IRREVERSIBILITY IN CLASSICAL MECHANICS

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Abstract

An explanation of the mechanism of irreversible dynamics was offered. The explanation was obtained within the framework of laws of classical mechanics by the expansion of Hamilton formalism. Such expansion consisted in adaptation of it to describe of the non-potential interaction of a systems. The procedure of splitting of a system into equilibrium subsystems, presentation of subsystem’s energy as the sum of energy of their relative motion and their internal energy was the basis of the approach which was used for the analysis of nonequilibrium systems. As a results the generalized Liouville equation and equation of subsystems interaction was obtained. Based on these equations, the irreversible transformation of energy of the relative motion of subsystems into their internal energy was proved. The formula which expresses the entropy via the work of subsystems’ interaction forces was submitted. The link between classical mechanics and thermodynamics was discussed.

1 Introduction

Collective properties of natural systems should be connected with laws of dynamics and properties of their elements. Searching of these connections is among the main tasks of physics. There are principal difficulties in connection with solving of this problem. Particularly they are consisted in absence of links between laws of classical mechanics and laws of the thermodynamics. The irreversibility problem which was formulated by Boltzmann about 150 years ago is the key problem among them [1-4]. The essence of this problem is that dynamics of natural systems is irreversible, while in accordance with Newton equation dynamics of elements of system is reversible.

Actually all attempts of irreversibility substantiation within the framework of canonical formalism of Hamilton were somehow or other stricken against Poincare’s theorem about reversibility. This theorem forbids the existence of irreversibility within Hamiltonian systems [5-8].

Study of irreversibility is often based on the Lorentz’s gas model [7-9]. This model represents point objects with certain masses. They are elastically scattered on various boundaries but do not interact between each other. Study of Lorentz’s gas allowed to find important laws of behavior of dynamic systems, and mixing is among them. But nevertheless the problem of irreversibility has remained unsolved. It was stricken against so-called ”coarse grain” of the phase space problem [8].

At the beginning of our irreversibility investigation we chose the most elementary system - system of hard disks. Taking collisions of disks among themselves into account was our first step in study of irreversibility. The motion equation of colliding hard disks was obtained. Based on it
we found out that forces of interaction of disks systems depend on its relative velocities, i.e. they are non-potential [10-11]. But in order to study such systems we had to expand the framework of Hamilton canonical formalism in such a way that it would be possible to use it for description of dynamics of systems with non-potential forces (polygenic forces [12]). Therefore Lagrange, Hamilton and Liouville equations for systems with non-potential forces acting between them were obtained [11, 15]. According to accepted terminology [12], we will call these equations and system-system interaction forces as "generalized equations" and "generalized forces".

The analysis of generalized Liouville equation led us to conclusion that irreversibility is possible only for non-potentially interacting systems. Using an equation of disks' motion and generalized Liouville equation we were succeeded in showing of existence of irreversible dynamics for the nonequilibrium system of disks which is presented in the form of two colliding subsystems. It was found out that the irreversibility is determined by decreasing of generalized forces [11].

The generality of results of researches of disks systems is limited to a condition of their absolute rigidity. Moreover, a series of assumptions at the proof of irreversibility have been used. It has essentially simplified the proof of irreversibility for systems of the disks. Therefore for generalization of these results on a real systems it was necessary to find such approach which would allow to remove the restriction connected with these assumptions and assumption about non-potentiality forces between elements of the system.

For this purpose we took into account that the presence of dependence of the systems interaction forces from velocities is the necessary condition for existence of irreversibility. This result allowed to reduced the problem concerning irreversibility of natural systems to the problem whether generalized forces acting between interacting systems are non-potential when forces acting between their elements are potential.

For analyzing generalized forces the fact that usually nonequilibrium systems can be represented in the form of set of equilibrium subsystems which are in motion relative to each other was used [2, §10]. It gave possibility to reduce problem of irreversible dynamics to the proof of non-potentiality of generalized forces and that these forces will be decreased. This proof was carried out in such way. In homogeneous space a closed nonequilibrium system of potentially interacting elements was prepared. This system was divided into a set of equilibrium subsystems. The energy of subsystem was presented in the form of the sum of internal energy, energy of relative motion and an interaction energy of the subsystem. After that the equation for energies' exchange between subsystems was obtained. In agreement with this equation we found out that kinetic energy of subsystems will be transformed both to potential and internal energy of subsystems. Then we showed that reverse transformation of internal energy of subsystems to energy of their motion is forbidden by the law of conservation of momentum. It provides relaxation of the system to equilibrium.

The connection of classical mechanics with thermodynamics follows from the fact that the work of generalized forces will change not only the energy of motion of a subsystem as a whole, but also its internal energy.

The fact that energy of subsystems' motion is irreversibly transformed to their internal energies allowed us to obtain the formula for the entropy deviation of the non-equilibrium system from equilibrium value.

Here a results of our investigation of the mechanism of irreversibility and interconnection between classical mechanics and thermodynamics are offered.
2 The generalized Liouville equation and irreversibility of a hard-disks system

The equation of motion for hard disks is deduced on the basis of collision matrix from laws of conservation of energy and momentum. This equation can be written as [17]:

\[ \dot{V}_k = \Phi_{kj} \delta(\psi_{kj}(t)) \Delta_{kj} \] (1)

where \( V_k = V_x + iV_y \) is a complexity form of velocity of \( k \)-disk along \( X \) and \( Y \) arcs consequently; \( \psi_{kj} = [1 - |l_{kj}|/|\Delta_{kj}|]; \Phi_{kj} = i(l_{kj}\Delta_{kj})/(|l_{kj}|\Delta_{kj}); \delta(\psi_{kj}) \) is a delta function; \( l_{kj}(t) = z_{0k}^0 + \int_0^t \Delta_{kj} dt \) are distances between centers of colliding disks; \( z_{0k}^0 - z_{0j}^0 \) and \( z_{0k}^0 \) are initial values of disks’ coordinates; \( k \) and \( j \) are numbers of colliding disks; \( i \) is an imaginary unit; \( t \) is a time; \( \Delta_{kj} = V_k - V_j \) are relative disks’ velocities; \( D \) is disks’ diameter. 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 \( k \) and \( j \) disks collisions are determined by \( \psi_{kj} = 0 \) equality.

