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Relation between classical mechanics and physics of condensed medium

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An equilibrium system of potentially interacting material points in a nonhomogeneous field is studied by numerical simulations, as well as criteria which are needed in order to switch from the quantified model to the thermodynamic one. This paper studies the system passing a potential barrier and factors which affect the change of the system's internal energy. These factors include width of the barrier, number of material points in the system, as well as initial conditions. The dependence between change in fluctuations of energy parameters of the system and the number of material points is also shown. The amount of dynamic entropy is estimated. The paper also defines and describes two critical values (N1 and N2). If the system includes more than N1 material points, then its dynamics becomes irreversible. If the number of material points is greater than N2, then thermodynamic model can be used. The results obtained by numerical simulations verified the theoretical conclusions.

Key words: Nonlinearity, classical mechanics, energy, thermodynamics, Lagrange equations, non-holonomic constraints, irreversibility.

INTRODUCTION

The possibility to derive the laws of thermodynamics, statistical physics and kinetics using the laws of classical mechanics is still considered as an open question. First of all, this is due to the fact that in the nature all processes are irreversible and dissipative. However, in accordance to the formalism of classical mechanics, the dynamics of systems are reversible. It is subject of one of the key problems of physics (Ginzburg, 2007; Bohr, 1958; Klein, 1961; Prigogine, 1980; Lebowitz, 1999; Zaslavsky, 1984). Up to the present time, clear criteria for the transition to the physics of continuous media are not set. For example, it is not possible to determine the exact number of elements a system should consist of, in order to become thermodynamically applicable, as well as the accuracy of any estimation which is done using the laws of thermodynamics. The abovementioned problems are not solved yet since until recently there was no rigorous explanation of irreversibility in the framework of the laws of classical mechanics, without introducing probabilistic hypotheses (Prigogine, 1980; Lebowitz, 1999; Zaslavsky, 1984; Smoluchowski, 1967; Cohen, 1998; Klimontovich, 1995; Kadomtsev, 1995; Sidharth, 2008). Indeed, today irreversibility is usually explained by the property of exponential instability of Hamiltonian systems and the hypothesis of the existence of fluctuations. The main idea of this explanation is as follows. According to the Poincare theorem on the reversibility of Hamiltonian systems, a system's coordinates in the phase space will

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be close enough to their initial values in a finite (although it can be very large) period of time (Prigogine, 1980; Zaslavsky, 1984; Smoluchowski, 1967). But if averaged over an arbitrarily small neighborhood of the phase space, the system will not return back to its initial position because of exponential instability. Arbitrarily small fluctuations in the system are equivalent to such averaging. Therefore, the existence of fluctuations in Hamiltonian systems is a sufficient condition for the occurrence of irreversibility. But the hypothesis of a roughening of the phase space due to fluctuations actually involves statistical laws which are alien to determinism of classical mechanics. Therefore, the question of justifiability of this hypothesis is still open.

A lot of attempts to explain the second law of thermodynamics on the basis of the laws of classical mechanics without the use of statistical hypotheses failed, so most probably it is impossible to solve this problem in the framework of the existing formalism of classical mechanics (Prigogine, 1980; Zaslavsky, 1984). This means either that there is no explanation in the framework of classical mechanics at all or that the formalism of classical mechanics requires expansion, for example by removing the limitations under which it was built (Prigogine, 1980).

In order to find an approach to solve the problem of irreversibility the dynamics of a system of hard discs has been studied firstly. Unlike other authors who studied the system of billiards, provided that they are Hamiltonian systems (Bird, 1976; Sinai, 1995), we considered the billiards in the approach of pair collisions of disks (Somsikov et al., 1999; Somsikov, 2004). As a result the irreversibility of the system of hard disks was found. It turned out that the exchange of momentum between the discs plays a key role in irreversibility. The Hamilton's and Lowville's equations describing equilibration in a system were obtained basing on these results (Somsikov, 2004). But a number of problems still remained. For example, the pair interaction in a real system is a special case which is valid only for fairly rarefied systems. Moreover, the interactions between the system's elements are potential. Therefore, the next step was the study of systems of potentially interacting material points (Somsikov, 2005).

It followed from the study of systems of hard discs that the mechanism of irreversibility cannot rely on the formalism of classical mechanics. Therefore, it was decided to look for an answer based on the energy equation for systems of potentially interacting elements, provided that Newton's laws are valid for each individual material point. As a result of these studies it was found that the system's dynamics is irreversible. Irreversibility was caused by the mutual transformation between the system's motion energy and its internal energy (Somsikov, 2014). But one problem still remains unsolved: Why formalisms of classical mechanics are reversible, while the dynamics of systems of material points is irreversible. This contradiction should be explained; it was found that in classical mechanics irreversibility has been lost while obtaining the Lagrange equations for systems of material points because of usage of the hypothesis of holonomic constraints (Somsikov, 2014). It turned out that this hypothesis excludes the possibility of describing the nonlinear transformation of energy between different degrees of freedom, which is responsible for the irreversibility.

It turned out that it is possible to explain irreversibility using Newton's laws by removing some of the limitations of classical mechanics formalism. The mechanics of structured particles (SP) was developed and a mechanism to explain irreversibility was offered. This mechanism was named deterministic as it uses the mechanics of SP without any probabilistic principles. The essence of this mechanism is as follows (Somsikov, 2014a; Somsikov, 2014b).

