Thermodynamics and classical mechanics

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Abstract. An explanation of the mechanism of irreversible dynamics in systems with mixing is offered. The procedure of splitting a system into subsystems in equilibrium and studying the dynamics of one of them as it interacts with the other subsystems is the basis of the approach to the analysis of nonequilibrium systems. The problem of “coarse-grain” dynamics is used. The “coarse-grain” problem on the phase space is eliminated with this method. The formula, that 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 a function $S$ named entropy, which can only grow for isolated systems, achieving a maximum in a state of equilibrium. But this contradicts reversibility in Newton’s equation and the potentiality of the fundamental forces [1, 2]. The irreversibility problem great importance for fundamental physics explains its big popularity among physicists. The history of its solution is very extensive and sometimes has been very dramatic. Therefore, let us reference only a few articles representative of this work, that would give a clear picture of the state of the art in the solution of the irreversibility problem [1, 3, 8, 17].

A first attempt to solve this contradiction was made by Boltzmann. From the $H$-theorem it follows that many-body systems should reach equilibrium. But to obtain this result, Boltzmann used probability principles. Therefore the contradiction was not overcome.

To overcome 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 for a hard-disks system. To avoid the condition imposed on the systems by the conservation laws and by their interactions through a potential [12-15].

To substantiate the mechanism for reaching an equilibrium state for a non-dissipative hard-disks system, the theory was based on the dependence of the disks interaction force on their relative velocities, and on the necessary condition for irreversibility [12]. The dependence of the disks interaction force on the velocities followed from their equation of motion. The existence of the irreversibility condition followed from the general Liouville equation. But in natural systems, the elementary particle interaction forces are due to a potential [2] and therefore the equation of motion is reversible. Thus there is a key question on a way to substantiate thermodynamics: is it possible to connect the fact of the elements interaction through a potential with the irreversibility found in real systems? The quest to answer this question is the purpose of this work.
The research is based on a similar method to the one used for a hard-disks system. A conservative system of interacting elements, out of equilibrium, is prepared. This system is then split into small subsystems that are accepted as being in equilibrium. The subsystem dynamics under the 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 showed that the forces between the selected subsystems, which we called the generalized forces, were dependent on the velocities. This result led us to the key point that on the base of the usual canonical Hamilton and Liouville equations, the fundamental problem of irreversibility cannot be solved. Instead we used the so-called generalized Hamilton and Liouville equations [12]. We discovered then, the condition of irreversible dynamics, which follows from the generalized Liouville equation.

Then the dynamics of the systems constructed from the elements with a potential derived interaction is analyzed. We will refer to them, as Newtonian systems. The equation of motion of the subsystem is obtained, in order to answer the questions of why and how the velocity dependence of generalized forces between subsystems appears when the forces between the elements are derived from a potential.

Then based on the equation for the energy exchange between subsystems, the essential link between thermodynamics and classical mechanics is analyzed, using the equation for the energy exchange between subsystems.

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 the 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 by [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 \( \pi \). After collision the transformation of disks velocities can be represented in the 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 the equations for colliding disks velocities change as:

\[ \begin{pmatrix} \delta V_k \\ \delta V_j \end{pmatrix} = \varphi_{kj} \begin{pmatrix} \Delta_{kj}^- \\ -\Delta_{kj}^+ \end{pmatrix} \] (1)

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 the changes of the disks velocities due to collisions, \( \varphi_{kj} = i\beta e^{i\vartheta_{kj}} \).

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

\[ \dot{V}_k = \Phi_{kj} \delta(\psi_{kj}(t)) \Delta_{kj} \] (2)
where $\psi_{kj} = [1 - |l_{kj}|/|\Delta_{kj}|]$; $\delta(\psi_{kj})$-delta function; $l_{kj}(t) = z_{kj}^0 + \int_0^t \Delta_{kj} dt$ 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; $\Phi_{kj} = i(l_{kj}\Delta_{kj})/(|l_{kj}||\Delta_{kj}|)$.

The Eq. (2) determines a redistribution of kinetic energy between 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 apply the generalized Hamilton equation to study the subsystem dynamics [12]:

$$\frac{\partial H_p}{\partial r_k} = -\dot{p}_k + F^p_k \quad (3)$$
$$\frac{\partial H_p}{\partial p_k} = V_k \quad (4)$$

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 of Eq. (3). These forces are not due to a potential.