The force of disks’ interaction, which is determined by the right side of eq. (1), depends on relative velocities of colliding disks and impact parameters. Therefore it is not a gradient of scalar function. As a force acting between any pair of disks depends on velocity, i.e. it is non-potential then forces acting between subsystems of disks are non-potential too and depend on velocities. Therefore for description of there dynamics it is impossible to use canonical equations of Lagrange, Hamilton and Liouville [12-14]. Hence, it is necessary to replace these equations by generalized ones which at least are applicable to the open systems with non-potential forces.

The generalized Liouville equation for subsystems was obtained in following way [15, 17]. We took a closed nonequilibrium system which consists of \( N \) elements. We divided this system into \( R \) equilibrium subsystems. Then we selected one of subsystems, which was called as \( m \)-subsystem. With the help of D’Alambert equation, the generalized Lagrange and Hamilton equations were obtained for \( m \)-subsystem at the basis of variational method. At obtains of these equations we considered, that forces between subsystems generally non-potential. On the basis of these equations the generalized Liouville equation was obtained. This equation can be written as [11,15]:

\[ \frac{df_m}{dt} = -f_m \frac{\partial}{\partial \tilde{p}_k} \tilde{F}_m \] (2)

Here \( f_m = f_m(\tilde{r}_k, \tilde{p}_k, t) \) is a normalized distribution function for \( m \)-subsystem elements; \( \tilde{F}_m \) is generalized force acting on \( m \)-subsystem, \( \tilde{F}_m = \sum_{k=1}^{L} \sum_{s=1}^{N-L} \tilde{F}_{ks}^m; k = 1, 2...L \) are disks of \( m \)-subsystem; \( s = 1, 2, 3,..., N - L \) are external disk acting on \( k \)-disk of \( m \)-subsystem; \( m = 1, 2, 3,..., R; \tilde{p}_k \) and \( \tilde{r}_k \) are momenta and coordinates of \( m \)-subsystem disks consequently.

The eq.(2) describes change of particles distribution function of the selected equilibrium subsystem on condition that non-potential forces are acting on it. This equation essentially differs from canonical Liouville equation. Actually canonical Liouville equation is suitable for description of potentially interacted systems on conditions for short enough intervals of time when it is possible to neglect an exchange of energy between systems [2].

The important step during generalization of Liouville equation was to refuse requirement of potentiality of forces acting between subsystems. It makes this equation applicable for study of irreversibility [11].

Let us note that the similar form of the generalized Liouville equation can be obtained if the forces is accepted to be dissipative [16]. But in this case generality of obtained equation
would be lost. It is so because postulating of dissipative forces is equivalent to postulating of irreversibility. Moreover acceptance dissipative forces essentially narrows field of applicability of this equation. Indeed, forces of interaction of disks’ systems are nondissipative though they are non-potential [17].

A physical essence of the right hand side of the eq. (2) that it is the integral of collisions which can be obtained with the help of the motion equations of elements. Both under condition of potentiality of forces, and equilibrium condition when relative motion of subsystems is absent, the right side of the eq. (2) is equal to zero.

Let us show, how it is possible to obtain possibility of existence of the irreversible dynamics under condition of non-potentiality forces acting between subsystems using the generalized Liouville equation [10].

Because the equality \( \sum_{m=1}^{R} F^m = 0 \) is correct then the following equation for Lagrangian of entire system, \( L_R, \frac{d}{dt} \frac{\partial L_R}{\partial \dot{v}_k} - \frac{\partial L_R}{\partial v_k} = 0 \) and the appropriate Liouville equation: \( \frac{\partial f_R}{\partial t} + \dot{v}_k \frac{\partial f_R}{\partial v_k} + \dot{p}_k \frac{\partial f_R}{\partial p_k} = 0 \) will have a place. Here \( f_R \) is distribution function which corresponds to entire system; \( \dot{v}_k \) is a velocity of \( k \)-disk. The entire system is conservative. Therefore we will have: \( \sum_{m=1}^{R} \text{div} \vec{J}_m = 0 \). Here \( \vec{J}_m = (\dot{r}_k, \dot{p}_k) \) is a generalized current vector of the \( m \)-subsystem in a phase space. This expression is equivalent to the following equality: \( \frac{d}{dt} (\sum_{m=1}^{R} \ln f_m) = \frac{d}{dt} (\prod_{m=1}^{R} f_m) = (\prod_{m=1}^{R} f_m)^{-1} \frac{d}{dt} (\prod_{m=1}^{R} f_m) = 0 \). So, \( \prod_{m=1}^{R} f_m = \text{const.} \) For equilibrium state we would have \( \prod_{m=1}^{R} f_m = f_R \). Because the equality \( \sum_{m=1}^{R} F^m = 0 \) is fulfilled at all times, we have the equality, \( \prod_{m=1}^{R} f_m = f_R \), as the integral of motion. This is in agreement with Liouville theorem about conservation of a systems’ phase space [2].

So, Liouville equation for entire non-equilibrium system is in accordance with the generalized Liouville equation for selected subsystems only in two cases: if the condition that \( \int_{0}^{t} \frac{\partial}{\partial p_k} F^m dt \to \text{const} \) is satisfied when \( t \to \infty \), or when \( \frac{\partial}{\partial p_k} F^m \) is a periodic function of time. The first case corresponds to irreversible dynamics, and the second case corresponds to reversible dynamics.