Newton built the mechanics for an abstract structureless material point (MP). Therefore, the external forces change only the position of MP. This fact defines Newton's second law. But all real bodies are not structure-less. Thus the external forces change not only the position of a body, but its internal energy as well. The internal energy is accounted for the motion of elements of the body with respect to its center of mass. This means that the dynamics of the system is defined by the principle of dualism of symmetry due to the fact that the system is not structure-less. The essence of the principle is that the dynamics of real bodies is determined by two types of symmetry: The symmetry of space and the symmetry of the body itself. The principle of dualism of energy follows from the principle of dualism of symmetry. The principle of dualism of energy claims that the dynamics of a real body is defined by splitting the body's total energy into its internal energy and the energy of motion. The equation of the body's motion follows from the principle of dualism of energy. This equation takes into account both the work needed to change the position of the body, and the work than changes the body's internal energy (Somsikov, 2014b).

Thus, the total energy of the body is an invariant which determines the body's dynamics; the energy of motion itself is not an invariant, so the motion of the body's mass center should be determined based on the invariance of the total energy.

According to classical mechanics, a body can be represented by a set of potentially interacting MPs (Goldstein, 1975; Landau, 1976). This means that the equation of motion of the body should be derived upon the condition that the motion of each MP is described by the laws of Newton. In general a body is an open non-equilibrium dynamic system. Such system in many cases could be considered as it is in a local thermodynamic equilibrium state (Klimontovich, 1995; Landau, 1976; Rumer and Rivkin, 1977). In this case, the body can be represented by a set of moving equilibrium subsystems;

each subsystem is in turn a set of potentially interacting MPs (Landau, 1976; Rumer and Rivkin, 1977). Let us name such a subsystem as a structured particle (SP). This means that the dynamics of an open non-equilibrium system should be defined based on the assumption that the system consists from a lot of SPs. Therefore, first of all, the mechanics of SPs should be built in order to describe the dynamics of real bodies.

As it turned out, the equation of motion of a SP allows explaining the mechanism of irreversibility without the use of probabilistic hypothesis of fluctuations (Somsikov, 2014a; Somsikov, 2014b). This is because the energy of motion is no longer an invariant for a SP, as it was for a MP. It has been found that the energy of the SP's motion is transformed into its internal energy in the non-homogeneous field of external forces. Increase in the internal energy is proportional to the gradient of the external forces. If the external field is weak enough, then the SP remains in equilibrium along its path. At the same time its internal energy can increase only, but it cannot be transformed into the energy of motion. This is the essence of deterministic irreversibility that is such irreversibility which follows from the deterministic laws of classical mechanics; unlike the irreversibility explained within the canonical framework of classical mechanics (Prigogine, 1980; Zaslavsky, 1984), the deterministic irreversibility does not need the hypothesis of fluctuations. Thus, the deterministic mechanism of irreversibility is caused by transformation of energy of a system's motion into its internal energy when the system is in a non-homogeneous field. The fact that in this case the energy of motion is not constant means that the time symmetry is broken. However, the sum of the energy of motion and the internal energy is constant. Hence it is clear that in order to explain the nature of deterministic irreversibility for a non-equilibrium system, the following should be done:

1. Represent a non-equilibrium system by a set of moving relative to each other equilibrium subsystems.
2. Represent the energy of these subsystems as the internal energy and the energy of motion.
3. Obtain the equation of motion of subsystems directly from the dual form of energy, thus preserving the nonlinear terms which are responsible for energy exchange different degrees of freedom.

Unlike the deterministic mechanism of irreversibility, the traditional statistical mechanism refers irreversibly in Hamiltonian systems to the hypothesis of the existence of arbitrarily small fluctuations. The point is that since the Hamiltonian systems are exponentially unstable, then the presence of such fluctuations results in irreversible dynamics. The presence of fluctuations in these systems or in the external limitations is a sufficient condition for the irreversibility.

The deterministic irreversibility is a strong argument in favor of determinism of nature. This is very important; just recall the fundamental debates of Bohr and Einstein's on determinism and randomness, which took place during creation of quantum mechanics (Ginzburg, 2007; Bohr, 1958;).

Due to the dualism of energy, the equation of a SP's motion is given by independent micro and macro variables. Moreover, micro variables define the motion of the MPs relative to the center of mass of the SP, while macro variables define the motion of the SP's center of mass itself. Deriving equation of motion of the SP in this way takes into account possible transformation of the energy of the SP's motion into its internal energy and requires no use of the hypothesis of holonomic constraints, which is the basis for deriving the canonical equation of Lagrange. Unlike the canonical equation of Lagrange, the equation of the SP's dynamics describes the nonlinear transformation of the SP's motion energy into its internal energy; this transformation breaks the symmetry of time (Somsikov, 2014a).

An oscillator passing through a potential barrier was studied, and it was found that the condition of holonomic constraints eliminates nonlinear terms in the equation, which are responsible for breaking of time symmetry (Somsikov and Denisenya, 2013). This issue is considered in more detail subsequently.

Existence of deterministic irreversibility leads to the concept of "deterministic entropy" (D-entropy) (Somsikov, 2014a; Somsikov, 2014b). D-entropy is a deterministic one, because it strictly follows from the laws of classical mechanics without use of the hypothesis of fluctuations in a system. It is defined as the relative change in the system's internal energy. Unlike the thermodynamic entropy, D-entropy for a system consisting of small number of MPs can be both positive and negative.

