The restrictions of classical mechanics in the description of dynamics of nonequilibrium systems and the way to get rid of them

V.M. Somsikov

Laboratory of Physics of the geoheliocosmic relation, Institute of Ionosphere, Almaty, Kazakstan.
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The reasons which restrict opportunities of classical mechanics at the description of nonequilibrium systems are discussed. The way of overcoming of the key restrictions is offered. This way is based on an opportunity of representation of nonequilibrium system as a set of equilibrium subsystems.

The equation of motion and the general Lagrange, Hamilton and Liouville equations for subsystems have been obtained. The way of a substantiation of thermodynamics is offered.

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I. INTRODUCTION

The development of the theoretical bases of physics of open nonequilibrium systems is collided with contradictions between classical mechanics and thermodynamics. These contradictions are most brightly displayed in a problem of a substantiation of the second law of thermodynamics or, in other words, explanations of irreversibility. Since L. Boltzmann and to this day the attempts to solve this problem are undertaken [1-4].

In the basis of the most widespread contemporary explanation of irreversibility the mixing property inherent at the Hamiltonian systems is used. The mixing leads to the irreversibility if one postulates averaging of phase space on physically small volume. But the explanation of the nature of such averaging within the framework of classical mechanics is impossible [2, 3].

With the purpose of search of solutions of these problems the hard disks systems were investigated [5, 6]. Its studying revealed that if the nonequilibrium system of disks has been represented by interacting equilibrium subsystems (IES) then equilibration is caused by the work of collective forces of IES. These forces are dependent on the disks velocities and their work transforms the motion energy of IES into the internal energy [6].

For generalization of results of researches of hard disks it was necessary to pass to the model of nonequilibrium systems of potentially interacting of elements. Studying of disks systems has shown that for this aim it is necessary to represent the model of nonequilibrium system as a set of interacting IES. That model possesses the big generality. Indeed, the base of statistical physics was created by Gibbs using that model [7]. In particular it has helped to introduce the distribution function into classical mechanics basing on concept of probability of beginning conditions for IES.

The method of Gibbs’s ensembles is applicable for studying equilibrium systems in the absence of an energy exchange between IES. But the exchange of energy between IES in case of nonequilibrium systems is responsible for an equilibration. Nevertheless the splitting of nonequilibrium system of potentially interacting elements into IES allows reducing the proof of irreversibility to the proof of existence of non-potential part of collective force between IES. It will be proved with the help of the equation of interaction of systems (UVS) which was obtained directly from the energy conservation law [8].

Basing on UVS and the model of nonequilibrium system as a set of IES the new approach to the analysis of nonequilibrium systems has been offered. The following assumptions and conditions are put into the basis of this approach: 1). IES energy should be submitted by the sum of internal energy and energy of IES motion as a whole; 2). Each element of system should be fixed for corresponding IES without dependence from its mixing; 3). During all process of equilibration all of subsystems are considered as equilibrium.

The first condition is necessary for introduction internal energy into the description of dynamics of systems, as the parameter which is necessary to correct describing an energy exchange between IES. The second condition allows avoiding a problem of redefinition IES due to mixing particles. Last condition is known from thermodynamics. It removes the problems connected to the description of system under condition of infringement of IES equilibrium.

Below the substantiation of this approach is submitted. The UVS equation and expression for dissipative force determining change of internal energy IES are obtained. It is shown how basing on UVS and D’Alambert principle, the obtaining of the generalized Liouville equations for IES is possible. Formulas for entropy of nonequilibrium systems are submitted. Connection between UVS and the basic equation of thermodynamics is analyzed. Here we also show how and why the offered approach has allowed to substantiate thermodynamics within the framework of laws of classical mechanics.

The problem of the description of nonequilibrium systems is a key problem for physics as a whole. Therefore alongside with mathematical calculations the discussion of the reasons why this problem could not be solved on the basis of canonical Hamilton equations is offered.