Thus irreversible dynamics is possible under condition of redistribution of phase-space volume between subsystems while full volume is an invariant. Reversibility exists if the system is placed near to equilibrium or it is located in cyclic points of phase-space. In the second case a periodic change of phase-space volume of subsystems takes place under condition of system phase-space volume preservation as a whole [9].

Thus generalized Liouville equation allows to describe dynamics of nonequilibrium systems within the framework of classical mechanics. According to this equation both reversible and irreversible dynamics take place. Irreversibility is possible only if motions of subsystems are presented and generalized forces depend on subsystems’ velocities. Presence of such dependence eliminates an interdiction of irreversibility which is dictated by the Poincare’s theorem about reversibility. Therefore to prove the existence of irreversibility first of all it is necessary to show presence of the relative motion of subsystems in nonequilibrium systems and non-potentiality of forces acting between subsystems.

For hard disks the irreversibility is possible because forces acting between subsystems are non-potential (necessary condition). Therefore if we show that these forces aspire to zero (sufficiently condition) then irreversibility for them will be proved.

Let’s take the nonequilibrium system of disks which consists of from two equilibrium subsys-
tems: $L$ and $K$ consequently. Let $L$-subsystem fly at $K$-subsystem. Let’s designate velocity of the center of mass $L$-subsystem as $\vec{V}_L$. Let’s assume that all disks collide simultaneously in and short enough intervals of time $\tau$. Such assumption does not have influence on qualitative characteristics of evolution. Then the equation of motion of disks (4) will be as follows [11]:

$$\dot{\vec{V}}_k^n = \Phi_{kj} \Delta_{kj}^{n-1} \tag{3}$$

Here $k = 1, 2, 3, \ldots L$ is $L$-subsystem disks’ numbers. $j$ number corresponds to each $k$ and point of time $t = n\tau$ there corresponds number $j$: $k \neq j$.

Taking accepted requirements into account it is possible to obtain the expression for the force acting on a subsystem by summing the equations (3) for all disks of $L$-subsystem. After such summation we will obtain:

$$\dot{\vec{V}}_L^n = \sum_{k=1}^{L} \Phi_{ks} \Delta_{ks}^{n-1} \tag{4}$$

Here we have taken into account that collisions of disks $L$-subsystem with external $s$-disks make contribution to the right side of eq. (4). This equation is written down in approach of pair collisions.

The eq. (4) describes change of a total momentum, effecting on 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 the force, acting on the part of external disks. Thus the eq. (4) determines changes of relative velocities of subsystem.

When $L \to \infty$ due to mixing the uniformity of distribution of impact parameters of disks takes place. Really, in accordance with the mixing condition we have the following [13]:

$$\mu(\delta)/\mu(d) = \delta/d \quad (a).$$

Here $\mu(\delta)$ is a measure which corresponds to the total value of impact parameter "$d$"; $\delta$ is an arbitrary interval of impact parameters and $\mu(\delta)$ is corresponding measure. The fulfillment of (a) condition means the proportionality between the number of collisions of disks which fall at the $\delta$ interval, and disk diameter-$d$. I.e. the distribution of impact parameters is homogeneous.

If (a) is correct then condition of decay of correlations is right. Therefore in accordance with eq. (4): $<\Phi_{ks} \Delta_{ks}^{n-1}> = <\Phi_{ks}> <\Delta_{ks}^{n-1}>$. As the first multiplier depends on impact parameters, and the second one depends on relative velocities the condition of decay of correlations is equivalent to condition of independence of coordinates and momentum [3, 13]. I.e., when $L \to \infty$ it is possible to turn from summation to integration of phase multiplier $\phi = <\Phi_{ks}>$ on impact parameter. Then we will have [11]:

$$\phi = \frac{1}{L} \lim_{L \to \infty} \sum_{k=1}^{L} \Phi_{ks} = \frac{1}{G} \int_0^\pi \Phi_{ks} d(cos \theta) = -\frac{2}{3},$$

where $G = 2$ is normalization factor; $(cos \theta) = d$ is impact parameter.

As relative velocities of subsystems are determined by velocities of centers of the mass we will have: $\vec{V}_L^n = <\Delta_{ks}^{n-1}>$. Therefore, we have: $\vec{V}_L^n = -\frac{2}{3}\vec{V}_L^{n-1} \quad (b)$.

Thus velocity of a subsystem is decreased. The rate of decreasing is determined by $2/3$ factor. The reason of such decreasing is related to chaotization of vectors of disks’ velocities. Thus, we have obtained that the nonequilibrium disks’ system is equilibrate.

Let us note that mathematical operations used by us are not connected neither with averaging of phase space nor with any other change of real nature of phenomenon which is under investigation.

Averaging of the phase space is usually used during irreversibility investigation on the basis of analysis of behaviour of phase trajectory. In the mixing systems phase trajectory eventually fills phase space very densely, it is infinitely closed to any accessible point. The irreversibility
relates to infinite fine splitting of the phase space by phase trajectory. It can be performed by averaging of the phase space i.e. by "coarse grain". But as a result of such operation the motion of phase trajectory becomes probabilistic and therefore irreversible [8]. I.e. operation of averaging of the phase space introduces irreversibility into a system. As the nature of the "coarse grain" of phase space is unknown and, most likely, there is no such nature, this approach does not solve a problem of irreversibility.