The equation of the SP's motion is nonlinear. It is almost impossible to do any analytical analysis in order to check the theoretical conclusions following from the equation. Hence numerical simulations are the only way to check the theoretical conclusions. Numerical simulations allow determining the criteria for switching from classical mechanics to thermodynamics, statistical physics, kinetics, as well as identifying the cases when the system is irreversible, depending on the properties of the system, etc.

So, the objective of the paper is to determine the basic dynamic properties of a system of potentially interacting MPs in a non-homogeneous external field using numerical simulations. The estimation of fluctuations of the system's internal energy depending on the number of MPs, as well as initial parameters of the system and the barrier has been done, dependence of change in the system's internal energy on the barrier's width, as well as D-entropy have been studied. This study made it possible to verify the theoretical conclusions about the dynamics of a SP, define the criteria needed to switch from the deterministic to the thermodynamic model for a system.

In addition, it made it possible to show how the important statistical laws of physics may result from the strict laws of classical mechanics, as well as define some cases when the mechanism of irreversibility is applicable.

AN OSCILLATOR PASSING A POTENTIAL BARRIER

Initially, the simplest system, more specifically a one-dimensional oscillator of two MPs connected by a spring, has been considered (Somsikov and Denisenya, 2013). The oscillator's total energy includes the energy of motion and the internal energy. These two types of energy are given in the independent micro and macro variables. Micro variables describe the oscillations, while macro variables determine the motion of the oscillator's mass center.

It was found that the presence of a non-homogeneous external field made the micro and macro variables dependent. As a result, mutual nonlinear transformation of the energy of motion into the internal energy was taken into account. This nonlinear transformation was lost when deriving the Lagrange equation because of use of the hypothesis of holonomic constraints (Somsikov, 2014b). This means that it is impossible to obtain the effects resulting from a nonlinear relation between the degrees of freedom within the formalism of Lagrange.

Let us explain on an example of two-body problem, how the uses of the hypothesis of holonomic constraints excludes the possibility of describing the energy exchange between different degrees of freedom. There are two ways of obtaining the motion equations of a system of two MPs. The first way is a traditional one. The motion equation for two MPs in the external field is given by Sinai (1995):

$$\dot{\nu}_1 = -F_{12} - F_1^0;\ \dot{\nu}_2 = -F_{21} - F_2^0 \quad (1)$$

Here F_1^0, F_2^0 are the external forces, acted on a first and second MP; F_{12} is the force of interaction of MPs
Let us add and subtract these equations. As a result, we obtain:

$$\dot{\nu}_1 + \dot{\nu}_2 = -(F_1^0 + F_2^0);\ \dot{\nu}_1 - \dot{\nu}_2 = -2F_{12} - F_{12}^0 \quad (2)$$

Where $F_{12}^0 = F_1^0 - F_2^0$
Equation (2) can be rewritten as:

$$2\dot{V} = -(F_1^0 + F_2^0);\ \dot{\nu}_{12} = -2F_{12} - F_{12}^0 \quad (3)$$

Where $V = \frac{1}{2}(\sum_{i=1}^{2} \nu_i)$; $\nu_{12} = \nu_1 - \nu_2$

Thus, according to the Equation (3), the motion of the system in the external field is an independent motion of the system's center of mass and the relative motion of MPs. The motion of the center of mass is defined by the sum of the external forces applied to it. Relative motion of MPs is determined by their interaction forces and the difference between the external forces acting on each MP. According to these equations, there are two invariant of motion. The first invariant is the energy of motion of the system as a whole, and the second invariant is the energy of the relative motion of MPs.

Now consider the derivation of the motion equation for a system basing on the energy equation. By differentiating the system's energy with respect to time, we get:

$$\nu_1(\dot{\nu}_1 + F_{12} + F_1^0) + \nu_2(\dot{\nu}_2 + F_{21} + F_2^0) = 0 \quad (4)$$

In general case the variables in Equation (4) cannot be separated. The sum is equal to zero not only when each term is equal to zero (as it is postulated by the hypothesis of holonomic constraints), but each term itself could be different from zero while their sum is zero. By regrouping the terms of equation (4), we obtain:

$$(\nu_1\dot{\nu}_1 + \nu_2\dot{\nu}_2) = -F_{12}\nu_{12} - \nu_1 F_1^0 - \nu_2 F_2^0 \quad (5)$$

By comparing this equation to Equation (3), using as the variables the velocity of the mass center and the relative velocities of MPs, the result obtained is:

$$2V\dot{V} + \frac{1}{2}\nu_{12}\dot{\nu}_{12} = -V(F_1^0 + F_2^0) - \frac{\nu_{12}}{2}(F_{12} + F_{12}^0) \quad (6)$$

It is equivalent to the following equation:

$$V\left[2\dot{V} + (F_1^0 + F_2^0)\right] + \frac{\nu_{12}}{2}\left[\dot{\nu}_{12} + 2F_{12} + F_{12}^0\right] \quad (7)$$

The terms in Equation (6) are grouped so that the first term determines the motion of the mass center, while the second term determines the change in the internal energy.

Equation (6) is equal to Equation (3) in the next cases: When $F_{12}^0 = 0$, when $\nu_{12} = 0$, and when external forces are linear. The first case is equivalent to the rigid connection between the MPs. The second case is equivalent to the homogeneity of the external field. The third case is associated with a linear dependence of external forces on the coordinates. Only in these cases the variables are separated. In general case of a non-homogeneous external field the variables of the Equation (6) cannot be separated and the hypothesis of holonomic constraints is not valid, that is, Equations (3) and (6) are not equivalent. Numerical simulations of an oscillator in a non-homogenous field have confirmed this conclusion (Somsikov, 2014b).