*Electronic address: nes@kaznet.kz
II. A SUBSTANTIATION OF THE APPROACH IDEA

The classical mechanics is based on the abstract concept of the elementary particle and the law of conservation of energy. Use of these concepts allows constructing classical mechanics on the basis of postulate: "Work of forces of reaction is always equal to zero on any virtual displacement which is not breaking set kinematics connections" [9]. Taking into account a condition of conservatism of the active forces leads to a principle of the least action, equations of Lagrange, Hamilton and Liouville [9-12]. These equations describe systems' dynamics in equilibrium states and near by. But all attempts to describe the dynamics of nonequilibrium systems with their help collide with a serious complexities. The analysis of these attempts allows assuming that some restrictions used at creation of a mathematical formalism of classical mechanics are unacceptable for the description of evolution of nonequilibrium systems. Our task is to determine these restrictions and to discover a way of construction of the theory allowing their elimination.

The evolutionary processes in nonequilibrium system are caused by internal forces and streams of energy created by them. These streams is impossible to describe with the help of a Hamilton formalism. One of the reasons is impossibility of application of a formalism of Hamilton for parts of system [9]. There is also other not less important reason. The Hamilton formalism is constructed on the basis of differential D'Alambert principle under condition of conservatism of collective forces [9]. This requirement excludes irreversibility automatically. But performance of a condition of conservatism of forces is strictly proved only for the equilibrium systems and in the approach of the theory of disturbances. In all other cases including a case of nonequilibrium systems, the strict proof of conservatism of collective forces is absent [9-12]. Therefore it is necessary to search for such approach to the analysis of nonequilibrium systems which allows to exclude the using of the requirement of potentiality of collective forces.

It was already mentioned that when the model of system of disks is presented by plurality IES, the irreversibility can be shown by analytical way. It is connected with non-potential collective forces between IES changing their internal energy [5, 6]. It means that for the analysis of nonequilibrium systems instead of model of system consisting of elementary particles it is necessary to use the model of system in the form of plurality of IES. For such model the solution of a problem of irreversibility is reduced to the proof of presence of non-potential forces between IES.

Necessity of splitting of system on a set of equilibrium subsystems at the description of its evolution follows from a statistical physics and a physical kinetics. In nonequilibrium systems for each physical point there corresponds the local velocity of a stream determining energy of a motion in this point. Besides in this point the internal energy is exist. This energy is determined by energy of the chaotic motions of particles. The nature of these two energies is various. The first is caused by transport of mass in the external field. The second energy is determined by a chaotic motion of particles. Therefore the distribution function at local equilibrium is determined by energy of a motion of IES center of masses (CM) and energy of a chaotic motion of particles [13]. The relative motion of IES disappears at an establishment of equilibrium. I.e. energy of motion of IES is the parameter describing a rate of a nonequilibrium.

It is possible to understand the necessity of splitting of IES energy on two types: internal energy and energy of CM motion from the analysis of two body system. As it is well known the problem of two bodies could not be solved directly in a laboratory coordinate system. It is related to the nonlinearity arising due to interaction between bodies. But the problem can be easily solved by transition into CM in which variables are parted. Such transition is equivalent to representation of energy in the two forms: energies of a motion of system as a whole and its internal energy. In the absence of exterior forces the motion energy of system is constant and a task is reduced to definition of the relative motion of particles. The problem can be solved by differentiation on time of the energy presented in the form of motion energy and an internal energy.

So, we will build the approach to analyzing of the dynamics of nonequilibrium systems within the frame of classical mechanics by the next way. A requirement of absolutely elasticity of the elements we will exclude by replacement of model of system of elementary particles on model of the system consisting from equilibrium structured particles, i.e. IES. Then, having presented of the IES energy as the sum of energies of its motion and an internal energy, we shall find the UVS. Using UVS the equations of Lagrange, Hamilton and Liouville will be obtained without use of the requirement of conservatism of collective forces.

III. THE SYSTEM MOTION EQUATION

Let us obtain the motion equation for particle in an external field. Let us presume that \( E = m \frac{v^2}{2} + U(r) = \text{const} \) is a particle energy. Here \( m \) is a mass; \( T = m \frac{v^2}{2} \) is a kinetic energy; \( U(r) \) is a potential energy. Then from eq. \( \dot{E} = 0 \), we will obtain:

\[
\nu (m \dot{v} + \frac{\partial U}{\partial r}) = 0 \tag{1}
\]

The eq. (1) is a balance equation of the kinetic and potential energies. It is carried out if the condition takes place:

\[
m \ddot{v} = - \frac{\partial U}{\partial r} \tag{2}
\]

It is Newton equation (NE). This equation is integrable because a variables were separated. The separation of
variables became possible in due to splitting of energy into kinetic and potential components, each of which depends on the different variables. We see that the sum of active and inertial forces is equal to zero. The particle moves lengthways of a gradient of potential. The work on the closed contour is equal to zero. Therefore the dynamics of a particle is reversible.