Using Eqs. (3,4), we can find the Liouville equation for $p$-subsystem. Let us therefor 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]:

$$\frac{df_p}{dt} = -f_p \sum_{k=1}^T \frac{\partial}{\partial p_k} F^p_k \quad (5)$$

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

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

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

Eq. (5) is obtained in the usual way. Therefore it is suitable for any interaction forces between subsystems, dissipative, as well as non-dissipative. For a hard-disks system the energy dissipation does not exist, it is only a redistribution of kinetic energy between colliding disks, thus, Eq. (5) can be used to analyze any open non-equilibrium system, because it takes into account the energy exchange between subsystems. Therefore it also explains irreversibility in the classical mechanics laws frame.

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 collisions integral obtained from the subsystem motion 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 the generalized forces are dependent on velocities. Therefore the relative subsystems velocities are distinguished from zero. This conclusion is in agreement with the fact, that the subsystems velocities in the non-equilibrium systems are non-zero [5]. This can only mean, that as the system goes to an equilibrium state, the relative velocities of the subsystems go to zero.

Let us consider the important relation between the dynamics of separate subsystems and for the whole system one. As the expression, $\sum_{p=1}^R \sum_{k=1}^T F^p_k = 0$, is carried out, the expression for the full system Lagrangian, $L_R$, becomes:

$$\frac{d}{dt} \frac{\partial L_R}{\partial V_k} - \frac{\partial L_R}{\partial r_k} = 0 \quad (6)$$
and the appropriate Liouville equation is: \( \frac{\partial f_R}{\partial t} + V_k \frac{\partial f_R}{\partial r_k} + \dot{p}_k \frac{\partial f_R}{\partial p_k} = 0. \) The function, \( f_R \), corresponds to the whole system, which is conservative, so that we have: \( \sum_{p=1}^{R} \text{div} J_p = 0. \)

This expression is equivalent to the next equality: \( \frac{d}{dt} \left( \sum_{p=1}^{R} \ln f_p \right) = \frac{d}{dt} \left( \ln \prod_{p=1}^{R} f_p \right) = 0. \) So, \( \prod_{p=1}^{R} f_p = \text{const}. \) In an equilibrium state we have \( \prod_{p=1}^{R} f_p = f_R. \)

Because the equality \( \sum_{p=1}^{R} F_p = 0 \) is fulfilled at all times, the equality, \( \prod_{p=1}^{R} f_p = f_R, \) is a motion integral, in agreement with Liouville theorem about phase space conservation [4].

Only in two cases does the Liouville equation for the whole non-equilibrium system agree with the general Liouville equation for selected subsystems: if the condition \( \int_0^T \left( \sum_{k=1}^{T} \frac{\partial}{\partial p_k} F_k \right) dt \rightarrow \text{const} \) (c) is satisfied when \( t \rightarrow \infty \), or when, \( \frac{d}{dt} \left( \sum_{k=1}^{T} \frac{\partial}{\partial p_k} F_k \right), \) 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 depend on their velocities, the irreversible dynamics is possible.

Dynamics of strongly rarefied systems of elements interacting through a potential are also described by the Eq. (2)[12]. For those systems, irreversibility is also possible.

Thus, the generalized Liouville equation allows us to describe the dynamics of non-equilibrium systems within the framework of classical mechanics. According to this equation the reversible and irreversible dynamics takes place. Irreversibility is possible only when there is a dependence of the generalized forces with the 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 it only applies to systems with conservative forces.

A necessary condition for irreversibility to occur, is the dependence of the generalized forces due to the subsystem interaction on their velocities. So, the question about irreversibility for Newtonian systems is reduced to that about the dependence of the forces between subsystems on the velocity.

For a hard-disks system and for strongly rarefied system of interacting elements through a potential, the presence of irreversibility is predetermined by Eq. (2). In these systems the interaction forces between the elements depend on their velocities. it is clear that the generalized forces will depend on velocities as well. But the forces between elements for Newtonian systems are conservative. 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. To answer this question will be one of the purposes of the next part of this paper.

3. The subsystems equation of motion

Let us analyze a Newtonian system. We take it, 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 taken to be 1.