As it turned out, in some cases the oscillator can pass the potential barrier even if its energy of motion is less than the height of the barrier (Figure 1).

In some cases the oscillator can also reflect, even if its

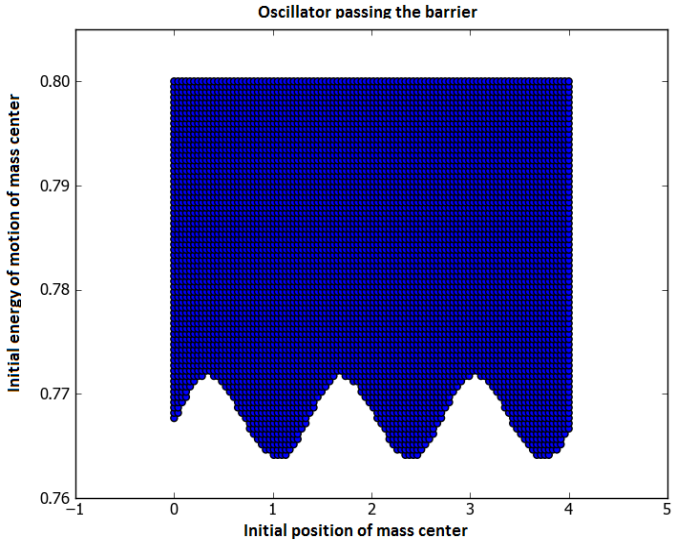

Figure 1. The filled area corresponds to the cases when the oscillator passes the barrier (depending on its initial energy of motion and phase).

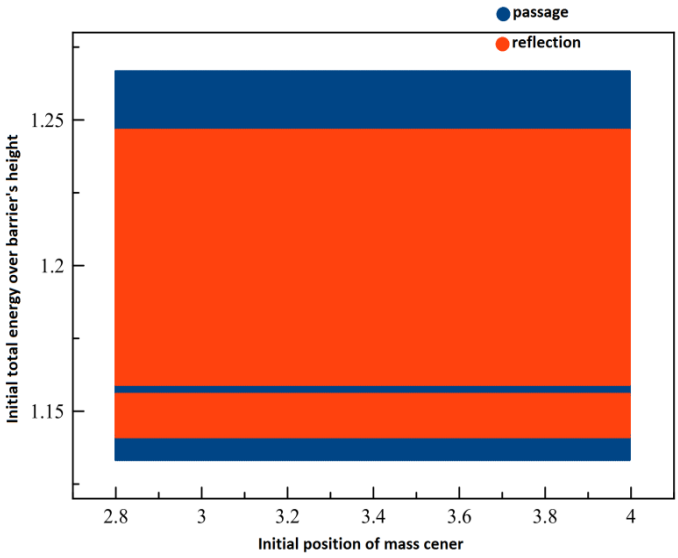

Figure 2. Oscillator's reflection / passage areas depending on its initial energy and position (red fill corresponds to reflection).

energy of motion is greater than the height of the barrier. Moreover, while gradually change the initial phase, it is possible to get interchangeable areas where the oscillator passes the barrier and where it is reflected (Somsikov and Denisenya, 2013) (Figure 2). These effects disappear if one neglects the nonholonomic constraints, that is, excludes consideration of the nonlinear mutual transformation of the oscillator's energy of motion into its internal energy.

At the moment when the oscillator is near the potential barrier, it is its phase that determines the sign of change in the internal energy (Figure 3). The result also depends on the height of the barrier, the oscillator's energy of motion, and other parameters. Thus, the calculation of oscillator's motion shows the important role of nonlinear effects in the dynamics of a system in a non-homogeneous field. These nonlinear effects can be studied only by using the principle of duality of symmetries, taking into account the transformation of the system's energy of motion into the energy of motion of the MPs relative to the system's center of mass.

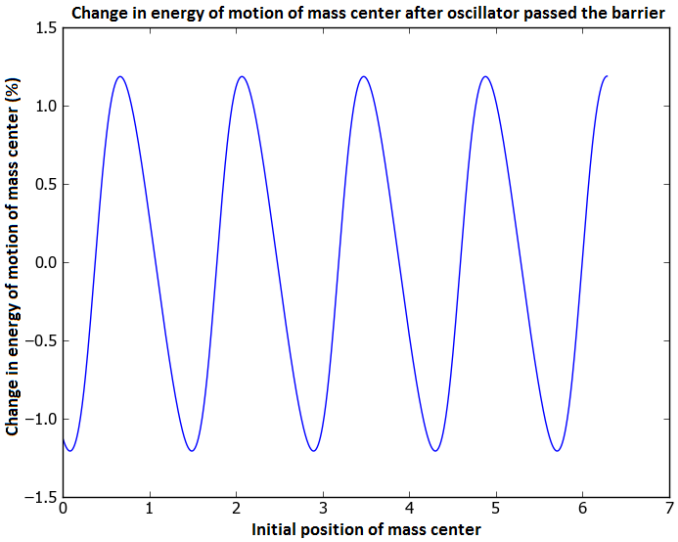

Figure 3. Change in the oscillator's energy of motion (% of its initial value) depending on its initial phase.