Let us consider a system consists of \( N \) potentially interacting elements; the mass of each element is equal to 1. The force between any two elements is a central and determined by the distance between them. Energy of system consist of the sum of kinetic energy of elements, \( T_N = \sum_{i=1}^{N} \frac{mv_i^2}{2} \), their potential energy in a field of external forces, \( -U_N^{env} \), and the potential energy of their interaction \( U_N(r_{ij}) = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} U_{ij}(r_{ij}) \), where \( r_{ij} = r_i - r_j \) - is a distance between elements \( i \) and \( j \). So, \( E = E_N + U^{env} = T_N + U_N + U^{env} = const \). The time derivative of the energy will be as follows:

\[
\sum_{i=1}^{N} v_i \dot{F}_i = 0 \quad (3)
\]

Where \( \dot{F}_i = m\ddot{v}_i + \sum_{j \neq i} F_{ij} + F_i^{env} \) is effective force for \( i \)

\[
\dot{U}^{env} = \sum_{i=1}^{N} v_i F_{i}^{env}; F_{ij} = \partial U_N / \partial r_{ij}; F_i^{env}(r_i) = \partial U^{env} / \partial r_i.
\]

The eq. (3) can be treated as orthogonality of the vector of effective forces with respect to the vector of velocities of elements of the system. If there are no restrictions imposed on the \( v_i \) directions, the requirement \( \dot{F}_i = 0 \) is satisfied [9]. Then from eq. (3) we obtain:

\[
m\ddot{v}_i = -\sum_{j \neq i} v_i \dot{F}_i + F_i^{env} \quad (4)
\]

It is NE for the system’s elements in non-homogeneous space. It leads to conclusion that the motion of an element of system is determined by the force which equal to the sum of vectors of forces, acting from all other particles and external force [11, 12].

Let us consider the motion of a system as the whole in a field of external forces. As well as for an elementary particle its kinetic energy is determined by the motion of CM. But except of this energy the system possess of internal energy. This energy has other nature because it is connected with interactions between particles but not with the external field of forces. The internal energy as well as energy of CM motion should vary due to the work of the external forces. Really, the external field will make work on change of internal energy due to motion of the particles relative to the CM. But velocity of CM motion does not depend on motion of elements inside of system. In connection with it, the energy of system should be presented as the sum of energy of motion of elements relative to the CM and the energy of CM motion. According with such dividing the system’s energy into two types, the external forces also will be represented by the sum of two forces: the force changing the velocity of CM and the force changing the internal energy.

Let us take into account the equality: \( T_N = \sum_{i=1}^{N} \frac{mv_i^2}{2} = M_N \dot{V}_N^2 + (m/N) \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} v_{ij}^2 \) (a), where \( V_N = \dot{R}_N = 1/N \sum_{i=1}^{N} \dot{r}_i \) -are velocities of the CM; \( R_N \) - are coordinates of the CM; \( v_i = \dot{r}_i \).

Let’s designate: \( E_N = T_N^{tr} + E_N^{ins} \) where \( E_N^{ins} = T_N^{ins} + U_N \) is entrance energy, \( T_N^{tr} \) is a CM kinetic energy. The velocity of elements is \( v_i = \dot{v}_i + V_N \) where \( \dot{v}_i \) is a velocity of particle relative to the CM. Then: \( T_N = M_N \dot{V}_N^2 + m \sum_{i=1}^{N} \dot{v}_i + \sum_{i=1}^{N} m\ddot{v}_i^2/2 \). Because \( \sum_{i=1}^{N} \dot{v}_i = 0 \) then from (a) we have: \( \sum_{i=1}^{N} m\ddot{v}_i^2/2 = 1/(2N) \sum_{i=1}^{N} \sum_{j=i+1}^{N} v_{ij}^2 \).