The Newton equation of motion for each element is:

\[
\ddot{v}_i = - \sum_{i=1,j \neq i}^{N} \frac{\partial}{\partial r_{ij}} U \tag{7}
\]
This equation in generally is nonlinear. For a two-body system using the center of mass coordinate system, the nonlinearity can be eliminated, as the system’s kinetic energy is excluded. As a result the system becomes integrated. For the systems of three and more bodies getting rid of the nonlinearity is generally impossible. Therefore they are non-integrable. Making the reason to split the non-equilibrium system into equilibrium subsystems, become clear. By such splitting we avoid the dynamics nonlinearity within the subsystems. If the system is in equilibrium, we do not need to split it into subsystems, since these subsystems will be motionless relative to each other [5]. To emphasize the absence of relative motion energy of the subsystems in the internal energy of the equilibrium system, we shall name the internal energy of the equilibrium system as a binding energy.

In order to describe the evolution of a non-equilibrium system, it is necessary to obtain an equation for the energy exchange between subsystems, which determines the generalized forces. We will take the laboratory coordinate system to represent the total subsystem energy as the sum of the kinetic energy of all subsystems, \( T^r_N \), the kinetic energy of its elements calculated from the center of mass coordinates, \( \tilde{T}^{ins}_N \), the potential energy of the elements in the subsystem, \( \tilde{U}^{ins}_N \), represents the interaction with other subsystems energy.

The energy, \( E^{ins}_N = \tilde{T}^{ins}_N + \tilde{U}^{ins}_N \), is a binding energy. The binding energy is the sum of particles kinetic energy from their relative motion and the energy due to their interaction through a potential. Its value is equal to the full energy of the system minus the potential energy of its interaction with other systems and the total kinetic energy the system. The binding energy, \( E^{ins}_N \), is determined by the relative velocity and the distance between particles. The energy, \( T^r_N \), is determined by the velocity of the center of mass of the system, and depends on the relative velocities of the subsystems, which in turn depend on the orderliness of the particles motion. Therefore the energy \( T^r_N \) will determine the degree of order in the system.

In absence of external forces, according to the law of momentum conservation for each system, the energies, \( T^r_N \), and \( E^{ins}_N \), are motion integrals.

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

\[
LV_L \dot{V}_L + \sum_{j=i+1}^{L} \sum_{i=1}^{L-1} \{v_{ij}[\dot{v}_{ij}/L + \partial U/\partial r_{ij}]\} = - \sum_{j=1}^{K} \sum_{i=1}^{L} v_{il} \partial U/\partial r_{iLJK} \tag{8}
\]

\[
KV_K \dot{V}_K + \sum_{j=i+1}^{K} \sum_{i=1}^{K-1} \{v_{ij}[\dot{v}_{ij}/K + \partial U/\partial r_{ij}]\} = - \sum_{j=1}^{K} \sum_{i=1}^{L} v_{jK} \partial U/\partial r_{iLJK} \tag{9}
\]

Here \( LV_L + KV_K = 0 \), \( V_L \) 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 each element belongs to.

The first term in the left hand side Eqs. (8, 9) respectively expresses the rate of change of kinetic energy for the subsystems, \( T^r_N \). The second term is related to the transformation of binding energy for the subsystems, \( E^{ins}_N \).

The right hand side in the Eqs. (8, 9) determines the energy of the subsystems interaction. The interaction causes the kinetic energy transformation of the subsystem motion, \( T^r_N \), into the binding energy.

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

\[
LV_i \left[ \dot{V}_L + \sum_{j=1}^{K} \sum_{l=1}^{L} \frac{\partial U}{\partial r_{ij,l,jK}} \right] + \sum_{j=i+1}^{L} \sum_{l=1}^{L-1} \left\{ \dot{v}_{ij} \frac{\tilde{v}_i}{L} + \frac{\partial U}{\partial r_{ij}} \right\} = - \sum_{j=1}^{K} \sum_{l=1}^{L} \sum_{j=1}^{L} \frac{\partial U}{\partial r_{ij,l,jK}} \tilde{v}_i L
\]  

(10)

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

Let us stress, that in the laboratory coordinate system, which in our case coincides with the center of mass of the complete system, interactions of the subsystems do not change the internal energy of a subsystem. Meaning that the transformation of the subsystems energy from the relative motion into the binding energy is a result of a reduction of order in the particles motion as the randomness of their velocity vectors increases. As we compare the Newton equation with equation (7), we can treat Newton equations as equations for forces. The work realized by these forces determine the transformation of the elements kinetic energy into potential energy. This transformation takes place at a transition of the system from one point of the configuration space to another. The force is given by the gradient of the particles potential energy. So the force and the particles potential energy are completely determined by the coordinates and the work of the potential derived forces on the closed contour is equal to zero, which corresponds to reversible dynamics.