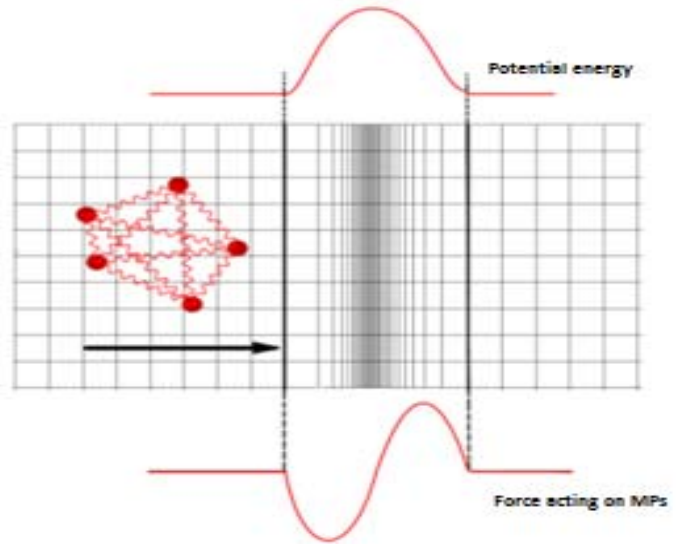

Figure 4. The scheme of numerical simulations of the system passing the potential barrier.

FORMULATION OF THE PROBLEM OF A SYSTEM PASSING A POTENTIAL BARRIER

A system of potentially interacting MPs in a nonhomogenous field has been considered (Figure 4). The initial parameters include the system's internal energy and the energy of motion of its center of mass. Coordinates and velocities of the MPs were set randomly. Their sums are equal to zero in the center of mass. The system is represented by a ball with a certain radius at which the potential energy of interaction of the MPs is equal to the total kinetic energy of the MPs.

The dual system of coordinates is used, that is the independent variables are the micro and macro variables. Microvariables determine the motion of each MP in the center of mass, while macro variables determine the motion of the center of mass itself. The barrier's height is chosen so that the system passes through it. Change in the system's internal energy, the system's motion energy, as well as D-entropy and other parameters of the problem are computed; the independent parameters include the number of MPs, the barrier's height and width,

as well as the initial conditions. The results obtained are compared with the statistical laws and with the theoretical conclusions obtained on the basis of the equations of motion of a SP (Somsikov, 2014a; Somsikov, 2014b):

$$M_N\vec{V}_N = -\vec{F}^{env} - \frac{(\Phi^{env} + E_N^{int})\vec{V}_N}{V_N^2} \quad (8)$$

Where $\vec{V}_N = \dot{\vec{R}}_N$ is velocity of the center of mass, $i = 1,2,3,\ldots,N$ - MP's count, $\vec{R}_N = \frac{1}{N}\sum_{i=1}^{N}\vec{r}_i$; $M_N = Nm$; $\vec{F}^{env} = \sum F_i^{env}(R_N, r_i)$, $E_N^{int} = \sum_{i=1}^{N} v_i\left(m\dot{v}_i + F(r_i)_i\right)$ - change in the system's internal energy, $\Phi^{env} = \sum v_i F_i^{env}(R_N, r_i)$, $\vec{F}_i^{env}(R_N, r_i)$ - external force acting on i^{th} MP, $r_i = R_N + \tilde{r}_i$, $\tilde{r}_i$, - MP's coordinates relative to the center of mass.

MPs interaction forces are given by Hooke's law. The external field is specified in the form of one period of a cosine $U(x_i) = U_b[cos(2\pi(x_i - R_b)/a) + 1]$, provided $\left(R_b - \frac{a}{2}\right) < x_i < \left(R_b + \frac{a}{2}\right)$. Hence the forces acting on each MP are given by:

$$F_i(x_i) = U_b sin(2\pi(x_i - R_b)/a) \quad (9)$$

Where U_b is the barrier's height; R_b is the position of the barrier's max height; a is the barrier's width; x_i is the distance between i^{th} MP and the center of mass; i - MP's count. According to Equation (9), the force is proportional to the barrier's height, and inversely proportional to its width.

The numerical simulations are done for various initial distributions of MPs and parameters of the problem in order to determine the nature of the changes in the energy of motion and the internal energy of the system, depending on the number of MPs and initial parameters.

CHANGE IN THE SYSTEM'S INTERNAL ENERGY AS A FUNCTION OF THE INITIAL PARAMETERS AND THE NUMBER OF MPS

According to the theoretical results, the dynamics of a conservative nonequilibrium system, represented by a set of equilibrium subsystems in a nonhomogeneous external field, should be irreversible due to the transformation of the system's kinetic energy into its internal energy (Somsikov, 2014b). A similar conclusion follows from the statistical methods of analysis of nonequilibrium systems (Landau, 1976; Rumer and Rivkin, 1977). Let us consider how much MPs a system should consist of in order to be described in terms of empirical equations of thermodynamics and statistical laws.

If the theoretical results derived from the equations of motion of systems are valid, then the numerical simulations should reveal that there is a certain number of MPs a system should consist of, such that the system's internal energy can increase only. This number (*N1*) can be taken as a first criterion for the system to be equilibrium. Obviously, this number should depend on the relative values of the internal energy, the energy of motion of the system, the potential barrier's height. Simulations have been done in order to verify existence of *N1* and study its behavior depending on the parameters of the system; the simulations estimated the change in the system's internal energy depending on the number of MPs.