We are searching for the mechanism of irreversibility by analyzing of the generalized force. Though this dynamic parameter is collective and equals sum of exterior forces acting on elements of subsystem, but it is strictly determined equation of motion also as well as a phase trajectory. During the analysis of the force we also had used mixing property. It has allowed us to use integration of forces instead of summation in thermodynamic limit. But in our case integration was carried out only for estimation of value of change of generalized force due to disks' collisions. Thus physical nature of the process was not distorted.

Let us note that according to offered mechanism of irreversibility the equilibrium state is asymptotically stable. I.e. on deviation of system from an equilibrium point the system returns back to it [11]. Really, on deviation of system from equilibrium the generalized force \( \vec{F}_L \) will appear. As it was shown (see eq. (b) ) this force is a decreasing force. Therefore equilibrium is asymptotically stable.

It is not difficult to determine characteristic time which is needed for system to return back to equilibrium on deviation from it. In accordance with expression (b) it can be written down as \( t_{din} \sim \int d\vec{V} \frac{\vec{F}_L}{|\vec{F}_L|} \). I.e., if the system leaves equilibrium due to exterior action then it will return back in characteristic time \( t_{din} \sim \frac{1}{|\vec{F}_L|} \).

Important conclusion follows from here. It consists in the fact that stability of equilibrium point causes restriction of probable fluctuations. Really, let's suppose that the system has deviated from equilibrium in a probable way. A time of deviation is determined by the probability laws. According to Smoluchowski formula [8, 22], for ergodic systems average resetting time, \( t_p \), or Poincare’s cycle time is equal to \( \tau = t_p (1 - P_0) / (P_0 - P_1) \), were \( P_1 \) -is a probability of return in \( t_p \) time; \( P_0 \) is a probability of initial phase region. But on deviation of system from equilibrium returning force \( \vec{F}_L \) appears. This force becomes bigger as system becomes farther from equilibrium. Therefore the amplitudes of possible fluctuations is restricted by this force. I.e. spontaneous deviation of system from equilibrium state is possible only for such points of phase space for which characteristic time \( t_{din} \) which is determined by field of generalized forces is more than characteristic time \( \tau \) which is necessary for spontaneous deviation. This condition determines the framework of applicability of probabilistic description of dynamics of systems with the mixing [10, 11].

Thus, in agreement with the generalized Liouville equation the dependence system-system interaction forces from their relative velocities is a necessary requirement of occurrence of irreversible dynamics. As pair interactions of disks depend on their velocities, the disks system-system interaction forces also depend on velocities. It causes an opportunity of existence of irreversibility. Such opportunity is realized because of decrease of forces of interaction of equilibrium subsystems of disks into which the nonequilibrium system is divide. In a result its system is equilibrates.

The conclusion about irreversibility for a hard-disks system will confirm further at the analysis of the more general case of dynamics of nonequilibrium systems of potentially interacting elements. For this purpose, using the procedure of splitting a system into equilibrium subsystems, presentation of their energies as the sum of their energy of motion and internal energy, the equation of interaction of such subsystems will be obtained. Based on it we will show, that
the reason of irreversible dynamics in nonequilibrium system of potentially interacting elements are a non-potentiality of the generalized forces of interaction of subsystems and decreasing of them.

3 The relative motion of subsystems

From generalized Liouville equation follows, that irreversibility is possible only when the forces of interaction of equilibrium subsystems are non-potential. Therefore it is clear, that if nonequilibrium system represents a set of equilibrium subsystems, which is in relative motion, the proof of irreversibility is reduced to the proof of decreasing of their relative velocities that is equivalent to decreasing of system-system interaction forces.

Representation of a nonequilibrium system in the form of set of selected equilibrium subsystems corresponds to local equilibrium approach which is used in statistical physics. Possibility of such representation is explained by the fact that the time of equilibration for a subsystem is much less than that for all system [2, 3]. Let’s show that such equilibrium subsystems will be characterized by relative motion. This fact will allow to reduce the proof of irreversibility for any systems to the proof of decrease of generalized forces without decrease of generality.

The proof of existence of relative motion of subsystems for nonequilibrium systems follows from [2, §10]. Let’s take the nonequilibrium system of disks which consists of \( R \) equilibrium subsystems. In accordance with [2] the entropy \( S \) for the system can be written down as:

\[
S = \sum_{m=1}^{R} S_m(E_m - T^{tr}_m) \tag{5}
\]

Here \( S_m \) is entropy for \( m \)-subsystem; \( E_m \) is full energy of \( m \)-subsystem; \( T^{tr}_m = P_m^2/2M_m \) is a kinetic energy of motion of \( m \)-subsystem; \( M_m \) is subsystem’s mass; \( P_m \) is momentum. The argument of \( S_m \) is internal energy of \( m \)-subsystem.

As the system is closed we have: \( \sum_{m=1}^{R} \vec{P}_m = \text{const}, \sum_{m=1}^{R} [\vec{r}_m \vec{P}_m] = \text{const} \). Here \( \vec{r}_m \) is a position vector of \( m \)-subsystem.

In equilibrium state the entropy as a function of momentum of subsystems is maximum. It is possible to determine necessary conditions of maximum using method of uncertain Lagrange multipliers; momentum derivatives from the following expression should be equal to zero:

\[
\sum_{m=1}^{R} \{S_m + aP_m + b[r_m P_m]\}, \tag{6}
\]

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

If we differentiate \( S_m \) with respect to \( P_m \) taking definition of temperature into account we will obtain: \( \frac{\partial}{\partial r_m} S_m(E_m - T^{tr}_m) = -P_m/(M_mT) = -v_m/T \). Hence, differentiating eq.(5) with respect \( P_m \), we shall have: \( v_m = u + [\Omega r_m] \) (a), where \( \Omega = bT, u = aT \), \( T \) is a temperature. From this fact follows that the entropy is maximum when velocities of all subsystems are determined by the formula (a). According to this formula all subsystems should move with identical translational velocities and to rotate with identical angular velocity in equilibrium. 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 (5), the rate of system’s deviation from equilibrium is determined by \( T^{tr}_m \) value. This energy can be selected by dividing the system into equilibrium
subsystems. In accordance with eq. (5) the process of equilibration is caused by transformation of energy $T_m^{tr}$ to internal energy of systems.

