equation [12, 13]. We showed that the irreversible dynamics really does follow from the generalized Liouville equation when forces between subsystems depend on velocities.

But studying of dynamics of disks was preliminary step on a way to understanding of the nature of irreversibility. Really, dynamics of disks is determined by non-Newtonian
forces. In a real systems fundamental forces is potential [2]. Therefore these results required generalization on a systems of potentially interacting elements.

The results of disks research have shown, that the question on irreversibility is reduced to a question on dependence of the forces of interaction of subsystems on velocities. This statement is in agreement with results, which was obtained in earlier works by a similar method: splitting the system into equilibrium subsystems and studying its dynamics near equilibrium state [5]. The macroscopically motion (it is similar to the subsystems motion in our case) was considered. By using of the method of Lagrange multiplier it has been strictly proved that equilibrium is possible when, \( T^{tr} = 0 \). Therefore it was necessary to find out, whether irreversible transformation of kinetic energy of relative motions of subsystems of potentially interacting elements is possibly. The equation of Newton for this purpose did not convenient. Really, it describes only such transformations of energy, which are connected to reversible transition of kinetic energy in potential. On the other hand, the equation of Newton is correct for any systems. It has led us to suggestion, that the Newton equation is not responsible for transformation of the energy, connected with work of non-potential forces. Became clear from here why the redistribution of energy caused by reduction of relative velocities of subsystems as a result of increase of a randomness of velocities of particles, is not described by canonical Liouville equation and why the coarse-grain is impossible. We came to the conclusion, that it is necessary to find a way of the description of process of transformation for two types of energy between systems. For this purpose analytical expression for an energy exchange between subsystems from the law of conservation of energy of system of potentially interacting elements has been obtained. From it expression followed, that the energy of relative motion of subsystems would be transformed to the binding energy as a result of disorder increasing of the vectors of velocities of particles. As a result, the relative velocities of subsystems will decrease. It has allowed offering the following mechanism of irreversible dynamics.

The nonequilibrium system is characterized by the greater orderliness of elements motions. It causes existence of relative motion of the equilibrium subsystems. As a result of mixing, the disorder of vectors of velocities of the particles is increase. It will lead to decrease of the subsystems velocities and increasing of the binding energy. The given process is irreversible because impossibly of increasing relative velocities of motion due to the binding energy. This conclusion is follows from the law of preservation of a subsystems momentum. As a result the kinetic energy of relative motion of subsystems will completely be transformed to the binding energy and system equilibrates.

The offered scenario of irreversibility cannot be obtained on the basis of the canonical equations of classical mechanics, as these equations do not describe work of non-potential forces, that reducing orderliness of motion of particles. Though mixing property underlies in the offered scenario of irreversibility, the coarse-grain problem of the phase space in it does not exist.

This scenario of irreversibility leads to a substantiation of thermodynamics. Really, the first thermodynamics law follows from the equations (8-10) which describe transformation energy of interacting subsystems. These equations are determined by presence of two qualitatively various types of energy: the binding energy and kinetic energy of relative motion of a subsystem as the whole. Irreversible transition of energy of motion
of a subsystem to their binding energy determines the contents of the second law of thermodynamics. I.e. the energy of the motion of subsystems as a result of amplification of chaos goes on increase of the entropy.

The further development of researches of irreversible dynamics on the basis of the offered approach represents significant interest. These researches will help explain connection between thermodynamic laws and classical mechanics. They are perspective also from the point of view of creation of the expanded formalism of the classical mechanics, which necessary for investigation of the open systems.

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