Thus the total kinetic energy of relative motion of particles is equal to the sum kinetic energies of their motions relative to CM. Because \( r_{ij} = \tilde{r}_{ij} = \tilde{r}_i - \tilde{r}_j \), where \( \tilde{r}_i, \tilde{r}_j \) - are coordinates of the elements with respect to the system’s CM then \( U_N(r_{ij}) = U_N(\tilde{r}_{ij}) = U_N(\tilde{r}_i) \) and \( \sum_{i=1}^{N} \sum_{j=i+1}^{N} v_{ij} F_{ij}(r_{ij}) = \sum_{i=1}^{N} \tilde{v}_i F_i(\tilde{r}_i), \) where \( F_i = \partial U_N / \partial \tilde{r}_i = \sum_{j \neq i} \partial U_N / \partial r_{ij}. \) Thus we have [14]:

\[
V_N M_N \dot{V}_N + \dot{E}_N^{ins} = -V_N F_N^{env} - \Phi^{env} \quad (5)
\]

Here \( F_N^{env} = \sum_{i=1}^{N} F_{i}^{env}(R, \tilde{r}_i), \dot{E}_N^{ins} = \sum_{i=1}^{N} \dot{v}_i (m \ddot{v}_i + F(\tilde{r}_i)), \Phi^{env} = \sum_{i=1}^{N} \tilde{v}_i F_i^{env}(R, \tilde{r}_i). \)

The eq. (5) represents balance of energy of system in a field of external forces. The first term in the left hand side determines change of kinetic energy of system. The second term determines the change of internal energy of system. The first term in the right hand side determines the work of forces changing energy of motion of system as a whole. The second term determines the work of forces changing internal energy of system. This work is connected with the motion particles of system relative to CM in the external field. Thus the work of external forces changes \( T_N^{tr} \) and \( E_N^{ins}. \)

When the external forces are absent the eq. (5) will split on two independent equations: the first is the equation of CM motion and the second is the equation of motion of particles relative to the CM.

Let us note that the eq. (5) can be obtained directly basing on the NE for elements. For this purpose we shall multiply the eq. (4) on the corresponding velocity. After summation the obtained equations for all particles we shall have the eq. (5) (if we have summarized the eq. (4)
without multiplying it on velocity in this case the internal forces in the second term of the eq. (5) will be lost [15]). It is confirms validity of the equation (5).

Let us compare dynamics of a particle and dynamics of system. As it follows from the eq. (1, 4) the force acting on the particle is potential. The particles dynamics is determined by kinetic and potential energies. Obviously it is impossible to find particles’ trajectory if not to divide the energy into the potential and kinetic parts.

In agreement with the eq.(5) the work of external forces determining motion of system goes both on changes of its CM velocity and on change of internal energy. This force can be divided on two forces. The first force is potential. The momentum of IES is change by this force. The second force changes the internal energy. It is non-potential force. Thus it is impossible to describe dynamics of system if not to divide the energy of system on three types: kinetic energy of motion of CM, internal energy and system’s potential energy in external field.

The equation of motion of system in an external field can be obtained from the eq. (5). It may be expressed as:

\[ M_N \ddot{V}_N = -F^{env} - [E^{ins}_N + \Phi^{env}]V_N/V^2 \]  

(6)

Let us call eq. (6) as generalized NE (GNE) for the structured particle. The GNE is reduced to the NE if one neglects the relative motion of elements, i.e. when the internal energy does not change. In this case the dynamics of system is similar to reversible dynamics of an elementary particle.

Thus, it is necessary to present the energy of a system as a sum of energy of motion and internal energy for determination a system dynamics in an external field. The external forces also need to be splitting into the forces changing these types of energies accordingly. Otherwise variables are not parted.

IV. THE EQUATION OF INTERACTION OF TWO SUBSYSTEMS

As it follows from the kinetic equations the dynamics properties of the nonequilibrium systems’ are determined by the energy of motion and internal energy in each physical points of the system [7, 13]. These parameters can be entered into the description of dynamics of system if the system is presented by a set of IES or, in other words, by a set of the structural particles. Using model of system as a set of IES help us ”select” nonequilibrium effects into interactions of IES. These interactions can be determined by the eq. (5) if external forces will be replaced by the forces between IES. Let us show how it can be done.