Figure 5 shows the results of 400 experiments for different number of MPs. Number of MPs correspond to a power of two (4, 8, 16, 32, 64, 128, 256, 512, 1024). Initial macro parameters are constant: the mass of the system equals 1 kg, the mass of each MP equals to $1/N$, the kinetic energy of the system's center of mass E_s equals 150 J, the system's velocity is directed along the coordinate axis X.

The potential barrier is located in the YZ plane and has a width along the X axis equal to 0.2 m, the barrier's height equals 130 J, the system's internal energy equals 100 J, links rigidity coefficient U_o equals 300000 N/m. Initial micro parameters, such that coordinates and velocities of the MPs, are set randomly. Each dot in the Figure 5 corresponds to the ratio of change in the system's internal energy to its initial kinetic energy ($\Delta E^{int}/E_0^{int}$).

The figure shows that if the number of MPs is greater than 64, then the change in the internal energy can be positive only. This means that for the given parameters of the problem and $N \geq 64$, the system's dynamics is irreversible. This conclusion is made based on the fact that the impossibility of transformation of the system's internal energy into its kinetic energy can be considered as the test for irreversibility. Let us name this number as the first critical number (*N1*). It is obvious that *N1* depends on the parameters of the problem, for example, on the barrier's width.

AREA OF APPLICABILITY OF D-ENTROPY

In accordance with the law of conservation of momentum, the internal energy of a system cannot be transformed into its kinetic energy, since it is not possible to change the system's momentum. This means that the system is irreversible.

The concept of D-entropy was introduced into the mechanics because of this irreversible energy transformation fora system in a nonhomogeneous external field. D-entropy equals the ratio of the increment of the system's internal energy to its initial value, as well as the entropy of Clausius. Consider a non-equilibrium system that can be represented by a set of SPs in the

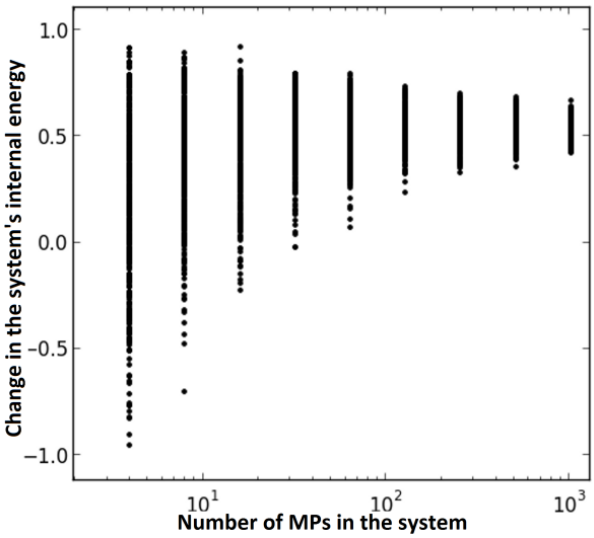

Figure 5. Fluctuations of the system's internal energy subject to the number of MPs.

approximation of local thermodynamic equilibrium; the increment of the D-entropy of this system is proportional to the energy of the relative motion of SPs, which is transforming into their internal energy. In this case, the change in the D-entropy is given by Somsikov (2014a; b):

$$\Delta S^d = \sum_{L=1}^{R}\left\{N_L \sum_{k=1}^{N_L}\left[\int \sum_s F_{ks}^L v_k dt\right]/E_L\right\} \quad (10)$$

where E_L is the internal energy of L^{th} SP; N_L is the number of MPs inside the L^{th} SP; L=1,2,3…,R- number of SPs; S - external MPs interacting with k^{th} MP in the L^{th} SP; F_{ks}^L- the force acting on k^{th} MP of one SP by S^{th} MP of another SP, and v_k- velocity of k^{th} MP.

Equation (10) is obtained based on the equation of motion of a SP, and determines the increment of the SP's internal energy comparing to its initial value. It is valid if the SP is in equilibrium along its path.

In our case L=1, so the Equation (10) is determined by a simple formula: $\Delta S^d = \Delta E^{ins}/E_0^{ins}$. This formula can be verified by numerical calculations of ΔE^{ins} for a system passing the potential barrier.

Figure 6 shows average values of change in the system's internal energy ΔE^{ins} over its initial kinetic energy (100 J), as well as confidence intervals for these values. Each confidence interval corresponds to the confidence level of 0.99 (400 experiments) and is calculated as standard deviation of the value multiplied by Student coefficient of 2.6. The values on Figure 6 are in fact the changes in D-entropy ΔS^d up to a constant factor. The calculations show that the value will be positive at $N \geq 8$ with the probability of 0.99; for smaller number of the MPs the value can be negative. As the number of MPs goes up, the fluctuation tends to zero, and even when $N \geq 10^3$, it becomes approximately equal to 0.1 of the absolute value of ΔS^d.

A further increase in the number of MPs does not change the increment of the internal energy, that is ΔE^{ins} reaches its limit at $N \approx 10^3$. If $N \geq 10^3$, then : $\Delta S^d = \Delta E^{ins}/E_0^{ins} \sim 0.55$. Since a further increase in the number of MPs does not affect the change in the thermodynamic parameters of the system, then $N = 10^3$ can be named as the second critical number (*N2*). This number determines the transition to the thermodynamic description for the problem.