As we consider now equation (10), it follows, that for non-equilibrium systems the relative motion kinetic energy of the subsystems exists, and is related to the order of the particles subsystems motion, and is, therefore determined by their distribution function. In contrast with conservative forces, the work of generalized forces will transform the motion’s kinetic energy of a subsystem not only into the subsystem potential energy as the whole, but also into the binding energy, which explains why the work realized by the generalized forces on a closed contour of the configuration space is different from zero. Actually at one particular point on the configuration space, for the same particle’s kinetic energy values, the subsystem’s motion kinetic energy can vary because of the particle’s motion orderliness. Thus, in non-equilibrium systems there is a new type of energy stream, connected to the relative motion of the subsystems. This energy is determined by the degree of the particles deviation from the velocity distribution function around the equilibrium point. The eq. (10) can be transformed into the Newton equation in three cases: in a state of equilibrium; if the subsystems can be taken as hard, showing no internal degree of freedom, and if all subsystems are conservative. The question arises as to why, for a closed particle system, the Newton equation Determines fairly if incompletely the system evolution towards equilibrium? the answer is because the work of the generalized forces determine the transformation of the relative motion of the subsystems kinetic energy into binding energy. This comes as a result when the velocity distribution function of the subsystems elements approaches equilibrium. So the subsystems relative motion kinetic energy disappears, even if the total kinetic energy of the whole particles system cannot vary. Really, in the center of mass coordinate system the particles velocities orderliness decreases as a result of the subsystems interaction. This leads to the reduction of relative velocities and the subsystems kinetic energy, as the binding energy increases. As a result the system reaches equilibrium. All this process is a consequence of disordering the particles velocities vectors. But the Newton equation determines only the transition of the particles kinetic energy into potential energy. So, the Newton equation “does not react” to such energy transformations, since it does not change the ratio between the particles kinetic and potential energy. Irreversibility is found because going back from the binding energy to kinetic energy is impossible for any subsystem, this
return could be possible only on the condition of the generalized forces spontaneous occurrence within a subsystem in equilibrium. But it would mean braking the spherical symmetry of the elements velocities distribution function. And it contradicts the momentum conservation law.

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

Having excluded from equation (7) the potential energy, we obtain the hard disks motion equation. Meaning that for both, hard disks systems and in systems of elements interacting through a potential, the nature of irreversibility is identical. Irreversibility is determined by the transformation of the subsystems relative motion energy into their binding energy, as a result of the disorder amplification.

In equilibrium, the subsystems relative velocities 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 as the generalized forces arising from the system deviation from equilibrium tend to zero. Hence, the system, having reached 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. Since the right hand side of these equations determines an energy exchange between subsystems as a result of their interaction. The first term of the left hand side of each equation determines the motion energy change of the subsystem as whole. In thermodynamics it corresponds to mechanical work done to a subsystem by an external influence. The second term of the left hand side corresponds to the subsystem binding energy increment. In thermodynamics this term corresponds to the thermal energy change in a system.

Let us now consider the essential 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]:

$$dE = dQ - PdY$$

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 complete energy change of a subsystem corresponds to $dE$.

The whole subsystem kinetic energy change, $dT^{tr}$, corresponds to the term $PdY$. Really,

$$dT^{tr} = V dV = V \dot{V} dt = V dr = P dY$$

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

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

$$dQ \approx T_0^{\text{ins}} [(dE^{\text{ins}}/T_0^{\text{ins}}) = T_0^{\text{ins}} (dv/v_0), \text{where } v_0 \text{ is the average velocity of an element, and } dv \text{ is its change. For subsystems in equilibrium, we have } dv/v_0 \sim d\Gamma_m/\Gamma_m, \text{ where } \Gamma_m \text{ is the phase volume of a subsystem, } d\Gamma_m \text{ that will increase as the binding energy value increases,}$$
By keeping the terms of the first order we get: $dQ \approx T_0^{\text{ins}} d\Gamma_m / \Gamma_m = T_0^{\text{ins}} d\ln \Gamma_m$. By definition $d\ln \Gamma_m = dS^{\text{ins}}$, where $S^{\text{ins}}$ is a subsystem entropy [5, 10]. So, near equilibrium we have $dQ \approx T_0^{\text{ins}} dS^{\text{ins}}$.