Let suppose the system consists of two IES - L and K. We take all elements to be identical and have the same weight 1, and L to be a number of elements in L - IES, K - is a number of elements in K - IES, i.e. \( L + K = N \), \( V_L = 1/L \sum_{i=1}^{L} v_i \) and \( V_K = 1/K \sum_{i=1}^{K} v_i \) - are IES’s velocities with respect to the CM of system. The velocity of the system’s CM we take equal to zero, i.e. \( L V_L + K V_K = 0 \).

We can represent the energy of the system as \( E_N = E_L + E_K + U^{int} = \text{const} \), where \( E_L \) and \( E_K \) are the IES energy, and \( U^{int} \) - is the energy of their interaction. According to the eq. (6), the energy of each IES can be represented as \( E_L = T^L_{tr} + E^{ins}_L, E_K = T^K_{tr} + E^{ins}_K \), where \( T^L_{tr} = M_L v_L^2/2, T^K_{tr} = M_K v_K^2/2, M_L = m L, M_K = m K \). \( E^{ins} \) is the internal energy of a IES. The \( E^{ins} \) consists of the kinetic energy of motion of the elements with respect to the CM of IES - \( T^{ins} \) and their potential energy - \( U^{ins} \), i.e. \( E^{ins} = T^{ins} + U^{ins} \), where \( U^{ins}_L = \sum_{i=1}^{L-1} \sum_{j=L+1}^{L} U_{iLjL}(r_{iLjL}) \), \( U^{ins}_K = \sum_{i_K=1}^{K-1} \sum_{j_K=1}^{K} U_{iKjK}(r_{iKjK}) \). The energy \( U^{int} \) is determined as \( U^{int} = \sum_{i=1}^{L} \sum_{j=1}^{K} U_{iLjK}(r_{iLjK}) \). Indexes \( j_K, j_L, i_K, i_L \) determine belonging of the elements to corresponding IES. In equilibrium we have: \( T^L_{tr} = 0 \). Hence, if the system aspirates to equilibrium, then \( T^{ins} \) energy for each IES will be transformed into the internal energy of IES.

We can obtain the equations of dynamics of \( L \) and \( K \) of IES in the following way. Let us differentiate energy of system on time. In order to find the equation for \( L - \) IES, at the left hand side of obtained equality we have kept only those terms which determine the change of the kinetic and potential energies of interaction of elements of \( L - \) IES. We replaced all other terms in the right hand side and combined the groups of terms in such a way when each group contains the terms with identical velocities. In accordance with NE (see eq. (5), the groups which contain terms with velocities of the elements from \( K - \) IES are equal to zero. As a result the right hand side of the equation will contain only the terms which determine the interaction of the elements \( L - \) IES with the elements \( K - \) IES. The equation for \( K - \) IES can be obtained in the same way. Then we execute replacement of variables: \( v_i = \dot{v}_i + V \) and take into account equality (a). As a result we will have [8, 14]:

\[ V_L M_L \ddot{V}_L + E^{ins}_L = -\Phi_L - V_L \Psi \]  

(7)

\[ V_K M_K \ddot{V}_K + E^{ins}_K = \Phi_K + V_K \Psi \]  

(8)

Here \( \Psi = \sum_{i=1}^{L} F^K_{ik} K, \Phi_L = \sum_{i=1}^{L} \dot{v}_i K F^K_{ik}, \Phi_K = \sum_{i_K=1}^{K} \dot{v}_i K F^K_{ik} K, F^K_{ik} = \sum_{j=1}^{K} F_{iLjK}, F^L_{jk} = \sum_{i=1}^{L} F_{iLjK}; \]

\[ E^{ins}_L = \sum_{i=1}^{L-1} \sum_{j=L+1}^{L} v_{iLjL} \left[ m \dot{v}_i L + \right] \]

\[ + F_{iLjL}], E^{ins}_K = \sum_{i_K=1}^{K-1} \sum_{j_K=1}^{K} v_{iKjK} \left[ \frac{m \dot{v}_i K K}{K} + \right] \]

\[ + F_{iKjK}], \]
The eqs. (7, 8) are the UVS. They describe energy exchange between IES. Independent variables of UVS are macroparameters, coordinates and velocities of IES motion, and also microparameters, coordinates and velocities of elements. UVS binds together two types of the description: at a macrolevel and at a microlevel. The description at a macrolevel determines IES dynamics as a whole and at a microlevel determines dynamics of IES elements.