CHANGE OF THE ENERGY OF THE SYSTEM PASSING THE BARRIER

Let us compare fluctuations of the system's internal energy depending on the number of MPs and their distribution function, with the law of statistical fluctuations of its mean square value. This comparison is a convincing proof of the possibility of justification of statistical laws based on the laws of mechanics. Let us recall the way it is usually proved that the relative fluctuation of any additive parameter of a system is inversely proportional to $\sqrt{N}$, where N is the number of elements in the system, on the basis of statistical laws (Landau, 1976).

The internal energy of the system (E^{ins}) is an additive value. If the system is divided into N subsystems, then the average value of its internal energy is equal to the sum of the average values of the internal energies of all subsystems, that is, $|E^{ins}| = \sum_{i=1}^{N}|E_i|$. Let us start from

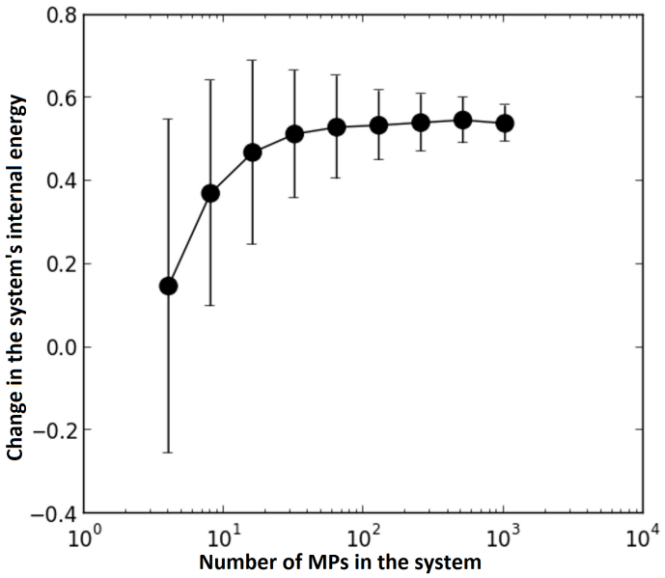

Figure 6. Change in the system's internal energy subject to the number of MPs.

the fact that the internal energy increases in proportion to the number of MPs. Then the mean square value of the fluctuations of the internal energy equals $|(\Delta E)^2| = |(\sum_{i=1}^{N} \Delta E_i)^2|$. If the fluctuations in the subsystems are independent, then $|(\Delta E)^2| = \sum_{i=1}^{N} |(\Delta E_i)^2|$. Hence the well-known law is obtained: $|(\Delta E)^2|^{1/2} \sim 1/N^{1/2}$.

Thus, if the calculated value of the relative fluctuations of E^{ins} varies inversely to $\sqrt{N}$, then this fact will serve as a proof of both the law of the fluctuations, and the possibility of the justification of this law by the laws of classical mechanics.

Figure 7 shows that dots, corresponding to the fluctuations of the internal energy, fit the curve corresponding to the statistical law of decrease of fluctuations in the system with the increase in the number of its elements (Landau, 1976).

This means, firstly, that the numerical simulations of the system passing through the barrier are correct, secondly, that the dualism of energy is reflected in the statistical laws, and thirdly, that the laws of classical mechanics are suitable not only for justification of the statistical laws, but also for determining the scope of their application depending on the parameters of the system.

The slight difference between the calculated fluctuations of ΔE^{ins} and the approximating line can be explained by the fact that the increase in the number of MPs results in a change of other parameters of the system that affect the value of ΔE^{ins} (for example, size of the system). Another reason for a certain deviation from the statistical law may be the fact that for a given number of MPs the system cannot be strictly considered as an equilibrium one. In general, the study of these deviations may be useful to identify the areas of applicability of statistical laws in the specific problems of dynamics.

CHANGE IN THE INTERNAL ENERGY SUBJECT TO THE WIDTH OF THE BARRIER

According to the equation of motion of the system, the change in the system's internal energy ΔE^{ins} nonlinearly depends on the micro and macro variables and is different from zero only when the scale of nonhomogeneity of the external field is about the scale of the system. The value of ΔE^{ins} should increase as the difference between the forces acting on different areas of the system goes up (Landau, 1976; Rumer and Rivkin, 1977). This conclusion is checked by calculating the dependence of ΔE^{ins} on the barrier's width. Figure 8 shows the results of these calculations.

The ordinate axis is the ratio of change in the internal energy to the initial energy of motion of the system's center of mass. The solid vertical line represents the standard deviation of coordinates of MPs (a measure of the system's size). The dotted line represents the maximum size of the system (the maximum distance between the MPs during the numerical experiment).

According to Figure 8, there is a decrease in the efficiency of transformation of the system's kinetic energy into its internal energy, with the increase in the barrier's width, that is, as gradient of the external field goes down,

