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## FROM THE LAWS OF CLASSICAL MECHANICS TO THE LAWS OF THERMODYNAMICS

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*It is shown that the laws of thermodynamics can be justified based on the laws of classical mechanics, relying on the mechanics of structured particles (SP). The difference between this mechanics and classical mechanics is that in the classical mechanics, the body model is used in the form of a material point (MP), and in the mechanics of the SP, a model in the form of a SP is used. As a SP, a system consisting of a sufficiently large number of potentially interacting MPs is taken. It is shown how the thermodynamic principle of energy is related to the energy duality, based on which the mechanics of the SP are constructed. It is explained what is the D-entropy. It is shown how the Boltzmann entropy formula is modified in accordance with the extended Liouville equation obtained in the mechanics of the SP.*

**Keywords:** classical mechanics, thermodynamics, irreversibility, entropy, structural particles.

### Introduction

The task of thermodynamics is to describe the behavior of systems which close to equilibrium, with a huge number of elements. The laws of thermodynamics answer the questions, what are the physical properties of the systems. However, the questions about the nature of these laws remain open [1]. The justification of thermodynamic laws is an actual problem of modern fundamental physics [2]. The main difficulty, which hitherto stood in the way of its solution, was connected with the fact that the laws of fundamental physics are reversible in time [3]. In particular, the motions of the material point (MP), as well as their combinations, determined by the laws of Newton and by the canonical formalisms of classical mechanics, are reversible. However, for thermodynamics the second law is valid, according to which all processes in real systems have a "time arrow", that is, they are irreversible [1]. Not so recently, a deterministic solution to the irreversibility problem has been found, which follows from the laws of classical mechanics and relies on the mechanics of the SP [4]. This opened up the possibility of substantiating thermodynamics.

Here, relying on the mechanics of the SP, a way of justifying the laws of thermodynamics in the framework of the fundamental laws of physics is proposed. First, a brief explanation of the mechanics of the SP is given. It is shown how the thermodynamic principle of energy is related to the principle of symmetry duality (PDS), based on which the mechanics of the SP were constructed. The essence of the PDS is that the dynamics of bodies is determined not only by the symmetries of space, but also by the symmetries of the body itself. From the PDS follows the duality of energy, based on which the equation of motion of the SP is obtained. It is explained what is D-entropy, which appearing in the mechanics of the SP. It is shown how the Boltzmann formula for entropy is modified in accordance with the extended Liouville equation obtained based on the mechanics of SP [12].

### 1. The main elements of the mechanics of the SP

In the SP mechanics, the SP is used as the basic model of the body. The SP is an equilibrium system of potentially interacting MPs. Since in the local thermodynamic equilibrium approximation the nonequilibrium system (NS) is representable by the set of SP [1, 7], the mechanics of the SP allow us to describe dissipative processes when the HC approaches equilibrium.

If we take into account the structure of the body, it will be possible to describe the mechanism of transformation of the energy of its motion into internal energy, relying on the laws of classical mechanics. The simplest example of such a transformation is the heating of a body due to friction when it slipping on the inclined surface.

The mechanics of the SP are constructed based on the principle of symmetry duality of the PDS. In accordance with the PDS, the total energy of the system based on which the equation of motion of the SP is derived is represented by the sum of the internal energy and energy of motion. This representation of energy is realized in micro- and macro variables. The micro variables determine the movement of the MPs relative to the center of mass of the system. The macro variables determine the movement of the SP in the space. Thus, in these variables the energy of the MP system automatically decays into the energy of its motion and internal energy. It can be written as [4, 5]:

$$E = E^{\text{int}} + E^{\text{tr}} \quad (1)$$

$E^{\text{int}}$  - is internal energy, determined by a group of micro variables,  $E^{\text{tr}}$  is the energy of motion of the SP, determined by a group of macro variables. Macro - and micro variables form two groups of independent variables [4]. This is easy to show if we take into account that the dynamics of the elements of the body does not affect in any way the dynamics of the body itself, in view of Galileo's principle of relativity.

The motion equation of SP is derived from the energy (1). It has the form [5]:

$$M_N \dot{V}_N = -F^{\text{env}} - \alpha_N V_N, \quad (2)$$

where  $\alpha_N$  - is a coefficient determined by the change in internal energy. It is a single-valued function of micro- and macro variables.