Thus, equilibrium is characterized by condition that $T_m^{tr} = 0$, which have a place on any splitting of the equilibrium system into subsystems. Therefore subsystems will have relative motion in nonequilibrium system. If the system goes to equilibrium then $T_m^{tr}$ energy should aspire to zero.

4 The subsystems dynamics

The proof of irreversibility for hard disks is based on dependence of velocity on disks’ interaction forces. But all fundamental forces in the nature are potential [20]. And according with generalized Liouville equation the presence of dependence of the generalized forces on velocities of motion of subsystems is necessary for existence of irreversibility in systems of potentially interacting elements. Therefore the problem concerning irreversibility of natural systems is reduced to the problem whether forces acting between systems are non-potential when forces acting between their elements are potential. It will be shown below that such dependence have place for nonequilibrium systems of potentially interacting elements.

We will solve this problem in such way. Let’s take a system of potentially interacting elements which was prepared as nonequilibrium. We represent it in the form of set of equilibrium subsystems. After that we obtain the equation for energies’ exchange between subsystems. We will search for this equation using requirement of existence for subsystems of not one, but two forms of energies - energies of their motion as a whole and their internal energy. The energy of interaction of systems will be introduced into the right part of the equation. The energy of subsystem we present in the form of the sum of its energy of a motion, an internal energy and an interaction energy. Internal energy will be represented in the form of the sum of a kinetic energy of motion of system’s particles concerning its centre of mass and a potential energy of interaction of particles inside of subsystem. Then time derivation from the energy presented thus will give the required equation which describes transformation of energy between subsystems. If we will obtain non-potentiality of the forces acting between subsystems from this equation then according to generalized Liouville equation the irreversible dynamics is possible.

Thus, as well as in the [18], we use a model of a simple system of particles. The basic distinction that our approach is non-statistical. It allows to determine the nature of nonconservative forces within the framework of classical mechanics and to analyze connection of the classical mechanics with the first and the second laws of thermodynamics.

Let’s take the system which consists of $N$ elements. Masses of elements are accepted to be equal to 1. We will present energy of the system as the sum of kinetic energy of motion of the system as a whole-$T_N^{tr}$ and the kinetic energy of the motion of its elements concerning the center of mass- $\tilde{T}_N^{ins}$; and their potential energy- $\tilde{U}_N^{ins}$. The energy $E_N^{ins} = \tilde{T}_N^{ins} + \tilde{U}_N^{ins}$ is internal energy of the system. It equals the sum of the kinetic energy of relative motion of elements and the energy of potential interaction. The $T_N^{tr}$ energy is determined by $\tilde{V}_N$ velocity of the center of mass. Therefore this energy is characterise the level of regularity of particles’ velocities because $\tilde{V}_N = \frac{1}{N} \sum_{i=1}^{N} \tilde{v}_i$.

When external forces are absent, $T_N^{tr}$ and $E_N^{ins}$ energies are constants. Due to the momentum preservation law these energies are the motion integrals.

The full energy of closed system of potentially interacting elements in homogeneous space can be presented as: $E_N = T_N + U_N = const$, where $T_N = \frac{1}{2} \sum_{i=1}^{N} \tilde{v}_i^2$ is a kinetic energy; $U_N(\vec{r}_{ij})$
is a potential energy; \( \vec{r}_{ij} = \vec{r}_i - \vec{r}_j \) is the distance between \( i \) and \( j \) elements.

The equation of motion for elements of system can be obtained by means of differentiation of expression of energy of systems with respect to time \([12]\). We will have: 
\[
    m \ddot{v}_i = - \sum_{i=1}^{N} \vec{F}_{ij},
\]
where \( \vec{F}_{ij} = \frac{\partial}{\partial \vec{r}_{ij}} U(c) \). It is a Newton equation.

Owing to splitting of nonequilibrium system into equilibrium subsystems, the problem concerning irreversibility nature is reduced to the problem concerning character of subsystems’ energy exchange. We will call the internal energy of equilibrium subsystem as “bound energy” to emphasize the absence of energy of relative motion of microsystems on which this subsystem can be divided.

To simplification let’s take the system which consists of two interacting equilibrium subsystems. They are \( L \) and \( K \)-subsystems. \( \vec{V}_L \) and \( \vec{V}_K \) are velocities of the centers of mass of corresponding subsystems. Number of elements in \( L \)-subsystem is equal to \( L \), and number of elements in \( K \)-subsystem is equal to \( K \). Let us suppose that \( L + K = N \) and \( L\vec{V}_L + K\vec{V}_K = 0 \), i.e. the center of mass of system is motionless.

Equations for energy exchange between subsystems can be obtained by means of differentiation of system energy with respect of time along with grouping terms which correspond to elements of different subsystems together.

Using summation of changes of kinetic and potential energies of elements in each subsystem we will obtain for \( L \)-subsystem:
\[
    \sum_{i_L=1}^{L} m \ddot{v}_{i_L} \vec{v}_{i_L} + \sum_{j_L=1}^{L} \sum_{i_L=1}^{L-1} \ddot{v}_{i_L,j_L} \vec{F}_{i_L,j_L} = - \sum_{j_K=1}^{K} \sum_{i_K=1}^{K-1} \ddot{v}_{i_K,j_K} \vec{F}_{i_K,j_K},
\]
(d), and for \( K \)-subsystem:
\[
    \sum_{i_K=1}^{K} m \ddot{v}_{i_K} \vec{v}_{i_K} + \sum_{j_K=1}^{K} \sum_{i_K=1}^{K-1} \ddot{v}_{i_K,j_K} \vec{F}_{i_K,j_K} = \sum_{j_L=1}^{L} \sum_{i_L=1}^{L-1} \ddot{v}_{i_L,j_L} \vec{F}_{i_L,j_L},
\]
(e).