5. Relation between entropy and generalized forces

If we consider the relation of the generalized forces field with entropy, according to the obtained results, and, in agreement with [5] the system equilibrium state is characterized by the absence of the subsystems relative motion energy, $T^{\text{tr}}_m$, of. I.e. energy $T^{\text{tr}}$, as a result of the work done by the generalized forces, will be redistributed between the subsystems as 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 increase $\Delta S$, can be determined as follows:

$$\Delta S = R \sum_{l=1}^{R} \{ m_l \sum_{k=1}^{m_l} \int \sum_{s} \frac{F_{k s} m_l v_k}{E^{m_l}_{s}} dt \}$$  \hspace{1cm} (12)

Here $E^{m_l}$, is the kinetic energy of subsystem; $m_l$ is the number of elements in subsystem "l"; $R$ is the number of subsystems; $s$ is number of external disks which collided with the internal disk $k$. The integral gives us the work realized by the force $F_{k s}$ during the relaxation towards equilibrium, and corresponds to Clausius phenomenological formula for entropy [5, 10]. So, Eq. (12) deduced entropy from the generalized force. Therefore we can use it to analyze different types of entropy [3, 16,].

Inherently Eq. (12) corresponds to the formula for entropy: $S = \sum_{l=1}^{R} S_l (E^{\text{ins}}_l + T^{\text{tr}}_l )$, (see, [5]).

In fact, if $E^{\text{ins}}_l \gg T^{\text{tr}}_l$, then $dS = \sum_{l=1}^{R} \frac{S_l}{T^{\text{tr}}_l} dT^{\text{tr}}_l$ which corresponds to Eq.(12).

Thus, Eq. (12) connects the force acting on the system with entropy. I.e. this formula establishes the connection between classical mechanics and thermodynamics parameters. It determines a measure of the systems deviation from equilibrium. Moreover, it shows the essence of the relationship between Boltzmann entropy definition, based on a measure of chaos, and Clausius entropy, based on the energy measure.

6. Discussion

Since the statement of an irreversibility problem, 150 years approximately have passed, and up to now, it was reduced to the phase space “coarse-grain” problem. All attempts to solve this problem within the framework of classical mechanics were unsuccessful as they encountered Poincaré’s theorem of reversibility, based on the strict canonical formalism of Hamilton. This, apparently, deprives us of any hope for the successful solution of the problem of irreversibility within the framework of classical mechanics [17]. Is it so?

Already with the three-body problem solution, there were doubts concerning the completeness of any known classical mechanics methods. The difficulty of its solution is, anyhow, connected with the problem to describe the nonlinear or the self-agreement process of an energy exchange between bodies. The same problem forced scientists to limit their researches only to systems in equilibrium, where it is possible to neglect an energy exchange between subsystems. In kinetic physics where energy and substances flows, play a basic role, phenomenological formulas based on statistical laws were used [7]. But it is the exchange of energy between particles and subsystems that determines the process for establishing equilibrium. This led us to conclude that it is impossible to solve an irreversibility problem without finding a way to describe the energy exchange process in the system within the framework of classical mechanics. It dictates the desire to try a Hamilton formalism expansion that will allow us an open system dynamics description.
The creation of the generalized formalism and the study of the mechanism of irreversibility were carried out by us in parallel [11-15]. To this end, a conservative system of interacting elements, out of equilibrium, was prepared. This system was then split into small subsystems that were accepted as being in equilibrium. Taking their interactions into account, the subsystem dynamics were analyzed based on the laws of classical mechanics.

First of all, the hard-disk systems dynamics was analyzed, using the motion equation for disks [11], we showed that the non-dissipative forces between the selected subsystems were dependent on the velocities. This result led us to the key point that based on the usual canonical Liouville equation, the irreversibility problem cannot be solved. Instead we had to use the so-called generalized Liouville equation [12, 13] to show that the irreversible dynamics do really follow from the generalized Liouville equation if the forces between subsystems are velocity dependent.

But studying the dynamics of disks was only a preliminary step on the way to understand the nature of irreversibility. The dynamics of disks is actually determined by non-Newtonian forces, and in real systems the fundamental forces are derived from a potential [2]. Therefore these results required a generalization to systems of interacting elements through a potential.

As a result, disks research has shown that the question on Irreversibility can be reduced to a question of how the forces depend on the subsystems velocities interaction. This statement is in agreement with results obtained in earlier works by a similar method: splitting the system into equilibrium subsystems and studying its dynamics near an equilibrium state [5]. The macroscopic motion (is similar to the subsystems motion in our case) was considered. Using the Lagrange multiplier method, it was strictly proved that equilibrium is possible when, $T_{tr} = 0$. Therefore it was necessary to find out, whether irreversible transformation of relative motion kinetic energy between subsystems of interacting elements through a potential is possible.