The first term on the right-hand side of (2) is the potential force changing the kinetic energy of the SP. The second term determines the change in the internal energy of the SP. Since the SP is in equilibrium, within a wide range its dynamics is determined by the internal energy and does not depend on the chaotic motion of each MP [2].

The symmetry of equation (2) differs from the symmetry of the time-reversible Newton's equation for MP, because of the presence of the second term on the right-hand side. This term is different from zero when SP motion in space with the inhomogeneous field of external force whose scale is comparable with the scale of the SP. It determines the transformation of the energy of the motion of the SP into its internal energy.

Let us compare the dynamics of MP and SP. While the work of external forces to move the MP only goes to its acceleration, for the SP the work of external forces goes both to accelerate the SP and to change of its internal energy. Moreover, if the energy of the motion of the SP is changed due to the sum of the forces acting on all of its MP, the internal energy varies due to the difference of these forces.

The motion energy of SP does not depend on internal energy. This allows one to describe unambiguously the dynamics of SP in two groups of independent micro- and macro variables. In a non-uniform field of external forces, terms appear that depend on the micro - and macro variables, which leads to violation of the invariance of the energy of motion. Such a violation of the invariance of the energy of motion means the irreversibility of the dynamics of the SP. The nature of the irreversibility of SP is described in detail in [4]. If we neglect the change in the internal energy, then equation (2) becomes an invertible Newton's equation.

Thus, a description of the irreversible dynamics of the SP is possible only if the structure of the body is taken into account. In general, the fact that equation (2) is built based on a dual representation of energy makes it possible to describe the processes of changing the internal energy of the system as it moves in an inhomogeneous field of forces. This, in turn, allows us to describe

systems with non-holonomic constraints, which include dissipative systems. Hence, it becomes possible to substantiate the laws of thermodynamics within the framework of the laws of fundamental physics. Let us show how and why, relying on the mechanics of SP, one can come to thermodynamics.

## 2. As thermodynamics follows from the mechanics of the SP

In the basics of thermodynamics lie empirical principles: the principle of temperature, the principle of energy (the first principle of thermodynamics); the principle of entropy (the second law of thermodynamics) and Nernst's postulate (the third law of thermodynamics). If in mechanics, the parameters of the system are coordinates and velocities, in thermodynamics this is the volume, pressure, temperature, entropy. The relationship between the thermodynamic parameters and the parameters of mechanics is established by integrating over the dynamic parameters of the microparticles that make up the body.

In the basics of thermodynamics lies the thermodynamic principle of energy. It can be written as follows [3]:

$$dU = \delta Q - \delta A \quad (3)$$

Where  $U$  - is the adiabatic potential,  $Q$  - is a thermal energy,  $A$  - is a work of external forces to change the volume of the system.

The mechanics of SP in accordance with the PDS is constructed based on the energy of the system. This energy is a sum of the internal energy and energy of motion. According to the energy equation of SP [4], the differential of the work of external forces with respect to the displacement of the SP can be written as follows:

$$dU^{sp} = \delta E^{int} + \delta E^{tr} \quad (4)$$

Where  $\delta E^{int}$  - is a change of the internal energy;  $\delta E^{tr}$  - is a change of the motion energy of SP.

By analogy with thermodynamics, expression (4) is called as the mechanical principle of energy. While the mechanical principle of energy is the complete work of external forces, the thermodynamic principle of energy includes only work on changing internal energy. It is equal to the sum of the work on changing the volume of the body and changing the thermal energy. Hence, for the adiabatic potential  $U$  we have equality  $U = E^{int}$ . This is quite natural, since the adiabatic potential corresponds to the law of conservation of the internal energy of the system.