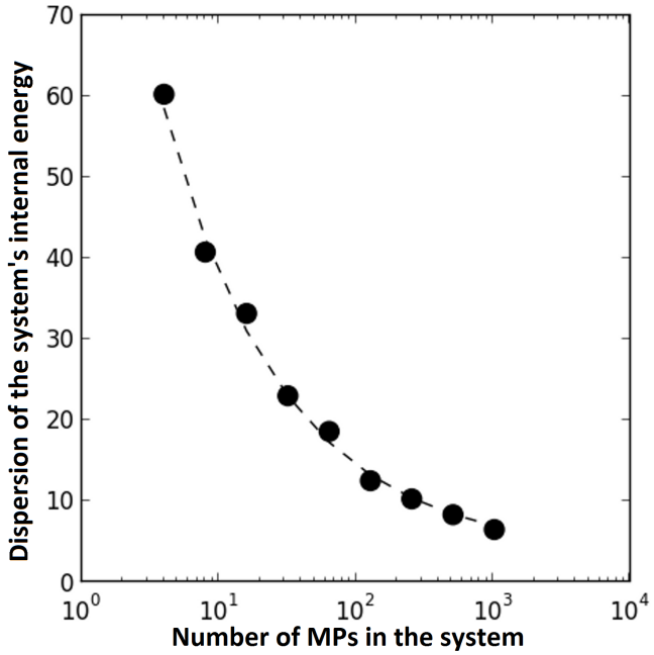

Figure 7. Dots: max amplitude of fluctuation of ΔE^{fluc} subject to number of MPs. Approximating line is given by $p + r/\sqrt{N}$, where p=3.5, r=110.

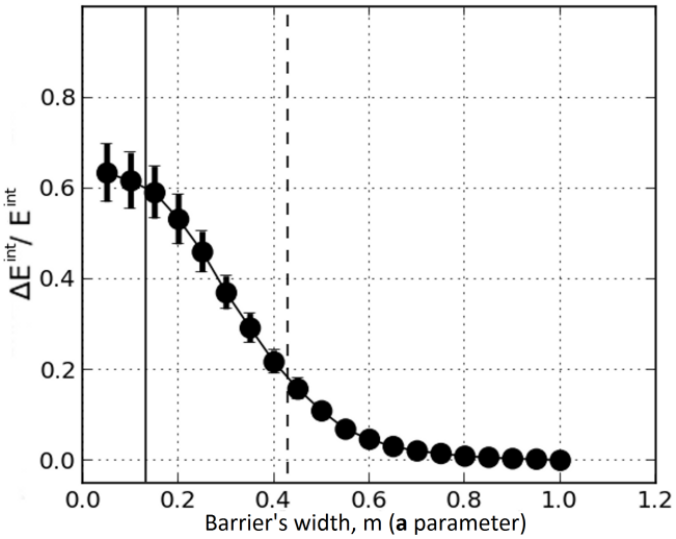

Figure 8. Change in the internal energy subject to the barrier's width, *a*.

then the change in the internal energy tends to zero. The law of diminishing is close to power-law dependence. The dependence of the internal energy on the gradient of the external forces follows from the Equation (8), if we expand the external force in the small parameter (Somsikov, 2014b).

All of the results of numerical simulations are obtained here only because the calculations were based on the concept of deterministic mechanism of irreversibility. Previously proposed D-entropy is calculated in accordance with this mechanism based on the rigorous equations of motion of systems (Somsikov, 2014b). The

D-entropy can be determined only if one uses the principle of symmetry dualism and consequent principle of energy dualism. The sum of the system's kinetic energy and its internal energy was constant during the calculations; this verified compliance with the law of conservation of energy.

CONCLUSION

Numerical simulations of dynamic parameters of motion of an equilibrium system of potentially interacting MPs in a nonhomogenous external field revealed the following patterns. A critical number of MPs is determined, such that the system's internal energy cannot go down for any given initial state of the system. In our case, this number, *N1* ~10^2. That is, when the number of SPs is greater than *N1*, then the system's dynamics becomes irreversible. This number specifies the minimum number of MPs in the system which is needed in order to apply a concept of D-entropy S^d.

Let us note that the value of $N>10^2$ is obtained for a specific model. In general, the value of *N1* should differ for a system with different parameters. But the main thing is not the exact value of *N1*, but the fact that it can be determined using the laws of Newton. This fact is a strong argument for an idea that the laws of thermodynamics can be obtained within the frameworks of classical mechanics without use of statistical hypotheses. Moreover, it supports the idea that the statistical laws themselves can be obtained using the laws of classical mechanics

The second critical value (*N2*) has been found. In our case $N2=10^3$. The increase in the system's internal energy ΔE^{tns} stabilizes if the number of its elements is greater than 10^3. In our case asymptotic value of $\Delta E^{tns}\sim 0.55$.The value of *N2* determines the transition to the thermodynamic description for the system.

It is shown that the relative fluctuations of E^{tns} goes down when the number of MPs goes up. The rate of this decrease is inversely proportional to $\sqrt{N}$. This relation for a systemis obtained on the basis of the equations of dynamics and this fact is an argument in favor of the idea that the statistical laws should be justifiable under the laws of classical mechanics. Since the law of fluctuations is the basis of statistical physics (Landau, 1976), this fact indicates the possibility of justification of statistical laws based on the laws of physics.

The efficiency of transformation of the system's kinetic energy into its internal energy goes down while the gradient of the external forces decrease. This dependence shows that the change in the internal energy is due to non-potential forces which themselves are proportional to the gradients of the external forces.

The numerical simulations carried out on the basis of the equation of SP's motion, allowed defining numerical criteria for the transition from a dynamic description to the thermodynamic model depending on the number of MPs. This opens the way for the justification of the laws of thermodynamics under the laws of classical mechanics.

Overall, the results confirm the need to describe the dynamics of systems in accordance with the principle of dualism of symmetry and use of the equation of SP's motion. Given that the real bodies are structured, it is dualism that allows identifying and study the connection between the laws of classical mechanics and the empirical laws of thermodynamics and statistical physics.

Conflict of Interest

The authors have not declared any conflict of interest.

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