Newton’s equation for this purpose was not suitable, because it only described such energy transformations, which were connected to a reversible transition of kinetic energy into potential. On the other hand, Newton’s equation holds for any system and has led us to suggest, that Newton’s equation is not responsible for energy transformation, connected with the work of non-conservative forces. Implying that the reason for the energy redistribution is caused by the subsystems relative velocities reduction, as a result of the increase in the randomness of the particles velocities, can not be described by the canonical Liouville equation, this also explains why the “coarse-grain” model is impossible. We came to the conclusion, that to find a way to describe the transformation process of the two types of energy between systems, an analytical expression for the energy exchange between subsystems derived from the law of energy conservation of interacting elements had to be obtained. From this expression it followed, that the subsystems relative motion energy had to be transformed into the binding energy as a result of the particles velocities vectors increasing disorder. As a result, the relative velocities of subsystems decrease. This allowed us to offer the following mechanism for irreversible dynamics. The non-equilibrium system is characterized by the greater orderliness of the elements motion, causing the existence of relative motion of the equilibrium subsystems, as a result of mixing, the disorder of the particles vectors velocities increases, leading to a decrease of the subsystems velocities and an increase of the binding energy. The given process is irreversible because it is impossible to increase the relative velocities due to the binding energy. This conclusion follows from the momentum conservation law for all subsystems. As a result the kinetic energy of the subsystems will be completely transformed into the binding energy and the system does reach equilibrium.

The offered scenario of irreversibility cannot be obtained from the canonical classical mechanics equations, since these equations do not describe the work realized by the non-conservative forces, the particles motion orderliness is reduced through the mixing property, underlying is the irreversibility scenario, where the “coarse-grain” problem of the phase space does not play any role because it does not exist.
In this scenario, irreversibility leads to a substantiation of thermodynamics. The first law follows from the equations (8-10) describing the transformation energy of interacting subsystems. This equation is determined by the presence of two qualitatively different types of energy: the binding energy and the complete subsystem kinetic energy of the relative motion. The second law of thermodynamics is determined by an irreversible transition of the subsystems energy of motion into their binding energy. I.e. the subsystems energy of motion, as a result of chaos amplification increases the entropy.

Further development of irreversible dynamics research with this approach is of significant interest. It will help explain the connection between thermodynamics and classical mechanical laws. They are also important for the creation of the classical mechanics expanded formalism, which is necessary for open systems investigation.

7. References

[1] Cohen E G D 1998 NATO Sci. Series, Series E: Applied Sciences. B 371 223
[2] Hooft T G 1980 Sci. American, 242 90
[3] Klimontovich Yu L 1995 Statistical theory of the open system (Yanus, Moscow)
[4] Lanczos C 1962 The variation principles of mechanics (Second edition University of Toronto Press)
[5] Landau L D & Lifshits Ye M 1976 Statistical Physics Part 1. (Nauka, Moscow)
[6] Landau L D & Lifshits Ye M 1973 Mechanics (Nauka, Moscow)
[7] Lifshits Ye M & Pitaevsky A P 1979 Phys. kinetics (Nauka, Moscow)
[8] Lebowitz J L 1993 Physics Today 32
[9] Petrosky T & Prigogine I 1997 Computers Math. Applic. 34 1
[10] Rumer Yu B & Ryvkin M Sh 1977 Thermodynamics. Stat. Physics and Kinetics (Nauka, Moscow)
[11] Somsikov V M 2001 Intern. Jour. Bifurc. And Chaos 11 2863
[12] Somsikov V M & Matesov D S 2001 Izv. MON RK. Ser. Phys 4 9
[13] Somsikov V M 2004 Intern. Jour. Bifurc. And Chaos 14 4027
[14] Somsikov V M 2004 The irreversibility and classical mechanics laws (Preprint cond-mat/0406449) 10
[15] Somsikov V M 2004 Jour. of the evolution of the open systems 6 (1) 40
[16] Tsallis C Baldovin F Cerbino R Pierobon P 2003 Introduction to Nonextensive Statistical Mechanics and Thermodynamics (Preprint cond-mat/03094093)
[17] Zaslavsky G M 1999 Physics Today 39