The subindexes \( K \) and \( L \) denote the subsystem to which elements belong.

Let’s transform the left side of the eqs. (d, e) using following equality:
\[
    \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{N} \ddot{v}_{ij} \vec{v}_{ij}, \quad \vec{V}_N = \frac{1}{N} \sum_{i=1}^{N} \ddot{v}_i; \quad \vec{v}_{ij} = \vec{v}_i - \vec{v}_j \text{ are relative velocities.}
\]

By grouping the terms which determine bound and motion energies of subsystems using relative velocities of elements, distances between elements and velocities of centers of mass of subsystems as variables we will obtain following equations with the help of eqs. (d, e) \([19]\):

\[
    Lm \ddot{V}_L + \sum_{j=i+1}^{L} \sum_{i=1}^{L-1} \{ \ddot{v}_{ij} \left[ \frac{m \ddot{v}_{ij}}{L} + \vec{F}_{ij} \right] \} = - \sum_{j_K=1}^{K} \sum_{i_K=1}^{K-1} \ddot{v}_{i_K,j_K} \vec{F}_{i_K,j_K} \quad \text{(7)}
\]

\[
    Km \ddot{V}_K + \sum_{j=i+1}^{K} \sum_{i=1}^{K-1} \{ \ddot{v}_{ij} \left[ \frac{m \ddot{v}_{ij}}{K} + \vec{F}_{ij} \right] \} = \sum_{j_L=1}^{L} \sum_{i_L=1}^{L-1} \ddot{v}_{i_L,j_L} \vec{F}_{i_L,j_L} \quad \text{(8)}
\]

Left sides in the eqs. (7, 8) determine changes of subsystems’ energies \( T_N^{tr} \) and \( E_N^{ins} \), as a result of interaction of subsystems. The first terms represent the change of kinetic energy of subsystems’ motion as a whole. The second terms describe transformation of the bound energy. The right sides of the eqs. (7, 8) describe the subsystems’ interaction and determine the rate of an energy exchange between subsystems.

Velocities of particles’ of any subsystem can be presented as the sum of velocities of the center of mass of the subsystem and their velocities in relation to the center of mass. I.e., 
\[
    v_i = \ddot{v}_i + V.
\]

Then after grouping both parts of eqs. (7, 8) in appropriate way, we will rewrite
eqs. (7, 8) as:

\[ L\dot{\vec{V}}_L \left[ m\dot{V}_L + \dot{\vec{\Psi}} \right] + \sum_{j=i+1}^L \sum_{i=1}^{L-1} \vec{v}_{ij} \left[ \frac{m\dot{v}_{ij}}{L} + \vec{F}_{ij} \right] = \vec{\Phi}_L \]  

(9)

\[ K\dot{\vec{V}}_K \left[ m\dot{V}_K - \dot{\vec{\Psi}} \right] + \sum_{j=i+1}^J \sum_{i=1}^{J-1} \vec{v}_{ij} \left[ \frac{m\dot{v}_{ij}}{K} + \vec{F}_{ij} \right] = \vec{\Phi}_K \]  

(10)

Here \( \dot{\vec{\Psi}} = - \sum_{j=1}^J \sum_{i=1}^J \vec{F}_{ij} \); \( \vec{v}_i = \vec{\tilde{v}}_i + \vec{V} \); \( \vec{\Phi}_L = - \sum_{j=1}^J \sum_{i=1}^J \vec{\tilde{v}}_{il} \vec{F}_{il,jK} \); \( \vec{\Phi}_K = \sum_{j=1}^J \sum_{i=1}^J \vec{\tilde{v}}_{jK} \vec{F}_{il,jK} \).

The eqs. (9, 10) determines the energy exchange between \( L \) and \( K \) subsystems. We will call this equation as the \textit{Equation of Systems Interaction}.

As it follows from the right side of eqs. (9, 10), the change of energy of \( L \)-subsystem as a result of its interaction with \( K \)-subsystem is determined by velocities of motion of \( L \)-subsystem’s particles in relation to its center of mass and potential interaction with particles of \( K \)-subsystem and vice versa.

The first terms of the left side of eqs. (9, 10) determines the change of the motion energy one subsystem as a wall in a potential field of another subsystem. The second term determines subsystems’ bound energy change as a result of motion of particles one subsystem in a field of particles of another subsystem.

Non-potentiality of forces of subsystems’ interaction is caused by transformation of kinetic energy of their motion not only into a potential energy of subsystems as a whole, but also into bound energy. Increase of a bound energy occurs as a result of decrease of ordered motion of particles or decrease of velocity of the relative motion of subsystems.

When \( \vec{V}_L = 0, \vec{V}_K = 0 \), energy of relative subsystems’ motion is absent. In this case the full systems’ energy is equal to the sum of bound energies of subsystems.

Let us explain, why bound energy is increasing only. Firstly we take an equilibrium system. If we divide this system into two subsystems by any way, they also will be equilibrium. Therefore generalized forces and relative subsystems velocities are equal to zero. It is clearly that in this case the spontaneous deviation from equilibrium is possibly only in the case of spontaneous occurrence of collective motion of particles which will lead to occurrence of relative motion of subsystems. It is equivalent to occurrence of momentum of a subsystem, which can arise only due to the internal energy. But the law of conservation of momentum forbids it.