Let us compare the thermodynamic and mechanical principles of energy. The common thing for these principles is that they take into account the role of the work of external forces, which is aimed at changing internal energy. However, there are differences. If the mechanical principle of energy is the complete work of external forces to move the system and change its internal energy, the thermodynamic principle includes only work on changing its internal energy. Moreover, this work is divided into work on changing the volume of the body and work on changing the thermal energy. That is, the mechanical principle of energy takes into account the complete work of external forces over the system. Such a definition of the mechanical principle of energy is because it is dictated by the nature of the violation of the symmetry of the SP time. The violation of the symmetry of time is associated with a violation of the invariance of the energy of the SP motion because of its transformation into internal energy. That is, in the mechanics of SP, unlike thermodynamics, the work of external forces is fully considered, including the work on moving the system. However, the work on changing internal energy for SP is not divided into work on changing its volume and its heat, as is done in thermodynamics.

In addition, in the mechanics of SP, the gradient of the external field of forces is taken into account, due to which a transformation of the energy of the motion of the SP into its internal energy

occurs. In thermodynamics, the potential energy of the entire system, as well as the inhomogeneity of the field of external forces, as well as the motion of the system in space, are excluded from consideration [2].

In general, these and other differences in the mechanics of SP from thermodynamics are not of a qualitative nature, as in the case of Newtonian mechanics for structureless bodies and mechanics of SP. This is because both in the mechanics of SP and in thermodynamics, structured bodies with internal energy are studied. Both the mechanics of SP and thermodynamics rely on the ideas of the molecular-kinetic theory [1]. In addition, although the thermodynamic principles of energy differ from the mechanical principle of energy, its corresponds to the PDS. Indeed, the work on changing the volume of the body corresponds to work on moving the SPs, by which the body can be modeling. In addition, thermal energy is equivalent to the internal energy of each of these SPs. Consequently, the thermodynamic and mechanical principles of energy in their physical essence coincide. Therefore, the differences in the mechanical and thermodynamic principles of energy, which connected, with differences of the parameters, using for analyses of the systems dynamic, are not an obstacle to the justification of thermodynamics within the fram of the laws of classical mechanics.

The generality of the mechanics of SP is much higher than the generality of thermodynamics. Indeed, all the collective parameters characterizing the thermodynamics of a gas can be obtained by integrating the dynamic parameters of the mechanics of the SP. This makes it possible not only to justify the laws of thermodynamics within the framework of the fundamental laws of physics, but also does not exclude the possibility of the development of nonequilibrium thermodynamics that allows describing nonequilibrium processes in continuous media on the basis of the equations of mass, energy, momentum, and entropy balance [1, 3].

### 3. Interrelation of entropy with dynamics

The duality of energy used in SP mechanics allows us to introduce the concept of entropy in it, as in thermodynamics, by defining it as [4, 5]:

$$\Delta S^d = \Delta E^{\text{int}} / E^{\text{int}} \quad (5)$$

This quantity is called the D-entropy. That is, the D-entropy determines the work of external forces by changing the internal energy of the system.

Since the NS can be given by a set of SP in motion relative to each other [6], the description of the dynamics of the NS can be performed within the framework of the mechanics of the SP. In this case, the tendency of the NS to equilibrium is determined by the transformation of the energy of the relative motions of the SP into their internal energy.

For a closed NS whose volume and energy are conserved, D-entropy determines the amount of energy of the relative motions of the SP, which has passed into their internal energy. This process of transforming the energies of the relative motions of the SP leads to the establishment of equilibrium. In this case, the D-entropy is equivalent to the Clausius entropy and for it; the analog of the second law of thermodynamics is valid, i.e.  $dS^d / dt \geq 0$ .

If we consider the establishment of an equilibrium in an NS composed of SP, then the change in its A-entropy can be determined as the sum of the entropies of all the SPs that make up the NS. This can be written as follows [4, 8]:

$$\Delta S^d = \sum_{L=1}^R \left\{ N_L \sum_{k=1}^{N_L} \left[ \int \sum_s F_{ks}^L v_k dt \right] / E_L \right\} \quad (6)$$

$E_L$  -is internal energy L-SP;  $F_{ks}^L$  -is a force, acting on the  $k$  -th MP of the SP from the side of the MP of the other SP;  $s$  - is external MPs with respect to  $L$  -SP, interacting with its  $k$  -i MP;  $v_k$  - is a speed of the  $i$ -th MP.

That is, the D-entropy determines the decrease in the energy of the relative motions of the SP because of its transformation into their internal energy.