The potential force, $\Psi$, determines motion of IES as a whole. This force is the sum of the potential forces acting on elements of one IES at the side of another IES. This force is the sum of the potential forces acting as a whole and at a microlevel determines dynamics of IES elements.

The forces which determined by the terms $\Phi_L$ and $\Phi_K$, transformed of the motion energy of IES to internal energy as a result of chaotic motion of elements of one IES in a field of the forces of another IES. They are non-potential forces which dependent on velocities and cannot be expressed as a gradient from any scalar function. These forces are equivalents to dissipative forces.

The motion eqs. for IES can be obtain from eqs. (7,8):

$$M_L \ddot{V}_L = -\Psi - \alpha_L V_L$$

$$M_K \ddot{V}_K = \Psi + \alpha_K V_K$$

(9)

(10)

where $\alpha_L = (\dot{E}_{ins}^L + \Phi_L)/V_L^2$, $\alpha_K = (\Phi_K - \dot{E}_{ins}^K)/V_K^2$.

The eqs. (9, 10) are GNE for interacting of systems. The second terms in the right hand side of the equations determine the forces changing internal energy of IES. These forces are equivalent to friction force. Its work consists of works of chaotic motion of elements one IES in a field of forces of another IES. The efficiency of transformation of energy of relative motion of IES into internal energy are determined by the factors $\"\alpha_L\"$, $\"\alpha_K\"$. If the relative velocities of IES elements are equal to zero the force of friction is also equal to zero.

For the description of dynamics of nonequilibrium systems we instead of traditional model of system have taken model of system as a set of interacting IES. Here a role of particles is carried out by IES. Their motion is determined by the eqs. (9, 10).

The state of system from a set of IES can be determined by the point in the phase space which consists of $6R - 1$ coordinates and momentum of IES, where $R$ is a number of IES. Let us call this space as $S$-space to distinguish it from usual phase space for elementary particles. Unlike usual phase space the $S$-space is compressible though total energy of all elements is a constant. The rate of compression of $S$-space is determined by the rate of transformation of motion energy of the IES into their internal energy. Thus the volume of compression of $S$-space is determined by energy of the IES motion.

Let us compare GNE and NE. The NE follows from representation of energy of an element as the sum of potential and kinetic energies. The transformation of one energy type to another is determined only by the potential force under condition of conservation of full energy.

The GNE determines motion of IES not only at transformation of kinetic and potential energies of IES, but also at transformation of IES internal energy. These transformations are determined by two forces. The potential part of force changes velocity of IES’s CM. The non-potential part of force changes its internal energy. Thus, for the structured particle external force will consist of two parts: potential and non-potential. Each of them has collective character.

The GNE passes into NE when the relative velocities of elements IES can be neglected. It is also have a place when distances between IES are big enough [16].

V. THE GENERALS OF LAGRANGE, HAMILTON AND LIOUVILLE EQUATIONS FOR IES

The dynamics of the nonequilibrium system submitted by a set of IES will be determined by generalized Lagrange, Hamilton and Liouville equations for IES. Before explaining a way of obtain of these equations, we shall remind under what conditions the canonical principle of Hamilton for system of elementary particles was deduced [9].

According to the differential principle of D’Alambert "the work of effective forces including inertial and active forces, at virtual motions elements of system is equal to zero for all reversible virtual motions compatible with restrictions on dynamics" [9]. From D’Alambert principle with the help of NE the integrated principle of Hamilton is deduced. For this purpose the integral on time of the virtual work made in system by effective forces is equated to zero. Integration on time is carried out provided that external forces possess power function. It means that the canonical principle of Hamilton is fair only for cases when $\sum F_i \delta R_i = -\delta U$ where $i$ is a number of particles, and $F_i$ - is a force acting on this particle [9]. But for IES we have no right to demand a carrying-out of a condition of conservatism of its forces. From the mathematical point of view it is because the $\sum F_i \delta R_i$ cannot be equal a full differential for IES. From the physical point of view it is due to the non-potential force which responds to the changes of the internal energy of IES. Therefore obtaining of the Hamilton equations should be carried out basing on GNE.

The principle D’Alambert for IES sounds so: the sum of works of all forces of interaction IES at their virtual motions compatible with restrictions on dynamics and in view of change of internal energy of IES is equal to zero.