In the second case we consider systems which consists of two subsystems in motion to each other. Their relative velocity cannot be increased due to their interaction energy as this energy is determined by velocity relative motion itself. As well as in the previous case the relative velocity of these subsystems cannot be increased due to their bound energy.

Thus, the decreasing of relative velocities of subsystems is possibly only. This decrease is caused by the fact that the work of generalized forces increases internal energy of subsystems due to kinetic energy of relative motion. The increasing of bound energy is non-potential as a result of decrease of orderliness of motion of particles, i.e. as a result of chaotization of vectors of particles’ velocities. As the inverse process is impossible, generalized forces can decrease only.

In the case when velocities of particles’ motion inside subsystems can be neglected (hard body systems approach) the right side term and the second term in the left side of Equation of Systems Interaction are equal to zero. It is easy to see that Equation of Systems Interaction in this case will be transformed to the Newton’s equations for two hard bodies: \( m\dot{V}_L = -\vec{\Psi} \) and \( m\dot{V}_K = \vec{\Psi} \).

It is not so difficult to check, that these equations can be obtained directly by summation of the Newton equations (c) for particles of each subsystem. As the sum of the forces inside
subsystems will be zero, the generalized forces will become the central subsystem-subsystem interaction forces. These forces will be potential as changes of bound energy of subsystems does not exist at such summation of the Newton equations (the total work of forces of interaction of elements in the closed system will be zero). Thus the Newton equations is follows from the Equation of Systems Interaction when we neglect particles’ motion in relation of the center of masses of corresponding subsystems.

5 Difference between particles dynamics and subsystems dynamics

The Newton equation (c) can be treated as equation for particles’ interaction forces. The work of these forces determine transformation of particles’ kinetic energy to their potential energy. This energy transformation takes place during transition of system from one point of configuration space into another [12,14]. Forces are determined by gradient of potential energy of particles. Thus, forces and potential energy of particles are completely determined by coordinates, and work of potential forces along closed contour is equal to zero. It corresponds to reversible dynamics.

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

The transition of subsystems’ bound energy into kinetic energy of subsystem is impossible. Really, this transition would be possible only under condition of spontaneous occurrence of generalized forces inside an equilibrium subsystem. But such occurrence means infringement of spherical symmetry of distribution function of elements velocities of equilibrium subsystems’ in relation to the center of mass. And it contradicts to the law of momentum preservation.

Thus, Equation of Systems Interaction as against the Newton equation describes process of transformation of systems’ energy which is caused not only by transformation of potential energy into kinetic energy, but also by change of distribution function of velocities of particles due to increase the rate of chaotic motion of particles.

There is a question why the Newton equation is suitable for description of particles’ dynamics, but nevertheless it does not determine systems’ equilibration? Let us offer the following answer. Dynamics of selected particles is unequivocally determined by the equation of Newton. A motion of any particle is reversible. But dynamics of subsystem is described by collective parameters such as bound energy, generalized forces etc. These parameters ambiguously depend on parameters of particles’ motion. Such ambiguity leads to occurrence of new collective systems’ laws which do not exist for separate particles. Let’s consider for example, velocity of motion of systems’ centre of masses, which is constant in the homogeneous space. This velocity is a collective parameter of system. It is determined by the sum of velocities of all particles of system. Therefore biunique conformity between velocity of center of mass and particles’ velocities does not exist. The impossibility of increase of motion energy of an equilibrium subsystem due to its bound energy is collective law which determines its dynamics. Therefore, inspite of reversibility of dynamics of separate particle, the subsystems dynamics can be irreversible.
Thus, irreversibility is a new property of systems which is absent in dynamics of their particles. Occurrence of this property within the frame of laws of classical mechanics becomes possible owing to ambiguous dependence of dynamics’ parameters of subsystems on parameters which determine dynamics of individual particles.

By exclusion of particles’ potential interaction from Equation of Systems Interaction with the help of eq. (1), we will obtain the Equation of Systems Interaction for elastic disks systems. It means that the nature of irreversibility is identical both for systems of elastic disks and for systems of potentially interacting elements.

6 Classical mechanics and thermodynamics

It is possible to come to thermodynamics with the help of the eqs. (7, 8). Actually, the right sides of these equations determine an exchange of energy between subsystems due to their interaction. The first term of the left side of each equation determines the change of the motion energy of subsystem as a whole. In thermodynamics this corresponds to mechanical work which is carried out by external forces acting on subsystem from inside. The second term of the left side corresponds to increase of 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 connection between eq. (7) and the basic equation of thermodynamics [2, 3]: 
\[ dE = dQ - PdY. \]
Here, \( E \) is energy of a subsystem as a whole; \( Q \) is thermal energy; \( P \) is pressure; \( Y \) is volume according to common terminology.

Change of energy of selected subsystem is due to the work carried out by external forces. Therefore, the change of full energy of a subsystem corresponds to \( dE \).

The change of kinetic energy of motion of subsystem as a whole, \( dT^{tr} \), corresponds to the \( PdY \) term. Really, 
\[ dT^{tr} = \vec{V}d\vec{V} = \vec{V}d\vec{V}dt = \vec{V}d\vec{r} = PdY \]

Let’s determine, what term in Equation of Systems Interaction corresponds to the change of bound energy. According to virial theorem [14, 21], if potential energy is a homogeneous function of second order of radiuses-vectors then 
\[ E^{ins} = 2T^{ins} = 2U^{ins}. \]
Lines denote averaging time. We have obtained above that bound energy, \( E^{ins} \), increases due to contribution of \( T^{tr} \) energy. But the opposite process is impossible. Therefore change of \( Q \) term corresponds to the change of \( E^{ins} \), bound energy.