The definition of D-entropy is applicable not only for SP, but also for the systems with a small number of MPs. In this case, the change in the D-entropy of a small system can turn out to be negative [8]. Numerical calculations have shown that for the D-entropy of systems moving in an inhomogeneous force field, the minimum number  $N_1$  of the number of MPs in the system is exist, for which the change in the D-entropy can only be positive. In addition, the second number  $N_2$  for the number of MPs in the system is exist also, after which the D-entropy ceases to change with increasing number of MP, i.e., goes to the asymptotic. This means that for such systems the concept of Clausius entropy is valid. Consequently, D-entropy allows us to determine the applications of thermodynamics based on the laws of classical mechanics [9].

Using the mechanics of SP, one can modify the expression for the Boltzmann entropy, which is determined through the distribution function of the system  $f_p$ .

The Boltzmann entropy looks like this [1]:

$$S^B = - \int f_p \ln f_p dpdq . \quad (7)$$

Differentiating the entropy with respect to time, we obtain:

$$\frac{dS^B}{dt} = \int (1 - \ln f_p) \frac{df_p}{dt} dpdq . \quad (8)$$

According to the canonical Liouville equation:  $df^p/dt = 0$ . Hence  $dS^B/dt = 0$ , which contradicts the second law of thermodynamics. In the framework of the probability mechanism of irreversibility, this contradiction is removed by coarsening of the phase space [2]. To do this, we introduce a coarsened distribution function, defined as follows:  $F = (\int f_p d\Gamma) / \delta\Gamma$ , where  $\delta\Gamma$  - is the region of coarsening of the phase space. For  $F$  the expression (8) is not zero. However, such a definition has a drawback. It is connected with non-certainty  $\delta\Gamma$ . Moreover, the nature of such averaging of the phase space is not known.

Let us show that in mechanics SP the  $S^B$  is different from zero without coarsening of the phase space [2]. According to the extended Liouville equation [12], which was obtained in the frame of the mechanics of SP, we have:

$$\frac{dS^B}{dt} = - \int (1 - \ln f_p) f_p \left( \sum_{k=1}^T \frac{\partial F_k^p}{\partial p_k} \right) dpdq \neq 0 \quad (9)$$

That is, the Boltzmann entropy follows from the mechanics of SP. Equation (9) corresponds to the physical meaning of entropy and the second law of thermodynamics. It is not equal to zero because for NS the value  $\sum_{k=1}^T \frac{\partial F_k^p}{\partial p_k} \neq 0$  [12].

The generality of the D-entropy is determined by the fact that the change in the entropy of the body is determined by integrating the dynamical parameters his elements. The rule of this integrating is follow from the laws of classical mechanics.

## Conclusion

The justification of the laws of thermodynamics within the framework of fundamental laws of physics became possible only thanks to the found mechanism of irreversibility. The explanation of this mechanism was obtained in the mechanics of the SP. In the mechanics of the SP, an equilibrium system is taken as a model of a body from a sufficiently large number of potentially

interacting MPs in the form of the equilibrium system, as well as thermodynamics is built on the principle of duality of energy, which follows from the PDS. Thus, the substantiation of thermodynamics in the frame of the laws of the classical mechanics became possible because of taking into account the structure of the bodies. Thanks to this, we can show that thermodynamics is a direct consequence of the fundamental laws that lie in the foundations of classical mechanics. This is the law of inertia, Galileo's principle; Newton's second and third laws.

According to the mechanics of SP, the second law of thermodynamics is due to the transformation of the energy of the body's motion into its internal energy. Such absorption takes place when the bodies move in inhomogeneous fields of external forces. It allowed us to propose in the mechanics of SP the definition of D-entropy. The D-entropy can be used to modification and justification of the Boltzmann entropy. This modification is based only on the fundamental laws of physics, the PDS principle, and following from the generalized Liouville equation. This eliminates the need to use the hypothesis of coarsening phase space. Previously, without this hypothesis, it was impossible to explain of this form of the Boltzmann's entropy.

The mechanics of SP can also be useful in the development of thermodynamics itself. For example, it allows us to evaluate the role of the inhomogeneity of the external force field in the thermodynamic description of processes. This is also necessary for the development of a nonequilibrium thermodynamics.

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