In according to the eqs. (9, 10) and Liouville formula from [6, 9], the generalized Liouville equations in $S$-space can be written as:

$$df/dt = -\frac{\partial F}{\partial V}$$

(11)

Here $f$ - is a distribution function for IES, $F$ - is a non-potential part of force acting on IES.
The right hand side of the eq. (11) is not equal to zero as forces of IES interaction which transformed of the energy of its relative motion in its internal energy, depend on velocities of elements. The S-space which determined by the coordinates and velocities of IES will be compressed. Thus system of IES will converge to equilibrium.

The impossibility of return of internal energy of IES in its energy of motion is caused by impossibility of change of IES motion due to motion of its elements. At an establishment of equilibrium the motion energy of IES will disappear. In this case the description in S-space coincides with the traditional description in usual phase space for elements of system.

VI. UVS AND THERMODYNAMICS

It is possible to come to the idea about necessity of replacement of model of elementary particles by the model of interacting IES from the analysis of the basic equation of thermodynamics. According to this equation the work of external forces acting on the system are splitting on two parts. The first part is connected to reversible work. It can be associated with change of energy of motion of system as a whole. Second part of energy will go on heating. It is connected to internal degrees of freedom of system. To this part of energy there corresponds internal energy of IES. Here we would like to show, how basing on the UVS it is possible to come to the thermodynamics from the classical mechanics.

Let us take the motionless nonequilibrium system consisting of "$R$" of IES. Each of IES consists of enough plenty of elements. Let $dE$ is a work which has been done at system. In thermodynamics that term is an internal energy of a system (do not confuse $E$ with the $E_{ins}$ - internal energy of IES). The $dE$ is determined by the basic equation of thermodynamics as: $dE = dQ - PdY$ [8]. Here, according to common terminology, $E$ is energy of a system; $Q$ is thermal energy; $P$ is pressure; $Y$ is volume.

As well as the basic equation of thermodynamics, UVS also is differential of two types of energy. According to the UVS the volume $dE$ is redistributed inside of the system in such a way that that one its part goes on change of energy of relative motion of IES, and another part changes its internal energy. The first term in the left hand side of UVS is a change of kinetic energy of motion of a IES as a whole, $dT_{tr}$. This term corresponds to the term $PdY$. Really, $dT_{tr} = VdV = \dot{V}Vdt = \dot{V}r = PdY$ [7].

If the potential energy is a homogeneous function of a second order of the radius-vectors, then in agreement with the virial theorem [10], we have: $\bar{E}_{ins} = 2\bar{T}_{ins} = 2\bar{U}_{ins}$. The line denotes the time average.

Let us consider the system near to equilibrium state. The average energy of each element is $E_{ins} = E_{ins}/N = \kappa T_{ins}$ where $N$ is a number of elements. As the increasing of the internal energy is determined by the volume $dQ$, then we will have: $dQ \approx T_0 dE_{ins}/T_0 \sim T_0 [dv_0/v_0]$, where $v_0$ is the average velocity of an element, and $dv_0$ is its change. For the system in the closed volume we have: $dv_0/v_0 \sim dV/T$, where $\Gamma$ is the phase volume of a system, $dV$ will increase due to increasing of the system’s energy on the value, $dQ$. By keeping the terms of the first order we get: $dQ \approx T_0 dV/T = T_0 d\ln \Gamma$. By definition $d\ln \Gamma = dS_{ins}$, where $S_{ins}$ is an entropy [8]. So, near to equilibrium state we have $dE_{ins} = dQ \approx T_0 dS_{ins}$.

The entropy increasing, $\Delta S$, for nonequilibrium system is completely determined by the energy $T_{tr}$ passing into $E_{ins}$. Therefore $\Delta S$ can be determined by the formula [7, 14]:

$$\Delta S = \sum_{L=1}^{R} \{ N_L \sum_{k=1}^{N_L} \int_{0}^{\infty} \sum_{s} \frac{F_{ks}^{L}v_k}{E^{L}} dt \}$$

Here $E^{L}$ is the kinetic energy of L-IES; $N_L$ is the number of elements in L-IES; $L = 1, 2, 3...R$; $R$ is the number of IES; $s$ is a number of the external element which interaction with element $k$ belonging to the L-IES; $F_{ks}$ is a force, acted on $k$-element; $v_k$ is a velocity of the $k$-element.