Let’s consider the system to be near to equilibrium. If the subsystem consists of \( N_m \) elements then average energy of each element can be written down as 
\[ \bar{E}^{ins} = E^{ins}/N_m = \kappa T_0^{ins}. \]

Now let us the bound energy be increased by \( dQ \). According to the virial theorem and keeping terms of the first order, we will have: 
\[ dQ \approx T_0^{ins}d(E^{ins}/T_0^{ins}) = T_0^{ins}d\bar{v}/\bar{v}_0, \]
where \( \bar{v}_0 \) is the average velocity of an element, and \( d\bar{v} \) is its change. For subsystems in equilibrium, we will have 
\[ d\bar{v}/\bar{v}_0 \sim d\Gamma_m/\Gamma_m, \]
where \( \Gamma_m \) is the phase volume of a subsystem, \( d\Gamma_m \) will be increased due to increase of the subsystem energy at \( dQ \) value. By keeping terms of the first order we will obtain: 
\[ dQ \approx T_0^{ins}d\Gamma_m/\Gamma_m = T_0^{ins}d\ln \Gamma_m. \]
According definition \( d\ln \Gamma_m = dS^{ins}, \) where \( S^{ins} \) is subsystem entropy. So 
\[ dQ \approx T_0^{ins}dS^{ins} \] near equilibrium.

Let’s consider the connection between generalized forces and entropy. According to eq. (2) the entropy production in non-equilibrium system is determined by transformation of kinetic energy of subsystems motion into bound energy. Eventually relative velocities of subsystems and generalized forces will comes to zero. As a result the energy of relative motion of subsystems completely transforms into bound energy and the system becomes equilibrate. It means that energy of motion of subsystem was spent on increase of entropy. Therefore the deviation of
entropy from equilibrium is determined by the following formula [19]:

$$\Delta S = \sum_{l=1}^{R} \left\{ m_l \sum_{k=1}^{m_l} \int \sum_{s} \frac{F_{ks} m_l v_k}{E^{m_l}} dt \right\}$$  \hspace{1cm} (11)

Here $E^{m_l}$ is a kinetic energy of subsystem; $m_l$ is a number elements in "l" subsystem; $R$ is a number of subsystems; $s$ is a number of external disks which were collided with internal disk $k$; $F_{ks}^{m_l}$ is a force, acting on $k$-disks; $v_k$ is a velocity of $k$- disk.

The integral in eq. (11) determines the work of $F_{ks}^{m_l}$ force, during the system’s relaxation to equilibrium. In equilibrium the energy of relative motion of subsystems and generalized forces are equal to zero. I.e. the integral in eq. (11) is determined by the energy of relative motion of subsystems. It corresponds to phenomenological Clauses formula for entropy [2, 3, 18]. So eq. (11) will be in accordance with the eq. (5). Really if $E^{m_s} \gg T^{tr}_l$, than we have:

$$dS = \sum_{l=1}^{R} \frac{\partial S_l}{\partial T_l^{tr}} dT_l^{tr}$$

It corresponds to eq. (11). Both in eq. (5) and eq. (11) entropy increasing is determined by change of the energy of relative motion of subsystems.

Thus, eq. (11) connects dynamic parameter which is generalized force acting on a subsystem, with entropy which is a thermodynamic parameter. I.e. eq.(11) 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.

7 Conclusion

As a result of investigation of a hard-disks system, the necessity of expansion of the canonical formalism of Hamilton for description of irreversible dynamics has been found out. This expansion consists in adaptation of the canonical formalism of Hamilton to non-potentially interacting systems. As a result of it expansion the generalized Liouville equation was obtained. Based on the this equation it was obtained that non-potentiality of generalized forces is the necessary condition for irreversible dynamics.

Using a method of splitting of nonequilibrium systems into the equilibrium subsystems and basing on generalized Liouville equation, the problem of irreversibility was transformed to the problem concerning character of behavior of generalized forces. In order to solve this problem the equation of subsystems interaction was obtained. The non-potentiality of the forces acting between subsystems and their tendency to zero has been found from this equation.

Following explanation of irreversibility can be offered. In spite of potentiality of fundamental forces, generalized forces are non-potential. The work of these forces irreversibly transforms energy of relative motion of subsystems to their bound energy. It is so because in accordance with the law of conservation of momentum, velocity of relative motion of a subsystem cannot be increased due to bound energy. Therefore these forces and relative velocities of subsystems are being decreased. The process of decreasing of the relative velocities of subsystems and increasing of bound energy is performed due to increase of chaotization of vectors of particles’ velocities. Thus irreversible decrease of energy of relative motion of subsystems due to its transformation to bound energy determines is essence of the irreversibility mechanism and of the equilibration process.

Since the non-potentiality of generalized forces is the essence of irreversibility, it is not possible to explain irreversibility within the framework of canonical Hamilton equations because of their inapplicability for description of dynamics of systems with non-potential forces [12].
The first law of thermodynamics follows from the subsystems’ interaction equation. This equation determines the transformation of the work of subsystem-subsystem interaction forces to the bound energy and the energy of subsystem motion.

The content of the second law of thermodynamics is determined by irreversible transformation of energy of motion of subsystems to their bound energy since amount of energy of subsystems’ motion, which is transformed to bound energy corresponds to increase of entropy.

The offered mechanism of irreversibility determines the horizon of probabilistic description of systems’ dynamics. In accordance with this mechanism it is impossible to use probabilistic description for nonequilibrium systems if characteristic time of equilibration due to generalized forces is less than probabilistic time of the occurrence of the system’s nonequilibrium state.

Thus, the results of irreversibility investigation given here confirm an opportunity of a substantiation of thermodynamics within the frame of classical mechanics.

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