In agreement with eq. (12), the entropy is determined by the energy of the relative motion of IES, transformed in an internal energy as a result of work of non-potential part of forces between IES.

To obtain equation for the entropy production we take into account that: $\Delta S = \Delta Q/T$. Thus $dS/dt = |dE_{ins}/dt|/(kE_{ins})$, where $k$ is a coefficient. It is possible to express this formula through the work of forces of interaction IES. Let $E_0$ is a full system’s energy, $E_{tr_0}$ is a beginning energy of relative motion of L-IES. In accordance with eqs. (10,11) the rate of increasing of the internal system’s energy is equal to: $\zeta = \sum_{L=1}^{R} \Phi_L$. The internal energy of a system is equal to: $E_{ins} = E_0 - \sum_{L=1}^{R} E_{tr}^{L}$, where $\sum_{L=1}^{R} E_{tr}^{L}$ is a sum of IES energy of relative motion. But $\sum_{L=1}^{R} E_{tr}^{L} = \zeta_0 - \int_{0}^{\infty} \zeta (t) dt$, where $\zeta_0 = \sum_{L=1}^{R} E_{tr_0}^{L}$. Then entropy production for the system, $\zeta_{prod} = dS/dt$, can be write:

$$\zeta_{prod} = D/(1 - D_0 + \int_{0}^{\infty} D(t) dt),$$

where $D = \zeta/E_0$, $D_0 = \zeta_0/E_0$.

The energy of $T_{tr}$ characterizes the rate of nonequilibrium system while $E_{ins}$ characterizes its degree of equilibrium.

For maintenance of nonequilibrium system in a stationary state, loss of energy $E_{tr}$ must be compensated by the inflow of external energy. It is possible to create with the help of contact of system with heater and due to outflow of radiation. Then the stationary state of nonequilibrium system is characterized by the formula: $\zeta_{prod} = |\varphi_-| - |\varphi_+|$, where $\varphi_-$ is entropy outflow, $\varphi_+$ is inflow of entropy, $\zeta_{prod}$ is entropy production, determined by the formula (12).
The process of transformation \( E^{ins} \) to the energy of IES motion is forbidden by the law of conservation of IES momentum [10]. Really, momentum of IES cannot be changed by the forces which change the internal energy. Therefore the work along the closed contour for IES not equal to zero. As a result the concept of entropy as the rate of increasing of IES internal energy due to energy of its relative motion will appear within the framework of classical mechanics. It is impossible to come to entropy concept in the frame of classical mechanics if base on the model of system as a set of elementary particles because for such model the determining of \( E^{ins} \) is impossible.

VII. CONCLUSION

To connect thermodynamics with classical mechanics it is necessary to refuse from the idealization of an elementary particle and a condition of conservatism of collective forces. It can be made by replacement of system of elementary particles on a system of IES.

Collective forces between IES are consisting of two parts. The potential part of force changes energy of IES motion. The non-potential part of force changes internal energy. The change of internal energy is caused by chaotic motion of particles of one IES in a field of forces of others IES. Therefore at equality to zero of velocities of particles in relative to CM of IES, the changes of its internal energy do not occur.

The Lagrange, Hamilton and Liouville equations on the basis of UVS are deduced. These equations describe dynamics of the nonequilibrium system in the compressible \( S \)-space where points are corresponds to the momentum and coordinates of the IES. We call this space as \( S \)-space in accordance with the entropy designation. Compressing of \( S \)-space is explained by the transition of energy of IES motion into their internal energy.

The following mechanism of irreversibility can be proposed: the energy of relative motion of IES is transformed into their internal energy as a result of the work of the non-potential part of a force between of IES. The system equilibrates when relative motion of IES disappears.

The explanation of the First law of thermodynamics is based on the fact that the work of subsystems’ interaction forces changes both the energy of their motion and their internal energy.

The explanation of the Second law of thermodynamics is based on the condition of irreversible transformation of the subsystems’ relative motion energy into their internal energy.

Thus within the limits of the accepted restrictions the offered approach has allowed to expand a formalism of classical mechanics on nonequilibrium systems and to connect it with thermodynamics.

Difficulties on a way of the solution of a problem of irreversibility are resolved at refusal of the assumption of absolute elasticity of particles and potentiality of collective forces between IES.

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